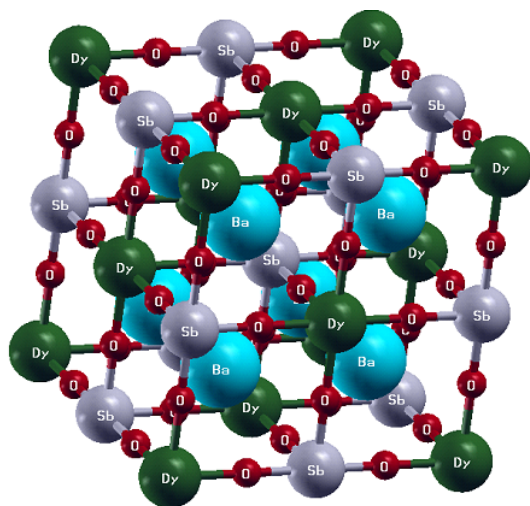


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 $\text{Ba}_2\text{DySbO}_6$: Applications in spintronic devices.

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Effect of energy loss on the lateral spread of MeV helium ions in C, Al, and Cu: Comparison with experimental data

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The Marwick-Sigmund model has been widely used to calculate the lateral spread of ions transmitted through matter. However, this model neglects the effect of ion energy loss within the target material. In this study, the model was employed to calculate the lateral spread distributions of MeV helium ions transmitted through carbon, aluminum, and copper targets. Ion energy loss was incorporated into the calculations using an approach analogous to that used for determining the angular distributions of transmitted ions. A comparison of our results with experimental data indicates that incorporating energy loss substantially enhances the overall agreement. Furthermore, this approach provides a rigorous method to account for lateral spread in depth resolution estimates for ion-beam analysis, particularly when nuclear stopping is a significant component of total stopping power.

Keywords: Lateral spread; multiple scattering; transport theory; interaction potential; energy loss; depth-resolution.

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1. Introduction

The study of ion-matter interactions constitutes a fundamental research area in many fields, including semiconductor device fabrication [1], nanotechnology [2], and radiation applications [3]. It involves processes such as ion energy loss and ion range, which govern particle transport and material modification. Therefore, a deep understanding of these processes is essential for the development of models that describe ion behavior in various media.

When an ion beam traverses matter, it undergoes electronic and nuclear interactions with target atoms, resulting in energy loss and angular deviation. The successive deflections due to the interactions with target atoms, known as multiple scattering, result in angular and lateral distributions of the ion beam. While lateral spread broadens the beam and introduces path-length fluctuations [4], understanding this phenomenon is crucial in various practical fields, including proton therapy [5], ion-beam imaging [6], external microbeam analysis of lithium batteries [7], high-resolution in-air ion-beam applications [8], nanofabrication [9, 10], and depth profiling [11]. In these domains, lateral spread imposes fundamental limits on achievable spatial resolution and introduces path-length fluctuations that directly contribute to the uncertainty of depth and energy measurements. For instance, in ion-beam analysis techniques such as RBS (Rutherford Backscattering Spectrometry) and ERDA (Elastic Recoil Detection Analysis), the lateral component of multiple scattering contributes to the energy spread of detected particles, thereby degrading depth resolution, particularly at large penetration depths. Accurate

quantification of this contribution, therefore, remains essential for interpreting and optimizing ion-beam experiments.

Although the theoretical foundations of the multiple scattering of charged particles in random media were established in early analytical works [12–15] and later reformulated [16–18], this theory continues to serve as a standard framework for interpreting experimental data on particle transport in matter [19–22]. Amsel *et al.* [23] provided a comprehensive review of the theory and its typical applications. Sigmund and Winterbon (SW) [17] and Marwick and Sigmund (MS) [18] developed two multiple scattering models to calculate the angular distribution and lateral spread of transmitted particles, respectively. These models, derived from transport theory, were formulated under the assumptions of a random medium, binary collisions with small scattering angles, and negligible energy loss. Subsequently, the SW model was generalized by Valdés and Arista (VA) [24] to incorporate energy loss into the angular distribution calculations. In contrast, incorporating energy loss into lateral spread calculations remains challenging, despite earlier attempts using the power-law potential [25]. In ion-beam analysis applications, the layered numerical formalism introduced by Szilágyi *et al.* [26] provides a computationally efficient framework for integrating continuous slowing-down effects into lateral-dispersion calculations. Serving as the computational kernel for the DEPTH code [26] and implemented in standard software such as SIMNRA [27] and WinDF [28], this formalism is essential for evaluating depth resolution and path-length fluctuations in RBS and ERDA measurements. However, comparisons with Monte Carlo and molecular dynam-

mics simulations indicated that this analytical approach exhibits systematic deviations at significant depths, attributed in part to the neglect of nuclear stopping power [29]. Moreover, Androutakaki *et al.* [30] have recently noted that applying this framework to the large penetration depths investigated in their study required extrapolating the theory beyond its original design limits.

Experimentally, angular distributions are evaluated using solid targets, whereas lateral spread measurements are commonly performed using gas targets. However, experimental data on the lateral spread in solid materials have been reported in only one study [31]. In that study, several carbon, aluminum, and copper targets were employed, and lateral spread measurements were performed using RBS or nuclear reaction techniques. Notably, this is one of the few studies that examine the lateral spread under conditions involving significant ion energy loss.

The present study represents a continuation of our comprehensive investigation into the effects of energy loss on ion multiple scattering [32–35]. Specifically, we analyze the lateral spread of helium ions transmitted through carbon, aluminum, and copper targets using the MS model, which we modified to account for ion energy loss in a manner analogous to the VA model's treatment of angular distributions. The main contribution is a comparison of calculated lateral-spread widths, as functions of penetration depth and ion energy, with the experimental data from Ref. [31].

2. Lateral spread theory

We consider a collimated beam of monoenergetic charged particles transmitted along the positive x -direction of an amorphous foil of thickness x (Fig. 1). The lateral distribution $G(x, \rho)$ of transmitted particles is given by [18]:

$$G(x, \rho) d^2\rho = \frac{\rho}{x} d\left(\frac{\rho}{x}\right) \int_0^\infty k dk J_0\left(\frac{k\rho}{x}\right) \times \exp\left[-\frac{Nx}{k} \int_0^k \sigma_0(k', E) dk'\right], \quad (1)$$

where $\rho = \sqrt{\rho_y^2 + \rho_z^2}$ is the lateral displacement. J_0 is the zero-order Bessel function of the first kind, N is the number of scattering centers per unit volume, E is the initial energy of the incident ion, and $\sigma_0(k', E)$, the transport cross section, is given by:

$$\sigma_0(k', E) = \int_0^\infty d\sigma(\phi) [1 - J_0(k'\phi)], \quad (2)$$

where ϕ is the single scattering angle defined in the laboratory frame and $d\sigma(\phi)$ is the differential cross section.

By introducing the reduced variables τ and $\tilde{\rho}$, which are defined in terms of the thickness x and the lateral displacement ρ as follows:

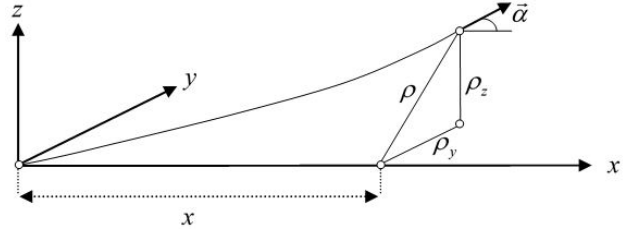


FIGURE 1. Geometry under consideration: The initial beam direction coincides with the positive x -axis. A lateral displacement ρ and an angular deviation $\tilde{\alpha}$ are considered after a penetration depth x .

$$\tau = \pi a^2 N x, \quad (3)$$

$$\tilde{\rho} = \pi a^2 N \frac{E a}{2 Z_1 Z_2 e^2} \rho, \quad (4)$$

where a is the screening radius, and Z_1 and Z_2 are the atomic numbers of the ion and the target atom, respectively. The function $G(x, \rho)$ can be represented in terms of the reduced lateral distribution function $g_1(\tau, \tilde{\rho})$ as follows:

$$G(x, \rho) d^2\rho = g_1(\tau, \tilde{\rho}) \tilde{\rho} d\tilde{\rho}, \quad (5)$$

with

$$g_1(\tau, \tilde{\rho}) = \frac{1}{\tau^2} \int_0^\infty z dz J_0\left(z \frac{\tilde{\rho}}{\tau}\right) \times \exp\left[-\frac{\tau}{z} \int_0^z d\gamma \Delta(\gamma)\right]. \quad (6)$$

The function $\Delta(\gamma)$, called the reduced transport cross section, is given by:

$$\Delta(\gamma) = \int_0^\infty \frac{d\tilde{\phi}}{\tilde{\phi}^2} f(\tilde{\phi}) [1 - J_0(\gamma\tilde{\phi})], \quad (7)$$

where $\tilde{\phi}$ is the reduced single scattering angle, and f is the scattering function determined by the interaction potential.

In the original MS model of lateral spread, ion energy loss was neglected during its entire trajectory within the target. This implies that the cross section $\sigma_0(k', E)$, defined by Eq. (2), is calculated at a fixed energy E corresponding to the ion's initial energy. For thin targets, which are related to low ion energy loss, this approximation is justified. However, as the target thickness increases and energy loss becomes significant, the assumption of negligible energy loss is no longer valid. In such cases, a more rigorous analysis is essential to consider the cross section at every possible instantaneous energy $E(x')$, corresponding to any path x' traversed by the ion inside the medium. To incorporate this, we apply the following substitution, previously introduced in the VA model [24], to Eq. (1):

$$x \sigma_0(k, E) \rightarrow \int_0^x \sigma_0(k, E(x')) dx', \quad (8)$$

or in terms of reduced quantities:

$$\tau \Delta(\gamma) \rightarrow \int_0^\tau \Delta(\gamma') d\tau'. \quad (9)$$

The new reduced transport cross section $\Delta(\gamma')$ is now expressed as:

$$\Delta(\gamma') = \int_0^\infty \frac{d\tilde{\phi}}{\tilde{\phi}^2} f(\tilde{\phi}) [1 - J_0(\gamma' \tilde{\phi})], \quad (10)$$

with:

$$\gamma' = \frac{E}{E(x')} \gamma. \quad (11)$$

The instantaneous energy $E(x')$ is expressed as:

$$E(x') = E - \int_0^{x'} \left(\frac{dE}{dx} \right) dx. \quad (12)$$

Here dE/dx is the total stopping power (electronic and nuclear).

It is important to note that the substitution given by Eq. (8) is valid under the condition that, for a given foil thickness x , the ion's path length L is considered equivalent to the foil thickness x . This approximation should be validated at high energy loss, where increased angular straggling can increase L/x .

3. Results and discussion

To verify that the ion path length L remains close to the foil thickness x , Monte Carlo simulations were performed using TRIM (SRIM 2013) [36] for 1-2 MeV ^4He ions and 1 MeV ^3He ions transmitted through carbon, aluminum, and copper targets. In the experimental systems of Möller and Williams [31], the largest relative energy loss values ($\Delta E/E$), where ΔE is the projectile's total energy loss in the target, were approximately 0.36 for ^4He in C, 0.22 for ^4He in Al, and 0.48 for ^3He in Cu. To test the validity of the approximation $L \approx x$ under conditions at least as severe as those in the

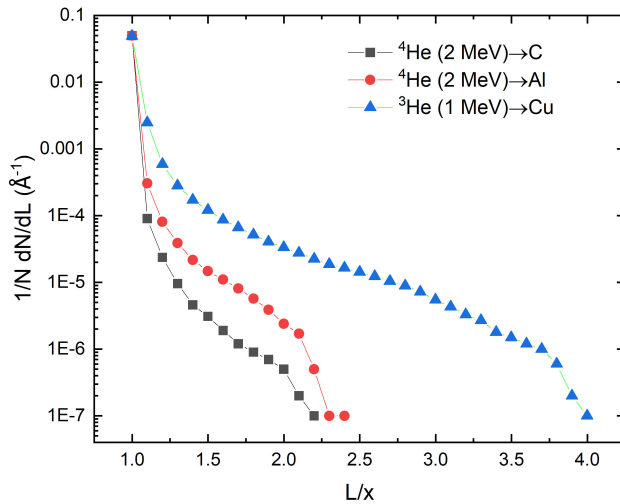


FIGURE 2. Path-length distribution as a function of L/x for He ions transmitted through C and Al films at 2 MeV (squares and circles, respectively), and through a Cu film at 1 MeV (triangles). The considered target thicknesses correspond to a relative energy loss $\Delta E/E = 0.5$.

experiments, we simulated target thicknesses corresponding to $\Delta E/E = 0.50$, slightly exceeding the maximum experimental value (0.48) reported in Ref. [31]. Figure 2 shows representative path-length distributions as a function of L/x , demonstrating that the vast majority of ions are transmitted with path lengths very close to x . These results support the validity of the $L \approx x$ approximation adopted in this study. Regarding the projectile charge state, the experimental study in Ref. [31] employed MeV $^3\text{He}^+$ and $^4\text{He}^+$ beams. However, the initial vacuum charge state need not be specified in the present treatment. MeV helium reaches charge equilibrium within a few to tens of nanometers [37, 38], a depth far smaller than the 0.3 – 20 μm targets used by Möller and Williams [31]. Ion spread is therefore governed by near-equilibrium charge states, in which helium projectiles behave effectively as nearly fully stripped He^{2+} ions [38, 39].

Using the MS model, the lateral distributions of helium ions with energies of 1 and 2 MeV transmitted through C, Al, and Cu targets were calculated. The projectile instantaneous energy $E(x')$ was computed numerically from Eq. (12) using the total stopping power (electronic and nuclear) obtained from the SRIM compilation [36]. The resulting $E(x')$ was fitted and substituted into Eq. (11) to calculate γ' . The lateral distribution $G(x, \rho)$ (Eq. (1)), or equivalently the reduced distribution $g_1(\tau, \tilde{\rho})$ (Eq. (6)), was computed using the reduced transport cross section $\Delta(\gamma)$ from Eq. (7) when energy loss is neglected, or $\Delta(\gamma')$ from Eq. (10) when energy loss is included. In all cases, the Thomas-Fermi-Molière (TFM) potential [40] was used to describe the interaction between He ions and the various targets. An example of these calculations is presented in Fig. 3, illustrating the case of 1 MeV ^3He ions transmitted through a Cu target of thickness $x = 700 \mu\text{g}/\text{cm}^2$. The areal thickness of the target (in $\mu\text{g}/\text{cm}^2$ units) was chosen to match the metric used in the experimental results of Ref. [31]. It can be observed that including energy loss affects the shape of the distribution, resulting in a

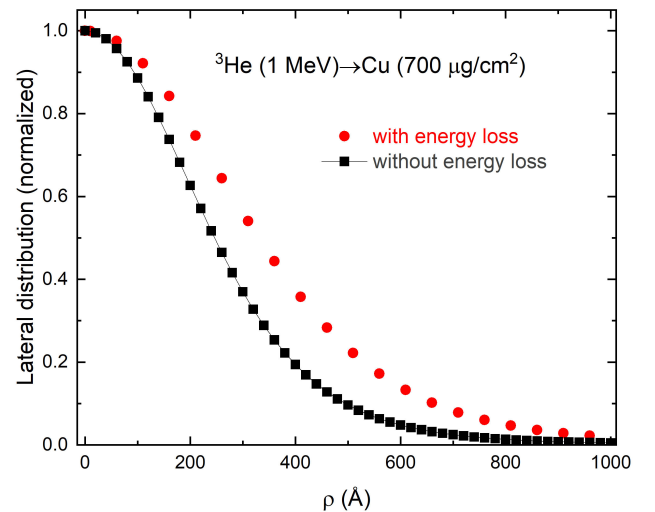


FIGURE 3. Lateral distributions of 1 MeV ^3He ions transmitted through a Cu target of $x = 700 \mu\text{g}/\text{cm}^2$ thickness.

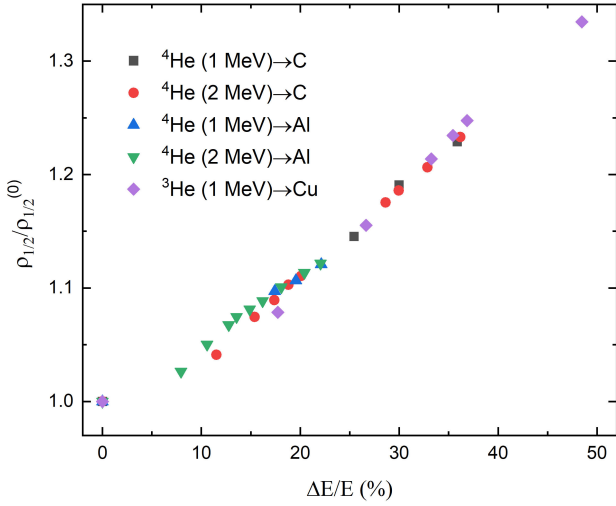


FIGURE 4. Variation of the ratio $\rho_{1/2}/\rho_{1/2}^{(0)}$ with the relative ion energy loss for different targets.

broader profile. These results are consistent with those obtained when energy loss is taken into account in the angular distribution calculations [24, 33]. It is worth noting that the relative ion energy loss $\Delta E/E$ in this case is approximately 50 %.

For comparison with the experiment, the half-width $\rho_{1/2}$, defined as the lateral displacement at which the distribution reaches half of its maximum value, was extracted from each calculated lateral distribution. It is defined by the condition:

$$G(x, \rho_{1/2}) = 0,5 G(x, 0). \quad (13)$$

After normalizing each distribution at zero lateral displacement, $\rho_{1/2}$ was determined numerically by interpolating the distribution near the half-maximum and extracting the corresponding lateral displacement. The symbols $\rho_{1/2}^{(0)}$ and $\rho_{1/2}$

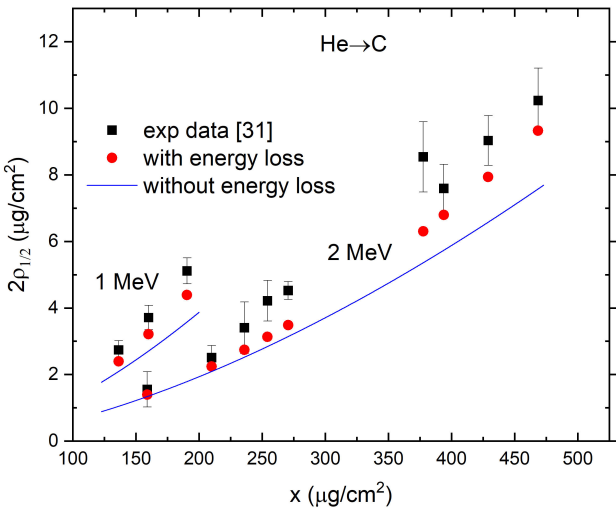


FIGURE 5. Variation of $2\rho_{1/2}$ as a function of target thickness x for ${}^4\text{He}$ ions transmitted through a C target. Squares: experimental data from [31]; solid lines: calculations without considering energy loss; circles: calculations including energy loss.

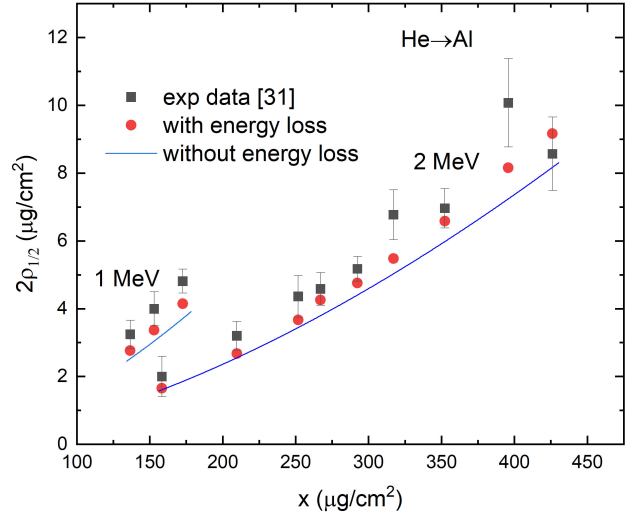


FIGURE 6. Same as Fig. 5 but for ${}^4\text{He}$ ions transmitted through an Al target.

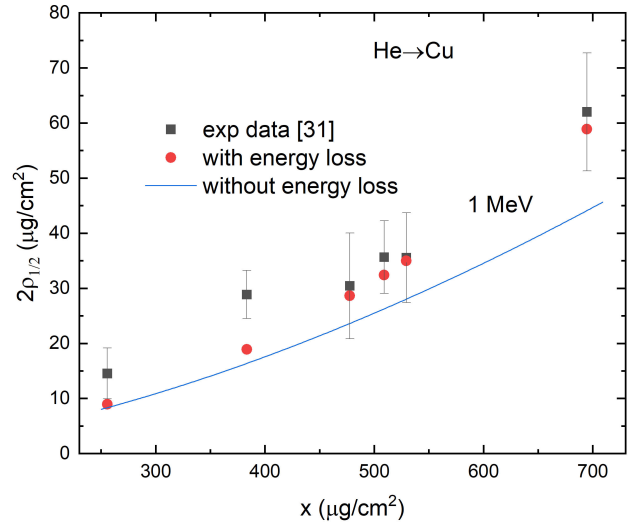


FIGURE 7. Same as Fig. 5 but for ${}^3\text{He}$ ions transmitted through a Cu target.

denote the values obtained without and with energy loss included, respectively. The half-widths, initially expressed in Å, were converted to $\mu\text{g}/\text{cm}^2$ using the corresponding target mass densities. Figure 4 shows the variation of the ratio $\rho_{1/2}/\rho_{1/2}^{(0)}$ with the relative ion energy loss. The results indicate that this ratio, which exhibits a uniform shape, increases with the energy loss. It appears to be almost independent of both the projectile energy and target material within the considered range of energy loss. A similar behavior was observed in the ratio of the half-maximum values of the angular distributions obtained with and without accounting for energy loss in the calculations [33].

Figures 5, 6 and 7 show a comparison between the calculated values of $2\rho_{1/2}$ (in $\mu\text{g}/\text{cm}^2$ units) as a function of target thickness, obtained with energy loss taken into account, and the experimental data from Ref. [31]. The results are presented for the following cases: ${}^4\text{He}$ ions with energies of 1

and 2 MeV on C and Al targets, and ^3He ions with 1 MeV energy on a Cu target, respectively. The corresponding calculated values obtained without considering energy loss are also included in the figures.

These figures clearly demonstrate that incorporating energy loss into the calculations significantly improves agreement with the experimental data across the entire range of target thicknesses. In contrast, calculations that neglect energy loss yield reasonable agreement only at small thicknesses, where the relative energy loss is low. However, as the

target thickness increases and the energy loss becomes more pronounced, deviations between these calculations and the experimental results become more significant. Incorporating energy loss into the calculations significantly improves model accuracy across all target materials. The maximum discrepancy between experimental and calculated values decreases from 26 % to 9 % for carbon, from 28 % to 19 % for aluminum, and from 29 % to 5 % for copper targets. Thus, beyond the qualitatively expected increase in lateral spread, explicitly treating energy loss yields quantitative improvements in predictive accuracy, particularly at large $\Delta E/E$. The present results demonstrate the importance of considering stopping effects in lateral-spread calculations, particularly for ions traversing substantial depths in matter. The proposed method enables depth-resolution evaluations in ion-beam analysis, particularly when nuclear stopping cons-

titutes a non-negligible fraction of the total stopping power, an effect not captured by the transformation approach of Szilágyi *et al.* [26].

4. Conclusions

In this study, a model based on transport theory was employed to calculate the lateral distributions of MeV He ions transmitted through carbon, aluminum, and copper targets. The assumption that the ion path length is equivalent to the foil thickness was rigorously tested using the TRIM code under conditions of high ion energy loss, demonstrating its applicability across all systems examined in this study. The effects of ion energy loss were added to the calculations using the VA model. The results show that when energy loss is taken into account, the calculated profiles change noticeably, becoming wider overall. Moreover, comparing the calculated half-widths of the lateral spread with experimental measurements highlights that including energy loss leads to much better agreement throughout the range of energy losses studied. This study emphasizes the necessity of incorporating energy loss into such calculations. Therefore, we recommend applying this method into future depth-resolution analyses, particularly in regimes where nuclear stopping cannot be neglected.

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Time evolution of contact-angle dynamics for water and sodium chloride solution droplets during evaporation

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In this work, the time evolution of the contact-angle dynamics of distilled water droplets and 0.9 % sodium chloride solution droplets placed on a solid glass surface was investigated experimentally during evaporation. The contact angle was determined using a simple geometric approach based on spherical-cap geometry from the droplet height and base diameter, without employing complex optical goniometric systems. The experiments were conducted under controlled environmental conditions, and the time-dependent variation of the contact angle was analyzed in detail. The results show that, for the 0.9 % sodium chloride solution droplet, the contact angle decreases faster and in an almost monotonic manner compared with the distilled water droplet. In contrast, the water droplet exhibits stick–slip behavior associated with contact-line pinning and depinning processes. The obtained results indicate that electrolyte ions influence wetting properties and contact-line dynamics. This study demonstrates the applicability of a simple geometric approach for contact-angle analysis without using complex goniometric systems. Furthermore, the obtained results for the 0.9 % NaCl solution may serve as useful reference data for modeling the evaporation behavior of physiological saline droplets on solid substrates.

Keywords: Contact angle; droplet evaporation; water; sodium chloride solution; wetting dynamics.

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1. Introduction

Evaporation of liquid droplets placed on a solid surface is one of the fundamental processes closely related to the physics of surface phenomena, heat and mass transfer, and wetting dynamics [1–3]. Such processes play an important role in many practical applications, including coating technologies, inkjet printing systems, microfluidics, biological assays, and materials processing [2, 4]. A macroscopic description of sessile-droplet evaporation is commonly based on the droplet geometry and its time evolution, where the contact angle emerges as a key physical parameter [3].

The contact angle is defined at the three-phase contact line where the liquid, solid surface, and gas phase meet, and it characterizes the degree of wetting of a surface by a liquid. Under equilibrium conditions, it is determined by the balance of interfacial tensions and is expressed by the classical Young equation [1]. However, during evaporation the droplet deviates from equilibrium; as a consequence, both the contact angle and the position of the contact line change dynamically with time [3–5]. Therefore, investigating the time-dependent evolution of the contact angle is necessary for a complete characterization of sessile-droplet evaporation [4, 5].

In previous studies, droplet evaporation is often interpreted in terms of two ideal limiting regimes: a constant contact radius (CCR) mode, in which the contact radius remains nearly unchanged while the contact angle decreases, and a constant contact angle (CCA) mode, in which the contact angle remains approximately constant while the contact line recedes [2, 3]. Under practical conditions, evaporation frequently proceeds in an intermediate, i.e., hybrid regime bet-

ween these two limits. In this case, temporary arrest and subsequent motion of the contact line are described by pinning–depinning processes, which lead to a nonlinear evolution of the contact angle [4, 6].

Many investigations of sessile-droplet evaporation have primarily focused on pure water droplets. These studies show that the evaporation rate and contact-angle dynamics of water droplets depend significantly on substrate properties, temperature, and relative humidity [3, 5]. In addition, a nonuniform distribution of evaporative flux along the droplet surface can induce internal capillary flows, thereby modifying the droplet shape and evaporation kinetics. This phenomenon has been widely studied in connection with the “coffee-ring” effect [5].

Compared to pure water, evaporation of electrolyte-solution droplets has been investigated to a lesser extent. The presence of ions in solution alters surface tension, vapor pressure, and wetting conditions, and can lead to the formation of concentration gradients inside the droplet during evaporation [7, 8]. As evaporation proceeds, the increasing salt concentration causes a redistribution of interfacial forces, which differentiates the contact-line dynamics and contact-angle evolution from the pure-water case both qualitatively and quantitatively [7, 9].

In this context, an aqueous sodium chloride solution with a concentration of 0.9 % is of particular interest. This specific concentration corresponds to standard physiological saline, making it highly relevant for medical and biological applications. Investigating the contact-angle dynamics of 0.9 % NaCl droplets provides useful reference data for modeling the evaporation behavior of physiological saline droplets on

solid surfaces.

In this work, the time evolution of the contact-angle dynamics of distilled water droplets and 0.9 % NaCl solution droplets placed on a solid glass surface is experimentally studied and comparatively analyzed during evaporation. The contact angle is determined using a simple geometric method based on measurements of the droplet height and base diameter, which enables real-time monitoring without employing complex optical goniometric systems. The main objective of this study is to identify differences in the contact-angle evolution between water and electrolyte-solution droplets and to experimentally evaluate the influence of ions on wetting and evaporation mechanisms.

2. Experimental setup and methods

2.1. Experimental setup and conditions

This study was carried out using a laboratory setup designed to investigate the contact-angle dynamics of sessile droplets during evaporation on a solid surface. Distilled water droplets and 0.9 % sodium chloride (NaCl) solution droplets, known as physiological saline, were selected as experimental objects due to their biological relevance. The experiments were performed on a smooth and transparent glass substrate.

The droplets were deposited using an automatic piston micropipette with an initial volume of $5.5 \mu\text{L}$, ensuring a stable shape close to a spherical cap (Fig. 1). To ensure minimal kinetic energy, the liquid was slowly extruded until a hanging drop gently made contact with the surface, effectively preventing splashing or artificial spreading.

The experiments were conducted in a specially constructed isolation chamber protected from external airflow and vibrations. To ensure thermal stability, the inner walls were lined with heat-reflecting foil. All experimental runs were performed at a constant ambient temperature of $23 \pm 0.5^\circ\text{C}$, maintained by a controlled heating panel and monitored using a digital thermohygrometer to ensure stable evaporation kinetics. Under these sealed and thermally regulated conditions, the relative humidity naturally stabilized at approximately 30 %. Maintaining a strictly constant relative humidity is critical, as evaporation kinetics and contact-angle dynamics are highly sensitive to ambient moisture levels. By conducting all measurements at this stable 30 % humidity baseline, the comparison between the two liquids was performed under identical environmental conditions. The general view of the experimental setup is shown in Fig. 2.



FIGURE 1. Automatic piston micropipette used for forming droplets and dispensing them onto the substrate surface (initial volume: $5.5 \mu\text{L}$).

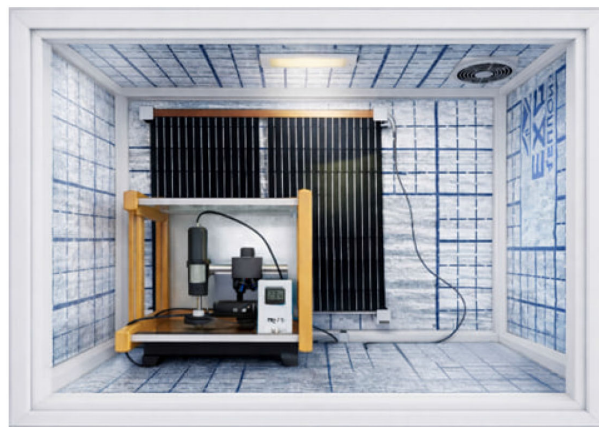


FIGURE 2. General view of the experimental setup designed to observe sessile-droplet evaporation under controlled conditions (isolated environment and arrangement of the measurement system).



FIGURE 3. Digital USB microscope system used for acquiring droplet images during evaporation. This figure illustrates the imaging device only; quantitative geometric measurements were performed on calibrated digital images, as shown in Fig. 4.

2.2. Observation and measurement of droplet geometry

The droplet evaporation process was observed from the side using a digital microscope (Fig. 3). The microscope enabled real-time imaging of the droplet side profile, while the droplet geometric parameters were determined from calibrated digital images (Fig. 4). During the experiments, the digital microscope was set to a fixed magnification of approximately 100x. This specific magnification level was chosen to ensure a clear, high-resolution view of the three-phase contact line while keeping the entire droplet profile within the field of view. Images of the evaporating droplet were acquired continuously at a fixed recording interval of 1 frame per minute (*i.e.*, one image every 60 seconds).

This specific acquisition interval was chosen to provide sufficient temporal resolution to accurately track the relatively slow macroscopic changes in the droplet profile and contact angle throughout the entire evaporation process.

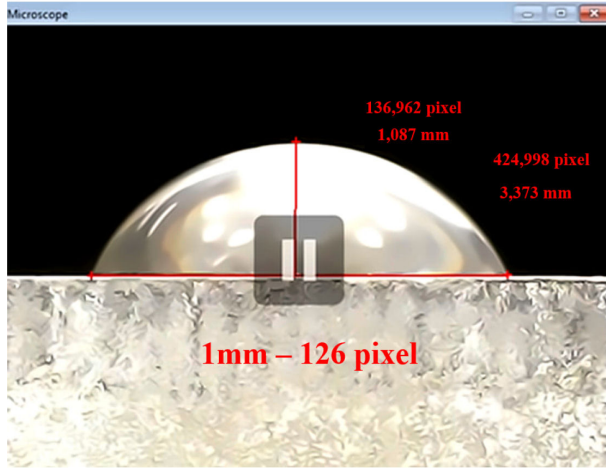


FIGURE 4. Example of measuring the droplet base diameter d and height h in the calibrated microscope image. The calibration factor was $1 \text{ mm} = 126 \text{ pixels}$.

The droplet geometric parameters—the base radius r at the droplet–substrate contact and the height h from the substrate surface to the droplet apex—were determined at each time interval during the evaporation process. To extract the geometric parameters, the acquired images were processed using the microscope’s dedicated measurement software, which was carefully calibrated using a standard micrometer scale prior to the experiments. Under the selected imaging conditions, the calibration factor was determined as $1 \text{ mm} = 126 \text{ pixels}$, which was used to convert pixel-based measurements into physical units. The image processing steps involved first defining the solid-liquid baseline (the substrate surface). Then, the base diameter d was determined by manually identifying and marking the two distinct three-phase contact points on this baseline. Following this, the droplet height h was measured by drawing a perpendicular vertical line from the center of the baseline to the highest boundary point (apex) of the droplet profile. These specific measurement steps were systematically repeated for each acquired frame to extract the continuous parameters required for the contact angle calculation.

The microscope system was calibrated in advance to ensure that all measurements were performed at the same scale. The proximity of the droplet shape to a spherical cap was visually monitored, and cases with noticeable geometric deviations were excluded from the analysis.

2.3. Method for determining the contact angle

To determine the contact angle, the droplet shape was treated as a spherical cap. This approach is justified by the fact that, for the selected droplet volume, surface-tension forces strongly dominate over gravitational effects. Quantita-

tively, this assumption is validated by evaluating the Bond number (Bo), which represents the ratio of gravitational forces to surface tension forces: $Bo = \rho g R^2 / \gamma$, where ρ is the liquid density, g is the gravitational acceleration, R is the droplet base radius, and γ is the surface tension. The physical properties of the liquids used in the experiments were determined at the controlled temperature of 23°C . For distilled water, the density was $\rho = 997,5 \text{ kg/m}^3$ and the surface tension was $\gamma = 72,3 \text{ mN/m}$. For the 0.9 % NaCl solution, the density and surface tension were slightly higher, at $\rho = 1004,6 \text{ kg/m}^3$ and $\gamma = 72,8 \text{ mN/m}$, respectively. These values were utilized to evaluate the Bond number (Bo), which characterizes the ratio of gravitational to surface-tension forces. For the distilled water droplet, taking $\rho = 1000 \text{ kg/m}^3$, $\gamma \approx 72 \text{ mN/m}$, and the maximum measured initial base radius $R \approx 1,69 \text{ mm}$, the calculated Bond number is $Bo \approx 0,39$. Additionally, the capillary length $l_c = \sqrt{\gamma / \rho g}$ for water is approximately 2.71 mm . Since the initial droplet radius ($1,69 \text{ mm}$) is strictly less than the capillary length, and the Bond number is well below unity ($Bo < 1$), gravitational flattening is negligible. Thus, the droplet firmly resides in the capillary regime, ensuring that its shape accurately conforms to a spherical cap throughout the evaporation process. Deviations from the spherical shape would only occur for significantly larger droplets where $Bo > 1$. The droplet side profile was analyzed in the plane as a part of a circular arc. Based on the droplet geometry, the contact angle θ is determined from the droplet height h and the base diameter d using the following expression:

$$\theta = \arccos \left(\frac{d^2 - 4h^2}{d^2 + 4h^2} \right). \quad (1)$$

This formula makes it possible to determine the angle between the tangent line to the droplet surface at the point of contact with the substrate and the substrate plane. The applied geometric method, based on the spherical-cap approximation, is a well-established technique in the study of wetting phenomena, particularly when surface tension dominates over gravity [2, 3]. Compared to more complex approaches such as polynomial fitting of the droplet profile or professional optical goniometry, this height-width method offers a practical and robust alternative for real-time monitoring under controlled laboratory conditions. It eliminates the need for sophisticated image-analysis algorithms while maintaining high accuracy for small sessile droplets ($Bo < 1$), where the profile remains inherently circular. Similar geometric approaches have been successfully utilized in previous studies to evaluate the evaporation kinetics of pure and multicomponent liquid droplets on various substrates [3, 4]. During the evaporation process, the contact angle was recalculated at each time point, and its time evolution was analyzed.

2.4. Data processing

To ensure a precise evaluation of the temporal resolution, the geometric parameters were extracted and the contact an-

gle was calculated at a strict time interval of 1 minute between consecutive analyzed images. This consistent 1-minute temporal resolution was maintained throughout the entire duration of the evaporation process for both liquids. The experiments were carried out under controlled laboratory conditions, with the relative humidity maintained at approximately 30 %. The obtained results were used to identify general trends in contact-line behavior, including monotonic and nonuniform decreasing regimes, as well as possible pinning and depinning effects. The presented data correspond to representative measurements obtained under the same experimental conditions for both liquids. To ensure the reproducibility of the experimental results, each evaporation test for both distilled water and 0.9 % NaCl solution was repeated three times under identical environmental conditions ($23 \pm 0,5^{\circ}\text{C}$ and 30 % RH). The data points presented in the results section correspond to the representative average values obtained from these runs. The maximum relative uncertainty in the determination of the contact angle was estimated to be approximately $\pm 1,5^{\circ}$, which primarily originates from the manual identification of the three-phase contact points and the substrate baseline during the digital image processing stage.

3. Results and discussion

3.1. Time evolution of the contact angle for a distilled water droplet

The visual evolution of the distilled water droplet profile during the 45-minute evaporation period is presented in Fig. 5. As observed, the droplet maintains a shape close to a spherical cap while both its height h and base diameter d decrease progressively over time. These side-profile images provide direct visual evidence of the geometric changes discussed in the following analysis.

During the evaporation of a distilled water droplet, the time variation of the contact angle θ was monitored over the interval 0 – 45 min. At the initial state, the droplet had a geo-

metry close to a spherical cap, and at $t = 0$ min the contact angle was $\theta \approx 65,19^{\circ}$. As evaporation proceeded, the droplet height h and the base radius r (diameter d) decreased steadily, and consequently $\theta(t)$ showed an overall decreasing trend.

At each time point, the contact angle was calculated from the droplet geometric parameters using the geometric method described above according to Eq. (1).

The measured base diameter, height, and the calculated contact-angle values for the water droplet are presented in Table I.

The time evolution of the contact angle for the distilled water droplet is presented in Fig. 6 (orange curve). The general trend of the curve indicates that the contact angle decreases with time; however, this decrease is not strictly linear over the entire process. In several time intervals, the rate of decrease becomes slower, and small short-term deviations from the overall trend are observed. Such behavior is consistent with possible contact-line pinning and depinning (“stick-slip”) effects, which are commonly encountered during sessile-droplet evaporation on solid substrates. These local deviations become more evident during the transition from a stage in which the contact line remains nearly pinned, corresponding approximately to the CCR regime, to a stage in which contact-line motion becomes more noticeable.

From a practical point of view, the evaporation process of the water droplet may be qualitatively divided into three stages. In the initial stage, the contact angle decreases relatively rapidly while the contact radius remains nearly stable, which is characteristic of behavior close to the CCR regime. In the intermediate stage, the decrease of θ becomes slower and stick-slip-like features appear more clearly, indicating alternating periods of temporary pinning and partial motion of the contact line. In the final stage, the droplet becomes flatter and the contact angle decreases more sharply as the droplet volume approaches its final stage of evaporation. These stages may be associated with the coupling between droplet geometry, evaporative mass loss, and contact-line dy-

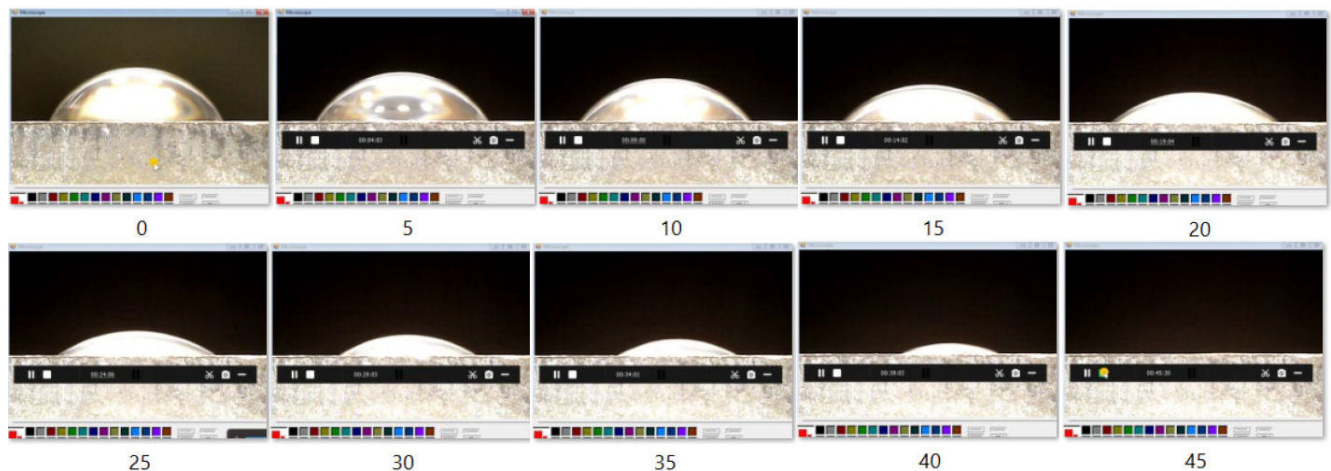


FIGURE 5. Side-profile microscope images of a distilled water droplet at representative time intervals (from $t = 0$ to $t = 45$ min) during evaporation on a glass surface at 23°C .

TABLE I. Time-dependent values of the geometric parameters and the contact angle θ during evaporation of a distilled water droplet.

Time (min)	Diameter (mm)	Height (mm)	θ ($^{\circ}$)	Time (min)	Diameter (mm)	Height (mm)	θ ($^{\circ}$)
0	3.381	1.081	65.194	23	3.095	0.508	36.347
1	3.373	1.040	63.321	24	3.048	0.484	35.238
2	3.365	1.016	62.252	25	3.016	0.460	33.928
3	3.357	0.992	61.167	26	2.976	0.445	33.300
4	3.349	0.960	59.652	27	2.929	0.437	33.230
5	3.333	0.929	58.275	28	2.794	0.429	34.142
6	3.325	0.905	57.124	29	2.651	0.413	34.612
7	3.317	0.889	56.385	30	2.571	0.397	34.324
8	3.310	0.865	55.188	31	2.524	0.365	32.262
9	3.302	0.849	54.428	32	2.437	0.349	31.965
10	3.302	0.833	53.546	33	2.389	0.341	31.865
11	3.294	0.786	51.024	34	2.333	0.325	31.137
12	3.286	0.778	50.677	35	2.262	0.317	31.315
13	3.286	0.730	47.912	36	2.119	0.278	29.405
14	3.270	0.714	47.182	37	2.064	0.262	28.490
15	3.262	0.691	45.921	38	1.944	0.222	25.731
16	3.254	0.651	43.615	39	1.873	0.206	24.811
17	3.254	0.635	42.640	40	1.786	0.199	25.126
18	3.246	0.619	41.753	41	1.746	0.159	20.644
19	3.238	0.587	39.858	42	1.675	0.127	17.245
20	3.214	0.571	39.122	43	1.587	0.103	14.792
21	3.190	0.548	37.923	44	1.524	0.087	13.027
22	3.119	0.532	37.673	45	1.111	0.040	8.237

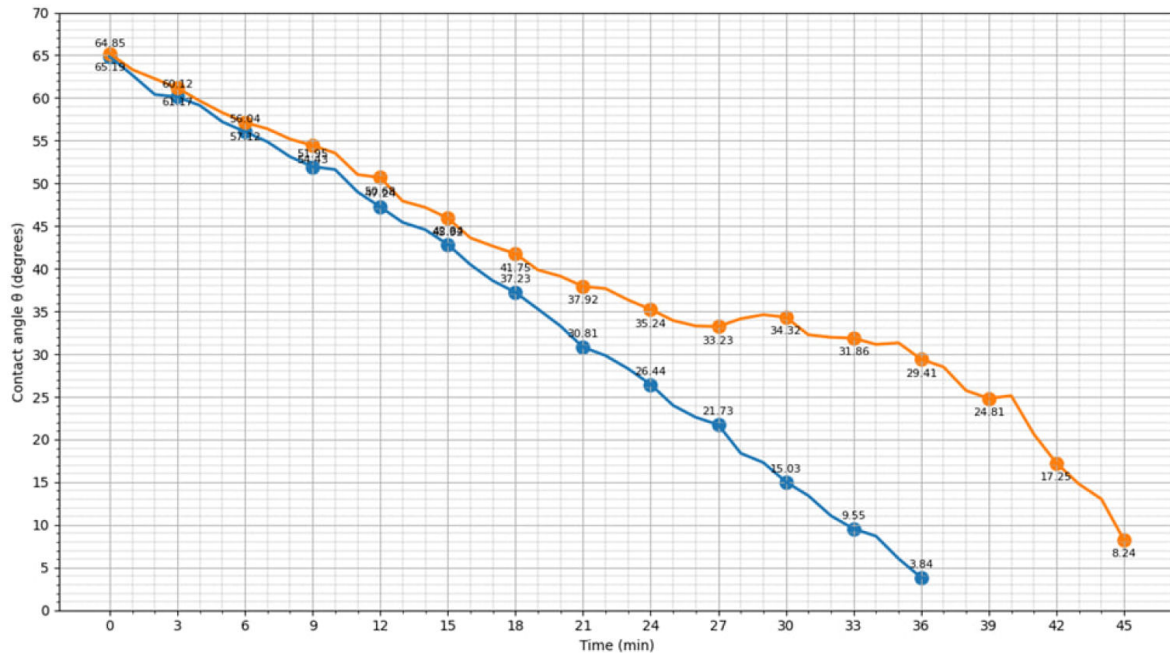


FIGURE 6. Comparative time evolution of the contact angle θ for distilled water (orange symbols) and 0.9 % NaCl solution (blue symbols) droplets during evaporation.

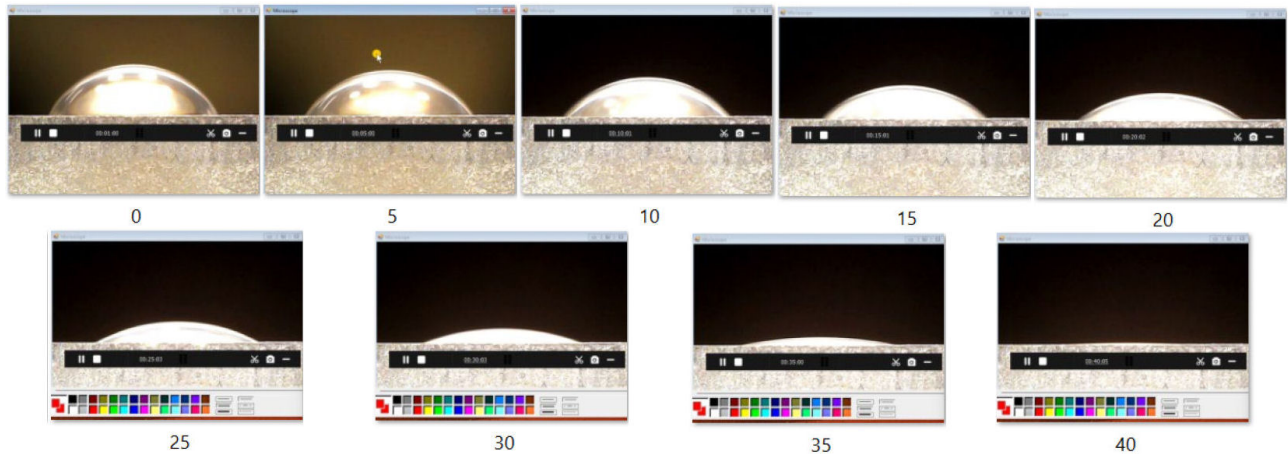


FIGURE 7. Side-profile microscope images of a 0.9 % NaCl solution droplet at representative time intervals (from $t = 0$ to $t = 40$ min) during evaporation, showing the characteristic pinning behavior.

namics. Thus, the water droplet exhibits a nonuniform evolution of the contact angle that reflects the complexity of the evaporation process even under controlled laboratory conditions. The observation of the distilled water droplet was concluded at 45 minutes. At this stage, the droplet had entered its final phase of evaporation, characterized by an extremely low height ($h \approx 0,040$ mm) and a very small contact angle ($\theta \approx 8,24^\circ$). Beyond this point, the droplet effectively becomes a thin, non-uniform liquid film where the spherical-cap geometry is no longer a valid approximation for precise contact-angle calculation. This endpoint is justified by the physical limits of the measurement technique, as the droplet profile transitions from a well-defined cap to a residual liquid

layer.

3.2. Contact-angle dynamics for the 0.9 % NaCl solution droplet

Figure 7 illustrates the side-profile evolution of the 0.9 % NaCl solution droplet during a 40-minute observation period. In contrast to pure water, the saline droplet exhibits a more pronounced pinning of the contact line, where the base diameter remains nearly constant for a longer duration while the height and contact angle decrease more sharply. This behavior is visually evident in the later stages of the evaporation process.

For the 0.9 % NaCl solution droplet, the contact-angle

evolution was measured over the interval 0–36 min. At the initial time, $\theta \approx 64,85^\circ$, indicating that the initial contact angle is very close to that of the distilled water droplet under the same experimental conditions. This similarity at the beginning of the experiment makes it possible to compare the subsequent evaporation behavior of the two droplets on a common basis. However, during the later stages of the process, the contact angle of the NaCl solution droplet decreases more rapidly than that of the water droplet and, by the end of the experiment, reaches the regime of very small angles. This behavior suggests that the temporal evolution of the droplet geometry is more pronounced in the presence of the saline solution. The measured geometric parameters and the corresponding calculated contact-angle values for the NaCl solution droplet are presented in Table II.

The contact angle dynamics for the NaCl solution are compared with water in Fig. 6 (blue curve). For the NaCl droplet, the decrease of $\theta(t)$ is smoother and almost monotonic compared with the water droplet, and short-term deviations are less pronounced. This suggests that, in the presence of the NaCl solution, the contact-line dynamics may differ from those observed for the water droplet. As evaporation proceeds, the increase in concentration may modify interfacial interactions and wetting conditions, which could contribute to a faster reduction of the contact angle.

3.3. Comparative analysis of distilled water and 0.9 % NaCl droplets

To directly compare the contact-angle dynamics of the water and NaCl droplets, Fig. 6 shows the combined $\theta(t)$ curves for both droplets in a single coordinate system. The presented curves correspond to representative measurements obtained under identical experimental conditions for both liquids. The comparative analysis shows that, although the initial contact angles are almost equal, at later stages of evaporation the contact angle of the NaCl solution droplet decreases faster than that of the water droplet and enters the small-angle regime much earlier. In the water droplet, the $\theta(t)$ curve exhibits more pronounced stick-slip-like features. This difference may be related to the influence of NaCl ions on surface tension, wetting behavior, and concentration changes occurring during evaporation.

3.4. Discussion of physical mechanisms

The obtained results suggest that the time evolution of the contact angle during evaporation is closely related to contact-line dynamics, interfacial interactions, and the redistribution of mass within the droplet. For the distilled water droplet, the nonuniform character of the $\theta(t)$ curve and the presence of

TABLE II. Time-dependent values of the geometric parameters and the contact angle θ during evaporation of a 0.9 % NaCl solution droplet.

Time (min)	Diameter (mm)	Height (mm)	θ ($^\circ$)	Time (min)	Diameter (mm)	Height (mm)	θ ($^\circ$)
0	3.397	1.079	64.85285	19	3.246	0.516	35.27402
1	3.389	1.032	62.68527	20	3.238	0.484	33.28807
2	3.381	0.984	60.40534	21	3.230	0.445	30.81021
3	3.373	0.976	60.11708	22	3.222	0.429	29.82299
4	3.357	0.952	59.12148	23	3.214	0.405	28.29050
5	3.349	0.913	57.20174	24	3.175	0.373	26.44483
6	3.341	0.889	56.04167	25	3.135	0.333	23.98724
7	3.333	0.865	54.86331	26	3.103	0.310	22.59856
8	3.333	0.833	53.11635	27	3.064	0.294	21.72666
9	3.325	0.810	51.95236	28	3.040	0.246	18.38632
10	3.317	0.802	51.61399	29	3.024	0.230	17.29864
11	3.310	0.754	48.98699	30	3.016	0.199	15.03496
12	3.302	0.722	47.24055	31	2.976	0.175	13.41521
13	3.302	0.691	45.42196	32	2.952	0.143	11.06749
14	3.294	0.675	44.57118	33	2.849	0.119	9.550584
15	3.278	0.643	42.84138	34	2.714	0.103	8.681166
16	3.270	0.603	40.48869	35	2.690	0.071	6.043462
17	3.262	0.571	38.58948	36	2.389	0.040	3.835873
18	3.254	0.548	37.22872				

short-term deviations are consistent with intermittent pinning and depinning of the contact line. Such behavior is typical of evaporation in a mixed or hybrid regime between the constant contact radius (CCR) and constant contact angle (CCA) limits, where temporary fixation of the contact line is followed by partial motion of the contact perimeter. In the initial stage

of evaporation, the behavior of the water droplet is close to the CCR regime, since the contact angle decreases while the contact radius remains nearly unchanged. At later stages, the appearance of local deviations and more noticeable contact-line motion suggests a transition toward a hybrid evaporation regime.

For the 0.9 % NaCl solution droplet, the decrease of the contact angle is smoother and closer to a monotonic trend. This behavior suggests that the presence of dissolved ions modifies the interfacial conditions and the mobility of the contact line. As evaporation proceeds, the local salt concentration near the contact line increases because the evaporative flux is generally higher near the droplet edge. This concentration increase may affect both the local surface tension and the balance of adhesive forces acting at the three-phase boundary. As a consequence, the contact-line dynamics may differ from those of the pure-water droplet, and the observed evolution becomes less irregular.

A possible physical interpretation is that the redistribution of ions during evaporation changes the coupling between surface tension, concentration gradients, and contact-line mobility. In evaporating saline droplets, concentration gradients may develop between the droplet center and the peripheral region, especially at later stages of evaporation. Such gradients can modify the local interfacial state and can contribute to a smoother recession of the droplet profile. In this sense, the faster decrease of the contact angle observed for the NaCl solution may be related not only to evaporation itself, but also to concentration-dependent changes in wetting behavior. This interpretation is consistent with previous studies showing that solute accumulation near the contact-line region can modify interfacial conditions and influence pinning–depinning behavior in evaporating saline droplets [8, 9].

In the saline droplet, evaporation leads to a gradual increase in salt concentration, particularly near the droplet edge where the evaporative flux is higher. This localized solute accumulation can enhance contact-line pinning and keep the droplet base nearly constant for a longer period, corresponding to behavior close to the CCR mode. Under such conditions, mass loss occurs while the contact line remains relatively constrained; therefore, the contact angle decreases more sharply in order to preserve the spherical-cap geometry. This interpretation also explains why the faster decrease of $\theta(t)$ in the 0.9 % NaCl droplet should not be directly attributed to a higher volumetric evaporation rate. Although dissolved ions may slightly reduce the vapor pressure and thus tend to slow evaporation, the observed $\theta(t)$ evolution is mainly associated with stronger three-phase contact-line pinning. In contrast, the distilled water droplet exhibits more frequent depinning events, which allows the contact angle to decrease at a slower overall rate.

The present observations are qualitatively consistent with previous studies on sessile-droplet evaporation. In particular, the nonuniform evaporation of pure-water droplets and the importance of pinning–depinning effects are in agreement with the general framework described for evaporating droplets on solid substrates [2–4]. In addition, the role of saline content in modifying evaporation behavior and interfacial processes is consistent with reports on evaporating salt-solution droplets [7–9]. At the same time, the present work differs from many previous studies in that the contact-angle evolution is determined here by a simple geometric method

based on direct measurements of droplet height and base diameter, without the use of complex optical goniometric systems. While previous models often focus on pure liquids, the main contribution of this study is the systematic evaluation of electrolyte influence on contact-line pinning using an accessible yet robust geometric approach. By bridging the gap between complex theoretical models and practical laboratory measurements, this research establishes a reliable framework for studying the wetting dynamics of saline solutions at physiologically relevant concentrations, which has remained less explored in recent literature.

4. Conclusion

A quantitative comparison of the evaporation kinetics reveals that the 0.9 % NaCl solution droplet reaches the low-contact-angle regime ($\theta < 10^\circ$) significantly faster than the distilled water droplet. Specifically, the saline droplet achieves this state at $t = 33$ min, while the water droplet requires approximately 44 min to reach a comparable angle, representing a 25 % reduction in the total duration of the spherical-cap stage. This accelerated decrease in $\theta(t)$ is consistent with the findings of Shahidzadeh *et al.* [8], who observed that solute accumulation at the contact line restricts the recession of the droplet base, thereby forcing a steeper decline in the contact angle to accommodate volume loss. Furthermore, the stick–slip behavior observed in our pure water samples, characterized by contact angle fluctuations of up to 2° – 3° (e.g., between $t = 27$ and $t = 30$ min), is markedly absent in the saline droplets, where the ions effectively stabilize the three-phase boundary. These observations provide a more detailed quantitative description of how electrolyte concentration influences wetting dynamics compared with previous qualitative descriptions.

In this study, the time evolution of the contact angle θ for distilled water droplets and 0.9 % NaCl solution droplets evaporating on a glass surface was investigated experimentally and comparatively analyzed. The contact angle was determined using a geometric approach based on the measured droplet parameters, and the $\theta(t)$ dynamics were evaluated at different stages of the evaporation process.

The experimental results showed that, for both liquids, the contact angle follows an overall decreasing trend during evaporation. However, the evolution of the contact angle appears to depend on the liquid composition. For the distilled water droplet, the variation of $\theta(t)$ is nonuniform and shows features consistent with stick–slip-type contact-line behavior. In contrast, for the 0.9 % NaCl solution droplet, the decrease of the contact angle is smoother and almost monotonic, and short-term fluctuations are less pronounced. These differences may be related to the influence of electrolyte ions on wetting conditions and contact-line dynamics.

The applied geometric approach makes it possible to determine the contact angle in real time using simple microscopic measurements, without employing complex optical goniometric systems. The obtained results show that this

methodology is practically useful for comparative evaluation of wetting dynamics during sessile droplet evaporation and for analyzing the influence of electrolyte solutions on the

contact-angle evolution under controlled conditions. A more detailed statistical analysis based on repeated measurements and uncertainty estimation will be considered in future work.

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Constructing the Hamiltonian for a free 1D KFGM particle in an interval

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We analyze the problem of a free 1D Klein-Fock-Gordon-Majorana (KFGM) particle in an interval. By free, we mean that there is no potential within the interval and that its walls are penetrable; hence, the pertinent energy current density does not vanish at the walls. Certainly, quantization in an interval is not trivial because certain restrictions imposed by the domains of the operators involved arise. Here, our objective is to obtain the Hamiltonian for these particles. In practice, the Feshbach-Villars (FV)—free Hamiltonian is the proper operator for characterizing them and is a function of the momentum operator. Additionally, a Majorana condition must also be imposed on the wavefunctions on which these two operators can act. Thus, we start by calculating the pseudo self-adjoint momentum operator. A three-parameter set of boundary conditions (BCs) constitutes its domain. Up to this point, the domain of the Hamiltonian is induced by the domain of the momentum operator; however, we ensure that only the BCs for which the energy current density has the same value at each end of the interval are in its domain. All these BCs essentially belong to a one-parameter set of BCs. Moreover, because the FV equation is invariant under the operation of parity, the parity-transformed wavefunction is also a solution of this equation, which further restricts the domain of the free FV Hamiltonian. Finally, knowing the most general three-parameter set of BCs for the pseudo self-adjoint FV Hamiltonian for a 1D KFGM particle in an interval, we find that only two BCs can remain within the domain of the FV—free Hamiltonian: the periodic BC and the antiperiodic BC. These BCs are satisfied by both the two-component FV wavefunction, with these components being related, and the one-component KFG wavefunction, which can be real or imaginary.

Keywords: Klein-Fock-Gordon-Majorana particles; Feshbach-Villars-Majorana particles; Klein-Fock-Gordon wave equation; Feshbach-Villars wave equation; pseudo self-adjoint operator; local observables; quantum boundary conditions.

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1. Introduction

As discussed in a few articles and books, for example, in Refs. [1–4], the Schrödinger Hamiltonian for a free one-dimensional (1D) Schrödinger particle moving in a penetrable or transparent-walled interval, *e.g.*, $\Omega = [a, b]$, is a function of its momentum operator squared. As a consequence, the boundary conditions (BCs) present in its domain are the same as those in the domain of the self-adjoint momentum operator, namely, $\Phi_S(b, t) = e^{i\theta} \Phi_S(a, t)$, with $\theta \in [0, 2\pi)$; however, in addition, $(\hat{p}_S \Phi_S)(x, t)$, *i.e.*, $\Phi'_S(x, t)$, must also satisfy this BC, *i.e.*, $\Phi'_S(b, t) = e^{i\theta} \Phi'_S(a, t)$ (the prime symbol is used to denote the first spatial derivative of a function hereinafter). Thus, we have a one-parameter general set of BCs for this Hamiltonian, which is also a self-adjoint operator [2]. Clearly, the well-known Dirichlet BC, *i.e.*, $\Phi_S(b, t) = \Phi_S(a, t) = 0$, is not included in this general set of BCs. Indeed, if this BC was included, the interval could not be considered penetrable but impenetrable; *i.e.*, the relation $j_S(b, t) = j_S(a, t) = 0$, *i.e.*, the so-called impenetrability condition at the extremes of the interval, would be verified, and the particle would not truly be a free particle. We recall that, as a consequence of the self-adjointness of the Hamiltonian, the usual probability current density $j_S = j_S(x, t) = \frac{\hbar}{m} \text{Im}(\Phi_S^* \Phi'_S)$ always satisfies the relation $j_S(b, t) = j_S(a, t)$ [1]. Thus, the local observable suitable for characterizing a 1D Schrödinger particle living in a finite interval (in an impenetrable interval or in an interval with

transparent walls) is precisely j_S .

The number of BCs characterizing a free 1D Schrödinger particle in an interval can be further restricted if one takes into account that the free Schrödinger equation has as its solution the wavefunction $\Phi_S(x, t)$ and its parity-transformed wavefunction $(\hat{\Pi}_S \Phi_S)(x, t) = \Phi_S(a + b - x, t)$. Thus, this fact leads to only two BCs: the periodic BC (*i.e.*, $\theta = 0$), $\Phi_S(b, t) = \Phi_S(a, t)$ and $\Phi'_S(b, t) = \Phi'_S(a, t)$; and the antiperiodic BC (*i.e.*, $\theta = \pi$), $\Phi_S(b, t) = -\Phi_S(a, t)$ and $\Phi'_S(b, t) = -\Phi'_S(a, t)$. Naturally, only for these two BCs is there no distinction between the two walls of the interval, as is to be expected for a particle moving freely within an interval (see Appendix A). For example, in Ref. [5], the antiperiodic BC was used in the description of a genuine free 1D Schrödinger particle in an interval; however, the domain of the (free) Hamiltonian operator was not given explicitly. Similarly, the problem of the free 1D Dirac particle in the finite interval was considered in Ref. [6]. Considering that the momentum operator under the parity operation must be transformed as a polar vector and that the Hamiltonian operator function of this operator must be self-adjoint and that it commutes with the combined operations of charge conjugation, parity and time reversal (*i.e.*, the free time-dependent Dirac equation is form invariant under this combined discrete symmetry), the periodic and antiperiodic BCs were also obtained. Certainly, the usual Dirac probability current density in these two physical situations does not vanish at the interval walls. Incidentally, the BCs for a 1D Weyl-Majorana particle

in an interval can be only the periodic and the antiperiodic BCs; that is, only these two BCs can be imposed on the wavefunctions that describe this type of particle (with a potential within the interval, or not) [7].

The nontrivial local observable that appears to be physically acceptable for completely characterizing a strictly neutral 1D Klein-Fock-Gordon (KFG) particle [8–10] (or a strictly neutral 1D Feshbach-Villars (FV) particle [11]), *i.e.*, a 1D KFG-Majorana (KFGM) particle [12, 13] (or a 1D FV-Majorana (FVM) particle) that lies within the interval $\Omega = [a, b]$ (confined to the interval or restricted in the interval with transparent walls), is given by

$$j_{\text{en}} = j_{\text{en}}(x, t) = -\frac{\hbar^2}{2m} \frac{1}{2} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Phi')^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi} - ((\hat{\tau}_3 + i\hat{\tau}_2)\Phi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi}' \right], \quad (1)$$

where $\Phi = \Phi(x, t)$ is a two-component FV wavefunction [14], $\dot{\Phi} = \partial\Phi/\partial t$ hereinafter, and $\hat{\tau}_2 = \hat{\sigma}_y$ and $\hat{\tau}_3 = \hat{\sigma}_z$ are Pauli matrices. We recall that the KFG and FV wave equations are completely equivalent, as long as the mass of the particle is not zero. The energy current density in Eq. (1) is a real quantity when it is calculated for a state Φ satisfying a Majorana condition, which is physically adequate [14]. Additionally, as a consequence of the pseudo self-adjointness (*i.e.*, generalized self-adjointness) of the Hamiltonian operator of the system, it follows that

$$j_{\text{en}}(b, t) = j_{\text{en}}(a, t). \quad (2)$$

A necessary condition for having a confined 1D KFGM particle to an interval is that the energy current density j_{en} (*i.e.*, the flow of energy) disappears at the walls of that interval, *i.e.*, $j_{\text{en}}(b, t) = j_{\text{en}}(a, t) = 0$. On the other hand, a necessary condition for having a free 1D KFGM particle in an interval is that j_{en} simply obeys the relation given in Eq. (2), *i.e.*, $j_{\text{en}}(b, t) = j_{\text{en}}(a, t)$. In the latter case, we say that the interval has transparent walls (or walls that allow leaks) [14]. Let us also note that we have not used here the usual KFG current density $j = j(x, t)$ (this density is $i\hbar/4m$ multiplied by the term in brackets in Eq. (1), but without any of the time derivatives). The reason is that this local observable vanishes everywhere whenever a Majorana condition is imposed on Φ . Therefore, j does not allow distinguishing between penetrable and impenetrable BCs if the particle is a 1D KFGM particle [14] (see Appendix B).

The main objective of our paper is to obtain the pseudo self-adjoint Hamiltonian operator that is physically adequate for characterizing a truly free 1D KFGM particle in an interval, *i.e.*, its specific domain (which includes the proper BCs). This operator, the FV—free Hamiltonian, is a function of the momentum operator for this particle; hence, the latter operator plays an important role in the construction of the Hamiltonian. Additionally, a Majorana condition must also be imposed on the two-component wavefunctions on which these two operators can act. Specifically, in the next section, we

obtain the domain of the pseudo self-adjoint momentum operator that is consistent with the Majorana condition. We find that a three-parameter general family of BCs constitutes the domain of this operator. In Sec. 3, we show how the domain of the free FV Hamiltonian is induced by the domain of the momentum operator. After that, we first ensure that, in the domain of the free FV Hamiltonian, only the BCs that satisfy the relation in Eq. (2) remain. Because the (free) FV equation is invariant under parity (*i.e.*, space reflection), the parity-transformed wavefunction is also a solution of this equation, which further restricts the domain of the Hamiltonian. To determine whether the BCs that emerge here (written in terms of the two-component FV wavefunction) can actually be in the domain of the pseudo self-adjoint-free Hamiltonian operator, we use the relation that connects the FV wavefunctions with the one-component KFG wavefunctions and transforms these BCs into BCs for the KFG wavefunction. The reason for this is that we already know the most general three-parameter set of BCs written in terms of the one-component KFG wavefunction for the pseudo self-adjoint FV Hamiltonian that describes a 1D KFGM particle in an interval. Thus, only BCs that are in this general three-parameter set can be part of the domain of the free FV Hamiltonian operator, which is also a pseudo self-adjoint operator. In the end, only two quantum BCs remain in the domain of the free FV Hamiltonian: the periodic BC and the antiperiodic BC. Finally, we discuss our results in Sec. 4 and complement what was mentioned in the second paragraph of this Introduction in Appendix A. Similarly, in Appendix B, we provide details that complement the ideas presented in the third paragraph of this Introduction, whereas a particular “extra” set of BCs that arises in Sec. 3 is analyzed in Appendix C.

2. The momentum operator for a 1D KFGM particle

The Hamiltonian operator describing a free 1D KFGM particle, *i.e.*, a free 1D KFG particle that is also strictly neutral, is the free FV Hamiltonian, namely,

$$\begin{aligned} \hat{h} &= (\hat{\tau}_3 + i\hat{\tau}_2) \frac{\hat{p}^2}{2m} + mc^2 \hat{\tau}_3 \\ &= (\hat{\tau}_3 + i\hat{\tau}_2) \frac{1}{2m} \hat{p} \hat{p} + mc^2 \hat{\tau}_3, \end{aligned} \quad (3)$$

where

$$\hat{p} = -i\hbar \hat{1}_2 \frac{\partial}{\partial x}, \quad (4)$$

is the momentum operator, $\hat{\tau}_2 = \hat{\sigma}_y$, $\hat{\tau}_3 = \hat{\sigma}_z$ and $\hat{1}_2$ is the 2×2 identity matrix [15, 16]. Moreover, the functions on which $\hat{p}$ (and $\hat{h}$) act are two-component wavefunctions of the form $\Phi = \Phi(x, t) = [\phi_1 \ \phi_2]^T = [\phi_1(x, t) \ \phi_2(x, t)]^T$ (the symbol T represents the transpose of a matrix) and must satisfy a Majorana condition, *i.e.*, $\Phi = \Phi_c \equiv \hat{\tau}_1 \Phi^*$ ($\Rightarrow \phi_2 = \phi_1^*$) or $\Phi = -\Phi_c = -\hat{\tau}_1 \Phi^*$ ($\Rightarrow \phi_2 = -\phi_1^*$), where

Φ_c is the charge-conjugate wavefunction, the asterisk denotes the complex conjugation operation and $\hat{\tau}_1 = \hat{\sigma}_x$ is a Pauli matrix. Clearly, the two components of Φ are not independent [13].

The formal generalized adjoint of $\hat{p}$ is defined as follows:

$$\hat{p}_{\text{adj}} \equiv \hat{\tau}_3 \hat{p}^\dagger \hat{\tau}_3 = -i\hbar \hat{1}_2 \frac{\partial}{\partial x}, \quad (5)$$

where $\hat{p}^\dagger$ is the usual formal Hermitian conjugate of $\hat{p}$. Clearly, the actions of $\hat{p}_{\text{adj}}$ and $\hat{p}$ are equal. The definition given in Eq. (5) leads to the following relation:

$$\langle\langle \hat{p}_{\text{adj}} \Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{p} \Phi \rangle\rangle, \quad (6)$$

where the indefinite (or improper) inner product is defined as follows:

$$\langle\langle \Psi, \Phi \rangle\rangle \equiv \int_{\Omega} dx \Psi^\dagger \hat{\tau}_3 \Phi = \langle\langle \Phi, \Psi \rangle\rangle^*, \quad (7)$$

($\Psi = [\psi_1 \ \psi_2]^T$ and $\Phi = [\phi_1 \ \phi_2]^T$). We assume that the particle lives in the interval $\Omega = [a, b]$. The inner product in Eq. (7) is defined over an indefinite inner product space; in our case, a $\hat{\tau}_3$ -space [17, 18]. The relation in Eq. (6) defines the generalized adjoint of $\hat{p}$ on the $\hat{\tau}_3$ -space, *i.e.*, $\hat{p}_{\text{adj}}$, where $\Psi \in \mathcal{D}(\hat{p}_{\text{adj}})$, the domain of $\hat{p}_{\text{adj}}$, and $\Phi \in \mathcal{D}(\hat{p})$, the domain of $\hat{p}$. These domains are linear subsets of the $\hat{\tau}_3$ -space on which we allow the operators $\hat{p}$ and $\hat{p}_{\text{adj}}$ to act. Certainly, BCs are a key part of these domains, and $\mathcal{D}(\hat{p})$ and $\mathcal{D}(\hat{p}_{\text{adj}})$ do not have to be the same.

If $\hat{p}$ satisfies the relation

$$\langle\langle \hat{p} \Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{p} \Phi \rangle\rangle, \quad (8)$$

the operator $\hat{p}$ is a generalized self-adjoint operator or a pseudo self-adjoint operator, *i.e.*, $\hat{p} = \hat{p}_{\text{adj}}$; hence, the actions of $\hat{p}$ and $\hat{p}_{\text{adj}}$ must be equal (in fact, they are equal), and their domains must also be the same. Specifically, by virtue of one integration by parts, $\hat{p}$ and $\hat{p}_{\text{adj}}$ satisfy the following relation:

$$\langle\langle \hat{p}_{\text{adj}} \Psi, \Phi \rangle\rangle = \langle\langle \Psi, \hat{p} \Phi \rangle\rangle + f[\Psi, \Phi; \Omega], \quad (9)$$

where the term evaluated at the boundaries of Ω is given by

$$\begin{aligned} f[\Psi, \Phi; \Omega] &= i\hbar \left[\Psi^\dagger \hat{\tau}_3 \Phi \right]_a^b \\ &= i\hbar \left\{ \begin{bmatrix} \psi_1(b, t) \\ \psi_2(a, t) \end{bmatrix}^\dagger \begin{bmatrix} \phi_1(b, t) \\ \phi_2(a, t) \end{bmatrix} \right. \\ &\quad \left. - \begin{bmatrix} \psi_2(b, t) \\ \psi_1(a, t) \end{bmatrix}^\dagger \begin{bmatrix} \phi_2(b, t) \\ \phi_1(a, t) \end{bmatrix} \right\}, \end{aligned} \quad (10)$$

(in the latter expression, we use the definition $[g]_a^b \equiv g(b, t) - g(a, t)$). Let us suppose initially that any wavefunction $\Phi \in \mathcal{D}(\hat{p})$ satisfies the BC $\Phi(a, t) = \Phi(b, t) = 0$, that is, $\phi_1(a, t) = \phi_2(a, t) = \phi_1(b, t) = \phi_2(b, t) = 0$. In this case, the boundary term $f[\Psi, \Phi; \Omega]$ in Eq. (10) vanishes, and Eq. (6) is verified without requiring any BC on the functions

$\Psi \in \mathcal{D}(\hat{p}_{\text{adj}})$. Thus, by initially choosing this BC, one has that $\mathcal{D}(\hat{p}) \neq \mathcal{D}(\hat{p}_{\text{adj}})$ (in fact, $\mathcal{D}(\hat{p}) \subset \mathcal{D}(\hat{p}_{\text{adj}})$); hence, $\hat{p}$ is not a pseudo self-adjoint operator.

If the operator $\hat{p}$ aims to be a pseudo self-adjoint operator, *i.e.*, $\hat{p} = \hat{p}_{\text{adj}}$, then $\mathcal{D}(\hat{p}) = \mathcal{D}(\hat{p}_{\text{adj}})$. Thus, we must allow every wavefunction Φ inside $\mathcal{D}(\hat{p})$ to satisfy some BCs that are less restrictive than the one used above. Let us propose the following general set of BCs that will be part of the domain $\mathcal{D}(\hat{p})$:

$$\begin{bmatrix} \phi_1(b, t) \\ \phi_2(a, t) \end{bmatrix} = \hat{N} \begin{bmatrix} \phi_2(b, t) \\ \phi_1(a, t) \end{bmatrix}, \quad (11)$$

where $\hat{N}$ is an arbitrary complex matrix. Substituting this relation into $f[\Psi, \Phi; \Omega]$ given in Eq. (10), we obtain the following expression:

$$\begin{aligned} f[\Psi, \Phi; \Omega] &= i\hbar \left\{ \begin{bmatrix} \psi_1(b, t) \\ \psi_2(a, t) \end{bmatrix}^\dagger \hat{N} \right. \\ &\quad \left. - \begin{bmatrix} \psi_2(b, t) \\ \psi_1(a, t) \end{bmatrix}^\dagger \right\} \begin{bmatrix} \phi_2(b, t) \\ \phi_1(a, t) \end{bmatrix}, \end{aligned} \quad (12)$$

and because $f[\Psi, \Phi; \Omega]$ must be zero, and we do not wish to use the initially chosen BC (because, for the latter, we have that $\hat{p} \neq \hat{p}_{\text{adj}}$), *i.e.*, $\phi_2(b, t) = \phi_1(a, t) = 0$ and $\phi_1(b, t) = \phi_2(a, t) = 0$, we have that

$$\begin{aligned} \begin{bmatrix} \psi_1(b, t) \\ \psi_2(a, t) \end{bmatrix}^\dagger \hat{N} &= \begin{bmatrix} \psi_2(b, t) \\ \psi_1(a, t) \end{bmatrix}^\dagger \\ \Rightarrow \begin{bmatrix} \psi_2(b, t) \\ \psi_1(a, t) \end{bmatrix} &= \hat{N}^\dagger \begin{bmatrix} \psi_1(b, t) \\ \psi_2(a, t) \end{bmatrix}. \end{aligned} \quad (13)$$

Because any wavefunction $\Psi \in \mathcal{D}(\hat{p}_{\text{adj}})$ would have to satisfy the same BCs that $\Phi \in \mathcal{D}(\hat{p})$ satisfies, *i.e.*, in addition to the BCs in Eq. (13), Ψ should also satisfy the BCs that are in Eq. (11), namely,

$$\begin{bmatrix} \psi_1(b, t) \\ \psi_2(a, t) \end{bmatrix} = \hat{N} \begin{bmatrix} \psi_2(b, t) \\ \psi_1(a, t) \end{bmatrix}. \quad (14)$$

Now, substituting this result into the result given in Eq. (13), we find that $\hat{N}$ is a unitary matrix, *i.e.*,

$$\hat{N}^\dagger = \hat{N}^{-1}. \quad (15)$$

This is the condition on $\hat{N}$ that ensures that any BC taken from the set given in Eq. (11), which is included in the domain of $\hat{p}$, is also in the domain of $\hat{p}_{\text{adj}}$. In this way, we make these two domains equal and ensure that $\hat{p} = \hat{p}_{\text{adj}}$, *i.e.*, that $\hat{p}$ is a pseudo self-adjoint operator. Because $\hat{N}$ is a unitary matrix, the result in Eq. (14) is a four-parameter general family of BCs.

Let us also note that the Dirac Hamiltonian operator in (1+1) dimensions $\hat{h}_D = c\hat{\alpha}\hat{p}$ ($\hat{p} = -i\hbar\hat{1}_2\partial/\partial x$), where $x \in \Omega = [a, b]$, in the Weyl representation ($\hat{\alpha} = \hat{\sigma}_z$), is a self-adjoint operator when its domain contains the general set of BCs given in Eq. (11), with $\hat{N}$ being a unitary matrix. In

this case, the operator $\hat{h}_D$ acts on two-component wavefunctions, and the scalar product for these wavefunctions is the usual one, *i.e.*, $\langle \Phi_D, \Psi_D \rangle \equiv \int_{\Omega} dx \Phi_D^\dagger \Psi_D$ (see, for example, Ref. [19] and references therein).

If we impose $\Psi = \Phi$ in Eq. (8) and in Eq. (9) with the result $\hat{p} = \hat{p}_{\text{adj}}$, we obtain the following condition:

$$f[\Phi, \Phi; \Omega] = i\hbar [\varrho]_a^b = 0 \Rightarrow \varrho(b, t) = \varrho(a, t), \quad (16)$$

where the usual KFG density is given by

$$\varrho = \varrho(x, t) = \Phi^\dagger \hat{\tau}_3 \Phi = |\phi_1|^2 - |\phi_2|^2. \quad (17)$$

Similar to the relation given in Eq. (9), the following relation between $\hat{p}$ and $\hat{p}_{\text{adj}}$ can also be written:

$$\langle \langle \hat{p}_{\text{adj}} \Psi, \hat{E} \Phi \rangle \rangle = \langle \langle \Psi, \hat{p} \hat{E} \Phi \rangle \rangle + f[\Psi, \hat{E} \Phi; \Omega], \quad (18)$$

where $\hat{E} = i\hbar \hat{1}_2 \partial/\partial t$ is the energy operator. Naturally, if $\Phi \in \mathcal{D}(\hat{p})$, then, automatically, $\hat{E} \Phi \in \mathcal{D}(\hat{p})$. If Φ satisfies a BC, then $\hat{E} \Phi$ satisfies that same BC. Consequently, any BC included in the general set of BCs, which we know leads to the cancellation of the boundary term in Eq. (10), must also cancel out the boundary term in Eq. (18) (compare the boundary terms in Eqs. (10) and (18) and note that if Φ satisfies a BC, then $\hat{E} \Phi$ also satisfies that BC). We recall that for any of the BCs that are within the general family of BCs, $\hat{p}$ is a pseudo self-adjoint operator, *i.e.*, $\hat{p} = \hat{p}_{\text{adj}}$ (*i.e.*, $\hat{p}$ acts the same as $\hat{p}_{\text{adj}}$ and $\mathcal{D}(\hat{p}) = \mathcal{D}(\hat{p}_{\text{adj}})$). Similarly, if we impose $\Psi = \Phi$ in Eq. (18) with the result $\hat{p} = \hat{p}_{\text{adj}}$, we obtain the following result:

$$\begin{aligned} f[\Phi, \hat{E} \Phi; \Omega] &= i\hbar [\varrho_{\text{en}}]_a^b = 0 \\ \Rightarrow \varrho_{\text{en}}(b, t) &= \varrho_{\text{en}}(a, t), \end{aligned} \quad (19)$$

where the (complex) KFG energy density is given by

$$\varrho_{\text{en}} = \varrho_{\text{en}}(x, t) = \Phi^\dagger \hat{\tau}_3 \hat{E} \Phi = i\hbar (\dot{\phi}_1^* \phi_1 - \dot{\phi}_2^* \phi_2), \quad (20)$$

where $\dot{\phi}_1 = \partial \phi_1 / \partial t$, etc., as usual [16]. The results given in Eqs. (16) and (19) are straightforward consequences of the pseudo self-adjointness of $\hat{p}$. In addition, j_{en} in Eq. (1) and ϱ_{en} in Eq. (20) satisfy a continuity equation (this situation is valid on-shell, *i.e.*, for solutions Φ of the FV equation. See Appendix B).

If we impose either of the two Majorana conditions on the four-parameter general set of BCs in Eq. (11), *i.e.*, $\phi_2 = \phi_1^* \Rightarrow \phi_1 = \phi_2^*$, or $\phi_2 = -\phi_1^* \Rightarrow \phi_1 = -\phi_2^*$ (with the condition given in Eq. (15)), then it becomes a three-parameter general set of BCs. This is because the unitary matrix $\hat{N}$ must also be a symmetric matrix, namely,

$$\hat{N} = \hat{N}^T. \quad (21)$$

Similarly, if a Majorana condition is imposed on the KFG density in Eq. (17), then it automatically vanishes, *i.e.*, $\varrho = 0$. Moreover, if a Majorana condition is imposed on the (complex) KFG energy density in Eq. (20), it becomes a real quantity, *i.e.*, $\varrho_{\text{en}} = \varrho_{\text{en}}^*$. Certainly, the general set of BCs given in

Eq. (11), with $\hat{N}$ being a unitary and symmetric matrix, can be written in terms of only one of the components of Φ (ϕ_1 or ϕ_2) and the other component can be obtained algebraically ($\phi_2 = \phi_1^*$ or $\phi_1 = \phi_2^*$, when $\Phi = \Phi_c$; and $\phi_2 = -\phi_1^*$ or $\phi_1 = -\phi_2^*$, when $\Phi = -\Phi_c$). All of these are general sets of BCs that make up the domain of the momentum operator $\mathcal{D}(\hat{p})$ for a 1D KFGM particle.

3. The Hamiltonian for a free 1D KFGM particle

The formal action of the Hamiltonian operator for a free 1D KFGM particle is given in Eq. (3), and its domain is essentially given by

$$\begin{aligned} \mathcal{D}(\hat{h}) &= \mathcal{D}(\hat{p}^2) = \mathcal{D}(\hat{p}\hat{p}) \sim \{ \Phi \mid \Phi \in \mathcal{D}(\hat{p}) \\ &\text{and } \hat{p}\Phi \in \mathcal{D}(\hat{p}) \} \subset \mathcal{D}(\hat{p}). \end{aligned} \quad (22)$$

Thus, the wavefunctions Φ belonging to $\mathcal{D}(\hat{h})$ must satisfy the same BCs that $\Phi \in \mathcal{D}(\hat{p})$ satisfy, *i.e.*, must satisfy any BC included in the set of BCs given in Eq. (11), with the matrix $\hat{N}$ satisfying Eqs. (15) and (21). Additionally, because $\hat{p}\Phi \in \mathcal{D}(\hat{p})$, the first spatial derivative of Φ , *i.e.*, ϕ_1' and ϕ_2' , must also satisfy the set of BCs in Eq. (11), with $\hat{N}$ fulfilling $\hat{N}^\dagger = \hat{N}^{-1}$ and $\hat{N} = \hat{N}^T$. The 2×2 unitary and symmetric matrix $\hat{N}$ depends on three real parameters and can be written as follows:

$$\hat{N} = e^{i\mu} \begin{bmatrix} m_0 - i m_3 & -i m_1 \\ -i m_1 & m_0 + i m_3 \end{bmatrix}, \quad (23)$$

where the real quantities m_0 , m_1 and m_3 satisfy $(m_0)^2 + (m_1)^2 + (m_3)^2 = 1$ (in this article, no parameter is labeled with the symbol m_2), and $\mu \in [0, \pi)$ ($\det(\hat{N}) = e^{i2\mu}$). Then, the wavefunctions Φ on which the Hamiltonian given in Eq. (3) can act, *i.e.*, the wavefunctions Φ that make up the domain of $\hat{h}$, $\mathcal{D}(\hat{h})$, can only satisfy BCs that are included in the following family of BCs:

$$\begin{aligned} \begin{bmatrix} \phi_1(b, t) \\ \phi_2(a, t) \end{bmatrix} &= \hat{N} \begin{bmatrix} \phi_2(b, t) \\ \phi_1(a, t) \end{bmatrix}, \quad \text{and} \\ \begin{bmatrix} \phi_1'(b, t) \\ \phi_2'(a, t) \end{bmatrix} &= \hat{N} \begin{bmatrix} \phi_2'(b, t) \\ \phi_1'(a, t) \end{bmatrix}. \end{aligned} \quad (24)$$

Up to this point, the domain of $\hat{h}$ is induced entirely by the domain of $\hat{p}$.

However, the Hamiltonian operator with the latter sets of BCs within its domain is not necessarily a pseudo self-adjoint operator. For example, the relation given in Eq. (2) is not necessarily verified. Certainly, if the latter relation holds for some BC, the Hamiltonian with this BC in its domain is not necessarily a pseudo self-adjoint operator; however, the equality $j_{\text{en}}(b, t) = j_{\text{en}}(a, t)$ is a consequence of the pseudo self-adjointness of $\hat{h}$. Thus, we can restrict the set of BCs in Eq. (24) by requiring the validity of that equality. To obtain the mathematical conditions that ensure that

$j_{\text{en}}(b, t) = j_{\text{en}}(a, t)$, it is convenient to first rewrite the family of BCs given in Eq. (24) as follows:

$$\begin{bmatrix} \phi_1(b, t) \\ \phi_2(b, t) \end{bmatrix} = \hat{V} \begin{bmatrix} \phi_1(a, t) \\ \phi_2(a, t) \end{bmatrix}, \quad \text{and} \quad (25)$$

$$\begin{bmatrix} \phi'_1(b, t) \\ \phi'_2(b, t) \end{bmatrix} = \hat{V} \begin{bmatrix} \phi'_1(a, t) \\ \phi'_2(a, t) \end{bmatrix},$$

where

$$\hat{V} = \frac{i}{m_1} \begin{bmatrix} -e^{i\mu} & m_0 - i m_3 \\ -(m_0 + i m_3) & e^{-i\mu} \end{bmatrix}, \quad (26)$$

and $m_1 \neq 0$ ($\det(\hat{V}) = 1$). Certainly, simple algebraic manipulations of the relations given in Eq. (24) lead to the results in Eqs. (25) and (26). On the other hand, the case $m_1 = 0$ is studied in Appendix C.

Then, evaluating the energy current density given in Eq. (1) at $x = b$, substituting into it the two relations given in Eq. (25) and their time derivatives $\dot{\Phi}(b, t) = \hat{V}\dot{\Phi}(a, t)$ and $\dot{\Phi}'(b, t) = \hat{V}\dot{\Phi}'(a, t)$, and finally equaling with $j_{\text{en}}(a, t)$ (see Eq. (2)), we obtain the result

$$\hat{V}^\dagger(\hat{\tau}_3 + i\hat{\tau}_2)^\dagger(\hat{\tau}_3 + i\hat{\tau}_2)\hat{V} = (\hat{\tau}_3 + i\hat{\tau}_2)^\dagger(\hat{\tau}_3 + i\hat{\tau}_2). \quad (27)$$

By substituting the matrix $\hat{V}$ in Eq. (26) into Eq. (27), the following three equations are obtained:

$$1 + m_0 \cos(\mu) + m_3 \sin(\mu) = (m_1)^2, \quad (28)$$

$$(e^{i\mu} + m_0 + i m_3)^2 = -(m_1)^2, \quad (29)$$

and

$$(e^{-i\mu} + m_0 - i m_3)^2 = -(m_1)^2. \quad (30)$$

From Eqs. (29) and (30), we obtain the same results, namely,

$$m_0 + \cos(\mu) = 0 \quad \text{and} \quad m_3 + \sin(\mu) = \pm m_1. \quad (31)$$

By substituting the latter two equations into Eq. (28), we obtain the result

$$m_3 = 0, \quad (32)$$

and the condition $(m_0)^2 + (m_1)^2 = 1$ is automatically satisfied, that is, $(-\cos(\mu))^2 + (\mp \sin(\mu))^2 = 1$ (we recall that $m_1 \neq 0$; hence, $\mu \neq 0$). Finally, the matrix $\hat{V}$ in Eq. (26) can be written as follows:

$$\hat{V} = \mp \frac{i}{\sin(\mu)} \begin{bmatrix} -e^{i\mu} & -\cos(\mu) \\ \cos(\mu) & e^{-i\mu} \end{bmatrix}, \quad (33)$$

where $\mu \in (0, \pi)$. The BCs that make up the domain of the free FV Hamiltonian in Eq. (3), thus far, are those given in Eq. (25), with the matrix $\hat{V}$ given in Eq. (33). That is, we have a one-parameter general family of BCs for this Hamiltonian operator, namely, $\Phi(b, t) = \hat{V}\Phi(a, t)$ with $\Phi'(b, t) = \hat{V}\Phi'(a, t)$. We recall that this one-parameter family of BCs satisfies the relation given in Eq. (2), *i.e.*, given a BC within

the one-parameter family of BCs, the energy current density has the same value at each end of the interval.

The 1D FV wave equation is given by

$$\hat{E}\Phi = \hat{h}\Phi \Rightarrow i\hbar \hat{1}_2 \frac{\partial}{\partial t} \Phi(x, t) = \left[-\frac{\hbar^2}{2m}(\hat{\tau}_3 + i\hat{\tau}_2) \frac{\partial^2}{\partial x^2} + mc^2 \hat{\tau}_3 \right] \Phi(x, t). \quad (34)$$

If $\Phi(x, t)$ is a solution of this equation, then

$$(\hat{\Pi}\Phi)(x, t) = \Phi(a + b - x, t), \quad (35)$$

is also a solution. The operator $\hat{\Pi}$ is the parity operator, and it reflects the wavefunction around the point $x = (a + b)/2$, *i.e.*, around the midpoint of the interval. In fact, $(\hat{\Pi}\Phi)(a, t) = \Phi(b, t)$, $(\hat{\Pi}\Phi)(b, t) = \Phi(a, t)$ and $(\hat{\Pi}\Phi)((a + b)/2, t) = \Phi((a + b)/2, t)$, as expected. To immediately see that $(\hat{\Pi}\Phi)(x, t)$ is also a solution of the free FV equation in Eq. (34), the formulas $\partial\Phi(u, t)/\partial u = -\partial\Phi(u(x), t)/\partial x$, and therefore, $\partial^2\Phi(u, t)/\partial u^2 = +\partial^2\Phi(u(x), t)/\partial x^2$, where Φ is a function of u and t and where u is a function of x (in fact, $u \equiv a + b - x$), can be used. Because $\Phi(x, t)$ and $(\hat{\Pi}\Phi)(x, t)$ are solutions of the free FV equation, this equation is parity invariant (hence, the Hamiltonian $\hat{h}$ commutes with $\hat{\Pi}$, *i.e.*, $\hat{h}(\hat{\Pi}\Phi) = \hat{\Pi}(\hat{h}\Phi)$ with $\hat{\Pi}\Phi \in \mathcal{D}(\hat{h})$). If $\Phi(x, t)$ and $\Phi'(x, t)$ satisfy a BC, then $(\hat{\Pi}\Phi)(x, t)$ and $(\hat{\Pi}\Phi)'(x, t)$ also satisfy it. Consequently, not only must the BCs given in Eq. (25) be in $\mathcal{D}(\hat{h})$, but the following must also be included:

$$(\hat{\Pi}\Phi)(b, t) = \hat{V}(\hat{\Pi}\Phi)(a, t) \quad \text{and}$$

$$(\hat{\Pi}\Phi)'(b, t) = \hat{V}(\hat{\Pi}\Phi)'(a, t), \quad (36)$$

where $(\hat{\Pi}\Phi)(x, t)$ at $x = a$ and $x = b$ are obtained from Eq. (35). Moreover, $(\hat{\Pi}\Phi)'(x, t) = (\partial/\partial x)(\Phi(a + b - x, t)) = -(\partial/\partial u)(\Phi(u, t))|_{u=a+b-x}$, *i.e.*, $(\hat{\Pi}\Phi)'(x, t) = -\Phi'(a + b - x, t)$; hence, $(\hat{\Pi}\Phi)'(a, t) = -\Phi'(b, t)$ and $(\hat{\Pi}\Phi)'(b, t) = -\Phi'(a, t)$. The BCs given in Eq. (36) can be written as follows:

$$\begin{bmatrix} \phi_1(a, t) \\ \phi_2(a, t) \end{bmatrix} = \hat{V} \begin{bmatrix} \phi_1(b, t) \\ \phi_2(b, t) \end{bmatrix}, \quad \text{and} \quad -\begin{bmatrix} \phi'_1(a, t) \\ \phi'_2(a, t) \end{bmatrix} = -\hat{V} \begin{bmatrix} \phi'_1(b, t) \\ \phi'_2(b, t) \end{bmatrix}, \quad (37)$$

where $\hat{V}$ is given in Eq. (33). Substituting the latter two relations into those given in Eq. (25), we obtain a new constraint on the matrix $\hat{V}$, namely,

$$\hat{V}^2 = \hat{1}_2. \quad (38)$$

By substituting the matrix $\hat{V}$ in Eq. (33) into Eq. (38), the following three equations are obtained:

$$\sin(\mu) \cos(\mu) = 0, \quad (39)$$

$$e^{i2\mu} - (\cos(\mu))^2 = -(\sin(\mu))^2, \quad (40)$$

and

$$e^{-i2\mu} - (\cos(\mu))^2 = -(\sin(\mu))^2, \quad (41)$$

and whose only common solution is given by

$$\mu = \frac{\pi}{2}. \quad (42)$$

Consequently, the matrix $\hat{V}$ in Eq. (33) takes the form

$$\hat{V} = \mp i \begin{bmatrix} -i & 0 \\ 0 & -i \end{bmatrix} = \mp \hat{1}_2, \quad (43)$$

and the BCs that are part of the domain of the free FV Hamiltonian are the following:

$$\begin{aligned} \begin{bmatrix} \phi_1(b, t) \\ \phi_2(b, t) \end{bmatrix} &= \mp \begin{bmatrix} \phi_1(a, t) \\ \phi_2(a, t) \end{bmatrix}, \quad \text{and} \\ \begin{bmatrix} \phi'_1(b, t) \\ \phi'_2(b, t) \end{bmatrix} &= \mp \begin{bmatrix} \phi'_1(a, t) \\ \phi'_2(a, t) \end{bmatrix}, \end{aligned} \quad (44)$$

that is, the periodic BC, $\Phi(b, t) = \Phi(a, t)$ and $\Phi'(b, t) = \Phi'(a, t)$, and the antiperiodic BC, $\Phi(b, t) = -\Phi(a, t)$ and $\Phi'(b, t) = -\Phi'(a, t)$. Owing to the Majorana conditions, it is sufficient to write these BCs in terms of only one of the components of Φ (the other component can be obtained algebraically). For example, in terms of ϕ_1 alone, the periodic BC is $\phi_1(b, t) = \phi_1(a, t)$ and $\phi'_1(b, t) = \phi'_1(a, t)$, and the antiperiodic BC is $\phi_1(b, t) = -\phi_1(a, t)$ and $\phi'_1(b, t) = -\phi'_1(a, t)$ (the BCs for ϕ_2 are obtained from the relation $\phi_2 = \phi_1^*$, when $\Phi = \Phi_c$, or from $\phi_2 = -\phi_1^*$, when $\Phi = -\Phi_c$). Finally, the wave equation for ϕ_1 is obtained from the FV equation and a Majorana condition, namely,

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \phi_1(x, t) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} [\phi_1(x, t) + \phi_1^*(x, t)] \\ &\quad + mc^2 \phi_1(x, t), \end{aligned} \quad (45)$$

when $\Phi = \Phi_c (\Rightarrow \phi_2 = \phi_1^*)$, or

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \phi_1(x, t) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} [\phi_1(x, t) - \phi_1^*(x, t)] \\ &\quad + mc^2 \phi_1(x, t), \end{aligned} \quad (46)$$

when $\Phi = -\Phi_c (\Rightarrow \phi_2 = -\phi_1^*)$ [13]. Because the latter two equations describe (strictly) neutral particles, they do not necessarily lead to the free 1D Schrödinger equation in the nonrelativistic limit, as one might expect. In fact, in this approximation, Eq. (45) leads to the result

$$\text{Re} \left[e^{-i\frac{mc^2}{\hbar}t} \left(-i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) (\phi_1)_{\text{NR}} \right] = 0, \quad (47)$$

(see Ref. [13]). Similarly, the nonrelativistic limit of Eq. (46) leads to the result

$$\text{Im} \left[e^{-i\frac{mc^2}{\hbar}t} \left(-i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) (\phi_1)_{\text{NR}} \right] = 0. \quad (48)$$

The latter equation can be obtained via the same procedure that led to Eq. (47). Certainly, because the terms enclosed in brackets do not have to be zero, the latter two equations are

not free 1D Schrödinger equations. However, if in Eqs. (47) and (48) the functions $(\phi_1)_{\text{NR}}$ and $(\phi_1)_{\text{NR}}^*$ are interpreted as independent solutions or fields, then these equations can yield the free Schrödinger equation for $(\phi_1)_{\text{NR}}$ and the equation that is the complex conjugate of the free Schrödinger equation for $(\phi_1)_{\text{NR}}^*$. The latter argument has been used and questioned when taking the nonrelativistic limit of certain real scalar field theories (see, for example, Refs. [20–23]).

In the free case, the relationship between the two-component FV wavefunction Φ and the corresponding one-component KFG wavefunction ϕ can be written as follows:

$$\begin{aligned} \Phi &= \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \phi + \frac{1}{mc^2} \hat{E} \phi \\ \phi - \frac{1}{mc^2} \hat{E} \phi \end{bmatrix} \\ \Rightarrow (\hat{\tau}_3 + i\hat{\tau}_2)\Phi &= \begin{bmatrix} \phi \\ -\phi \end{bmatrix}, \end{aligned} \quad (49)$$

(see, for example, Refs. [15, 16]). The latter matrix relation precisely leads to the complete equivalence between the KFG and FV wave equations; certainly, the mass of the particle cannot be zero. Thus, by virtue of the relation on the right-hand side in Eq. (49), the two BCs given in Eq. (44), *i.e.*, $(\hat{\tau}_3 + i\hat{\tau}_2)\Phi(b, t) = \mp(\hat{\tau}_3 + i\hat{\tau}_2)\Phi(a, t)$ and $(\hat{\tau}_3 + i\hat{\tau}_2)\Phi'(b, t) = \mp(\hat{\tau}_3 + i\hat{\tau}_2)\Phi'(a, t)$, lead us to the following two BCs for the one-component wavefunction ϕ :

$$\phi(b, t) = \mp\phi(a, t), \quad \text{and} \quad \phi'(b, t) = \mp\phi'(a, t), \quad (50)$$

namely, the periodic BC (positive signs) and the antiperiodic BC (negative signs). Certainly, the one-component KFG wavefunction ϕ is real, or purely imaginary, depending on the Majorana condition chosen. Finally, because the two BCs in Eq. (50) are included in the most general three-parameter set of BCs for which the FV Hamiltonian operator for a 1D KFGM particle in an interval is pseudo self-adjoint, the free FV Hamiltonian operator for a 1D KFGM particle in an interval with these two BCs is a pseudo self-adjoint operator (see BCs (vii) and (viii) in Sec. 4 of Ref. [14]).

4. Final discussion

A truly free 1D KFGM particle in an interval is a strictly neutral 1D particle that is located in a finite region but is not confined to that region, nor is it subject to any external field. Consequently, the energy current density j_{en} does not vanish at the walls of that region; however, there are infinitely many BCs that satisfy this requirement. To distinguish between all these BCs, we restrict the domain of the free FV Hamiltonian operator, which is a function of the domain of the pseudo self-adjoint momentum operator (we calculate the latter domain first) by requiring that, given a BC within the domain of the Hamiltonian, the energy current density has the same value at each end of the interval. Then, a one-parameter general family of BCs must lie within the domain of the free FV Hamiltonian. Because the FV wave equation is invariant under the operation of parity, the parity-transformed wavefunction

is also a solution of this equation, which further restricts the domain of the free FV Hamiltonian. Finally, knowing what BCs are inside the domain of the pseudo self-adjoint FV Hamiltonian operator for a 1D KFGM particle in an interval, we find that only two quantum BCs can remain in the domain of the free FV Hamiltonian: the periodic BC and the antiperiodic BC. These BCs are satisfied by both the two-component FV wavefunction and the one-component KFG wavefunction. Furthermore, as a consequence of imposing a Majorana condition, the two components of the FV wavefunction are not independent, and the KFG wavefunction is either real or imaginary. Owing to the Majorana conditions, it is sufficient to write these BCs in terms of only one of the components of the FV wavefunction. The first-order equation in time for the chosen component is obtained from the FV wave equation and a Majorana condition.

The physical interpretation of the periodic BC imposed on the wavefunctions ϕ , Φ , ϕ_1 or $\phi_2 = \pm\phi_1^*$, is that it simulates the motion of a 1D KFGM particle over a complete circle (360°), *i.e.*, the particle reaches one wall and reappears at the other wall. In contrast, the physical interpretation of the antiperiodic BC is that it simulates the motion of the particle over half of a Möbius strip (180°), *i.e.*, the particle reaches one wall and reappears at the other wall but “upside down.”

Naturally, when the domain of the momentum operator $\hat{p}$ contains only the periodic (antiperiodic) BC, *i.e.*, $\Phi(b, t) = \Phi(a, t)$ ($\Phi(b, t) = -\Phi(a, t)$), then automatically the domain of the free FV Hamiltonian operator $\hat{h}$ that is a function of $\hat{p}$ times $\hat{p}$ contains only the periodic (antiperiodic) BC, that is, $\Phi(b, t) = \Phi(a, t)$ and $\Phi'(b, t) = \Phi'(a, t)$ ($\Phi(b, t) = -\Phi(a, t)$ and $\Phi'(b, t) = -\Phi'(a, t)$). Certainly, both this momentum operator and the free FV Hamiltonian operator are pseudo self-adjoint operators, and the periodic (antiperiodic) BC is invariant under the parity operation, *i.e.*, it is a $\hat{\Pi}$ -symmetric BC. These results can be extended to the problem of a truly free 1D KFGM particle moving in the real line with, for example, the point $x = 0$ excluded. The two BCs for this problem can be obtained from the two BCs for the truly free 1D KFGM particle on the interval by making the replacements $x = a \rightarrow 0+$ and $x = b \rightarrow 0-$. Certainly, the two nonconfining BCs define transparent or penetrable barriers at $x = 0$.

Finally, to obtain our results, we use only a few simple concepts found in the general theory of linear operators over an indefinite inner product space and, of course, some algebraic procedures to construct the families and subfamilies of BCs. Furthermore, the main result of the article—that is, the result given in Eq. (44) along with the discussion in the two paragraphs following that equation—does not appear to have been published previously. We believe that our work will be of interest to all those interested in the fundamental aspects of relativistic quantum mechanics.

Appendix A

The free 1D Schrödinger equation

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Phi_S(x, t) &= \hat{h}_S \Phi_S(x, t) = \frac{\hat{p}_S^2}{2m} \Phi_S(x, t) \\ &= \frac{\hat{p}_S \hat{p}_S}{2m} \Phi_S(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Phi_S(x, t), \end{aligned} \quad (\text{A.1})$$

has as its solution the wavefunction $\Phi_S(x, t)$, but the parity-transformed wavefunction $(\hat{\Pi}_S \Phi_S)(x, t) = \Phi_S(a + b - x, t)$ is also a solution. The procedure used in the paragraph following Eq. (35) can be repeated here to verify this result. The Hamiltonian $\hat{h}_S$ essentially has the following domain:

$$\begin{aligned} \mathcal{D}(\hat{h}_S) &= \mathcal{D}(\hat{p}_S^2) = \mathcal{D}(\hat{p}_S \hat{p}_S) \\ &\sim \{ \Phi_S \mid \Phi_S \in \mathcal{D}(\hat{p}_S) \text{ and } \hat{p}_S \Phi_S \in \mathcal{D}(\hat{p}_S) \}. \end{aligned} \quad (\text{A.2})$$

Thus, $\Phi_S \in \mathcal{D}(\hat{p}_S)$ and $\hat{p}_S \Phi_S \in \mathcal{D}(\hat{p}_S)$; therefore, $\Phi_S(b, t) = e^{i\theta} \Phi_S(a, t)$ and $\Phi'_S(b, t) = e^{i\theta} \Phi'_S(a, t)$ (with $\theta \in [0, 2\pi)$), respectively. Moreover, because $(\hat{\Pi}_S \Phi_S)(x, t)$ is also a solution of the equation in (A.1), we have the following restrictions: $\hat{\Pi}_S \Phi_S \in \mathcal{D}(\hat{p}_S)$ and $\hat{p}_S(\hat{\Pi}_S \Phi_S) \in \mathcal{D}(\hat{p}_S)$; therefore, $(\hat{\Pi}_S \Phi_S)(b, t) = e^{i\theta} (\hat{\Pi}_S \Phi_S)(a, t)$ and $(\hat{\Pi}_S \Phi_S)'(b, t) = e^{i\theta} (\hat{\Pi}_S \Phi_S)'(a, t)$, respectively. The latter two BCs become the following two BCs: $\Phi_S(a, t) = e^{i\theta} \Phi_S(b, t)$ and $\Phi'_S(a, t) = e^{i\theta} \Phi'_S(b, t)$, respectively. Finally, only two BCs satisfy the two pairs of BCs mentioned above and therefore only they can be in the domain of the free 1D Schrödinger Hamiltonian: the periodic and antiperiodic BCs, *i.e.*, $\Phi_S(b, t) = \Phi_S(a, t)$ plus $\Phi'_S(b, t) = \Phi'_S(a, t)$; and $\Phi_S(b, t) = -\Phi_S(a, t)$ plus $\Phi'_S(b, t) = -\Phi'_S(a, t)$, respectively.

Appendix B

The FV Hamiltonian operator for a 1D KFG particle in the interval $\Omega = [a, b]$ is given by

$$\hat{h} = \frac{\hat{p}^2}{2m} (\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \hat{\tau}_3. \quad (\text{B.1})$$

The formal generalized adjoint of $\hat{h}$ is given by

$$\hat{h}_{\text{adj}} \equiv \hat{\tau}_3 \hat{h}^\dagger \hat{\tau}_3 = \frac{\hat{p}^2}{2m} (\hat{\tau}_3 + i\hat{\tau}_2) + mc^2 \hat{\tau}_3. \quad (\text{B.2})$$

Clearly, the actions of $\hat{h}$ and $\hat{h}_{\text{adj}}$ are equal. The latter definition leads automatically to the following relation:

$$\langle \langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle \rangle = \langle \langle \Psi, \hat{h} \Phi \rangle \rangle, \quad (\text{B.3})$$

where the scalar product is defined in Eq. (7). The latter relation defines the operator $\hat{h}_{\text{adj}}$ on a $\hat{\tau}_3$ -space, where $\Psi \in \mathcal{D}(\hat{h}_{\text{adj}})$, the domain of $\hat{h}_{\text{adj}}$, and $\Phi \in \mathcal{D}(\hat{h})$, the domain of $\hat{h}$. By applying the method of integration by parts twice, the following relation can be demonstrated [24]:

$$\langle \langle \hat{h}_{\text{adj}} \Psi, \Phi \rangle \rangle = \langle \langle \Psi, \hat{h} \Phi \rangle \rangle + g[\Psi, \Phi; \Omega], \quad (\text{B.4})$$

where the boundary term is given by

$$g[\Psi, \Phi; \Omega] = -\frac{\hbar^2}{2m} \frac{1}{2} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Psi')^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Psi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi' \right]_a^b. \quad (\text{B.5})$$

Using the relationship between the two-component FV wavefunction Φ and the corresponding one-component KFG wavefunction ϕ given in Eq. (49) and another similar relationship for Ψ and ψ , we can write $g[\Psi, \Phi; \Omega]$ in terms of only ψ and ϕ , namely,

$$g[\Psi, \Phi; \Omega] = -\frac{\hbar^2}{2m} [(\psi')^* \phi - \psi^* \phi']_a^b. \quad (\text{B.6})$$

The most general family of BCs for a 1D KFG particle in an interval, characterized by four real parameters and leading to the disappearance of $g[\Psi, \Phi; \Omega]$, was obtained in Ref. [24], namely,

$$\begin{bmatrix} \phi(b, t) - i\lambda\phi'(b, t) \\ \phi(a, t) + i\lambda\phi'(a, t) \end{bmatrix} = \hat{U} \begin{bmatrix} \phi(b, t) + i\lambda\phi'(b, t) \\ \phi(a, t) - i\lambda\phi'(a, t) \end{bmatrix}, \quad (\text{B.7})$$

where $\phi = \phi_1 + \phi_2$ (see Eq. (49)), λ is a real parameter and the unitary matrix $\hat{U}$ is given by

$$\hat{U} = e^{i\theta} \begin{bmatrix} n_0 - i n_3 & -n_2 - i n_1 \\ n_2 - i n_1 & n_0 + i n_3 \end{bmatrix}, \quad (\text{B.8})$$

where $\theta \in [0, \pi)$, and the real parameters n_0, n_1, n_2 and n_3 satisfy $(n_0)^2 + (n_1)^2 + (n_2)^2 + (n_3)^2 = 1$. By imposing a Majorana condition on the general family of BCs given in Eqs. (B7) and (B8) ($\Phi = \Phi_c = \hat{\tau}_1 \Phi^* \Rightarrow \phi = \phi^*$ or $\Phi = -\Phi_c = -\hat{\tau}_1 \Phi^* \Rightarrow \phi = -\phi^*$), the result $n_2 = 0$ is obtained. Thus, the four-parameter family of BCs becomes a three-parameter family of BCs. Indeed, the latter family is for a 1D KFGM particle in an interval [13]. For all BCs included in the general set of BCs given in Eqs. (B.7) and (B.8), $\hat{h}$ is a pseudo self-adjoint operator, *i.e.*,

$$\langle \langle \hat{h}\Psi, \Phi \rangle \rangle = \langle \langle \Psi, \hat{h}\Phi \rangle \rangle. \quad (\text{B.9})$$

Thus, $\hat{h} = \hat{h}_{\text{adj}}$, *i.e.*, the actions of $\hat{h}$ and $\hat{h}_{\text{adj}}$ are equal, and $\mathcal{D}(\hat{h}) = \mathcal{D}(\hat{h}_{\text{adj}})$. If we make $\Psi = \Phi$ in Eq. (B.9) and in Eq. (B.4) with the result $\hat{h} = \hat{h}_{\text{adj}}$, we obtain the following condition [24]:

$$g[\Phi, \Phi; \Omega] = i\hbar [j]_a^b = 0 \Rightarrow j(b, t) = j(a, t), \quad (\text{B.10})$$

where the usual KFG current density is given by

$$j = j(x, t) = \frac{i\hbar}{2m} \frac{1}{2} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Phi')^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi - ((\hat{\tau}_3 + i\hat{\tau}_2)\Phi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\Phi' \right]. \quad (\text{B.11})$$

The operators $\hat{h}$ and $\hat{h}_{\text{adj}}$ also satisfy the following relation:

$$\langle \langle \hat{h}_{\text{adj}}\Psi, \hat{E}\Phi \rangle \rangle = \langle \langle \Psi, \hat{h}\hat{E}\Phi \rangle \rangle + g[\Psi, \hat{E}\Phi; \Omega], \quad (\text{B.12})$$

where $\hat{E} = i\hbar \hat{1}_2 \partial/\partial t$ is the energy operator. If $\Phi \in \mathcal{D}(\hat{h})$, then automatically, $\hat{E}\Phi \in \mathcal{D}(\hat{h})$. Thus, any BC within the general set of pseudo self-adjoint BCs given in Eqs. (B.7) and (B.8) that leads to the disappearance of the boundary term $g[\Psi, \Phi; \Omega]$ in Eq. (B.4) must also lead to the disappearance of $g[\Psi, \hat{E}\Phi; \Omega]$ in Eq. (B.12). If we make $\Psi = \Phi$ in Eq. (B.12) with the result $\hat{h} = \hat{h}_{\text{adj}}$, we obtain the following result [14]:

$$g[\Phi, \hat{E}\Phi; \Omega] = i\hbar [j_{\text{en}}]_a^b = 0 \Rightarrow j_{\text{en}}(b, t) = j_{\text{en}}(a, t), \quad (\text{B.13})$$

where the (complex) KFG energy current density is precisely the result given in Eq. (1), namely,

$$j_{\text{en}} = j_{\text{en}}(x, t) = -\frac{\hbar^2}{2m} \frac{1}{2} \left[((\hat{\tau}_3 + i\hat{\tau}_2)\Phi')^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi} - ((\hat{\tau}_3 + i\hat{\tau}_2)\Phi)^\dagger (\hat{\tau}_3 + i\hat{\tau}_2)\dot{\Phi}' \right]. \quad (\text{B.14})$$

The results given in Eqs. (B.10) and (B.13) are direct consequences of the pseudo self-adjointness of $\hat{h}$. Moreover, j is equal to zero everywhere and j_{en} is a real quantity when j and j_{en} are calculated for a state Φ satisfying a Majorana condition.

The following relations are also obtained:

$$\frac{d}{dt} \langle \langle \Psi, \Phi \rangle \rangle = -\frac{1}{i\hbar} g[\Psi, \Phi; \Omega], \quad (\text{B.15})$$

and

$$\frac{d}{dt} \langle \langle \Psi, \hat{E}\Phi \rangle \rangle = -\frac{1}{i\hbar} g[\Psi, \hat{E}\Phi; \Omega], \quad (\text{B.16})$$

where Ψ and Φ in Eqs. (B.15) and (B.16) must also satisfy the 1D FV wave equation. If $\hat{h}$ is a pseudo self-adjoint operator, then the boundary terms in Eqs. (B.15) and (B.16) vanish; consequently, $\langle \langle \Psi, \Phi \rangle \rangle$ and $\langle \langle \Psi, \hat{E}\Phi \rangle \rangle$ are time-independent quantities. Moreover, if we make $\Psi = \Phi$ in Eqs. (B.15) and (B.16), the following results are obtained:

$$\frac{d}{dt} \langle \langle \Phi, \Phi \rangle \rangle = \frac{d}{dt} \left(\int_{\Omega} dx \varrho \right) = -[j]_a^b, \quad (\text{B.17})$$

and

$$\frac{d}{dt} \langle \langle \Phi, \hat{E}\Phi \rangle \rangle = \frac{d}{dt} \left(\int_{\Omega} dx \varrho_{\text{en}} \right) = -[j_{\text{en}}]_a^b, \quad (\text{B.18})$$

where the definition of the indefinite scalar product indefinite scalar product definition in Eq. (7) was also used. If $\hat{h}$ is a pseudo self-adjoint operator, *i.e.*, if the results in Eqs. (B.10) and (B.13) are imposed, then $\langle \langle \Phi, \Phi \rangle \rangle = \int_{\Omega} dx \varrho = \text{const}$ and $\langle \langle \Phi, \hat{E}\Phi \rangle \rangle = \int_{\Omega} dx \varrho_{\text{en}} = \text{const}$ (on-shell results). In fact, the results in Eqs. (B.17) and (B.18) are obtained by integrating the continuity equations $\hat{E}\varrho - \hat{p}j = 0$ and $\hat{E}\varrho_{\text{en}} - \hat{p}j_{\text{en}} = 0$, respectively, over the interval Ω .

The usual Lorentz two-vector current density is given by

$$j^\mu = j^\mu(x, t) = \frac{i\hbar}{2m} [\phi^*(\partial^\mu \phi) - (\partial^\mu \phi^*) \phi], \quad (\text{B.19})$$

where $\phi = \phi(x, t)$ is a one-component KFG wavefunction, $j^0 = c\rho$ and $j^1 = j$. In (1+1) dimensions, Greek indices $\mu, \nu, \dots$ take the values 0 and 1, and the metric tensor is $g^{\mu\nu} = \text{diag}(1, -1)$. The continuity equation then takes the usual form $\partial_\mu j^\mu = 0$ [15]; therefore, $\hat{E}\rho - \hat{p}j = 0$ (where $\hat{E} = i\hbar c \partial_0$ and $\hat{p} = -i\hbar \partial_1$). We introduce the following second-rank Lorentz tensor:

$$K^\mu_\nu = K^\mu_\nu(x, t) = \frac{i\hbar}{2m} \times [\phi^* (\partial^\mu (i\hbar \partial_\nu \phi)) - (\partial^\mu \phi^*) (i\hbar \partial_\nu \phi)], \quad (\text{B.20})$$

where $K^0_0 = \rho_{\text{en}}$ and $K^1_0 = j_{\text{en}}/c$; also, $K^{01} = K^{10}$ when ψ satisfies a Majorana condition ($\phi = \phi^*$, or $\phi = -\phi^*$), *i.e.*, in this case, $K^{\mu\nu}$ is a symmetric tensor. The latter tensor is an unusual energy-momentum tensor. However, K^μ_ν and the commonly used energy-momentum tensor [25]

$$T^\mu_\nu = T^\mu_\nu(x, t) = \frac{\hbar^2}{2m} [(\partial_\nu \phi^*) (\partial^\mu \phi) + (\partial^\mu \phi^*) (\partial_\nu \phi)] - \frac{\hbar^2}{2m} \left[(\partial^\alpha \phi^*) (\partial_\alpha \phi) - \frac{m^2 c^2}{\hbar^2} \phi^* \phi \right] g^\mu_\nu, \quad (\text{B.21})$$

are linked via the following relation:

$$K^\mu_\nu = T^\mu_\nu + \frac{\hbar^2}{2m} \left[(\partial^\alpha \phi^*) (\partial_\alpha \phi) - \frac{m^2 c^2}{\hbar^2} \phi^* \phi \right] g^\mu_\nu - \frac{\hbar^2}{2m} \partial_\nu (\phi^* (\partial^\mu \phi)). \quad (\text{B.22})$$

Using the free KFG equation,

$$\left(\partial^\alpha \partial_\alpha + \frac{m^2 c^2}{\hbar^2} \right) \phi = 0, \quad (\text{B.23})$$

the following result can be obtained from Eq. (B22):

$$\partial_\mu K^\mu_\nu = \partial_\mu T^\mu_\nu. \quad (\text{B.24})$$

As is well known, $\partial_\mu T^\mu_\nu = 0$ [25], consequently,

$$\partial_\mu K^\mu_\nu = 0. \quad (\text{B.25})$$

By choosing $\nu = 0$, the latter equation gives us a specific continuity equation, *i.e.*, $\partial_0 K^0_0 + \partial_1 K^1_0 = 0$; therefore, $\hat{E}\rho_{\text{en}} - \hat{p}j_{\text{en}} = 0$, as expected.

Appendix C

The BCs corresponding to the case $m_1 = 0$ can be obtained from the general family of BCs given in Eq. (24) with the matrix $\hat{N}$ given in Eq. (23). After setting $m_1 = 0$, the following two-parameter family of BCs is obtained:

$$\begin{aligned} \hat{V}_1 \begin{bmatrix} \phi_1(b, t) \\ \phi_2(b, t) \end{bmatrix} &= \hat{V}_2 \begin{bmatrix} \phi_1(a, t) \\ \phi_2(a, t) \end{bmatrix}, \quad \text{and} \\ \hat{V}_1 \begin{bmatrix} \phi'_1(b, t) \\ \phi'_2(b, t) \end{bmatrix} &= \hat{V}_2 \begin{bmatrix} \phi'_1(a, t) \\ \phi'_2(a, t) \end{bmatrix}, \end{aligned} \quad (\text{C.1})$$

where

$$\begin{aligned} \hat{V}_1 &= \begin{bmatrix} 1 & -e^{i\mu}(m_0 - i m_3) \\ 0 & 0 \end{bmatrix}, \quad \text{and} \\ \hat{V}_2 &= \begin{bmatrix} 0 & 0 \\ 1 & -e^{-i\mu}(m_0 - i m_3) \end{bmatrix}, \end{aligned} \quad (\text{C.2})$$

where $(m_0)^2 + (m_3)^2 = 1$, and $\mu \in [0, \pi)$ ($\det(\hat{V}_1) = \det(\hat{V}_2) = 0$). The latter set of BCs may be called “separated” because each of the relations arising from Eq. (C.1) is always evaluated at a single point, that is, at $x = a$ or at $x = b$.

Then, evaluating the energy current density given in Eq. (1) at $x = b$, substituting into there the relations $\phi_1(b, t) = e^{i\mu}(m_0 - i m_3)\phi_2(b, t)$ and $\phi'_1(b, t) = e^{i\mu}(m_0 - i m_3)\phi'_2(b, t)$ (obtained from the two relations in Eq. (C.1)) and their time derivatives, we obtain the result

$$\begin{aligned} j_{\text{en}}(b, t) &= -\frac{\hbar^2}{m} [1 + m_0 \cos(\mu) + m_3 \sin(\mu)] \\ &\times \left[(\phi'_2)^*(b, t) \dot{\phi}_2(b, t) - (\phi_2)^*(b, t) \dot{\phi}'_2(b, t) \right]. \end{aligned} \quad (\text{C.3})$$

Similarly, evaluating the energy current density given in Eq. (1) at $x = a$, substituting into it the relations $\phi_1(a, t) = e^{-i\mu}(m_0 - i m_3)\phi_2(a, t)$ and $\phi'_1(a, t) = e^{-i\mu}(m_0 - i m_3)\phi'_2(a, t)$ (obtained from the two relations in Eq. (C.1)) and their time derivatives, we obtain the result

$$\begin{aligned} j_{\text{en}}(a, t) &= -\frac{\hbar^2}{m} [1 + m_0 \cos(\mu) - m_3 \sin(\mu)] \\ &\times \left[(\phi'_2)^*(a, t) \dot{\phi}_2(a, t) - (\phi_2)^*(a, t) \dot{\phi}'_2(a, t) \right]. \end{aligned} \quad (\text{C.4})$$

Because the latter two results must be equal (see Eq. (2)), we have that $m_3 \sin(\mu) = 0$; hence,

$$m_3 = 0, \quad \mu = 0 \quad \text{and} \quad m_0 = \pm 1. \quad (\text{C.5})$$

Therefore, the BCs that emerge from the latter restrictions are given by

$$\begin{aligned} \begin{bmatrix} 1 & \mp 1 \\ 0 & 0 \end{bmatrix} \Phi(b, t) &= \begin{bmatrix} 0 & 0 \\ 1 & \mp 1 \end{bmatrix} \Phi(a, t), \quad \text{and} \\ \begin{bmatrix} 1 & \mp 1 \\ 0 & 0 \end{bmatrix} \Phi'(b, t) &= \begin{bmatrix} 0 & 0 \\ 1 & \mp 1 \end{bmatrix} \Phi'(a, t), \end{aligned} \quad (\text{C.6})$$

where the upper (lower) sign corresponds to $m_0 = +1$ ($m_0 = -1$). Note that if $m_0 = +1$, then the two components of $\Phi(x, t)$, $\phi_1(x, t)$ and $\phi_2(x, t)$, are equal at $x = b$, and their first derivatives, $\phi'_1(x, t)$ and $\phi'_2(x, t)$, are also equal there; the same holds at $x = a$. If $m_0 = -1$, then the components of $\Phi(x, t)$ and their first spatial derivatives have opposite signs at $x = b$, and the same occurs at $x = a$. The BCs in Eq. (C.6) can be written in terms of the one-component KFG wavefunction ϕ (indeed, we use the equivalence between the KFG and FV wave equations). Evaluating the wavefunction Φ at $x = b$ and $x = a$ in the relation on the left side of Eq. (49)

and substituting these quantities into Eq. (C.6), we obtain the following two sets of BCs:

$$\begin{aligned}\dot{\phi}(b, t) &= \dot{\phi}(a, t) = 0, \quad \text{and} \\ \dot{\phi}'(b, t) &= \dot{\phi}'(a, t) = 0,\end{aligned}\quad (\text{C.7})$$

($m_0 = +1$). These BCs are the time derivatives of the Dirichlet and Neumann BCs, and

$$\begin{aligned}\phi(b, t) &= \phi(a, t) = 0, \quad \text{and} \\ \phi'(b, t) &= \phi'(a, t) = 0,\end{aligned}\quad (\text{C.8})$$

($m_0 = -1$). These BCs are the Dirichlet and Neumann BCs.

The energy current density given in Eq. (1) can also be written in terms of the wavefunction ϕ [14], namely,

$$j_{\text{en}} = j_{\text{en}}(x, t) = -\frac{\hbar^2}{2m} \left[(\phi')^* \dot{\phi} - \phi^* \dot{\phi}' \right]. \quad (\text{C.9})$$

Clearly, if j_{en} is evaluated at the walls of the interval and the BCs given in Eq. (C.7) are used, then the impenetrability condition is obtained, *i.e.*, $j_{\text{en}}(b, t) = j_{\text{en}}(a, t) = 0$. The same applies if the BCs given in Eq. (C.8) are used. Therefore, these two BCs do not characterize a truly free 1D KFGM particle moving in an interval. Indeed, the case $m_1 = 0$ does not generate new nonconfining BCs. On the other hand, these two sets of BCs, *i.e.*, the BCs in Eq. (C.7) (or the BCs in Eq. (C.6)

with the upper sign) and the BCs in Eq. (C.8) (or the BCs in Eq. (C.6) with the lower sign), are not included in the most general three-parameter family of BCs for the pseudo self-adjoint FV Hamiltonian operator that describes a 1D KFGM particle in an interval (see Sec. 4 of Ref. [14]). Consequently, these two quantum BCs cannot be part of the domain of the pseudo self-adjoint-free FV Hamiltonian operator and must be discarded.

Conflicts of interest

The authors declare no conflicts of interest.

Data availability statement

No datasets were generated or analyzed during the current study.

Authors' contributions

Conceptualization, T.K. and S.DeV.; methodology, S.DeV.; formal analysis, T.K. and S.DeV.; investigation, T.K. and S.DeV.; resources, T.K. and S. DeV.; writing—original draft, S.DeV.; writing—review and editing, T.K. and S.DeV.; supervision, S.DeV. Both authors have read and agreed to the current version of the manuscript.

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Hermitian hamiltonians and imaginary eigenvalues beyond the Hilbert space

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In a quantum system initially in the n -th eigenstate, an adiabatic evolution of the Hamiltonian ensures that the system remains in the corresponding instantaneous eigenstate while acquiring a phase factor. This phase has two components: one resulting from standard time evolution and another associated with the dependence of the eigenstate on the varying Hamiltonian, known as the Berry phase. In this work, we explore the concept of geometric amplitudes in the context of a Hermitian Hamiltonian. We introduce the notion of geometric amplitude and provide a novel derivation of this concept. Our study reveals that a system undergoing cyclic evolution under adiabatic conditions acquires an additional amplitude factor of purely geometric origin. To illustrate this idea, we apply it to a concrete case: a generalized inverted harmonic oscillator. Although a pseudo-inner product can be introduced to make resonance states formally normalizable, this procedure relies on a non-unitary metric operator and defines a modified Hilbert space; it does not restore normalizability nor self-adjointness in the standard $L^2(R)$ framework.

In memory of my father, Maamache Leulmi-Amar, my mother, and my uncle, Djabou Zoulikha and Djabou Amar.

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1. Introduction

Quantum mechanics (QM), the fundamental theory governing microscopic phenomena, is built upon a rigorous mathematical framework that ensures its consistency and wide applicability across physics. One of its central objectives is the prediction of time evolution in Hamiltonian systems, a task essential for understanding a vast range of physical processes.

A cornerstone of the standard formulation of QM is the requirement that observables be represented by self-adjoint operators on a Hilbert space. This condition guarantees the reality of the spectrum and the unitarity of time evolution in closed systems [1]. However, it is important to emphasize that these properties are rigorously ensured only when the operator is truly self-adjoint on an appropriate domain [2, 3]. Formal Hermiticity alone is not sufficient.

The inverted harmonic oscillator provides a paradigmatic illustration of this subtlety [4–8]. Although its Hamiltonian is formally Hermitian, the associated potential is unbounded from below, which drastically modifies its spectral properties compared to the standard harmonic oscillator. While the conventional oscillator possesses a discrete, non-degenerate, equally spaced spectrum with square-integrable eigenfunctions, the inverted oscillator exhibits a purely continuous spectrum covering the entire real axis. Its generalized eigenstates are not square-integrable and therefore lie outside the Hilbert space $L^2(R)$.

In such contexts, the spectral problem must be formulated beyond the usual Hilbert space framework, typically within a rigged Hilbert space or resonance theory. Upon analytic continuation of the frequency parameter $\omega \rightarrow i\omega$, one formally obtains a discrete set of purely imaginary eigenvalues, $E_n = i\hbar\omega(n + 1/2)$.

These quantities do not correspond to stationary bound-state energies. Rather, they are associated with resonant (Gamow) states and appear as poles of the scattering matrix in the complex energy plane, encoding the intrinsic instability of the system.

This situation leads to a conceptual tension. A fundamental statement in quantum mechanics asserts that Hermitian (self-adjoint) operators have real eigenvalues [1]. Yet, in certain physically relevant extensions of the spectral problem, one encounters purely imaginary eigenvalues associated with formally Hermitian Hamiltonians. The resolution of this apparent paradox lies in the fact that these eigenvalues correspond to generalized, non-normalizable states that do not belong to the Hilbert space on which the operator is self-adjoint. Consequently, the usual expectation-value arguments ensuring spectral reality no longer apply.

If a Hermitian operator were to admit an eigenvalue

$$H|n\rangle = iE_n|n\rangle, \quad E_n \in \mathbb{R}, \quad (1)$$

within the Hilbert space, the expectation value $\langle\psi, H\psi\rangle$ would become purely imaginary, contradicting its guaranteed reality. The appearance of imaginary eigenvalues therefore signals that one is working outside the standard L^2 -framework.

Despite the Hermiticity of H , such eigenvalues induce non-unitary time evolution. The evolution operator, $U(t) = \exp(-iHt)$ generates exponential decay or growth rather than a pure phase rotation. Accordingly, the quantum state evolves as:

$$|\Psi_n(t)\rangle = e^{E_n t}|n\rangle, \quad (2)$$

where we have set $\hbar = 1$ throughout. In this case, the norm of the state is not preserved: $\langle\Psi_n(t)|\Psi_n(t)\rangle \neq 1$. Such evolution is non-unitary and reflects dynamical instability rather

than observable stationary energies. This clearly violates unitarity, which is expected for Hermitian dynamics. To restore a consistent probabilistic interpretation, one may introduce a modified scalar product using a metric operator η such that the inner product $\langle \Psi_n(t) | \eta | \Psi_n(t) \rangle$ remains conserved in time and generalizes conventional quantum mechanics.

We emphasize that the imaginary eigenvalues discussed here do not originate from non-Hermiticity, PT symmetry, or pseudo-Hermiticity. Unlike the non-Hermitian Hamiltonians introduced by Carl M. Bender and collaborators [9, 10] in the context of PT -symmetric quantum mechanics, whose spectral reality arises from unbroken PT symmetry, the phenomena considered here emerge from the extension of the spectral problem to generalized states. Similarly, while pseudo-Hermitian formulations—developed notably by Ali Mostafazadeh [11]—allow one to define modified inner products ensuring spectral reality in certain non-Hermitian systems, our analysis starts from formally Hermitian Hamiltonians and attributes complex eigenvalues solely to the non-normalizable nature of the associated states.

The inverted harmonic oscillator thus serves as a canonical example of a Hermitian system exhibiting continuous spectra, resonance phenomena, and dynamically unstable modes. It plays an important role in diverse areas such as quantum instability, tunneling, scattering theory, and quantum chaos.

The situation becomes even more intriguing when the Hamiltonian is time-dependent. The adiabatic theorem—originally formulated by Paul Ehrenfest [12]—states that a system governed by a slowly varying Hamiltonian remains in its instantaneous eigenstate up to a phase factor, provided suitable spectral conditions are satisfied. The Hermiticity of the Hamiltonian is crucial in the standard proof of this theorem, as it ensures real instantaneous eigenvalues and orthonormal eigenstates.

In 1984, Michael Berry [6] demonstrated that adiabatic cyclic evolution leads to an additional geometric phase factor, now known as the Berry phase. This phase has profound geometrical and topological significance and has been observed in numerous physical systems. However, all standard formulations of the adiabatic theorem and geometric phase assume that the instantaneous eigenvalues are real. This naturally leads to the central question addressed in the present work. What becomes of adiabatic evolution and geometric phases when the Hamiltonian admits purely imaginary eigenvalues associated with generalized states?

The purpose of this paper is to clarify the mathematical status and physical interpretation of imaginary eigenvalues arising in formally Hermitian systems, to distinguish them from genuinely non-Hermitian spectral phenomena, and to analyze their implications for dynamical stability and adiabatic quantum evolution.

As mentioned, a fundamental fact in quantum mechanics is that Hermitian (or self-adjoint) operators have only real eigenvalues. However, one may encounter Hermitian Hamiltonians with imaginary eigenvalues.ⁱ Such cases involving

imaginary eigenvalues have not been widely explored in the literature and will be one of the key topics discussed in this paper.

Before proceeding with the discussion, let us first recall a representative example that illustrates this theme: the inverted harmonic oscillator, characterized by the Hamiltonian

$$H = \frac{1}{2} \left[\frac{p^2}{m} - m\omega^2 q^2 \right], \quad (3)$$

$\omega > 0$, $m > 0$ are real constants. This is the same form as the standard harmonic oscillator, but with a negative sign in front of the potential term. It represents an unstable (repulsive) potential: $-(1/2)m\omega^2 q^2$.

Mathematically, the generalized harmonic oscillator and its inverted counterpart exhibit closely related structures, allowing the solutions of one system to be derived almost directly from those of the other through appropriate transformations. This formal similarity, however, masks profound physical differences. The harmonic oscillator displays a discrete, non-degenerate, and equally spaced energy spectrum with normalizable eigenfunctions in the standard Hilbert space. By contrast, the inverted harmonic oscillator has a doubly degenerate continuous spectrum ranging from $-\infty \rightarrow +\infty$, and its eigenfunctions are not normalizable in the conventional sense. Nevertheless, the introduction of a nontrivial metric allows one to endow the state space with a well-defined pseudo-inner product, thereby providing a generalized notion of normalizability for the wave functions. We finally emphasize that the eigenvalues associated with the inverted harmonic oscillator are purely imaginary, reflecting the intrinsically unstable nature of this system.

Let's first look at the classical dynamics to understand the appearance of imaginary frequencies. The equation of motion associated with the Hamiltonian (3) is:

$$\ddot{q} = \omega^2 q \Rightarrow q(t) = Ae^{\omega t} + Be^{-\omega t}. \quad (4)$$

The classical solution is exponential, not oscillatory. This is equivalent to saying that the system has a purely imaginary frequency: $\omega \rightarrow \pm i\omega$. This is a hallmark of dynamical instability: the system does not return to equilibrium but instead undergoes unbounded growth or decay.

On the quantum level, solving the time-independent Schrödinger equation leads to solutions governed by the parabolic cylinder equation. The resulting wavefunctions are expressed in terms of Weber functions (or modified Airy functions at asymptotic limits). However, due to the inverted potential, these solutions grow exponentially at spatial infinity and are not square-integrable, the spectrum is continuous, not discrete.

This example challenges the standard assumption that Hermiticity guarantees unitary evolution. It also highlights the need for generalized mathematical frameworks, such as rigged Hilbert spaces or effective non-Hermitian formulations, even when starting from a formally Hermitian Hamiltonian.

When the Hamiltonian becomes explicitly time-dependent, the situation becomes even more intricate. In such cases, approximation techniques become essential. One particularly powerful method is the adiabatic theorem [12]. It applies to quantum systems whose Hamiltonian $H(t)$ varies slowly with time and asserts that the system remains in its instantaneous eigenstate up to a phase factor, provided the spectral gap condition is satisfied.

The Hermiticity of the Hamiltonian plays a crucial role in the validity of the adiabatic theorem, as shown in various foundational studies [2–5]. In the following, we build on this concept by introducing Berry's adiabatic phase [6] and the associated notion of geometric phase, which provides further insight into the topological and geometric aspects of quantum evolution in the presence of slow parameter variations. This phenomenon can be described by "global change without local change". Berry points out the geometrical character of this phase which is not negligible because of its nonintegrable character. Since this much work has been done to this issue and the so-called Berry phase is now well established, theoretically as well as experimentally.

The adiabatic theorem, a fundamental result in quantum theory, states that for a Hamiltonian $H(t)$ that varies slowly over time, the solution of the time-dependent Schrödinger equation can be approximated using the eigenstates $|n(t)\rangle$ of the instantaneous Hamiltonian

$$H(t) |n(t)\rangle = E_n(t) |n(t)\rangle, \quad (5)$$

with energies $E_n(t)$ ($n = 0, 1, \dots$). This eigenvalue equation implies no relation between the phases of the eigenstates $|n(t)\rangle$ at different t .

The adiabatic theorem concerns states $|\Psi_n(t)\rangle$ satisfying the time-dependent Schrödinger equation

$$i \frac{\partial}{\partial t} |\Psi_n(t)\rangle = H |\Psi_n(t)\rangle, \quad (6)$$

and asserts that if a quantum system with a time-dependent non-degenerate Hamiltonian $H(t)$ is initially in the n th eigenstate $|n(0)\rangle$ of $H(0)$, and if $H(t)$ evolves slowly enough, then the state at time t remains in the n th instantaneous eigenstate of $H(t)$ up to a multiplicative phase factor.

This phase factor

$$\varphi_n(t) = - \int_0^t dt' \langle n(t') | H(t') - i\hbar \frac{\partial}{\partial t'} | n(t') \rangle \quad (7)$$

consists of two contributions: a dynamical phase and a geometric phase. Consequently, the quantum state $|\Psi_n(t)\rangle$ can be expressed as:

$$|\Psi_n(t)\rangle = e^{i \int_0^t dt' \langle n(t') | i \frac{\partial}{\partial t'} - H(t') | n(t') \rangle} |n(t)\rangle. \quad (8)$$

The geometric phase manifests itself in a wide variety of physical phenomena, such as the evolution of light polarization in optical fibers and the precession of neutrons subjected to magnetic fields. Furthermore, the concept of geometric

phase has been extended to systems with continuous spectra [11, 21] as well as to non-Hermitian Hamiltonians [22–29].

Up to this point, all discussed cases assume that the energy eigenvalues are real, either discrete or continuous. A natural and intriguing question then arises: What happens when the eigenvalues of the Hamiltonian are imaginary?

The aim of this work is fourfold. First, we seek to clarify the mathematical status of imaginary eigenvalues in operators that are formally Hermitian, with particular attention to issues of self-adjointness and domain. Second, we aim to distinguish such situations from genuinely non-Hermitian frameworks, including those exhibiting PT symmetry. Third, we analyze the implications of imaginary eigenvalues for the time evolution of quantum states, especially regarding the breakdown of unitarity. Finally, we investigate how the notion of geometric phase, in particular the Berry phase, is modified in this nonstandard context.

2. Solution of the Schrödinger equation

We consider a quantum system described by a Hamiltonian $H(\vec{R}(t))$ that depends on a real time dependent parameter $\vec{R}(t)$ which parametrizes the environment of the system and such that $\vec{R}(T) = \vec{R}(0)$. The time evolution is described by the time-dependent Schrödinger equation (6). At any instant, the natural basis consists of the eigenstates $|n(\vec{R}(t))\rangle$ associated with imaginary energies $iE_n(\vec{R}(t))$, defined by the eigenvalue equation

$$H(\vec{R}(t)) |n(\vec{R}(t))\rangle = iE_n(\vec{R}(t)) |n(\vec{R}(t))\rangle. \quad (9)$$

Assume that the system is initially prepared in the n -th eigenstate of the Hamiltonian, *i.e.*, $|\Psi_n(\vec{R}(0))\rangle = |n(\vec{R}(0))\rangle$. The adiabatic theorem states that if the Hamiltonian $H(\vec{R}(t))$ evolves slowly (adiabatically), the system remains in the corresponding instantaneous eigenstate $|n(\vec{R}(t))\rangle$ throughout the evolution. In other words, no transitions occur to other eigenstates, although the eigenenergy itself may change over time.

Under this adiabatic assumption, we consider the ansatz:

$$|\Psi_n(t)\rangle = C_n(t) |n(\vec{R}(t))\rangle, \quad (10)$$

where $C_n(t)$ is a time-dependent prefactor.

The eigenfunctions of the Hamiltonian $H(\vec{R}(t))$ do not generally belong to L^2 and, as a result, do not form a complete set of orthonormal functions $\langle m(\vec{R}(t)) | n(\vec{R}(t)) \rangle \neq \delta_{mn}$. A key question arising from the current interest in Hermitian quantum mechanics with imaginary eigenvalues is: What are the necessary and sufficient conditions for obtaining normalizable solutions? To address this, we propose introducing a metric $\eta(t)$, inspired by the pseudo-Hermitian framework, to define a scalar product that guarantees a well-defined and positive norm,

$$\langle m(\vec{R}(t)) | \eta(t) | n(\vec{R}(t)) \rangle = \delta_{mn}. \quad (11)$$

Substituting the expression (10) into the time-dependent Schrödinger equation and projecting the result onto the eigenstate weighted by the time-dependent metric $\eta(t)$: *i.e.*, $\langle n(\vec{R}(t)|\eta(t)$, yields a differential equation that governs the evolution of $C_n(t)$.

As a result, the time-evolved wave function takes the form:

$$|\Psi_n(t)\rangle = e^{\int_0^t E_n(t) dt} e^{\gamma_n(t)} |n(\vec{R}(t))\rangle. \quad (12)$$

This expression includes both a dynamical term (from the imaginary eigenvalue $iE_n(t)$) and a geometric contribution arising from the nontrivial time dependence of the eigenbasis and the metric $\eta(t)$

$$\gamma_n(t) = \int_0^t \langle n(\vec{R}(t')) | \eta(t') \frac{\partial}{\partial t'} | n(t') \rangle dt'. \quad (13)$$

The total amplitude factor can thus be written as:

$$\phi = \underbrace{e^{\int_0^t E_n(t) dt}}_{\text{dynamical amplitude}} + \underbrace{e^{\gamma_n(t)}}_{\text{Geometrical amplitude}}. \quad (14)$$

The geometric term $\gamma_n(t)$, which depends only on the path followed in Hilbert space, is analogous to the Berry phase encountered in Hermitian systems under cyclic adiabatic evolution. Meanwhile, the first exponential captures the familiar dynamical contribution.

The orthonormality relation in Eq. (11) does not directly extend to the time-evolved states $|\Psi_n(t)\rangle$, due to the time-dependent prefactor. To restore a consistent normalization framework, we define a rescaled metric: $\tilde{\eta}(t) = \eta(t)e^{-2\int_0^t E_n(t) dt} e^{-2\gamma_n(t)}$. With this definition, the time-evolved states remain orthonormal in the modified inner product:

$$\langle \Psi_m(t) | \tilde{\eta}(t) | \Psi_n(t) \rangle = \delta_{mn}. \quad (15)$$

3. Example: inverted generalized harmonic oscillator

Consider the quantum system defined by the following Hamiltonian:

$$H(t) = \frac{1}{2} [Z(t)p^2 + Y(t)(pq + qp) + X(t)q^2]. \quad (16)$$

usually called a generalized harmonic oscillator [30] which depends on the set of external parameters $(X, Y, Z) \in \mathbb{R}^3$. For fixed values of the parameters, H corresponds to the Hamiltonian of the harmonic oscillator with purely imaginary frequency provided $XZ \lessgtr Y^2$ and we assume henceforth that this remains the case as X, Y, Z vary.

The Hamiltonian of the inverted generalized harmonic oscillator is defined by Eq. (16). In contrast to the standard harmonic oscillator, its spectral properties are markedly different due to the quadratic potential being unbounded from below. As a consequence, the system exhibits several distinctive features. First, its energy spectrum is continuous and extends

over the entire real line ($E \in \mathbb{R}$). In particular, the Hamiltonian does not admit a ground state, since the potential diverges to $-\infty$ as $|q| \rightarrow \infty$.

The generalized eigenstates associated with this continuous spectrum are not square-integrable and therefore do not belong to the Hilbert space $L^2(\mathbb{R})$. Instead, they are understood as scattering states within an extended framework, such as the rigged Hilbert space formalism. Each energy value is, in general, doubly degenerate, a degeneracy that has a clear physical interpretation in terms of scattering solutions corresponding to left- and right-moving waves in the repulsive quadratic potential.

If one formally performs an analytic continuation of the frequency parameter ($\omega \rightarrow i\omega$), one obtains a discrete set of purely imaginary energy values of the form $E_n = i(n + [1/2])\omega$. However, these quantities do not represent physical energies of stationary bound states. Rather, they are associated with resonant (Gamow) states and correspond to poles of the scattering matrix in the complex energy plane, thereby encoding the intrinsic instability and decay properties of the system.

The inverted generalized harmonic oscillator therefore provides a paradigmatic example of a quantum system characterized by a continuous spectrum, non-normalizable eigenstates, and resonance phenomena. For this reason, it plays an important role in the study of quantum instability, tunneling processes, and various aspects of quantum chaos.

The eigenvalue equation takes the following form

$$\left[-\frac{Z}{2} \frac{\partial^2}{\partial q^2} - iYq \frac{\partial}{\partial q} + \left(\frac{Xq^2 - iY}{2} \right) \right] \psi_n = E_n \psi_n, \quad (17)$$

To determine the eigenfunctions ψ_n and the eigenvalues, we introduce the following unitary transformation

$$\psi_n^r(q) = U\psi_n(q) = \exp \left[\frac{iY}{2Z} q^2 \right] \psi_n(q), \quad (18)$$

(r indicates reversed) such as

$$U^\dagger q U = q, \quad U^\dagger p U = p - \frac{Y}{Z} q, \quad (19)$$

and let us note that the transformed Hamiltonian H^r

$$H^r = U^\dagger H U = \frac{1}{2} \left[Zp^2 + \frac{(XZ - Y^2)}{Z} q^2 \right], \quad (20)$$

corresponds to the Hamiltonian of the inverted harmonic oscillator with purely imaginary frequency $i\sqrt{(Y^2 - XZ)} = i\omega$.

Therefore, this replacement transforms the eigenfunctions ψ_n into generalized eigenvectors ψ_n^r of the inverted harmonic oscillator (20)

$$\begin{aligned} \psi_n^r(q) &= \left(\frac{i\omega m}{\pi} \right)^{\frac{1}{4}} \exp \left[-\frac{i}{2} \frac{Y}{Z} q^2 \right] \chi_n \left[\left(\frac{i\omega}{2} \right)^{\frac{1}{2}} q \right] \\ &= \exp \left[-\frac{i}{2} \frac{Y}{Z} q^2 \right] V^{-1} \left\{ \left(\frac{\omega m}{\pi} \right)^{\frac{1}{4}} \chi_n \left[\left(\frac{\omega}{2} \right)^{\frac{1}{2}} q \right] \right\}, \end{aligned} \quad (21)$$

where the operator $V = \exp[-(\pi/8)(qp + pq)]$ changes the coordinate q and momentum p operators as

$$\begin{aligned} \exp\left[\frac{\pi}{8}(qp + pq)\right] q \exp\left[-\frac{\pi}{8}(qp + pq)\right] &= qe^{-i\frac{\pi}{4}}, \\ \exp\left[\frac{\pi}{8}(qp + pq)\right] p \exp\left[-\frac{\pi}{8}(qp + pq)\right] &= pe^{i\frac{\pi}{4}}, \end{aligned} \quad (22)$$

and its action on a wave function in the q representation reads $Vf(q) = e^{i\frac{\pi}{8}}f(qe^{i\frac{\pi}{4}})$. The so-called n th Hermite function $\chi_n(q)$ satisfies the following equation:

$$\frac{\partial^2 \chi_n}{\partial q^2} + 2(n + 1 - q^2)\chi_n(x) = 0, \quad (23)$$

and the corresponding energies are exactly given by

$$E_n = \left(n + \frac{1}{2}\right)\omega = i\left(n + \frac{1}{2}\right)\sqrt{(Y^2 - XZ)}. \quad (24)$$

It is straightforward to verify that the norm associated with the solution (21) is not well-defined. Specifically, when calculating the squared norm of these functions, we observe that $\langle \psi_n^r | \psi_n^r \rangle \neq 1$. This suggests introducing the metric operator

$$\begin{aligned} \eta &= \exp\left[-\frac{i}{2\hbar}\frac{Y}{Z}q^2\right] \\ &\times \exp\left[\frac{\pi}{4}(xp + px)\right] \exp\left[\frac{i}{2\hbar}\frac{Y}{Z}q^2\right], \end{aligned} \quad (25)$$

such that the squared norm $\langle \psi_n^r | \eta | \psi_n^r \rangle = 1$ is finite. Note that the metric operator is not unique, in the sense that infinitely many operators can possibly be implemented.

Inserting the wave function (18) and the metric (25) into the formula (13) defining the geometric quantity, one finds

$$\gamma_n(C) = -\left(n + \frac{1}{2}\right) \oint_C \frac{Z}{\omega} d\left(\frac{Y}{Z}\right), \quad (26)$$

where the following property of the Hermite functions $\int_{-\infty}^{+\infty} \zeta^2 \chi_n^2[\zeta] d\zeta = (n + [1/2])$, has been used. Thus $\gamma_n(C)$ given by a circuit integral in parameter space is imaginary. Thus the time-evolved wave can be written as:

$$\begin{aligned} |\Psi_n(q, t)\rangle &= e^{\int_0^t E_n(t) dt} e^{\gamma_n(t)} \exp\left[-\frac{i}{2}\frac{Y}{Z}q^2\right] \\ &\times V^{-1} \left\{ \left(\frac{\omega m}{\pi}\right)^{\frac{1}{4}} \chi_n\left[\left(\frac{\omega}{2}\right)^{\frac{1}{2}} q\right] \right\}, \end{aligned} \quad (27)$$

the first exponential is the dynamical amplitude and the second exponential (the geometrical amplitude) is the object of attention in this paper.

4. Conclusion

In quantum mechanics, the reality of the eigenspectrum plays a central role, as it guarantees the physical observability and stability of measurable quantities such as energy,

momentum, and angular momentum. Within the conventional framework, this property follows from the Hermiticity of the Hamiltonian operator, which ensures a real spectrum and unitary time evolution. Real eigenvalues therefore represent physically meaningful states and form a fundamental basis for the predictive consistency of quantum theory.

Recent developments in non-Hermitian quantum mechanics have considerably broadened this perspective. It is now well established that certain classes of non-Hermitian operators, including those possessing PT symmetry or belonging to the class of pseudo-Hermitian Hamiltonians, may still exhibit entirely real spectra under appropriate conditions. It is not generally true that all PT -symmetric Hamiltonians possess entirely real eigenvalue spectra; this holds only when the PT symmetry is unbroken. When PT symmetry is spontaneously broken, complex conjugate eigenvalue pairs can emerge. Conversely, the presence of a real spectrum does not imply that a Hamiltonian is PT -symmetric, as there exist non- PT -symmetric operators with entirely real eigenvalues. Therefore, PT symmetry is neither a necessary nor a sufficient condition for spectral reality. These extensions provide powerful theoretical tools for describing open quantum systems, dissipative dynamics, and gain-loss mechanisms, while maintaining a consistent probabilistic interpretation through generalized inner-product structures.

Within this context, the adiabatic theorem remains a fundamental principle governing the evolution of quantum states under slowly varying Hamiltonians. When a system initially prepared in an instantaneous eigenstate evolves adiabatically along a closed path in parameter space, the state acquires not only the usual dynamical phase but also an additional geometric contribution known as the Berry phase. This geometric phase depends exclusively on the geometry of the path traced in parameter space and has profound implications across many areas of physics.

In the present work, we revisited the geometric aspects of adiabatic evolution and explored their extension beyond the conventional phase structure. In particular, we introduced the notion of a geometric amplitude, which generalizes the concept of geometric phase in situations where the spectral or normalization properties of the eigenstates differ from those encountered in standard Hermitian systems. We have shown that, under cyclic and adiabatic evolution, the quantum state may acquire an additional amplitude factor of purely geometric origin. This contribution arises from the structure of the parameter space and from the normalization properties of the instantaneous eigenstates, and is therefore distinct from the dynamical evolution generated by the Hamiltonian.

To illustrate this mechanism, we applied the formalism to a generalized harmonic oscillator with time-dependent parameters and an effective negative frequency. This model provides a useful framework for investigating unstable quantum dynamics. In particular, it exhibits features such as continuous spectra, non-normalizable eigenstates, and resonance-like behavior, which are commonly encountered in problems involving quantum instability, tunneling processes, and

aspects of quantum chaos.

Although the generalized harmonic oscillator and the inverted harmonic oscillator are mathematically related through suitable transformations, their physical interpretations remain fundamentally different. The ordinary harmonic oscillator possesses a discrete, non-degenerate, and equally spaced energy spectrum with square-integrable eigenfunctions forming a complete orthonormal basis in Hilbert space. By contrast, the inverted harmonic oscillator is characterized by a continuous spectrum extending from $-\infty$ to $+\infty$, and its eigenfunctions are not square-integrable in the conventional sense.

This apparent difficulty can be consistently addressed within extended frameworks such as rigged Hilbert spaces or generalized inner-product structures, which allow the proper treatment of non-normalizable states, including scattering and resonance states. Within this broader setting, the unstable nature of the inverted oscillator manifests through exponen-

tially growing or decaying solutions, reflecting the intrinsic dynamical instability of the potential rather than a breakdown of the quantum formalism.

In summary, the present work highlights the rich geometric structure underlying adiabatic quantum evolution in systems that depart from the standard Hermitian paradigm. In particular, the introduction of the geometric amplitude extends the conventional framework of geometric effects in quantum mechanics and provides new insight into the role of geometry in the dynamics of unstable or non-standard quantum systems. Our main result shows that adiabatic cyclic evolution can generate not only a geometric phase but also a geometric amplitude, thereby revealing a deeper geometric structure in quantum dynamics beyond the traditional Berry-phase description.

I dedicate this work to my grandchildren Mohamed and Racim Cheboudi, Taim-Abderahmane Maamache and Sadjed-Yazen Bendib

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- i. A simple example may illustrate the issue: consider quantum mechanics on the real line and the quantum mechanical operator $O = q^3 p + p q^3$. This operator is hermitian (or symmetric) but it still has an eigenvalue $(-i\lambda)$ with a square-integrable eigenfunction $\chi_\lambda(q) = 1/|q|^{3/2} e^{-\lambda/4q^2}$.
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Dimensional consistency in fractional differential equations with non singular kernels

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The purpose of this article is to address the issues of dimensional consistency that arise in the process of replacing the ordinary time derivative operator by a fractional derivative operator in order to write a fractional differential equation. We show that by performing a simple change of variables fulfilling certain conditions ensures the consistency in physical dimensions for fractional differential equations with non singular kernels. An example of the proposed method is given.

Keywords: Fractional calculus; Caputo-Fabrizio fractional derivative; RC circuit.

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1. Introduction

From a mathematical point of view, fractional calculus was introduced as a generalization of classical calculus and has become a powerful tool for modeling complex dissipative phenomena, attracting the interest of scientists and being currently the subject of many theoretical and experimental investigations [1-3]. Among the various definitions of fractional derivatives, Riemann-Liouville and Caputo operators, based on power-law kernels, are widely used to capture memory effects with algebraic decay [4]. However, these kernels are singular at the origin, which can lead to difficulties in handling initial conditions and interpreting physical processes. To overcome these limitations, Caputo and Fabrizio proposed a fractional derivative with smooth non-singular exponential kernels, which have the ability to describe material heterogeneities and multi-scale fluctuations [5]. Despite these kernel design development, incorporating fractional derivatives into physical models introduces additional challenges related to dimensional consistency.

Fractional derivatives, whether defined with singular or non-singular kernels, are incorporated into differential equations to model physical phenomena through fractional differential equations (FDEs). Through these formulations, non-integer models have been applied to systems such as the parallel RLC circuit or the damped harmonic oscillator [6]. However, the straightforward replacement of an integer order derivative by a fractional order derivative in equations involving physical variables leads to dimensional imbalance that raises questions about the interpretability of the models [7].

To address this issue, some strategies are implemented, such as introducing a scaling parameter or characteristic constant that restores the dimensional homogeneity in the equations. For example, Gómez-Aguilar *et al.* [8,9], and Bachuin [10] introduced an auxiliary parameter σ that repre-

sents the fractional time components of the system, naming the non-local time as the *cosmic time*. This parameter allows the fractional derivative to be dimensionally consistent with its classical counterpart, even though its physical interpretation remains challenging, as it typically carries units such as $\text{sec}^{-\alpha}$ that are not directly measurable in practice.

Alternatively, Vaz and Capelas de Oliveira [7] describe a dimensional regularization technique for the fractional derivative of Caputo, where a multiplicative term involving the independent variable is introduced to maintain the original physical dimension of the problem. This approach avoids the arbitrariness of auxiliary parameters by systematically balancing the dimensions through characteristic scales.

Other methods include normalization procedures that transform variables into dimensionless forms to avoid dimensional balancing, but when reintroducing physical dimensions into fractional form, some problems are encountered when interpreting the terms of the FDE [7].

The main goal of this article is to answer the question on how physical dimensions in a fractional derivative operator has to be taken into account to model real problems and to have dimensional consistency in the fractional differential system.

2. Dimensional consistency in fractional derivative operators

The simplest procedure for constructing a fractional differential equation consists of simply replacing all conventional derivative operators of a given system by the fractional derivative operator. The replacement of an integer order derivative operator by a fractional derivative operator in a differential equation leads to a dimensional inconsistency. For example, let us consider the definition of the classical Caputo

fractional derivative, which is given by

$${}^C D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_a^t \frac{df(s)}{ds} \frac{1}{(t-s)^\alpha} ds, \quad (1)$$

with $\alpha \in (0, 1]$ and $a \in [-\infty, t]$ and $f(t) \in H^1(a, b)$ for $b > a$, where $H^1(a, b)$ denotes a Sobolev space. If we do such replacements we have a dimensional inconsistency since the time dimension of ${}^C D_t^\alpha$, i.e. the Caputo fractional derivative, is $\text{sec}^{-\alpha}$ while that of d/dt is sec^{-1} . For achieving dimensional consistency, Gómez *et al.* introduce the following simple rule which consists of replacing the ordinary time derivative operator by the fractional one in the following way

$$\frac{d}{dt} \rightarrow \frac{1}{\sigma^{1-\alpha}} {}^C D_t^\alpha \quad \text{where} \quad 0 < \alpha \leq 1, \quad (2)$$

where $\sigma > 0$ is a new parameter which has the dimension of time, i.e. $[\sigma] = s$. Using this procedure, it is easy to write down the fractional differential equation of any given system. Note that the dimensions of d/dt and $(1/\sigma^{1-\alpha}) {}^C D_t^\alpha$ are now consistent.

However, there are many different definitions of fractional derivatives in the literature. Traditional definitions of fractional derivatives, such as the Caputo operator, employ power-law kernels with singularities at the origin. Although these kernels effectively represent long-range memory, their singular behavior often leads to analytical difficulties, numerical instabilities, and ambiguity in the physical interpretation of initial conditions. In order to overcome these limitations, Caputo and Fabrizio proposed a new fractional derivative in 2015 characterized by a non-singular and nonlocal exponential kernel. This formulation preserves the memory effect inherent to fractional calculus while ensuring improved regularity and computational tractability. Caputo and Fabrizio proposed changing the kernel $(t-s)^{-\alpha}$ in the Caputo fractional derivative by the exponential function $\exp[-(\alpha t/(1-\alpha))]$ and $1/\Gamma(1-\alpha)$ by $(2-\alpha)M(\alpha)/2(1-\alpha)$, to obtain the following definition for the fractional derivative with non singular kernel of the Caputo-Fabrizio type given by

$${}^{CF} D_t^\alpha f(t) = \frac{(2-\alpha)M(\alpha)}{2(1-\alpha)} \int_0^t \frac{df(s)}{ds} \times \exp\left[-\frac{\alpha(t-s)}{1-\alpha}\right] ds, \quad (3)$$

where $M(\alpha)$ is a normalization function such that $M(\alpha) = 2/(2-\alpha)$.

The Caputo-Fabrizio derivative satisfies several fundamental properties that make it suitable for theoretical and applied mathematical physics. The Caputo-Fabrizio operator satisfies the following mathematical properties

Linearity. For any functions $f, g \in C^1([0, T])$ and constants $a, b \in \mathbb{R}$,

$${}^{CF} D_t^\alpha (af(t) + bg(t)) = a {}^{CF} D_t^\alpha f(t) + b {}^{CF} D_t^\alpha g(t). \quad (4)$$

Derivative of a constant. If $f(t) = C$, where C is a constant, then

$${}^{CF} D_t^\alpha C = 0, \quad (5)$$

which is consistent with classical differentiation and advantageous for physical modeling.

Limit cases. The Caputo-Fabrizio derivative interpolates between classical operators:

$$\begin{aligned} \lim_{\alpha \rightarrow 0} {}^{CF} D_t^\alpha f(t) &= f(t) - f(0), \\ \lim_{\alpha \rightarrow 1} {}^{CF} D_t^\alpha f(t) &= \frac{df(t)}{dt}. \end{aligned} \quad (6)$$

Laplace transform. Let $\mathcal{L}\{f(t)\}(s) = F(s)$. The Laplace transform of the Caputo-Fabrizio derivative is given by

$$\mathcal{L}\{{}^{CF} D_t^\alpha f(t)\}(s) = \frac{1}{1-\alpha} \frac{sF(s) - f(0)}{s + \frac{\alpha}{1-\alpha}}, \quad (7)$$

which facilitates the analytical solution of fractional differential equations.

Due to its non-singular kernel, well-defined initial conditions, and favorable analytical properties, the Caputo-Fabrizio derivative has been extensively employed in the formulation and analysis of fractional differential equations. Applications include stability analysis of dynamical systems, reaction-diffusion processes, and control problems, where it provides a mathematically consistent and physically interpretable alternative to classical fractional operators. The operator (2) is nonlocal, as the value of the derivative at time t depends on the entire history of the function over $[0, t]$. However, unlike power-law kernels, the exponential kernel induces a memory with finite persistence, which is often more realistic in applied models.

From Eq. (2) we see that the Caputo-Fabrizio fractional derivative is a dimensionless operator, therefore in order to write down the corresponding fractional differential operator we need to introduce a new dimensionless parameter given by

$$\tau(t, \alpha) = \int_0^t \frac{dt}{\varphi(t, \alpha)}, \quad (8)$$

where $\varphi(t, \alpha)$ is a function that has to have the dimension of time in order for τ to be a dimensionless function and also has to be chosen in such a way so that $\tau(t, \alpha)$ is a strictly monotonic increasing function. Therefore, we can replace the ordinary time derivative operator by the following one

$$\frac{d}{dt} \rightarrow \frac{d\tau}{dt} \frac{d}{d\tau} \rightarrow \frac{1}{\varphi(t(\tau), \alpha)} {}^{CF} D_\tau^\alpha. \quad (9)$$

In order to obtain the ordinary time derivative in Eq. (9) when $\alpha = 1$ we must impose the following condition:

$$\frac{1}{\varphi(t, 1)} \frac{d}{d\tau} = \frac{d}{dt}. \quad (10)$$

Therefore, if we would like to solve the fractional differential equation, using the Caputo-Fabrizio fractional derivative operator, equivalent to a first order differential equation with constant coefficients given by

$$\frac{dx}{dt} + Px(t) = Q, \quad (11)$$

where P and Q are constants, we proceed to solve the following fractional differential equation

$${}^{CF}D_{\tau}^{\alpha}x(\tau) + P\varphi(t(\tau), \alpha)x(\tau) = Q\varphi(t(\tau), \alpha). \quad (12)$$

Substituting Eq. (2) into Eq. (12) we have

$$\frac{e^{-\alpha\tau/(1-\alpha)}}{1-\alpha} \int_0^{\tau} e^{\alpha u/(1-\alpha)} x'(u) du + P\varphi(t(\tau), \alpha)x(\tau) = Q\varphi(t(\tau), \alpha). \quad (13)$$

Differentiating both sides of Eq. (13) with respect to τ and simplifying, we get

$$\frac{dx}{d\tau} = (1-\alpha) \frac{d}{d\tau} [Q\varphi(t(\tau), \alpha) - P\varphi(t(\tau), \alpha)x(\tau)] + \alpha [Q\varphi(t(\tau), \alpha) - P\varphi(t(\tau), \alpha)x(\tau)], \quad (14)$$

which can be rearranged as

$$[(1-\alpha)P\varphi(t(\tau), \alpha) + 1] x'(\tau) + [(1-\alpha)P\varphi(t(\tau), \alpha)\dot{\varphi} + \alpha P\varphi(t(\tau), \alpha)] x(\tau) - [(1-\alpha)Q\varphi(t(\tau), \alpha)\dot{\varphi} + \alpha Q\varphi(t(\tau), \alpha)] = 0, \quad (15)$$

where $\dot{\varphi} = d\varphi/dt$. Equation (15) has the following integrating factor [11]

$$\mu(\tau) = \exp \int \frac{\alpha P\varphi(t(\tau), \alpha)}{1 + (1-\alpha)P\varphi(t(\tau), \alpha)} d\tau. \quad (16)$$

Therefore, multiplying Eq. (15) by $\mu(\tau)$ and integrating we arrive to the solution of Eq. (12) which is given by

$$x(\tau) = \Xi(\tau) \left(C + \int \mu(\tau) [(1-\alpha)Q\dot{\varphi} + \alpha Q]\varphi(t(\tau), \alpha) d\tau \right), \quad (17)$$

where

$$\Xi(\tau) = \frac{1}{[(1-\alpha)P\varphi(t(\tau), \alpha) + 1] \mu(\tau)}, \quad (18)$$

3. Example: Analysis of an RC circuit

We are now interested in the modeling and study of a simple electrical circuit consisting of a resistor and a capacitor within the framework of the fractional derivative with a non singular kernel [12-17]. Using the Kirchhoff voltage law in

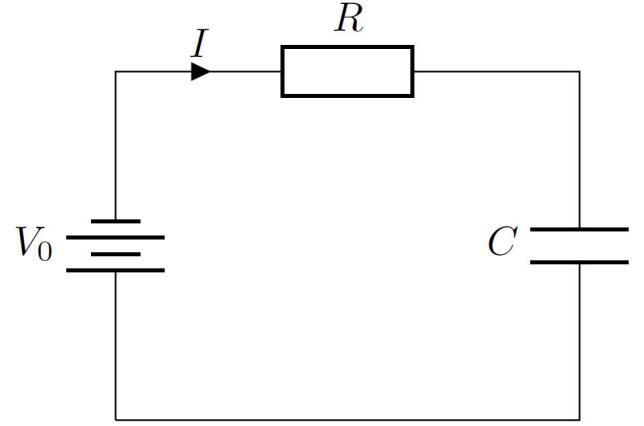


FIGURE 1. The figure shows the RC circuit.

the circuit shown in Fig. 1, we get the following fractional differential equation

$${}^{CF}D_t^{\alpha}q(t) + \Gamma q(t) = \Gamma q_0, \quad (19)$$

where $\Gamma = 1/RC$ and $q_0 = V_0C$.

In order to have dimensional consistency in Eq. (19), several authors include an auxiliary parameter σ , which has the dimension of seconds and is associated with the temporal components in the system to maintain the dimensional consistency of the fractional differential equation, which is valid for the case of singular kernels [18-24].

For the case of differential equations with non singular kernels we have to introduce an auxiliary function φ in order to have dimensional consistency in Eq. (19), therefore in this example we are going to use our method by using two different dimensionless functions $\tau(t, \alpha)$. For the first case we are going to use $\varphi(t, \alpha) = e^{-(1-\alpha)\Gamma t}/\Gamma$ and for the second case we are going to use $\varphi(t, \alpha) = (1 + \Gamma(1-\alpha)t)/\Gamma$, respectively.

3.1. Case 1

We are going to use the following function $\varphi(t, \alpha) = e^{-(1-\alpha)\Gamma t}/\Gamma$ which has the unit of second and using Eq. (8) we get the following dimensionless function

$$\tau(t, \alpha) = \frac{e^{(1-\alpha)\Gamma t} - 1}{1 - \alpha}. \quad (20)$$

Note that $\tau(t, \alpha)$ is a strictly monotonic increasing function and satisfies Eq. (10). Using Eq. (12) we have the following fractional differential equation for the RC circuit

$${}^{CF}D_{\tau}^{\alpha}q(\tau) + \frac{q}{1 + (1-\alpha)\tau} = \frac{q_0}{1 + (1-\alpha)\tau} \quad \text{where } 0 < \alpha \leq 1. \quad (21)$$

Using Eqs. (17) and (18) we find the solution of the fractional differential equation given in Eq. (21) which is given by

$$q(\tau, \alpha) = q_0 + C_0(1 + (1-\alpha)\tau) \times (2 - \alpha + (1-\alpha)\tau)^{1/(\alpha-1)}. \quad (22)$$

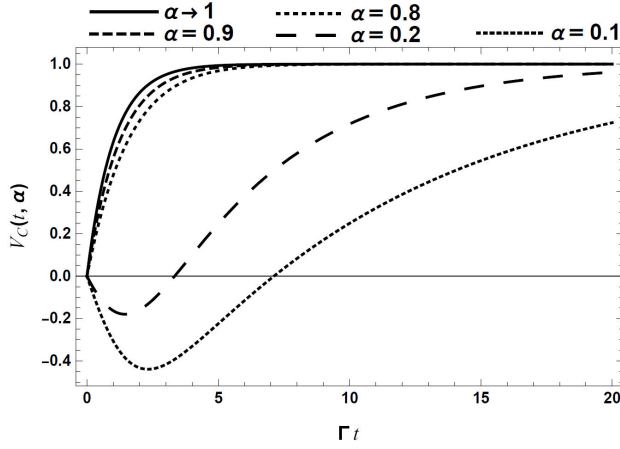


FIGURE 2. The figure shows the voltage across the capacitor for the case when the DC voltage is $V_0 = 1$ V.

Using the initial condition $q(0, \alpha) = 0 = q_0 + C_0(2 - \alpha)^{1/(\alpha-1)}$ and using Eq. (20) we can write the solution in terms of the ordinary time and the initial condition which is given by

$$q(t, \alpha) = q_0 \times \left(1 - e^{(1-\alpha)\Gamma t} \left[\frac{2-\alpha}{(1-\alpha) + e^{(1-\alpha)\Gamma t}} \right]^{1/(1-\alpha)} \right). \quad (23)$$

The voltage across the capacitor while it is charging is given by

$$V_C(t, \alpha) = V_0 \times \left(1 - e^{(1-\alpha)\Gamma t} \left[\frac{2-\alpha}{(1-\alpha) + e^{(1-\alpha)\Gamma t}} \right]^{1/(1-\alpha)} \right). \quad (24)$$

It is easy to verify the solution by taking $\alpha \rightarrow 1$ in Eq. (24) in order to get

$$V_C(t, 1) = V_0 (1 - e^{-\Gamma t}), \quad (25)$$

which is the expected solution for an RC circuit connected to a DC battery.

In Fig. 2 we show the graph of the voltage across the capacitor given by Eq. (24) for different values of α . The results given in Fig. 2 shows that when $\alpha \rightarrow 1$ the system displays the classical behavior. However, for values of $0 < \alpha < 1$, the solution describes a dissipative system due to the fact that the fractional differentiation with respect to time represents a non-local effect of dissipation of energy (internal friction) represented by the fractional order α .

3.2. Case 2

We are going now to use the following function $\varphi(t, \alpha) = (1 + \Gamma(1 - \alpha)t)/\Gamma$ which has the unit of time and using Eq. (8) we get the following dimensionless function

$$\tau(t, \alpha) = \frac{1}{1-\alpha} \ln [1 + \Gamma(1 - \alpha)t]. \quad (26)$$

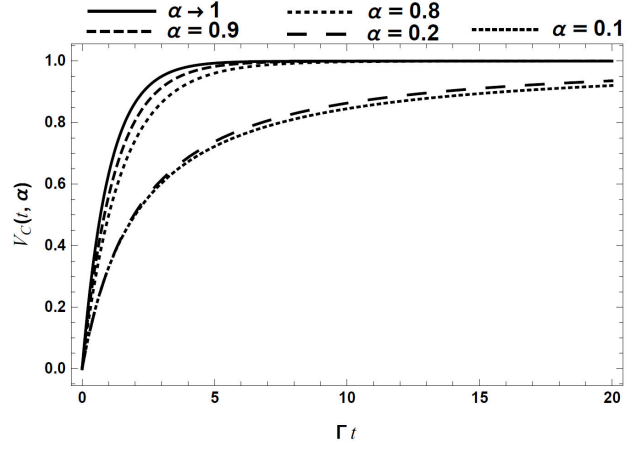


FIGURE 3. The figure shows the voltage across the capacitor for the case when the DC voltage is $V_0 = 1$ V.

Note that $\tau(t, \alpha)$ satisfies Eq. (10). Using Eq. (12) we have the following fractional differential equation for the RC circuit

$${}^{CF}D_\tau^\alpha q(\tau) + qe^{(1-\alpha)\tau} = q_0 e^{(1-\alpha)\tau} \quad \text{where } 0 < \alpha \leq 1. \quad (27)$$

Using Eqs. (17) and (18) we find the solution of the fractional differential equation given in Eq. (27) which is given by

$$q(\tau, \alpha) = q_0 + \frac{C_0}{[1 + (1 - \alpha)e^{(1-\alpha)\tau}]^{1+\alpha/(1-\alpha)^2}}. \quad (28)$$

Using the initial condition $q(0, \alpha) = 0 = q_0 + C_0(2 - \alpha)^{-1-\alpha/(1-\alpha)^2}$ and using Eq. (26) we can write the solution in terms of the ordinary time and the initial condition which is given by

$$q(t, \alpha) = q_0 \left(1 - \frac{1}{\left[1 + \frac{\Gamma(1-\alpha)^2}{(2-\alpha)} t \right]^{1+\alpha/(1-\alpha)^2}} \right). \quad (29)$$

The voltage across the capacitor while it is charging is given by

$$V_C(t, \alpha) = V_0 \left(1 - \frac{1}{\left[1 + \frac{\Gamma(1-\alpha)^2}{(2-\alpha)} t \right]^{1+\alpha/(1-\alpha)^2}} \right). \quad (30)$$

It is easy to verify the solution by taking $\alpha \rightarrow 1$ in Eq. (30) in order to get

$$V_C(t, 1) = V_0 (1 - e^{-\Gamma t}), \quad (31)$$

which is the expected solution for an RC circuit connected to a DC battery.

4. Conclusions

A systematic way to construct fractional differential equations with non singular kernels has been proposed. The relevant aspect of this work is the method for setting up the fractional differential equations with nonsingular kernels while keeping the dimensionality of the physical parameters. A new function has been introduced, that depends on the order of the derivative being considered *i.e.* $0 < \alpha \leq 1$, to keep the dimensionality of the physical parameters. An example of this new approach has been given for the case of an RC circuit connected to a DC battery. The results presented in this

paper can be easily extended to non singular fractional derivatives of higher order. We should point out that there might be other functions φ that could result in a different fractional differential equation and that will result in other classes of solutions with different behavior.

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Systematic analysis of fermionic masses and flavor mixings: a model-independent approach

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In a model-independent context, we perform a systematic and detailed study of the fermion flavor masses and mixings. In this analysis, we present a most general parameterization form of the 3×3 mass matrix, as well as the Pontecorvo-Maki-Nakagawa-Sakata flavor mixing matrix, in terms of the fermionic masses and some free parameters. A likelihood test using the χ^2 statistic is implemented to evaluate whether the theoretical expressions for the leptonic flavor mixing angles also reproduce the experimental data. The results of the χ^2 fit show that the theoretical expressions obtained for the Pontecorvo-Maki-Nakagawa-Sakata mixing matrix correctly reproduce the actual experimental data on neutrino oscillations.

Keywords: Fermionic mass matrix; fermionic mixing matrix.

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1. Introduction

The fermionic sector of particle physics deserves an in-depth exploration beyond the Standard Model for several fundamental reasons. The Standard Model, although successful, has critical gaps in that sector [1-4], as it does not explain why exactly three generations of fermions exist, nor does it predict their specific masses [1,5]. The hierarchy of fermionic masses, from the neutrino to the top quark, spans more than 12 orders of magnitude without a satisfactory theoretical explanation. The mixing patterns in the fermionic sector reveal structures that suggest deeper underlying physics. The CKM matrix for quarks and the PMNS matrix for neutrinos show mixing angles that appear to follow specific patterns, but the Standard Model offers no fundamental explanation for these values. In concordance with experiments [6,7], neutrinos oscillation is given by implying the massive neutrinos [1]. On the other hand, the CP violation observed in the fermionic sector is insufficient to explain the matter-antimatter asymmetry of the universe. This suggests that additional sources of CP violation exist in extended fermionic sectors. Many dark matter candidates are fermionic (such as neutralinos in supersymmetry). Exploration of the extended fermionic sector could reveal stable particles that constitute dark matter. Standard Model fermions naturally fit into representations of larger symmetry groups (such as SO(10) or E6), suggesting that they are part of more fundamental structures. Exploration of the fermionic sector transcends current limitations and could reveal the fundamental architecture of physical reality, connecting from microscopic structure to the deepest cosmological mysteries.

Within the SM framework, neutrinos were originally con-

sidered massless particles, since they do not interact with the Higgs field in the same way as other particles. However, in SM minimal extensions, such as the See-Saw mechanism, a natural explanation is introduced for the extremely small neutrino masses. In this model, neutrinos acquire mass through mixing with heavier particles, which results in neutrino masses being much smaller compared to other particles [8]. Although the absolute neutrino mass has not yet been directly measured, very low upper limits ($O(\text{eV})$) have been set by experiments such as KATRIN [9]. These experiments confirm that neutrinos have an extremely small, but nonzero, mass.

This paper is organized as follow: Section 2 is addressed to the fermionic mixing matrices, whereas Sec. 3 shows the fermionic general mass matrix and its analysis; the orthogonal matrix associated to the diagonalization of the general mass matrix is shown in Sec. 4. The analytic lepton flavor mixing matrix and numerical analysis is provided in Sec. 5. Finally, in Sec. 6 are given the conclusions.

2. Fermionic Mixing matrices

CKM matrix

The CKM matrix V_{CKM} (Cabibbo, Kobayashi, Maskawa) is of the order 3×3 that describes quark mixings in SM context. This one specifically refers how up (u , c , t)-down (d , s , b) quarks mix through the weak interaction. This mixing is related with disintegration processes mediated for $W^\pm$ gauge bosons (charged currents) and quarks flavor changing. The V_{CKM} has the form [1]:

$$\mathbf{V}_{\text{CKM}} = \mathbf{U}_u \mathbf{U}_d^\dagger = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}, \quad (1)$$

where $\mathbf{U}_u$ and $\mathbf{U}_d$ are unitary matrices that diagonalize the mass matrix of the up- and down-quarks, respectively. The elements of the CKM matrix $[\mathbf{V}_{\text{CKM}}]_{ij}$ are complex numbers that describe the transition probability from a quark i -th to a quark j -th. Since the CKM matrix $\mathbf{V}_{\text{CKM}}$ is unitary, guarantees the conservation of probability in transitions between

quarks. In an angle-phase parameterization, the matrix elements are related to three mixing angles (θ_{12} , θ_{23} , θ_{13}), and one Charge-Parity (CP)-violating phase, δ_{CP} . These mixing angles determine the magnitude of mixing between quarks, while the phase is responsible for CP symmetry violation in weak interactions. The complex phase of the $\mathbf{V}_{\text{CKM}}$ is the source that introduces CP violation in the SM, a phenomenon related to the fact that the laws of physics are not completely symmetric under charge and parity inversion.

In the standard PDG parameterization, the $\mathbf{V}_{\text{CKM}}$ is written as [1]

$$\mathbf{V}_{\text{CKM}} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix}, \quad (2)$$

where $s_{ij} \equiv \sin \theta_{ij}$ and $c_{ij} \equiv \cos \theta_{ij}$. The meaning of the mixing angles are: θ_{12} represents the mixing between the first and second generation of quarks, whereas θ_{23} angle represents the mixing between the second and third generation of quarks, and θ_{13} angle represents the mixing between the first and third generation of quarks. This angle is associated with the complex phase δ_{CP} , which is crucial for CP violation. The elements of the CKM matrix are related to three mixing angles in the following form [10],

$$\begin{aligned} \sin^2 \theta_{12} &= \frac{|V_{us}|^2}{1 - |V_{ub}|^2}, \\ \sin^2 \theta_{23} &= \frac{|V_{cb}|^2}{1 - |V_{ub}|^2}, \\ \sin^2 \theta_{13} &= |V_{ub}|^2. \end{aligned} \quad (3)$$

On the other hand, the Jarlskog invariant is a scalar quantity that measures the magnitude of CP symmetry violation in the quark sector of the Standard Model. It is defined from the elements of the CKM matrix; specifically, the Jarlskog invariant is expressed as [11]:

$$\mathcal{J} = \text{Im} \{ V_{ud} V_{cs} V_{us}^* V_{cd}^* \}. \quad (4)$$

This invariant is particularly important because it does not depend on the choice of the phase in the CKM matrix. Its value is proportional to the magnitude of CP symmetry violation in quark interactions, serving as a direct indicator of this phenomenon. In terms of the mixing angles, we have

$$\mathcal{J} = \frac{1}{8} \sin 2\theta_{12} \sin 2\theta_{23} \sin 2\theta_{13} \cos \theta_{13} \sin \delta_{CP}. \quad (5)$$

Thus, the phase factor in terms of the elements of the $\mathbf{V}_{\text{CKM}}$ can be written as:

$$\sin \delta_{CP} = \frac{\mathcal{J} (1 - |V_{ub}|^2)}{|V_{cb}| |V_{tb}| |V_{ub}| |V_{ud}| |V_{us}|}. \quad (6)$$

To arrive at the above expression, the fact that the $\mathbf{V}_{\text{CKM}}$ is unitary was used.

PMNS matrix

The PMNS matrix (Pontecorvo-Maki-Nakagawa-Sakata) is analogous to the CKM matrix but applies to the lepton sector instead of the quark sector (it is crucial for describing how neutrinos change from one type to another, a phenomenon known as neutrino oscillation). The PMNS matrix relates the flavor states of leptons to their mass states. The leptonic flavor mixing matrix PMNS arises from the mismatch between the diagonalization of the charged lepton and neutrino mass matrices, and is defined as [1],

$$\mathbf{V}_{\text{PMNS}} = \mathbf{U}_\ell^\dagger \mathbf{U}_\nu = \begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{pmatrix}, \quad (7)$$

where $\mathbf{U}_\ell$ and $\mathbf{U}_\nu$ are unitary matrices that diagonalize the mass matrices of the charged leptons and neutrinos, respectively. Each element $U_{\alpha i}$ of the PMNS matrix describes the probability amplitude for a neutrino with flavor α (where α can be e , μ , or τ) to be in the mass state i (where $i = 1, 2$, or 3). In the symmetric parametrization of the PMNS matrix, three mixing angles (θ_{12} , θ_{23} , θ_{13}) and three CP-violating phases (ϕ_{12} , ϕ_{13} , ϕ_{23}) are included [12]. In this parametrization, the PMNS matrix is written as [1]

$$\mathbf{V}_{\text{PMNS}} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13}e^{-i\phi_{12}} & s_{13}e^{-i\phi_{13}} \\ -s_{12}c_{23}e^{i\phi_{12}} - c_{12}s_{23}s_{13}e^{-i(\phi_{23}-\phi_{13})} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{-i(\phi_{23}+\phi_{12}-\phi_{13})} & s_{23}c_{13}e^{-i\phi_{23}} \\ s_{12}s_{23}e^{i(\phi_{23}+\phi_{12})} - c_{12}c_{23}s_{13}e^{i\phi_{13}} & -c_{12}s_{23}e^{i\phi_{23}} - s_{12}c_{23}s_{13}e^{-i(\phi_{12}-\phi_{13})} & c_{23}c_{13} \end{pmatrix}, \quad (8)$$

where $s_{ij} = \sin \theta_{ij}$ and $c_{ij} = \cos \theta_{ij}$. The relations between the mixing angles and the entries of the PMNS matrix are

$$\begin{aligned}\sin^2 \theta_{12} &= \frac{|U_{e2}|^2}{1 - |U_{e3}|^2}, \\ \sin^2 \theta_{23} &= \frac{|U_{\mu 3}|^2}{1 - |U_{e3}|^2}, \\ \sin^2 \theta_{13} &= |U_{e3}|^2.\end{aligned}\quad (9)$$

In case of neutrino oscillations, the Jarlskog invariant is defined as

$$\mathcal{J} = \text{Im} \{ U_{e1} U_{\mu 3} U_{e3}^* U_{\mu 1}^* \}, \quad (10)$$

which in the symmetric parametrization takes the form

$$\mathcal{J} = \frac{1}{8} \sin 2\theta_{12} \sin 2\theta_{23} \sin 2\theta_{13} \cos \theta_{13} \sin \delta, \quad (11)$$

where $\delta = \phi_{13} - \phi_{23} - \phi_{12}$. In addition, the invariants

$$\begin{aligned}\mathcal{I}_1 &= \text{Im} \{ U_{e2}^2 U_{e1}^{*2} \}, \\ \mathcal{I}_2 &= \text{Im} \{ U_{e3}^2 U_{e1}^{*2} \},\end{aligned}\quad (12)$$

associated with the Majorana phase factors [10] in the symmetric parametrization take the form

$$\begin{aligned}\mathcal{I}_1 &= \frac{1}{4} \sin^2 2\theta_{12} \cos^4 \theta_{13} \sin(-2\phi_{12}), \\ \mathcal{I}_2 &= \frac{1}{4} \sin^2 2\theta_{13} \cos^2 \theta_{12} \sin(-2\phi_{13}).\end{aligned}\quad (13)$$

Then, the phase factors associated with CP violation can be written as

$$\begin{aligned}\sin \delta &= \frac{\mathcal{J} (1 - |V_{e3}|^2)}{|U_{e1}| |U_{e2}| |U_{e3}| |U_{\mu 3}| |U_{\tau 3}|}, \\ \sin(-2\phi_{12}) &= \frac{\mathcal{I}_1}{|U_{e1}|^2 |U_{e2}|^2}, \\ \sin(-2\phi_{13}) &= \frac{\mathcal{I}_2}{|U_{e1}|^2 |U_{e3}|^2}.\end{aligned}\quad (14)$$

The equivalence between the standard PDG parametrization and the symmetric one can be expressed as $\mathbf{U}_{\text{PDG}} = \mathbf{K} \mathbf{U}_{\text{sim}}$, where $\mathbf{K} = \text{diag}(1, e^{i(\alpha_{21}/2)}, e^{i(\alpha_{21}/2)})$. Here, the Dirac-type phase takes the form $\delta = \phi_{13} - \phi_{23} - \phi_{12}$, while the Majorana-type phases are $\alpha_{21} = -2\phi_{12}$ and $\alpha_{31} = -2(\phi_{12} + \phi_{23})$.

3. Fermionic general mass matrix

In general, in the physics of elementary particles, the fermionic mass matrix, $\mathbf{M}_f$, does not have any particular internal symmetry. Therefore, to diagonalize it through a unitary transformation, bilinear forms must be constructed as follows:

$$\mathbf{M}_f \mathbf{M}_f^\dagger \quad \text{and} \quad \mathbf{M}_f^\dagger \mathbf{M}_f, \quad (15)$$

which are Hermitian matrices. The matrices in Eq. (15) can be brought to their diagonal form through the following unitary transformations:

$$\begin{aligned}\mathbf{V}_f \mathbf{M}_f \mathbf{M}_f^\dagger \mathbf{V}_f^\dagger &= \Delta_{f,\lambda} \quad \text{and} \\ \mathbf{U}_f \mathbf{M}_f^\dagger \mathbf{M}_f \mathbf{U}_f^\dagger &= \Delta_{f,\lambda},\end{aligned}\quad (16)$$

where $\mathbf{U}_f$ and $\mathbf{V}_f$ are unitary matrices. Additionally, $\Delta_{f,\lambda} = \text{diag}(\lambda_{f1}, \lambda_{f2}, \lambda_{f3})$, where the λ_{fi} are the real eigenvalues of the matrices $\mathbf{M}_f \mathbf{M}_f^\dagger$ and $\mathbf{M}_f^\dagger \mathbf{M}_f$. Therefore, from the expressions in Eq. (16), we obtain

$$\mathbf{V}_f \mathbf{M}_f \mathbf{U}_f^\dagger = \Delta_{f,\Sigma}, \quad \text{or} \quad \mathbf{M}_f = \mathbf{V}_f^\dagger \Delta_{f,\Sigma} \mathbf{U}_f, \quad (17)$$

where $\Delta_{f,\Sigma} = \text{diag}(\Sigma_{f1}, \Sigma_{f2}, \Sigma_{f3})$. The $\Sigma_{fi} \equiv \sqrt{\lambda_{fi}}$ are the singular values of the matrix $\mathbf{M}_f$, which may be complex quantities.

In order to determine the explicit form of the unitary matrices $\mathbf{U}_f$ and $\mathbf{V}_f$, we will consider two possible internal symmetries of the mass matrix $\mathbf{M}_f$. The first is to consider the mass matrix as a Hermitian matrix, and the second is to consider it as a complex symmetric matrix. In the case of representing the mass matrix through a Hermitian matrix, the condition $\mathbf{M}_f = \mathbf{M}_f^\dagger$ must be satisfied. Then, from Eq. (17), the self-adjoint matrix of the fermion mass matrix can be written as

$$\mathbf{M}_f^\dagger = \mathbf{U}_f^\dagger \Delta_{f,\Sigma}^\dagger \mathbf{V}_f. \quad (18)$$

By comparing the matrices in Eqs. (17) and (18), it follows that the unitary matrices satisfy the relation $\mathbf{U}_f = \mathbf{V}_f$. Moreover, $\Delta_{f,\Sigma} = \Delta_{f,\Sigma}^\dagger$, which implies that the elements of the matrix $\Delta_{f,\Sigma}$ are real quantities. Consequently, and in accordance with the singular value decomposition theorem, in this particular case the fermion mass matrix in Eq. (17) takes the form

$$\mathbf{M}_f = \mathbf{U}_f^\dagger \Delta_{f,m} \mathbf{U}_f \quad \Rightarrow \quad \mathbf{U}_f \mathbf{M}_f \mathbf{U}_f^\dagger = \Delta_{f,m}, \quad (19)$$

where $\Delta_{f,m} = \text{diag}(m_{f1}, m_{f2}, m_{f3})$. In this case, the singular values and the eigenvalues of the matrix $\mathbf{M}_f$ are equal. Therefore, the $m_{fi} = \Sigma_{fi}$ are the physical masses of the fermions.

On the other hand, when representing the fermion mass matrix through a complex symmetric mass matrix, the condition $\mathbf{M}_f = \mathbf{M}_f^\top$ must hold. Then, starting from Eq. (17), the transpose of the fermion mass matrix can be written as

$$\mathbf{M}_f^\top = \mathbf{U}_f^\top \Delta_{f,\Sigma}^\top \mathbf{V}_f^*. \quad (20)$$

By comparing the matrices in Eqs. (17) and (20), it follows that the unitary matrices satisfy the relation $\mathbf{U}_f^\top = \mathbf{V}_f^\dagger$ or $\mathbf{U}_f = \mathbf{V}_f^*$. Furthermore, the relation $\Delta_{f,\Sigma} = \Delta_{f,\Sigma}^\top$ is automatically satisfied because the matrix $\Delta_{f,\Sigma}$ is a diagonal

matrix. Consequently, the fermion mass matrix in Eq. (17) takes the form

$$\mathbf{M}_f = \mathbf{U}_f^\top \Delta_{f,\Sigma} \mathbf{U}_f. \quad (21)$$

In general, the elements of the matrix $\Delta_{f,\Sigma}$ are complex quantities, so it can be written as

$$\Delta_{f,\Sigma} = \mathbf{K}_f \Delta_{f,m} \mathbf{K}_f, \quad (22)$$

where $\Delta_{f,m} = \text{diag}(m_{f1}, m_{f2}, m_{f3})$ and $\mathbf{K}_f = \text{diag}(e^{i(\varphi_{f1}/2)}, e^{i(\varphi_{f2}/2)}, e^{i(\varphi_{f3}/2)})$, with $m_{fi} = |\Sigma_{fi}|$ and $\varphi_{fi} = \arg\{m_{fi}\}$. From Eq. (22), the fermion mass matrix in equation (21) can be expressed as

$$\mathbf{M}_f = \mathcal{U}_f^\top \Delta_{f,m} \mathcal{U}_f \Rightarrow \mathcal{U}_f^* \mathbf{M}_f \mathcal{U}_f^\dagger = \Delta_{f,m}, \quad (23)$$

where $\mathcal{U}_f = \mathbf{K}_f \mathbf{U}_f$. The phase factors present in the diagonal matrix $\mathbf{K}_f$ can be absorbed into the spinors of the mass terms. It is common to associate these phase factors with the CP-violating phases of the Majorana type.

In summary, the mass matrices given in Eqs. (19) and (23) can be expressed in the following compact form:

$$\mathbb{V}_f^j \mathbf{M}_f \mathbb{U}_f^{j\dagger} = \Delta_{f,m}, \quad j = 1, 2, \quad (24)$$

where

$$\begin{aligned} \mathbb{U}_f^1 &= \mathbf{U}_f, & \mathbb{V}_f^1 &= \mathbf{U}_f, & \text{for } \mathbf{M}_f &= \mathbf{M}_f^\dagger, \\ \mathbb{U}_f^2 &= \mathcal{U}_f, & \mathbb{V}_f^2 &= \mathcal{U}_f^*, & \text{for } \mathbf{M}_f &= \mathbf{M}_f^\top, \end{aligned} \quad (25)$$

with $\mathcal{U}_f = \mathbf{K}_f \mathbf{U}_f$.

3.1. Fermion mass matrix 3×3

The general fermion mass matrix of 3×3 can be written in the following expression:

$$\mathbf{M}_f = \begin{pmatrix} m_{11}^f & m_{12}^f & m_{13}^f \\ m_{21}^f & m_{22}^f & m_{23}^f \\ m_{31}^f & m_{32}^f & m_{33}^f \end{pmatrix}, \quad (26)$$

where the superscript $f = u, d, \ell, \nu$ denotes the up quarks, down quarks, charged leptons, and neutrinos, respectively. The elements m_{ij}^f of the matrix $\mathbf{M}_f$, with $i, j = 1, 2, 3$, are complex quantities. The fermion mass matrix $\mathbf{M}_f$ can be rotated via the orthogonal transformation

$$\mathbf{M}_{Rf} = \mathbf{R}_{\beta_f} \mathbf{M}_f \mathbf{R}_{\beta_f}^\top \quad \text{or} \quad \mathbf{M}_f = \mathbf{R}_{\beta_f}^\top \mathbf{M}_{Rf} \mathbf{R}_{\beta_f}. \quad (27)$$

In these expressions, $\mathbf{R}_{\beta_f}$ is a real symmetric rotation matrix given as

$$\mathbf{R}_{\beta_f} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \beta_f & \sin \beta_f \\ 0 & -\sin \beta_f & \cos \beta_f \end{pmatrix}. \quad (28)$$

On the other hand, in order to generate a zero in the $(1, 3)$ entry of the matrix $\mathbf{M}_{Rf}$, it is required that the relation

$$\tan \beta_f = \frac{m_{13}^f}{m_{12}^f}, \quad (29)$$

whereas, to generate a zero in the $(3, 1)$ entry of the matrix $\mathbf{M}_{Rf}$, the relation must be hold

$$\tan \beta_f = \frac{m_{31}^f}{m_{21}^f}. \quad (30)$$

By comparing the expressions in Eqs. (29) and (30), it can be observed that both refer to the same rotation angle β_f , and therefore, the relation

$$\frac{m_{13}^f}{m_{12}^f} = \frac{m_{31}^f}{m_{21}^f}. \quad (31)$$

In order for the definition of the angle β_f to be a real quantity, and corresponds to a pure rotation, the relation must hold

$$\begin{aligned} \arg\{m_{13}^f\} &= \arg\{m_{31}^f\}, \\ \arg\{m_{21}^f\} &= \arg\{m_{12}^f\}. \end{aligned} \quad (32)$$

Thus, the rotated mass matrix, $\mathbf{M}_{Rf}$, takes the form

$$\mathbf{M}_{Rf} = \begin{pmatrix} m_{11}^f & A_f & 0 \\ A_f' & B_f' & C_f \\ 0 & C_f' & D_f' \end{pmatrix}, \quad (33)$$

here in the following expressions $t_{\beta_f} \equiv \tan \beta_f$,

$$\begin{aligned} A_f &= m_{12}^f \sqrt{1 + t_{\beta_f}^2}, & A_f' &= m_{21}^f \sqrt{1 + t_{\beta_f}^2}, \\ B_f' &= \frac{m_{22} + m_{33} t_{\beta_f}^2 + (m_{23} + m_{32}) t_{\beta_f}}{1 + t_{\beta_f}^2}, \\ C_f &= \frac{m_{23} - m_{32} t_{\beta_f}^2 + (m_{33} - m_{22}) t_{\beta_f}}{1 + t_{\beta_f}^2}, \\ C_f' &= \frac{m_{32} - m_{23} t_{\beta_f}^2 + (m_{33} - m_{22}) t_{\beta_f}}{1 + t_{\beta_f}^2}, \\ D_f' &= \frac{m_{33} + m_{22} t_{\beta_f}^2 - (m_{23} + m_{32}) t_{\beta_f}}{1 + t_{\beta_f}^2}. \end{aligned} \quad (34)$$

Motivated by the hierarchical pattern of fermion masses and mixings, where direct first–third family couplings are suppressed with respect to nearest–neighbour interactions, we work in an intermediate weak basis in which the $(1, 3)$ and $(3, 1)$ entries of the mass matrix vanish. Such a structure can arise from approximate flavour symmetries or from vacuum alignment conditions following the minimization of extended Higgs potentials. Exploiting weak–basis freedom, the fermion mass matrix is therefore cast into a canonical form with $M_{13} = M_{31} = 0$, which should be regarded as a basis choice rather than a dynamical texture assumption. Requiring this transformation to be implemented by a single real rotation leads to the consistency conditions in Eqs. (31) and (32), ensuring that both entries are simultaneously eliminated. The resulting matrix, given in Eq. (33), represents

the most general mass matrix within this canonical class. The analysis is then performed in two complementary scenarios, Hermitian and complex symmetric mass matrices, corresponding to Dirac and Majorana fermion mass terms, respectively. The general Dirac mass matrices can be diagonalized through bi-unitary transformations, equivalently associated with the diagonalization of Hermitian mass combinations carrying the same physical content [1,13-26].

In this analysis of the mass matrices and flavor mixing, two possible internal symmetries in the fermion mass matrices will be considered. The first internal symmetry to consider is representing the fermion mass matrix as a Hermitian matrix, $\mathbf{M}_f = \mathbf{M}_f^\dagger$. An immediate consequence of this internal symmetry is that the rotated matrix satisfies $\mathbf{M}_{Rf} = \mathbf{M}_{Rf}^\dagger$. Thus, the elements of the matrix $\mathbf{M}_{Rf}$ fulfill the relations $A'_f = A_f^*$, $C'_f = C_f^*$, $B'_f = B_f^*$, and $D'_f = D_f^*$. From the previous expressions, it can be concluded that the diagonal elements are real quantities, $m_{11}^f = m_{11}^{f*}$, $m_{22}^f = m_{22}^{f*}$, $m_{33}^f = m_{33}^{f*}$, and that the off-diagonal elements satisfy $m_{21}^f = m_{12}^{f*}$, $m_{31}^f = m_{13}^{f*}$, $m_{32}^f = m_{23}^{f*}$. The second internal symmetry that will be considered here is to treat the fermion mass matrix as a complex symmetric matrix, $\mathbf{M}_f = \mathbf{M}_f^\top$. An immediate consequence of the previous symmetry is that the rotated matrix satisfies the relation $\mathbf{M}_{Rf} = \mathbf{M}_{Rf}^\top$. Therefore, the elements of this matrix satisfy $A'_f = A_f$ and $C'_f = C_f$. Additionally, the off-diagonal elements of the matrix $\mathbf{M}_f$ satisfy the conditions $m_{12}^f = m_{21}^f$, $m_{13}^f = m_{31}^f$, $m_{23}^f = m_{32}^f$.

The matrix $\mathbf{M}_{Rf}$ can be expressed in polar form, therefore,

$$\mathbf{M}_{Rf} = \mathbf{Q}_f \bar{\mathbf{M}}_{Rf} \mathbf{P}_f, \quad (35)$$

where $\mathbf{Q}_f = \mathbf{P}_f^\dagger$ for the case when $\mathbf{M}_f$ is Hermitian, and $\mathbf{Q}_f = \mathbf{P}_f^\top$ for when $\mathbf{M}_f$ is a complex symmetric matrix. The explicit form of the phase factor matrix is

$$\begin{aligned} \mathbf{P}_f &= \text{diag} \left\{ 1, e^{i\vartheta_{f,a}}, e^{i(\vartheta_{f,c} + \vartheta_{f,a})} \right\} \text{ for } \mathbf{M}_f = \mathbf{M}_f^\dagger, \\ \mathbf{P}_f &= \text{diag} \left\{ 1, e^{i\vartheta_{f,a}}, e^{i(\vartheta_{f,c} - \vartheta_{f,a})} \right\} \text{ for } \mathbf{M}_f = \mathbf{M}_f^\top, \end{aligned} \quad (36)$$

where $\vartheta_{f,a} = \arg \{A_f\}$ and $\vartheta_{f,c} = \arg \{C_f\}$. Additionally, for the case $\mathbf{M}_f = \mathbf{M}_f^\top$, the following relations must hold: $\arg \{B_f\} = 2 \arg \{A_f\}$ and $\arg \{D_f\} = 2(\arg \{C_f\} - \arg \{A_f\})$. The real symmetric matrix, $\bar{\mathbf{M}}_{Rf}$, can be written as

$$\bar{\mathbf{M}}_{Rf} = m_{11}^f \mathbb{I}_{3 \times 3} + \mathcal{M}_f, \quad (37)$$

where $\mathbb{I}_{3 \times 3} = \text{diag}(1, 1, 1)$,

$$\mathcal{M}_f = \begin{pmatrix} 0 & \mathcal{A}_f & 0 \\ \mathcal{A}_f & \mathcal{B}_f & \mathcal{C}_f \\ 0 & \mathcal{C}_f & \mathcal{D}_f \end{pmatrix}, \quad (38)$$

where for both internal symmetries in the fermion mass matrix, it holds that $\mathcal{A}_f = |A_f|$, $\mathcal{B}_f = B_f$, $\mathcal{C}_f = |C_f|$,

$\mathcal{D}_f = D_f$. For a Hermitian mass matrix $\mathbf{M}_f$,

$$\begin{aligned} \mathcal{A}_f &= |m_{12}^f| \sqrt{1 + t_{\beta_f}^2}, \\ \mathcal{B}_f &= \frac{m_{22} + m_{33} t_{\beta_f}^2 + (m_{23} + m_{23}^*) t_{\beta_f}}{1 + t_{\beta_f}^2} - m_{11}^f, \\ \mathcal{C}_f &= \left| \frac{m_{23} - m_{23}^* t_{\beta_f}^2 + (m_{33} - m_{22}) t_{\beta_f}}{1 + t_{\beta_f}^2} \right|, \\ \mathcal{D}_f &= \frac{m_{33} + m_{22} t_{\beta_f}^2 - (m_{23} + m_{23}^*) t_{\beta_f}}{1 + t_{\beta_f}^2} - m_{11}^f. \end{aligned} \quad (39)$$

On the other hand, a complex symmetric mass matrix $\mathbf{M}_f$,

$$\begin{aligned} \mathcal{A}_f &= |m_{12}^f| \sqrt{1 + t_{\beta_f}^2}, \\ \mathcal{B}_f &= \left| \frac{m_{22} + m_{33} t_{\beta_f}^2 + 2m_{23} t_{\beta_f}}{1 + t_{\beta_f}^2} \right| - m_{11}^f, \\ \mathcal{C}_f &= \left| \frac{m_{23} (1 - t_{\beta_f}^2) + (m_{33} - m_{22}) t_{\beta_f}}{1 + t_{\beta_f}^2} \right|, \\ \mathcal{D}_f &= \left| \frac{m_{33} + m_{22} t_{\beta_f}^2 - 2m_{23} t_{\beta_f}}{1 + t_{\beta_f}^2} \right| - m_{11}^f. \end{aligned} \quad (40)$$

Without loss of generality, here m_{11}^f is considered a real quantity. This is possible because the matrix $\mathbf{P}_f$ always allows a phase factor to be factored out, which would be absorbed by the spinors of the mass term. With the help of the expressions in Eqs. (35) and (37), the mass matrix in Eq. (27) can be rewritten as

$$\mathbf{M}_f = \mathbf{R}_{\beta_f}^\top \mathbf{Q}_f \left(m_{11}^f \mathbb{I}_{3 \times 3} + \mathcal{M}_f \right) \mathbf{P}_f \mathbf{R}_{\beta_f}. \quad (41)$$

The real symmetric matrix $\mathcal{M}_f$ can be diagonalized through the following orthogonal transformation

$$\mathcal{M}_f = \mathbf{O}_f \Delta_{f,\sigma} \mathbf{O}_f^\top, \quad (42)$$

where $\Delta_{f,\sigma} = \text{diag}(\sigma_{f1}, \sigma_{f2}, \sigma_{f3})$, here the σ_{fi} are the eigenvalues of the real symmetric matrix $\mathcal{M}_f$ and are known as the running masses of the fermions [27]. Thus,

$$\mathbf{M}_f = \mathbf{R}_{\beta_f}^\top \mathbf{Q}_f \mathbf{O}_f \left(m_{11}^f \mathbb{I}_{3 \times 3} + \Delta_{f,\sigma} \right) \mathbf{O}_f^\top \mathbf{P}_f \mathbf{R}_{\beta_f}. \quad (43)$$

From the above mass matrix, Eq. (43), for the quark sector when the mass matrix is represented by a Hermitian matrix, it takes the form

$$\mathbf{M}_q = \mathbf{U}_q^\dagger \Delta_{q,m} \mathbf{U}_q, \quad (44)$$

where $q = u, d$ denotes the up-type and down-type quarks, and $\mathbf{U}_q = \mathbf{O}_q^\top \mathbf{P}_q \mathbf{R}_{\beta_q}$ is the unitary matrix that diagonalizes the quark mass matrix. While in the case when the quark mass matrix is represented by a complex symmetric matrix, we have

$$\mathbf{M}_q = \mathbf{U}_q^\top \Delta_{q,m} \mathbf{U}_q, \quad (45)$$

with $q = u, d$ denotes the up-type and down-type quarks, and $\mathbf{U}_q = \mathbf{O}_q^\top \mathbf{P}_q \mathbf{R}_{\beta_q}$ is the unitary matrix that diagonalizes the quark mass matrix. Furthermore, in the previous expressions $\Delta_{q,m} = \text{diag}(m_{q1}, m_{q2}, m_{q3})$ is a diagonal matrix of the physical masses of the quarks.

In contrast, for the lepton sector when the mass matrix is represented by a Hermitian matrix, the expression in Eq. (43) can be rewritten as

$$\mathbf{M}_l = \mathbf{U}_l \Delta_{l,m} \mathbf{U}_l^\dagger, \quad (46)$$

where $l = \ell, \nu$ denotes the charged leptons and neutrinos. Furthermore, $\mathbf{U}_l = \mathbf{R}_{\beta_l}^\top \mathbf{P}_l^\dagger \mathbf{O}_l$ is the unitary matrix that diagonalizes the lepton mass matrix. For the case when the lepton mass matrix is represented by a complex symmetric matrix,

$$\mathbf{M}_l = \mathbf{U}_l \Delta_{l,m} \mathbf{U}_l^\top, \quad (47)$$

where $l = \ell, \nu$ denotes the charged leptons and neutrinos. Additionally, $\mathbf{U}_l = \mathbf{R}_{\beta_l}^\top \mathbf{P}_l^\top \mathbf{O}_l$ is the unitary matrix that diagonalizes the lepton mass matrix. Thus, in the previous expressions, $\Delta_{l,m} = \text{diag}(m_{l1}, m_{l2}, m_{l3})$ is a diagonal matrix of the physical masses of the leptons.

The hierarchy between fermionic masses is taken into account considering the normal hierarchy (NH), it is assumed that the first two fermions have small masses and are closer to each other, while the third is considerably heavier.

$$m_{f,1} < m_{f,2} \ll m_{f,3}, \text{ with } f = l, \nu. \quad (48)$$

In the inverted hierarchy (IH), consistent just with neutrinos, the two heavier fermions are nearly degenerate, while the third is considerably lighter. In terms of the mass differences:

$$m_{\nu 3} \ll m_{\nu 1} < m_{\nu 2}. \quad (49)$$

Despite this scenario is less intuitive as NH, it is compatible with the experimental data available so far. It has not yet been confirmed which of the two mass hierarchies is correct, but future experiments such as DUNE (Deep Underground Neutrino Experiment) [28] and JUNO (Jiangmen Underground Neutrino Observatory) aim to determine the neutrino hierarchy as one of their main objectives.

From the expression in Eq. (43), we obtain

$$\sigma_{fi} = s_i m_{fi} - m_{11}^f, \quad (50)$$

which relates the physical masses of the fermions with their running masses. In this expression, the s_i ($i = 1, 2, 3$) is a sign that takes values ± 1 , such that $\mathcal{A}_f^2 \geq 0$ is guaranteed. Changing the sign of one of the eigenvalues is equivalent to performing a rotation in the eigenvalue space. In other words, for fermion fields, the sign of the mass is irrelevant, as the sign can be changed via a chiral transformation: $f_R \rightarrow f'_R = e^{i\gamma_5(\pi/2)} f_R$ and $f_L \rightarrow f'_L = e^{i\gamma_5(\pi/2)} f_L$. These transformations change the sign of the eigenvalues, but leave invariant the rest of the Lagrangian.

4. Orthogonal matrix in terms of the fermion masses

The square of the matrix $\mathcal{M}_f$ is

$$\begin{aligned} \mathcal{M}_f^2 &= \mathcal{M}_f^\dagger \mathcal{M}_f \\ &= \begin{pmatrix} \mathcal{A}_f^2 & \mathcal{A}_f \mathcal{B}_f & \mathcal{A}_f \mathcal{C}_f \\ \mathcal{A}_f \mathcal{B}_f & \mathcal{A}_f^2 + \mathcal{B}_f^2 + \mathcal{C}_f^2 & \mathcal{B}_f \mathcal{C}_f + \mathcal{C}_f \mathcal{D}_f \\ \mathcal{A}_f \mathcal{C}_f & \mathcal{B}_f \mathcal{C}_f + \mathcal{C}_f \mathcal{D}_f & \mathcal{C}_f^2 + \mathcal{D}_f^2 \end{pmatrix}. \end{aligned} \quad (51)$$

Therefore, $\mathcal{M}_f^2 = \mathbf{O}_f^\top \Delta_{f,\sigma}^2 \mathbf{O}_f$ where $\Delta_{f,\sigma}^2 = \text{diag}(\sigma_{f1}^2, \sigma_{f2}^2, \sigma_{f3}^2)$. The invariants of the matrix $\mathcal{M}_f$ satisfy the relations

$$\text{Tr}\{\mathcal{M}_f\} = \text{Tr}\{\Delta_{f,\sigma}\} \Rightarrow \mathcal{B}_f + \mathcal{D}_f = \sigma_{f1} + \sigma_{f2} + \sigma_{f3},$$

$$\det\{\mathcal{M}_f\} = \det\{\Delta_{f,\sigma}\} \Rightarrow -\mathcal{A}_f^2 \mathcal{D}_f = \sigma_{f1} \sigma_{f2} \sigma_{f3},$$

$$\chi\{\mathcal{M}_f\} = \frac{1}{2} \left(\text{Tr}\{\mathcal{M}_f^2\} - \text{Tr}\{\mathcal{M}_f\}^2 \right),$$

$$\mathcal{A}_f^2 - \mathcal{B}_f \mathcal{D}_f + \mathcal{C}_f^2 = -\sigma_{f1} \sigma_{f2} - \sigma_{f1} \sigma_{f3} - \sigma_{f2} \sigma_{f3}. \quad (52)$$

Thus, the elements of the real symmetric matrix $\mathcal{M}_f$ in terms of the running masses of the fermions take the form

$$\mathcal{A}_f = \sqrt{\frac{\sigma_{f1} \sigma_{f2} \sigma_{f3}}{\mathcal{D}_f}}, \quad (53a)$$

$$\mathcal{B}_f = s_3 \sigma_{f3} + s_2 \sigma_{f2} + s_1 \sigma_{f1} - \mathcal{D}_f, \quad (53b)$$

$$\mathcal{C}_f = \sqrt{\frac{(s_3 \sigma_{f3} - \mathcal{D}_f)(\mathcal{D}_f - s_2 \sigma_{f2})(\mathcal{D}_f - s_1 \sigma_{f1})}{\mathcal{D}_f}}. \quad (53c)$$

The parameters m_{11}^f and $\mathcal{D}_f$ must satisfy the conditions:

For a normal hierarchy in the fermion mass spectrum: $\sigma_{f3} > \sigma_{f2} > \sigma_{f1}$

$$\begin{aligned} m_{f1} &> m_{11}^f, \\ \sigma_{f3} &> \mathcal{D}_{\{ > \sigma_{\{ \in}, & \mathcal{D}_{\{ \neq -\sigma_{\{\infty} + \sigma_{\{\in} + \sigma_{\{\in}, & \text{for } \Downarrow_{\{\infty} \rightarrow -|\Downarrow_{\{\infty}|, & s_{\infty} = -\infty, s_{\in} = +\infty, s_{\in} = +\infty, \\ \sigma_{f3} &> \mathcal{D}_{\{ > \sigma_{\{\infty}, & \mathcal{D}_{\{ \neq +\sigma_{\{\infty} - \sigma_{\{\in} + \sigma_{\{\in}, & \text{for } \Downarrow_{\{\in} \rightarrow -|\Downarrow_{\{\in}|, & s_{\infty} = +\infty, s_{\in} = -\infty, s_{\in} = +\infty, \\ \sigma_{f2} &> \mathcal{D}_{\{ > \sigma_{\{\infty}, & \mathcal{D}_{\{ \neq +\sigma_{\{\infty} + \sigma_{\{\in} - \sigma_{\{\in}, & \text{for } \Downarrow_{\{\in} \rightarrow -|\Downarrow_{\{\in}|, & s_{\infty} = +\infty, s_{\in} = +\infty, s_{\in} = -\infty. \end{aligned} \quad (54)$$

For an inverted hierarchy in the fermion mass spectrum:

$$\sigma_{f2} > \sigma_{f1} > \sigma_{f3}$$

$$\begin{aligned} m_{f3} &> m_{11}^f, \\ \sigma_{f2} &> \mathcal{D}_{\{ > \sigma_{\{\in}, & \mathcal{D}_{\{ \neq -\sigma_{\{\infty} + \sigma_{\{\in} + \sigma_{\{\in}, & \text{for } \Downarrow_{\{\infty} \rightarrow -\Downarrow_{\{\infty}, & s_{\infty} = -\infty, s_{\in} = +\infty, s_{\in} = +\infty, \\ \sigma_{f1} &> \mathcal{D}_{\{ > \sigma_{\{\in}, & \mathcal{D}_{\{ \neq +\sigma_{\{\infty} - \sigma_{\{\in} + \sigma_{\{\in}, & \text{for } \Downarrow_{\{\in} \rightarrow -\Downarrow_{\{\in}, & s_{\infty} = +\infty, s_{\in} = -\infty, s_{\in} = +\infty, \\ \sigma_{f2} &> \mathcal{D}_{\{ > \sigma_{\{\infty}, & \mathcal{D}_{\{ \neq +\sigma_{\{\infty} + \sigma_{\{\in} - \sigma_{\{\in}, & \text{for } \Downarrow_{\{\in} \rightarrow -\Downarrow_{\{\in}, & s_{\infty} = +\infty, s_{\in} = +\infty, s_{\in} = -\infty. \end{aligned} \quad (55)$$

In agreement with experimental data on neutrino oscillations, the inverted hierarchy is only present in the neutrino mass spectrum.

The real symmetric matrix $\mathcal{M}_f$ can be brought to its diagonal form by means of the orthogonal transformation in Eq. (42). The orthogonal matrix $\mathbf{O}_f$ is constructed using the eigenvectors of the matrix $\mathcal{M}_f$, and it has the following expression:

$$\mathbf{O}_f = (s_1|M_1\rangle, s_2|M_2\rangle, s_3|M_3\rangle). \quad (56)$$

The form of the eigenvector for a general matrix $\mathbf{M}_f$, Eq. (26), is [29]:

$$|M_k\rangle = \frac{1}{N_i} \begin{pmatrix} (\lambda_i - m_{22})m_{13} + m_{12}m_{23} \\ (\lambda_i - m_{11})m_{23} + m_{21}m_{13} \\ (\lambda_i - m_{11})(\lambda_i - m_{22}) - m_{12}m_{21} \end{pmatrix}. \quad (57)$$

In this expression, λ_i ($i = 1, 2, 3$) correspond to the eigenvalues of the matrix $\mathbf{M}_f$, and $N_i \equiv \sqrt{\langle \mathbf{M}_i | \mathbf{M}_i \rangle}$ are the normalization constants. The orthogonal matrix $\mathbf{O}_f$ that diagonalizes the mass matrix $\mathcal{M}_f$ takes the expression

$$\begin{pmatrix} s_1 \sqrt{\frac{\sigma_{f2}\sigma_{f3}\xi_{f1}}{\mathcal{D}_{f1}}} & s_2 \sqrt{\frac{\sigma_{f1}\sigma_{f3}\xi_{f2}}{\mathcal{D}_{f2}}} & s_3 \sqrt{\frac{\sigma_{f1}\sigma_{f2}\xi_{f3}}{\mathcal{D}_{f3}}} \\ \sqrt{\frac{\sigma_{f1}\mathcal{D}_f\xi_{f1}}{\mathcal{D}_{f1}}} & \sqrt{\frac{\sigma_{f2}\mathcal{D}_f\xi_{f2}}{\mathcal{D}_{f2}}} & \sqrt{\frac{\sigma_{f3}\mathcal{D}_f\xi_{f3}}{\mathcal{D}_{f3}}} \\ -\sqrt{\frac{\sigma_{f1}\xi_{f3}\xi_{f2}}{\mathcal{D}_{f1}}} & s_1 s_2 \sqrt{\frac{\sigma_{f2}\xi_{f3}\xi_{f1}}{\mathcal{D}_{f2}}} & s_3 \sqrt{\frac{\sigma_{f3}\xi_{f1}\xi_{f2}}{\mathcal{D}_{f3}}} \end{pmatrix}, \quad (58)$$

where $\sigma_{f1} = s_1 m_{f1} - m_{11}^f$, $\sigma_{f2} = s_2 m_{f2} - m_{11}^f$, $\sigma_{f3} = s_3 m_{f3} - m_{11}^f$, $\xi_{f1} = (\mathcal{D}_f - s_1 \sigma_{f1})$, $\xi_{f2} = s_3 (\mathcal{D}_f - s_2 \sigma_{f2})$, $\xi_{f3} = (\sigma_{f3} - s_3 \mathcal{D}_f)$,

$$\begin{aligned} \mathcal{D}_{f1} &= \mathcal{D}_f (\sigma_{f2} + s_3 \sigma_{f1}) (\sigma_{f3} + s_2 \sigma_{f1}), \\ \mathcal{D}_{f2} &= \mathcal{D}_f (\sigma_{f3} + s_1 \sigma_{f2}) (\sigma_{f2} + s_3 \sigma_{f1}), \\ \mathcal{D}_{f3} &= \mathcal{D}_f (\sigma_{f3} + s_1 \sigma_{f2}) (\sigma_{f3} + s_2 \sigma_{f1}). \end{aligned} \quad (59)$$

5. Lepton flavor mixing matrix

In this case, the unitary matrix that diagonalizes the mass matrix of the leptons takes the form

$$\begin{aligned} \mathbf{U}_l &= \mathbf{R}_{\beta_l}^\top \mathbf{P}_l^\dagger \mathbf{O}_l, & \text{for } \mathbf{M}_l = \mathbf{M}_l^\dagger, \\ \mathbf{U}_l &= \mathbf{R}_{\beta_l}^\top \mathbf{P}_l^\top \mathbf{O}_l, & \text{for } \mathbf{M}_l = \mathbf{M}_l^\top. \end{aligned} \quad (60)$$

Therefore, the lepton flavor mixing matrix, PMNS, which is defined as $\mathbf{V}_{\text{PMNS}} = \mathbf{U}_\ell^\dagger \mathbf{U}_\nu$ [1], takes the form

$$\begin{aligned} \mathbf{V}_{\text{PMNS}} &= \mathbf{O}_\ell^\top \mathbf{P}_\ell \mathbf{R}_{\beta_{\ell\nu}} \mathbf{P}_\nu^\dagger \mathbf{O}_\nu, & \text{for } \mathbf{M}_l = \mathbf{M}_l^\dagger, \\ \mathbf{V}_{\text{PMNS}} &= \mathbf{O}_\ell^\top \mathbf{P}_\ell^\dagger \mathbf{R}_{\beta_{\ell\nu}} \mathbf{P}_\nu \mathbf{O}_\nu, & \text{for } \mathbf{M}_l = \mathbf{M}_l^\top. \end{aligned} \quad (61)$$

In the above expressions, we have

$$\mathbf{R}_{\beta_{ud}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\beta_\ell - \beta_\nu) & \sin(\beta_\ell - \beta_\nu) \\ 0 & -\sin(\beta_\ell - \beta_\nu) & \cos(\beta_\ell - \beta_\nu) \end{pmatrix}. \quad (62)$$

In the particular case when the rotation angle is the same in both lepton sectors, $\beta_\ell = \beta_\nu$, the matrices in Eq. (61) take the form

$$\mathbf{V}_{\text{PMNS}} = \mathbf{O}_\ell^\top \mathbf{P}_{\ell\nu} \mathbf{O}_\nu, \quad (63)$$

where $\mathbf{P}_{\ell\nu} = \mathbf{P}_\ell \mathbf{P}_\nu^\dagger$ for $\mathbf{M}_l = \mathbf{M}_l^\dagger$, while $\mathbf{P}_{\ell\nu} = \mathbf{P}_\ell^\dagger \mathbf{P}_\nu$ for $\mathbf{M}_l = \mathbf{M}_l^\top$. In explicit form

$$\begin{aligned} \mathbf{P}_{\ell\nu} &= \text{diag}(1, e^{i\Phi_a}, e^{i\Phi_c}) & \text{for } \mathbf{M}_l = \mathbf{M}_l^\dagger, \\ \mathbf{P}_{\ell\nu} &= \text{diag}(1, e^{i\Phi_a}, e^{i\Phi_c}) & \text{for } \mathbf{M}_l = \mathbf{M}_l^\top. \end{aligned} \quad (64)$$

Here, $\Phi_a = \vartheta_{\ell,a} - \vartheta_{\nu,a}$ and $\Phi_c = \vartheta_{\ell,c} - \vartheta_{\nu,c}$ for $\mathbf{M}_l = \mathbf{M}_l^\dagger$, and $\Phi_a = \vartheta_{\nu,a} - \vartheta_{\ell,a}$ and $\Phi_c = \vartheta_{\nu,c} - \vartheta_{\ell,c}$ for $\mathbf{M}_l = \mathbf{M}_l^\top$. The difference between representing the mass matrix of the leptons with a Hermitian matrix or with a complex symmetric matrix mainly lies in the diagonal phase factor matrix $\mathbf{P}_{ud}$. However, as the lepton flavor mixing matrix PMNS is defined in Eq. (63), it is not possible to obtain direct information

about whether the mass matrix is complex symmetric or Hermitian.

The values of the mass ratios of the quarks are more stable with respect to changes in the energy scale than the masses of the quarks themselves. In other words, the value of the mass ratios of the quarks has the same order of magnitude regardless of the energy scale [27,30]. In this work, the mass matrices, as well as the PMNS flavor mixing matrix, are normalized with respect to the masses of the heavier leptons. The charged leptons are normalized with respect to m_τ , obtaining $\tilde{\sigma}_e = \tilde{m}_e - \tilde{m}_{11}^\ell$, $\tilde{\sigma}_\mu = \tilde{m}_\mu + \tilde{m}_{11}^\ell$, $\tilde{\sigma}_\tau = 1 - \tilde{m}_{11}^\ell$, $\tilde{\xi}_{\ell 1} = \tilde{\mathcal{D}}_\ell - \tilde{\sigma}_e$, $\tilde{\xi}_{\ell 2} = \tilde{\mathcal{D}}_\ell + \tilde{\sigma}_\mu$, $\tilde{\xi}_{\ell 3} = \tilde{\sigma}_\tau - \tilde{\mathcal{D}}_\ell$,

$$\begin{aligned}\tilde{\mathcal{D}}_{\ell 1} &= \tilde{\mathcal{D}}_\ell (\tilde{\sigma}_\mu + \tilde{\sigma}_e) (\tilde{\sigma}_\tau - \tilde{\sigma}_e), \\ \tilde{\mathcal{D}}_{\ell 2} &= \tilde{\mathcal{D}}_\ell (\tilde{\sigma}_\tau + \tilde{\sigma}_\mu) (\tilde{\sigma}_\mu + \tilde{\sigma}_e), \\ \tilde{\mathcal{D}}_{\ell 3} &= \tilde{\mathcal{D}}_\ell (\tilde{\sigma}_\tau + \tilde{\sigma}_\mu) (\tilde{\sigma}_\tau - \tilde{\sigma}_e),\end{aligned}\quad (65)$$

where $\tilde{m}_e = m_e/m_\tau$, $\tilde{m}_\mu = m_\mu/m_\tau$, $\tilde{m}_{11}^\ell = m_{11}^\ell/m_\tau$, $\tilde{\sigma}_e = \sigma_e/m_\tau$, $\tilde{\sigma}_\mu = \sigma_\mu/m_\tau$, $\tilde{\sigma}_\tau = \sigma_\tau/m_\tau$, $\tilde{\xi}_{\ell 1} = \xi_{\ell 1}/m_\tau$, $\tilde{\xi}_{\ell 2} = \xi_{\ell 2}/m_\tau$, $\tilde{\xi}_{\ell 3} = \xi_{\ell 3}/m_\tau$, $\tilde{\mathcal{D}}_\ell = \mathcal{D}_\ell/m_\tau$. In the case of neutrinos with a normal hierarchy, $m_{\nu 3} > m_{\nu 2} > m_{\nu 1}$, in the mass spectrum we have $\tilde{\sigma}_{\nu 1} = \tilde{m}_{\nu 1} - \tilde{m}_{11}^\nu$, $\tilde{\sigma}_{\nu 2} = \tilde{m}_{\nu 2} + \tilde{m}_{11}^\nu$, $\tilde{\sigma}_{\nu 3} = 1 - \tilde{m}_{11}^\nu$, $\tilde{\xi}_{\nu 1} = \tilde{\mathcal{D}}_\nu - \tilde{\sigma}_{\nu 1}$, $\tilde{\xi}_{\nu 2} = \tilde{\mathcal{D}}_\nu + \tilde{\sigma}_{\nu 2}$, $\tilde{\xi}_{\nu 3} = \tilde{\sigma}_{\nu 3} - \tilde{\mathcal{D}}_\nu$,

$$\begin{aligned}\tilde{\mathcal{D}}_{\nu 1} &= \tilde{\mathcal{D}}_\nu (\tilde{\sigma}_{\nu 2} + \tilde{\sigma}_{\nu 1}) (\tilde{\sigma}_{\nu 3} - \tilde{\sigma}_{\nu 1}), \\ \tilde{\mathcal{D}}_{\nu 2} &= \tilde{\mathcal{D}}_\nu (\tilde{\sigma}_{\nu 3} + \tilde{\sigma}_{\nu 2}) (\tilde{\sigma}_{\nu 2} + \tilde{\sigma}_{\nu 1}), \\ \tilde{\mathcal{D}}_{\nu 3} &= \tilde{\mathcal{D}}_\nu (\tilde{\sigma}_{\nu 3} + \tilde{\sigma}_{\nu 2}) (\tilde{\sigma}_{\nu 3} - \tilde{\sigma}_{\nu 1}),\end{aligned}\quad (66)$$

where $\tilde{m}_{\nu 1} = m_{\nu 1}/m_{\nu 3}$, $\tilde{m}_{\nu 2} = m_{\nu 2}/m_{\nu 3}$, $\tilde{m}_{11}^\nu = m_{11}^\nu/m_{\nu 3}$, $\tilde{\sigma}_{\nu 1} = \sigma_{\nu 1}/m_{\nu 3}$, $\tilde{\sigma}_{\nu 2} = \sigma_{\nu 2}/m_{\nu 3}$, $\tilde{\sigma}_{\nu 3} = \sigma_{\nu 3}/m_{\nu 3}$, $\tilde{\xi}_{\nu 1} = \xi_{\nu 1}/m_{\nu 3}$, $\tilde{\xi}_{\nu 2} = \xi_{\nu 2}/m_{\nu 3}$, $\tilde{\xi}_{\nu 3} = \xi_{\nu 3}/m_{\nu 3}$, and $\tilde{\mathcal{D}}_\nu = \mathcal{D}_\nu/m_{\nu 3}$. In the case of neutrinos with an inverted hierarchy, $m_{\nu 2} > m_{\nu 1} > m_{\nu 3}$, in the mass spectrum we have $\tilde{\sigma}_{\nu 1} = \tilde{m}_{\nu 1} - \tilde{m}_{11}^\nu$, $\tilde{\sigma}_{\nu 2} = 1 + \tilde{m}_{11}^\nu$, $\tilde{\xi}_{\nu 1} = \tilde{\mathcal{D}}_\nu - \tilde{\sigma}_{\nu 1}$, $\tilde{\sigma}_{\nu 3} = \tilde{m}_{\nu 3} - \tilde{m}_{11}^\nu$, $\tilde{\xi}_{\nu 2} = \tilde{\mathcal{D}}_\nu + \tilde{\sigma}_{\nu 2}$, $\tilde{\xi}_{\nu 3} = \tilde{\sigma}_{\nu 3} - \tilde{\mathcal{D}}_\nu$,

$$\begin{aligned}\tilde{\mathcal{D}}_{\nu 1} &= \tilde{\mathcal{D}}_\nu (\tilde{\sigma}_{\nu 2} + \tilde{\sigma}_{\nu 1}) (\tilde{\sigma}_{\nu 3} - \tilde{\sigma}_{\nu 1}), \\ \tilde{\mathcal{D}}_{\nu 2} &= \tilde{\mathcal{D}}_\nu (\tilde{\sigma}_{\nu 3} + \tilde{\sigma}_{\nu 2}) (\tilde{\sigma}_{\nu 2} + \tilde{\sigma}_{\nu 1}), \\ \tilde{\mathcal{D}}_{\nu 3} &= \tilde{\mathcal{D}}_\nu (\tilde{\sigma}_{\nu 3} + \tilde{\sigma}_{\nu 2}) (\tilde{\sigma}_{\nu 3} - \tilde{\sigma}_{\nu 1}),\end{aligned}\quad (67)$$

where $\tilde{m}_{\nu 1} = m_{\nu 1}/m_{\nu 2}$, $\tilde{m}_{\nu 3} = m_{\nu 3}/m_{\nu 2}$, $\tilde{m}_{11}^\nu = m_{11}^\nu/m_{\nu 2}$, $\tilde{\sigma}_{\nu 1} = \sigma_{\nu 1}/m_{\nu 2}$, $\tilde{\sigma}_{\nu 2} = \sigma_{\nu 2}/m_{\nu 2}$, $\tilde{\sigma}_{\nu 3} = \sigma_{\nu 3}/m_{\nu 2}$, $\tilde{\xi}_{\nu 1} = \xi_{\nu 1}/m_{\nu 2}$, $\tilde{\xi}_{\nu 2} = \xi_{\nu 2}/m_{\nu 2}$, $\tilde{\xi}_{\nu 3} = \xi_{\nu 3}/m_{\nu 2}$, and $\tilde{\mathcal{D}}_\nu = \mathcal{D}_\nu/m_{\nu 2}$. For the particular case of performing a chiral rotation on the second eigenvalue, $m_{f2} = -|m_{f2}|$, which implies that $s_1 = +1$, $s_2 = -1$ and $s_3 = +1$, the PMNS matrix takes the form

$$\mathbf{V}_{\text{PMNS}}^{\text{th}} = \begin{pmatrix} V_{e1}^{\text{th}} & V_{e2}^{\text{th}} & V_{e3}^{\text{th}} \\ V_{\mu 1}^{\text{th}} & V_{\mu 2}^{\text{th}} & V_{\mu 3}^{\text{th}} \\ V_{\tau 1}^{\text{th}} & V_{\tau 2}^{\text{th}} & V_{\tau 3}^{\text{th}} \end{pmatrix}, \quad (68)$$

The elements of the PMNS mixing matrix are expressed as

$$\begin{aligned}V_{e1}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_\mu \tilde{\sigma}_\tau \tilde{\sigma}_{\nu 2} \tilde{\sigma}_{\nu 3} \tilde{\xi}_{\ell 1} \tilde{\xi}_{\nu 1}}{\tilde{\mathcal{D}}_{\ell 1} \tilde{\mathcal{D}}_{\nu 1}}} + \sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_{\nu 1}}{\tilde{\mathcal{D}}_{\ell 1} \tilde{\mathcal{D}}_{\nu 1}}} \left(\sqrt{\tilde{\mathcal{D}}_\ell \tilde{\mathcal{D}}_\nu \tilde{\xi}_{\ell 1} \tilde{\xi}_{\nu 1}} e^{i\Phi_a} + \sqrt{\tilde{\xi}_{\ell 2} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 2} \tilde{\xi}_{\nu 3}} e^{i\Phi_c} \right), \\ V_{e2}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_\mu \tilde{\sigma}_\tau \tilde{\sigma}_{\nu 1} \tilde{\sigma}_{\nu 3} \tilde{\xi}_{\ell 1} \tilde{\xi}_{\nu 2}}{\tilde{\mathcal{D}}_{\ell 1} \tilde{\mathcal{D}}_{\nu 2}}} + \sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_{\nu 2}}{\tilde{\mathcal{D}}_{\ell 1} \tilde{\mathcal{D}}_{\nu 2}}} \left(\sqrt{\tilde{\mathcal{D}}_\ell \tilde{\mathcal{D}}_\nu \tilde{\xi}_{\ell 1} \tilde{\xi}_{\nu 2}} e^{i\Phi_a} + \sqrt{\tilde{\xi}_{\ell 2} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 1} \tilde{\xi}_{\nu 3}} e^{i\Phi_c} \right), \\ V_{e3}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_\mu \tilde{\sigma}_\tau \tilde{\sigma}_{\nu 1} \tilde{\sigma}_{\nu 2} \tilde{\xi}_{\ell 1} \tilde{\xi}_{\nu 3}}{\tilde{\mathcal{D}}_{\ell 1} \tilde{\mathcal{D}}_{\nu 3}}} + \sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_{\nu 3}}{\tilde{\mathcal{D}}_{\ell 1} \tilde{\mathcal{D}}_{\nu 3}}} \left(\sqrt{\tilde{\mathcal{D}}_\ell \tilde{\mathcal{D}}_\nu \tilde{\xi}_{\ell 1} \tilde{\xi}_{\nu 3}} e^{i\Phi_a} - \sqrt{\tilde{\xi}_{\ell 2} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 1} \tilde{\xi}_{\nu 2}} e^{i\Phi_c} \right), \\ V_{\mu 1}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_\tau \tilde{\sigma}_{\nu 2} \tilde{\sigma}_{\nu 3} \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 1}}{\tilde{\mathcal{D}}_{\ell 2} \tilde{\mathcal{D}}_{\nu 1}}} + \sqrt{\frac{\tilde{\sigma}_\mu \tilde{\sigma}_{\nu 1}}{\tilde{\mathcal{D}}_{\ell 2} \tilde{\mathcal{D}}_{\nu 1}}} \left(\sqrt{\tilde{\mathcal{D}}_\ell \tilde{\mathcal{D}}_\nu \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 1}} e^{i\Phi_a} + \sqrt{\tilde{\xi}_{\ell 1} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 2} \tilde{\xi}_{\nu 3}} e^{i\Phi_c} \right), \\ V_{\mu 2}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_\tau \tilde{\sigma}_{\nu 1} \tilde{\sigma}_{\nu 3} \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 2}}{\tilde{\mathcal{D}}_{\ell 2} \tilde{\mathcal{D}}_{\nu 2}}} + \sqrt{\frac{\tilde{\sigma}_\mu \tilde{\sigma}_{\nu 2}}{\tilde{\mathcal{D}}_{\ell 2} \tilde{\mathcal{D}}_{\nu 2}}} \left(\sqrt{\tilde{\mathcal{D}}_\ell \tilde{\mathcal{D}}_\nu \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 2}} e^{i\Phi_a} + \sqrt{\tilde{\xi}_{\ell 1} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 1} \tilde{\xi}_{\nu 3}} e^{i\Phi_c} \right), \\ V_{\mu 3}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_\tau \tilde{\sigma}_{\nu 1} \tilde{\sigma}_{\nu 2} \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 3}}{\tilde{\mathcal{D}}_{\ell 2} \tilde{\mathcal{D}}_{\nu 3}}} + \sqrt{\frac{\tilde{\sigma}_\mu \tilde{\sigma}_{\nu 3}}{\tilde{\mathcal{D}}_{\ell 2} \tilde{\mathcal{D}}_{\nu 3}}} \left(\sqrt{\tilde{\mathcal{D}}_\ell \tilde{\mathcal{D}}_\nu \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 3}} e^{i\Phi_a} - \sqrt{\tilde{\xi}_{\ell 1} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 1} \tilde{\xi}_{\nu 2}} e^{i\Phi_c} \right),\end{aligned}$$

$$\begin{aligned}
V_{\tau 1}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_\mu \tilde{\sigma}_{\nu 2} \tilde{\sigma}_{\nu 3} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 1}}{\tilde{D}_{\ell 3} \tilde{D}_{\nu 1}}} + \sqrt{\frac{\tilde{\sigma}_\tau \tilde{\sigma}_{\nu 1}}{\tilde{D}_{\ell 3} \tilde{D}_{\nu 1}}} \left(\sqrt{\tilde{D}_\ell \tilde{D}_\nu \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 1}} e^{i\Phi_a} - \sqrt{\tilde{\xi}_{\ell 1} \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 2} \tilde{\xi}_{\nu 3}} e^{i\Phi_c} \right), \\
V_{\tau 2}^{\text{th}} &= -\sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_\mu \tilde{\sigma}_{\nu 1} \tilde{\sigma}_{\nu 3} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 2}}{\tilde{D}_{\ell 3} \tilde{D}_{\nu 2}}} + \sqrt{\frac{\tilde{\sigma}_\tau \tilde{\sigma}_{\nu 2}}{\tilde{D}_{\ell 3} \tilde{D}_{\nu 2}}} \left(\sqrt{\tilde{D}_\ell \tilde{D}_\nu \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 2}} e^{i\Phi_a} - \sqrt{\tilde{\xi}_{\ell 1} \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 1} \tilde{\xi}_{\nu 3}} e^{i\Phi_c} \right), \\
V_{\tau 3}^{\text{th}} &= \sqrt{\frac{\tilde{\sigma}_e \tilde{\sigma}_\mu \tilde{\sigma}_{\nu 1} \tilde{\sigma}_{\nu 2} \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 3}}{\tilde{D}_{\ell 3} \tilde{D}_{\nu 3}}} + \sqrt{\frac{\tilde{\sigma}_\tau \tilde{\sigma}_{\nu 3}}{\tilde{D}_{\ell 3} \tilde{D}_{\nu 3}}} \left(\sqrt{\tilde{D}_\ell \tilde{D}_\nu \tilde{\xi}_{\ell 3} \tilde{\xi}_{\nu 3}} e^{i\Phi_a} + \sqrt{\tilde{\xi}_{\ell 1} \tilde{\xi}_{\ell 2} \tilde{\xi}_{\nu 1} \tilde{\xi}_{\nu 2}} e^{i\Phi_c} \right).
\end{aligned} \quad (69)$$

The parameter $\tilde{D}_l$, with $l = \ell, \nu$, for a normal hierarchy in the neutrino mass spectrum, must satisfy the condition:

$$\begin{aligned}
\tilde{m}_{11}^f < \tilde{m}_{f1}, \quad \tilde{\sigma}_{l3} > \tilde{D}_l > \tilde{\sigma}_{l1}, \\
\tilde{D}_l \neq +\tilde{\sigma}_{l1} - \tilde{\sigma}_{l2} + \tilde{\sigma}_{l3} \quad \text{for } m_{l2} \rightarrow -|m_{l2}|.
\end{aligned} \quad (70)$$

For an inverted hierarchy in the neutrino mass spectrum, the next condition must be satisfied:

$$\begin{aligned}
\tilde{m}_{11}^\nu < \tilde{m}_{\nu 3}, \quad \tilde{\sigma}_{\nu 1} > \tilde{D}_\nu > \tilde{\sigma}_{\nu 3}, \\
\tilde{D}_\nu \neq +\tilde{\sigma}_{\nu 1} - \tilde{\sigma}_{\nu 2} + \tilde{\sigma}_{\nu 3} \quad \text{para } m_{\nu 2} \rightarrow -|m_{\nu 2}|.
\end{aligned} \quad (71)$$

5.1. Numerical analysis

To evaluate how well the theoretical expressions fit the experimental data, a likelihood fit is implemented here, where the χ^2 statistic is used as the measure. The χ^2 statistic measures the difference between the observed and expected values according to the theoretical model. The method seeks the optimal values of the model parameters that minimize the error between the data and the model.

In this case, the χ^2 statistic takes the form:

$$\chi^2 = \sum_{i < j}^3 \frac{(\sin^2 \theta_{ij}^{\text{exp}} - \sin^2 \theta_{ij}^{\text{th}})^2}{\sigma_{\theta_{ij}}^2}. \quad (72)$$

In this expression for the χ^2 statistic, the superscript “th” is used to denote the theoretical expressions of the mixing angles of the leptons, which are obtained from the expressions:

$$\begin{aligned}
\sin^2 \theta_{12}^{\text{th}} &= \frac{|V_{e2}^{\text{th}}|^2}{1 - |V_{e3}^{\text{th}}|^2}, \quad \sin^2 \theta_{23}^{\text{th}} = \frac{|V_{\mu 3}^{\text{th}}|^2}{1 - |V_{e3}^{\text{th}}|^2}, \\
\sin^2 \theta_{13}^{\text{th}} &= |V_{e3}^{\text{th}}|^2.
\end{aligned} \quad (73)$$

Meanwhile, the terms with the superscript “exp” denote the experimental data with an uncertainty $\sigma_{\theta_{ij}}$ for the mixing angles of the leptons.

For this likelihood analysis, the results from the global fit of neutrino oscillation parameters reported in Refs. [31,32] are considered. The values of the differences of the squares of the neutrino masses, $\Delta m_{ij}^2 = m_{\nu i}^2 - m_{\nu j}^2$, at BFP $\pm 1\sigma$ are

$$\begin{aligned}
\Delta m_{21}^2 (10^{-5} \text{ eV}^2) &= 7,50_{-0,20}^{+0,22}, \\
\Delta m_{31}^2 (10^{-3} \text{ eV}^2) &= 2,55_{-0,03}^{+0,02} \quad \text{for NH}, \\
\Delta m_{13}^2 (10^{-3} \text{ eV}^2) &= 2,45_{-0,03}^{+0,02} \quad \text{for IH}.
\end{aligned} \quad (74)$$

The values of the differences in the mixing angles of the leptons at BFP $\pm 1\sigma$ are

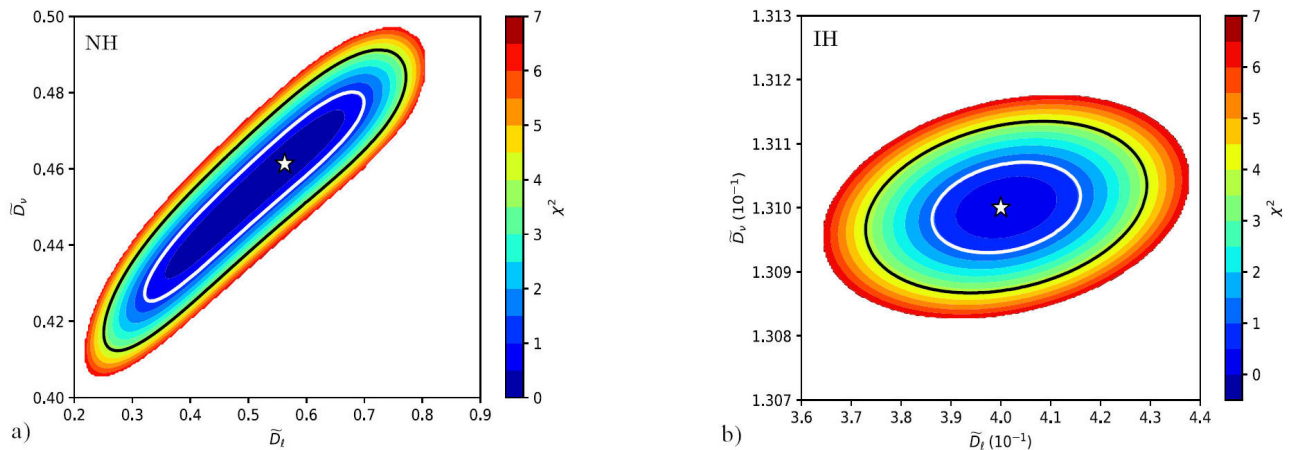


FIGURE 1. Regions of parameters for $\tilde{D}_\ell$ and $\tilde{D}_\nu$, where the white star represents the best fit point (BFP). The regions delimited by the white and black lines represent the allowed region at 1σ and 2σ C.L., respectively.

$$\begin{aligned}
\sin^2 \theta_{12}^{\text{exp}} (10^{-1}) &= 3,18 \pm 0,16, \\
\sin^2 \theta_{23}^{\text{exp}} (10^{-1}) &= 5,74 \pm 0,14 \text{ for NH}, \\
\sin^2 \theta_{23}^{\text{exp}} (10^{-1}) &= 5,78_{-0,17}^{+0,10} \text{ for IH}, \\
\sin^2 \theta_{13}^{\text{exp}} (10^{-2}) &= 2,200_{-0,062}^{+0,069} \text{ for NH}, \\
\sin^2 \theta_{13}^{\text{exp}} (10^{-2}) &= 2,225_{-0,070}^{+0,064} \text{ for IH}.
\end{aligned} \tag{75}$$

From the definition of Δm_{ij}^2 , two of the neutrino masses can be written as

$$\left. \begin{aligned} m_{\nu 2} &= \sqrt{\Delta m_{21}^2 + m_{\nu 1}^2} \\ m_{\nu 3} &= \sqrt{\Delta m_{31}^2 + m_{\nu 1}^2} \end{aligned} \right\} \text{ for NH}, \tag{76}$$

$$\left. \begin{aligned} m_{\nu 1} &= \sqrt{\Delta m_{13}^2 + m_{\nu 3}^2} \\ m_{\nu 3} &= \sqrt{\Delta m_{21}^2 + \Delta m_{13}^2 + m_{\nu 3}^2} \end{aligned} \right\} \text{ for IH},$$

where $m_{\nu 1}$ and $m_{\nu 3}$ are the mass of the lightest neutrino for NH and IH, respectively. Furthermore, for each type of hierarchy, this neutrino mass is considered the only free parameter in the previous expressions, as the Δm_{ij}^2 are determined by the experiment.

From the expressions in Eqs. (65)-(67), (69) and (73), it is easy to conclude that for the normal [inverted] hierarchy, the χ^2 statistic depends on the parameters $\tilde{m}_e$, $\tilde{m}_\mu$, $\tilde{m}_{\nu 1[3]}$, $\tilde{m}_{\nu 2[1]}$, $\tilde{m}_{11}^\ell$, $\tilde{m}_{11}^\nu$, $\tilde{D}_\ell$, $\tilde{D}_\nu$, Φ_a , and Φ_c . However, in this likelihood analysis, the parameters $\tilde{m}_e$, $\tilde{m}_\mu$, and $\tilde{m}_{\nu 2[1]}$ will not be considered as free parameters since their values are determined by experimental data.

So, the statistic parameter χ^2 depends of seven free parameters:

$$\chi^2 = \chi^2 \left(\tilde{m}_{\nu 1[3]}, \tilde{m}_{11}^\ell, \tilde{m}_{11}^\nu, \tilde{D}_\ell, \tilde{D}_\nu, \Phi_a, \Phi_c \right). \tag{77}$$

However, the χ^2 statistic depends only on three experimental values, which correspond to the leptonic flavor mixing angles. Therefore, if the seven parameters are simultaneously considered as free in the likelihood analysis, we can

only determine the values of these parameters at the best-fit point (BFP). To search for the BFP through likelihood fitting, we will consider the following values for the charged lepton masses [1]

$$\begin{aligned} m_e &= 0,51099895000 \pm 0,0000000015 \text{ MeV}, \\ m_\mu &= 105,6583755 \pm 0,0000023 \text{ MeV}, \\ m_\tau &= 1776,93 \pm 0,09 \text{ MeV}. \end{aligned} \tag{78}$$

To minimize the χ^2 statistic, we perform a scan of the parameter space in which the differences of the squares of the neutrino masses and the charged lepton masses are fixed at their central values, which are given in Eqs. (75) and (78). For a normal hierarchy, we obtain the following values at the BFP for the seven free parameters and the mixing angles, with a value of the χ^2 statistic equal to $3,6184 \times 10^{-3}$:

$$\begin{aligned} m_{\nu 1} &= 4,09 \times 10^{-3} \text{ eV}, \quad \tilde{m}_{11}^\ell = 2,98 \times 10^{-7}, \\ \tilde{m}_{11}^\nu &= 1,15 \times 10^{-5}, \quad \tilde{D}_\ell = 5,54871 \times 10^{-1}, \\ \tilde{D}_\nu &= 4,60288 \times 10^{-1}, \quad \Phi_a = 39^\circ, \quad \Phi_a = 300^\circ, \\ \sin^2 \theta_{12}^{\text{th}} &= 3,17242 \times 10^{-1}, \quad \sin^2 \theta_{13}^{\text{th}} = 2,20018 \times 10^{-2}, \\ \sin^2 \theta_{23}^{\text{th}} &= 5,74517 \times 10^{-1}. \end{aligned} \tag{79}$$

On the other hand, for an inverted hierarchy we obtain the following for a value of the χ^2 statistic equal to $6,26357 \times 10^{-3}$:

$$\begin{aligned} m_{\nu 3} &= 2,82 \times 10^{-2} \text{ eV}, \quad \tilde{m}_{11}^\ell = 1,02 \times 10^{-6}, \\ \tilde{m}_{11}^\nu &= 3,60 \times 10^{-1}, \quad \tilde{D}_\ell = 4,00000 \times 10^{-1}, \\ \tilde{D}_\nu &= 1,31000 \times 10^{-1}, \quad \Phi_a = 87^\circ, \quad \Phi_a = 248,5^\circ, \\ \sin^2 \theta_{12}^{\text{th}} &= 3,18278 \times 10^{-1}, \quad \sin^2 \theta_{13}^{\text{th}} = 2,22517 \times 10^{-2}, \\ \sin^2 \theta_{23}^{\text{th}} &= 5,79041 \times 10^{-1}. \end{aligned} \tag{80}$$

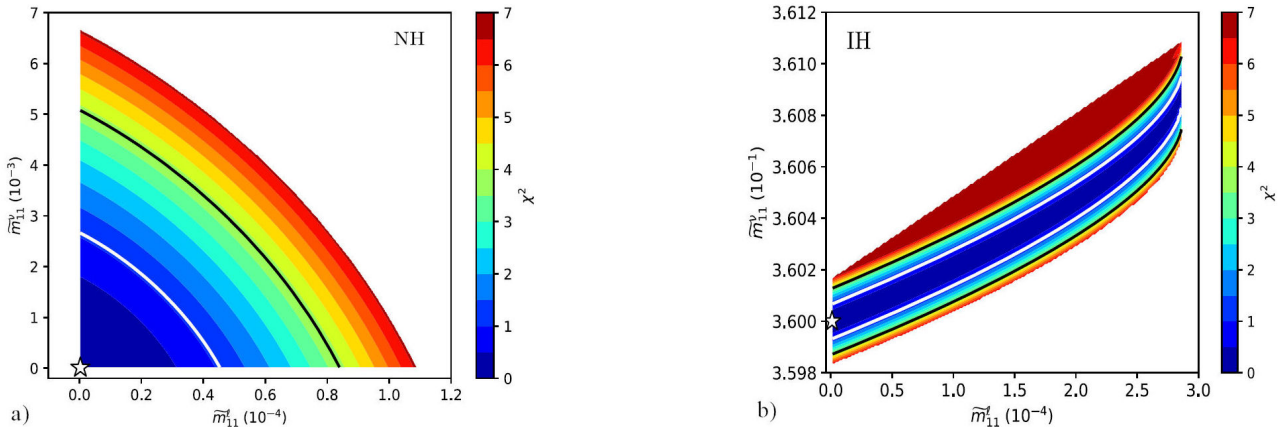
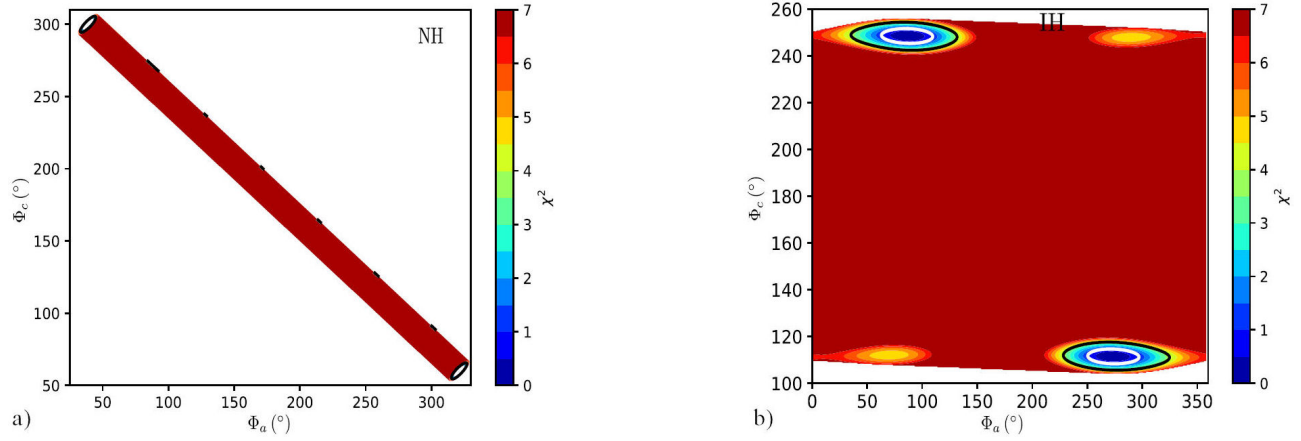


FIGURE 2. Parameter regions for $\tilde{m}_{11}^\ell$ and $\tilde{m}_{11}^\nu$, where the white star represents the BFP. The regions bounded by the white and black lines represent the allowed region at 1σ and 2σ C.L., respectively.

FIGURE 3. Parameter regions for Φ_a and Φ_c .

Now, since we already know the numerical values of the seven free parameters at the BFP, the next step is to perform new likelihood fits in which the values of five or six free parameters are fixed so that the χ^2 statistic has one or two degrees of freedom.

In order to determine the allowed regions of the free parameters, the values of Δm_{ij}^2 and the charged lepton masses are fixed at the BFP values given in Eqs. (74) and (78). Meanwhile, $\tilde{m}_{\nu 1[3]}$, $\tilde{m}_{11}^\ell$, $\tilde{m}_{11}^\nu$, $\tilde{D}_\ell$, $\tilde{D}_\nu$, Φ_a , and Φ_c are fixed at the values given in Eqs. (79) and (80).

Thus, in the case where the statistic is $\chi^2 = \chi^2(\tilde{D}_\ell, \tilde{D}_\nu)$, this implies one degree of freedom, yielding the following results at 1σ C.L.

$$\begin{aligned} \tilde{D}_\ell &= \begin{cases} (5,549_{-2,339}^{+1,428}) \times 10^{-1} \text{ for NH,} \\ (4,00_{-0,14}^{+0,16}) \times 10^{-1} \text{ for IH,} \end{cases} \\ \tilde{D}_\nu &= \begin{cases} (4,603_{-0,349}^{+0,196}) \times 10^{-1} \text{ for NH,} \\ (1,3100_{-0,0007}^{+0,0008}) \times 10^{-1} \text{ for IH.} \end{cases} \end{aligned} \quad (81)$$

For the normal and inverted hierarchies, we obtain $\chi^2 = 5,41 \times 10^{-3}$ and $\chi^2 = 3,59 \times 10^{-4}$ respectively. In Fig. 1, we show the parameter regions for $\tilde{D}_\ell$ and $\tilde{D}_\nu$, where the white star represents the BFP. The regions bounded by the white and black lines represent the allowed region at 1σ and 2σ C.L., respectively. The left panel corresponds to the normal hierarchy, with both parameters of order 10^{-1} . The right panel corresponds to the inverted hierarchy, where both parameters are also of order 10^{-1} .

In the case where the statistic is $\chi^2 = \chi^2(\tilde{m}_{11}^\ell, \tilde{m}_{11}^\nu)$, this implies one degree of freedom, yielding the following

results at 1σ C.L.

$$\begin{aligned} \tilde{m}_{11}^\ell &= \begin{cases} (2,98_{-2,88}^{+451,65}) \times 10^{-7} \text{ for NH,} \\ (1,02_{-1,00}^{+286,55}) \times 10^{-6} \text{ for IH,} \end{cases} \\ \tilde{m}_{11}^\nu &= \begin{cases} (1,15_{-1,14}^{+265,81}) \times 10^{-5} \text{ for NH,} \\ (3,600_{-0,007}^{+0,010}) \times 10^{-1} \text{ for IH.} \end{cases} \end{aligned} \quad (82)$$

For the normal and inverted hierarchies, we obtain $\chi^2 = 3,20 \times 10^{-3}$ and $\chi^2 = 5,98 \times 10^{-3}$, respectively. In Fig. 2, we show the parameter regions for $\tilde{m}_{11}^\ell$ and $\tilde{m}_{11}^\nu$, where the white star represents the BFP. The regions bounded by the white and black lines represent the allowed region at 1σ and 2σ C.L., respectively. The left panel corresponds to the normal hierarchy, where the parameter $\tilde{m}_{11}^\ell$ is of order 10^{-4} and the parameter $\tilde{m}_{11}^\nu$ is of order 10^{-3} . The right panel corresponds to the inverted hierarchy, where the parameter $\tilde{m}_{11}^\ell$ is of order 10^{-4} and the parameter $\tilde{m}_{11}^\nu$ is of order 10^{-1} .

In the case where the statistic is $\chi^2 = \chi^2(\Phi_a, \Phi_c)$, this implies one degree of freedom, yielding the following results at 1σ C.L.

$$\begin{aligned} \Phi_a &= \begin{cases} (39_{-3,0}^{+4,0})^\circ \text{ for NH,} \\ (87_{-17}^{+28})^\circ \text{ for IH,} \end{cases} \\ \Phi_c &= \begin{cases} (300_{-3,0}^{+2,0})^\circ \text{ for NH,} \\ (248,5 \pm 3,0)^\circ \text{ for IH.} \end{cases} \end{aligned} \quad (83)$$

For the normal and inverted hierarchies, we obtain $\chi^2 = 2,58 \times 10^{-3}$ and $\chi^2 = 6,33 \times 10^{-3}$, respectively. In Fig. 3, we show the complete parameter regions for the phase factors Φ_a and Φ_c . In Fig. 4, we show a zoom-in of the parameter regions for Φ_a and Φ_c , where the white star represents the BFP. The regions bounded by the white and black lines represent the allowed region at 1σ and 2σ C.L., respectively. The left panel corresponds to the normal hierarchy. The right panel corresponds to the inverted hierarchy.

In the case where the statistic is $\chi^2 = \chi^2(m_{\nu 1[3]})$, this implies two degrees of freedom, yielding the following results at 1σ C.L.

$$\begin{aligned} m_{\nu 1} &= \left(4,09^{+0,13}_{-0,12}\right) \times 10^{-3} \text{ eV for NH,} \\ m_{\nu 3} &= (2,82 \pm 0,01) \times 10^{-2} \text{ eV for IH.} \end{aligned} \quad (84)$$

For the normal and inverted hierarchies, we obtain $\chi^2 = 3,39 \times 10^{-3}$ and $\chi^2 = 6,15 \times 10^{-3}$, respectively.

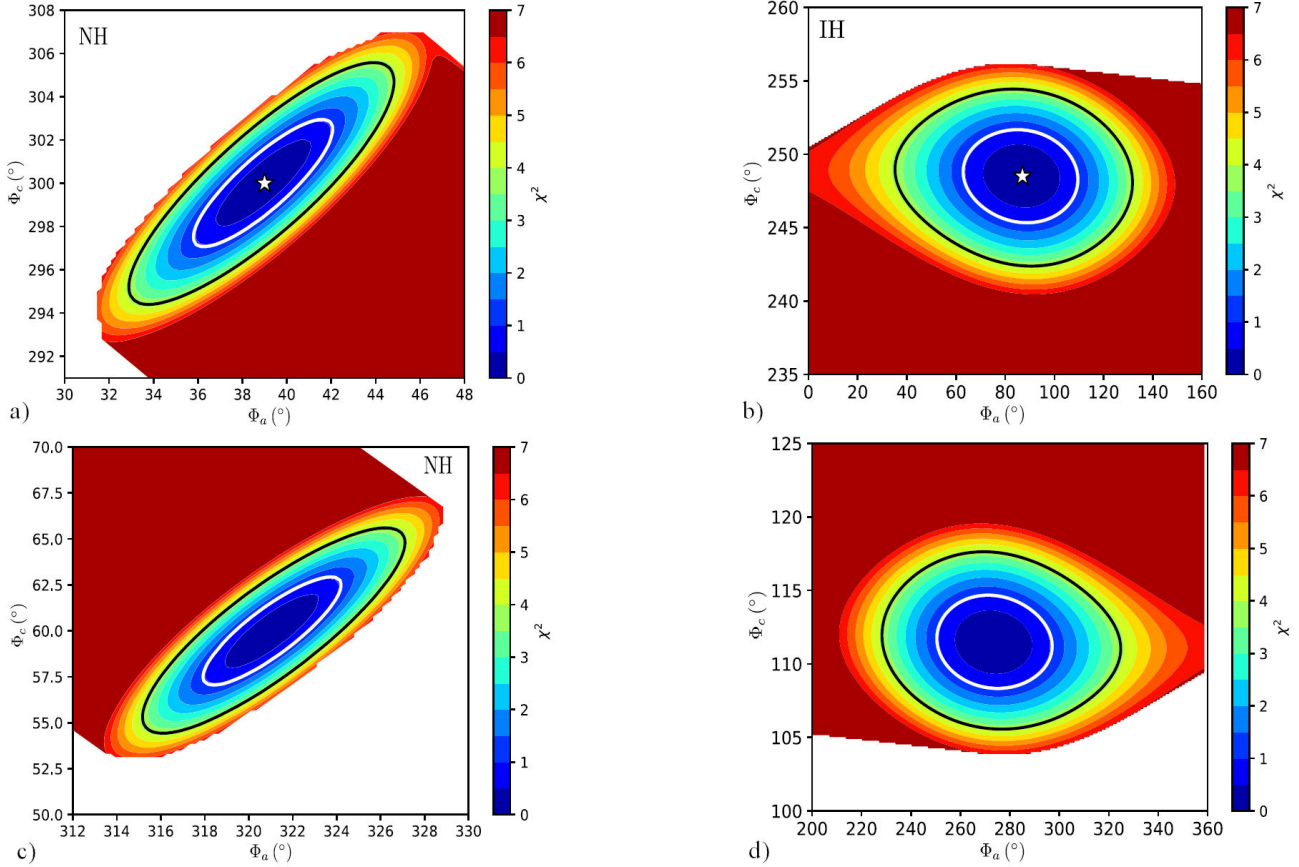


FIGURE 4. Amplification of the parameter regions for Φ_a and Φ_c , where the white star represents the BFP. The regions bounded by the white and black lines represent the allowed region at 1σ and 2σ C.L., respectively.

From the results obtained in the previous likelihood fits, for a normal hierarchy, the leptonic mixing angles have the following average values at 1σ C.L.

$$\begin{aligned} \sin^2 \theta_{12}^{\text{th}} &= \left(3,172^{+0,051}_{-0,057}\right) \times 10^{-1}, \\ \sin^2 \theta_{13}^{\text{th}} &= \left(2,199^{+0,046}_{-0,066}\right) \times 10^{-2}, \\ \sin^2 \theta_{23}^{\text{th}} &= \left(5,744^{+0,054}_{-0,097}\right) \times 10^{-1}, \end{aligned} \quad (85)$$

whereas for an inverted hierarchy at 1σ C.L.

$$\begin{aligned} \sin^2 \theta_{12}^{\text{th}} &= \left(3,183^{+0,054}_{-0,060}\right) \times 10^{-1}, \\ \sin^2 \theta_{13}^{\text{th}} &= (2,225 \pm 0,069) \times 10^{-2}, \\ \sin^2 \theta_{23}^{\text{th}} &= \left(5,787^{+0,073}_{-0,059}\right) \times 10^{-1}. \end{aligned} \quad (86)$$

With these values for the flavor mixing angles, it can be seen that the current experimental values for neutrino oscillations are correctly reproduced.

6. Conclusions

A systematic and detailed model-independent analysis of fermionic flavor masses and mixings was developed. First, we have demonstrated that fermion mass matrices can be consistently cast into a canonical weak-basis form with vanishing (1, 3) and (3, 1) entries, motivated by the hierarchical structure of fermion masses and mixings and without invoking dynamical texture assumptions. This formulation naturally encompasses both Hermitian and complex symmetric cases, providing a unified description of Dirac and Majorana fermion mass terms. Then, it is required that the rotated matrix satisfies the internal symmetry of being either Hermitian

or complex symmetric, in order to express it in polar form and factor out the phases. Both the real symmetric matrix and the PMNS flavor mixing matrix are expressed in terms of the fermion masses and some free parameters.

To evaluate how well the theoretical expressions for the leptonic flavor mixing angles reproduce experimental data, a likelihood test using the χ^2 statistic was implemented. The

results of the χ^2 fit show that the theoretical expressions obtained for the PMNS flavor mixing matrix correctly reproduce the current experimental data on neutrino oscillations. The difference between representing the lepton mass matrix as Hermitian or as complex symmetric lies solely in the form of the diagonal matrix of phase factors.

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A charged black string wormhole with disclinations: Ray and wave optics

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This study investigates the optical behavior of photon rays and scalar waves in a three-dimensional static Black String Charged Wormhole (BSCWH) spacetime featuring topological disclinations. By analyzing null geodesics and the scalar Helmholtz equation, we present a unified treatment of light and wave propagation in curved spacetime with geometric defects. The disclination parameter accounts for angular deficits due to topological defects, the wormhole parameter governs throat geometry, and the Neveu-Schwarz (NS) charge introduces a string-inspired field contribution. These factors jointly influence light bending, photon orbits, and scalar wave modes. Scalar wave propagation reduces to a Schrödinger-like equation with an effective potential, from which we derive a spatially and frequency-dependent effective refractive index. We obtain a closed-form weak-field deflection angle in terms of the geometric parameters and the disclination, and demonstrate that the trivial redshift function inherent to the BSCWH geometry precludes the formation of a photon sphere, yielding instead a critical impact parameter set by the throat radius. In the wave-optics sector, we show that the effective potential diverges at the throat, enforcing total reflection of scalar waves and producing frequency-dependent phase shifts characteristic of a dispersive analogue-gravity medium. Our findings reveal how curvature, charge, and topological features modify optical signatures, with implications for gravitational lensing, analogue gravity experiments, and optical media design. This work highlights the role of string-inspired effects and spacetime defects in shaping wave dynamics near wormholes.

Keywords: Geodesic motion; optical propagation; effective refractive index; Helmholtz equation; effective potential; deflection angle; disclination; analogue gravity.

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1. Introduction

Wormholes (WHs) are theoretical solutions to the Einstein Field Equations (EFE), representing bridges that may connect distant regions of the same universe or entirely different universes. Characterized by a finite-radius throat, these structures are sustained by matter-energy configurations that may uphold or violate classical energy conditions. The concept originated with early developments in General Relativity (GR), notably the Einstein-Rosen bridge proposed by Einstein and Rosen as a connection between two asymptotically flat space-times [1, 2]. Subsequent models include the Ellis-Bronnikov solution [3, 4], as well as Reissner-Nordström and Kerr-type WHs, which were later explored in Euclidean contexts [5, 6]. A major advancement came with the Morris-Thorne wormhole (MTW), a static, spherically symmetric solution that requires exotic matter violating the null and weak energy conditions at the throat [7]. To address this, various studies have proposed WH solutions that avoid exotic matter within both standard GR and modified gravity frameworks [10–12]. Additionally, WHs have been examined as potential

time machines, where a time shift between the mouths allows for temporal travel [13]. Traversable WHs have also been studied in cosmological settings, including de Sitter and anti-de Sitter space-times [15, 16]. Beyond these static charged configurations, recent work has enlarged the catalogue of exact rotating wormholes. Within Einstein-Maxwell-dilaton (EMD) theory, traversable solutions carrying electric, magnetic, and NS-type charges have been built and shown to keep their ring singularity causally hidden behind the throat, a property named wormhole cosmic censorship [18–21]. Rotating traversable WHs in Einstein-Maxwell theory, together with their NUT-charged generalizations, have further clarified the role of Misner strings and the separation of angular momentum from gravitomagnetic charge in these geometries [22–25].

Black strings (BS) are extended gravitational objects that arise by augmenting higher-dimensional BH solutions [26–35] with additional flat spatial directions. This construction leads to horizon topologies of the form $S^{d-2} \times \mathbb{R}$. A seminal investigation into the stability of these configurations was conducted by Gregory and Laflamme [36, 37], who demonstrated that neutral BS in dimensions greater than four

are susceptible to a long-wavelength instability. This phenomenon, now known as the Gregory-Laflamme (GL) instability, occurs when perturbation modes along the string direction grow exponentially over time, provided their wavelength exceeds a critical threshold. The standard neutral BS metric is obtained by extending the Schwarzschild-Tangherlini BH solution [38] along an additional spatial dimension that is translationally invariant. These uniform BS solutions possess event horizons that are either infinite or compactified periodically, maintaining translational symmetry along the extended direction. However, the onset of GL instability breaks this symmetry and may lead to a transition toward non-uniform BS [39,40] or localized BH phases. In the context of string theory and supergravity, analogous instabilities have been observed in systems such as near-extremal or smeared $\mathcal{D}$ -branes wrapped on transverse circles [41-43]. These scenarios are often connected to neutral Kaluza-Klein BH phases via dualities and Lorentz boosts. An important theoretical development in this area is the Gubser-Mitra conjecture, which postulates a correspondence between thermodynamic and classical (dynamical) instabilities in extended gravitational configurations. This conjecture has been extensively studied in the context of smeared branes, supporting the interpretation of GL-type instabilities as manifestations of underlying thermodynamic instability [41]. Furthermore, phase transitions between BS and BH have been explored within strongly coupled thermal field theories, particularly through holographic duality and compactified supersymmetric Yang-Mills models [42]. These phenomena carry significant implications for braneworld scenarios. In models with large extra dimensions [44,45], or in warped geometries such as those proposed in the Randall-Sundrum framework [46,47], BS solutions are expected to form and exhibit GL-like instabilities, mirroring the behavior observed in higher-dimensional gravitational systems. Thin-shell WHs constructed from charged BS spacetimes [48], as well as embeddings of WHs and dyonic BS in warped braneworlds [49], have further enriched the landscape of extended gravitational objects. Charged BS and black branes have also been studied in higher-curvature Lovelock theories [50], while wave equations governing perturbations of rotating charged BS have been analyzed in Ref. [51]. In the string-theoretic context, massless BH and charged WH solutions have been constructed [52], providing a natural arena for exploring the interplay between gauge fields and topology.

The study of ray and wave optics in curved manifolds provides a powerful framework for understanding how spacetime geometry influences electromagnetic radiation. Within the context of GR, mass and energy curve spacetime, thereby affecting light propagation through phenomena such as gravitational lensing (GL) [53], wave interference patterns [54], and modifications in scattering amplitudes [55]. These effects are particularly evident in features like photon rings observed near compact astrophysical objects [56]. However, direct experimental verification remains difficult due to gravity's inherently weak coupling, requiring astronomical distances for

measurable deviations. To address this limitation, analogue gravity systems have been developed to replicate relativistic geometries in controlled laboratory environments [57,58]. These analogues span diverse platforms, including the observation of Hawking-like radiation in Bose-Einstein condensates [59], simulations of relativistic orbits using refractive-index-engineered optical materials [60], and photonic setups that mimic GL [61]. Another complementary approach involves reducing the spatial dimensionality of curved space-times (from $\mathcal{D}$ to $3\mathcal{D}$), thereby facilitating experimental access to curvature-induced wave phenomena [62]. This geometrically inspired modeling approach was significantly advanced by Batz *et al.* [63], whose foundational work established a non-linear Schrödinger-type framework for describing light propagation on surfaces of constant Gaussian curvature. Their theory deepens the connection between geometry and wave dynamics and has inspired research across classical optics, plasmonics [64], and quantum wave transport [65]. In particular, their model elucidates how curvature directly governs wave evolution in structured optical environments [66,67]. In parallel, the geometrical optics of topological defects such as disclinations has been explored in condensed-matter analogues [68], while surface-plasmon models of BH and WH optics [69] and metamaterial platforms for ray optics [70] have demonstrated that curved-space optical phenomena can be faithfully reproduced in laboratory settings. Classical optics for charged BH spacetimes has also been developed in a rigorous mathematical framework [71], and wave-optics effects in GL of gravitational waves have been probed as signatures of dark-matter substructure [72]. Recent developments in the fields of photonics and quantum physics have led to significant advances in understanding wave propagation and particle interactions in complex media. Dos S. Azevedo *et al.* [73] have demonstrated novel nonlinear optical phenomena in engineered materials, highlighting new avenues for controlling light at the nanoscale. Complementing this, Xu *et al.* [74] analyzed light manipulation techniques within advanced photonic structures, emphasizing applications in optical communication and sensing. Meanwhile, Shao *et al.* [75] provided valuable insights into wave dynamics in disordered systems, revealing mechanisms behind localization and enhanced scattering effects. On a theoretical and fundamental physics level, Dogan *et al.* have made substantial contributions through a series of works [76-78] focusing on quantum field theoretic approaches to particle behavior in curved spacetime and non-trivial geometries, including ray geodesics and wave propagation on WH-like surfaces [79]. Their research sheds light on how topological and geometric effects influence particle spectra and interaction cross-sections, thereby opening new possibilities for exploring physics beyond the Standard Model. Moreover, Ahmed *et al.* [80,81] have advanced the understanding of symmetry-breaking mechanisms and their implications for particle mass generation and vacuum stability. Their investigations provide crucial theoretical foundations that may guide future experimental searches for new physics phenomena. Collectively, these interdisciplinary efforts

demonstrate the rich interplay between optical physics and high-energy theory, driving forward the frontier of modern physics.

In this paper, we investigate a three-dimensional static traversable black string charged wormhole (BSCWH) space-time embedded with disclinations. We explore both ray optics and wave optics in this curved space-time background. For ray optics, we analyze null geodesic (NG) motion to determine the behavior of photon trajectories. For wave optics, we examine the scalar Helmholtz equation and, by employing a suitable ansatz for the scalar field, recast it into a Schrödinger-like form. This transformation allows us to identify an effective potential that governs the wave dynamics. From this potential, we derive an effective refractive index (RI) that depends on both spatial coordinate and wave frequency. We demonstrate how geometric parameters, such as the throat radius, the NS charge, the curvature scale, and the disclination affect the photon paths and the RI profile in the WH geometry. In addition, we derive a closed-form weak-field approximation for the deflection angle, identify the critical impact parameter governing photon capture, and present numerical tables that quantify the dependence of key optical observables on the spacetime parameters.

The structure of this paper is as follows: In Sec. 2, we introduce a three-dimensional, static, and circularly symmetric charged BSCWH with disclinations. In Sec. 3, we analyze NG motion and derive the corresponding photon trajectories, including the critical impact parameter and the weak-field deflection angle. Section 4 is devoted to the study of wave optical properties in this curved space-time background, where we obtain an effective RI. Finally, in Sec. 5, we summarize our findings and present concluding remarks. Throughout this work, we adopt natural units where $c = 1 = 8\pi G = \hbar$.

2. Three-dimensional BSCWH with disclinations

In this section, we introduce the three-dimensional static and circularly symmetric BSCWH with disclinations. In the subsequent sections, we investigate its ray and wave optical properties and analyze how the geometric parameters influence these characteristics.

In Ref. [82], the author proposed 3D traversable WH metric analogue to the MTW 4D case [7,11]. The line element is described by the circular symmetry in the chart (t, r, ϕ) as,

$$ds^2 = -e^{2\Phi(r)} dt^2 + \frac{dr^2}{1 - \frac{b(r)}{r}} + r^2 d\phi^2, \quad (1)$$

where $\Phi(r)$ is a redshift function and $b(r)$ is a shape function of a traversable WH. The flare-out condition is given by $|r b'(r) - b(r)|_{r=r_0} < 0$, while a throat of WH is defined as $b(r = r_0) = r_0$.

In Ref. [83], the authors considered a logarithmic dilaton profile, $\phi = -\ln(r/\ell)$, as the dual of a constant dilaton with

a trivial redshift function $\Phi(r) = 0$, and used this to generate a static, circularly symmetric 3D charged BSCWH. By adding suitable matter sources-including the dilaton scalar, they arrived at a line element of the form with disclinations given by

$$ds^2 = -dt^2 + \frac{dr^2}{f(r)} + \alpha^2 r^2 d\phi^2, \quad (2)$$

where the metric function $f(r)$ is given by

$$f(r) = 1 - b(r)/r, \quad b(r) = b_0 - \frac{Q^2 \ell^4}{4r}. \quad (3)$$

For completeness, we recall the theory that produces the line element (2). It descends from the three-dimensional low-energy effective action of string theory [83], which in the string frame reads

$$S = \frac{1}{2} \int d^3x \sqrt{-g} e^{-2\varphi} \left[R + 4(\nabla\varphi)^2 + \frac{4}{\ell^2} - \frac{1}{12} H_{\mu\nu\rho} H^{\mu\nu\rho} \right], \quad (4)$$

with φ the dilaton (distinct from the redshift function Φ), ℓ the curvature (string) length, and $H_{\mu\nu\rho} = \partial_{[\mu} B_{\nu\rho]}$ the NS three-form field strength. In three dimensions the antisymmetric three-form must be proportional to the Levi-Civita tensor, $H_{\mu\nu\rho} = Q \sqrt{-g} \epsilon_{\mu\nu\rho}$, so the whole NS sector enters through the single charge Q . Taking the logarithmic dilaton $\varphi = -\ln(r/\ell)$ of Ref. [83], dual to a constant dilaton with trivial redshift $\Phi(r) = 0$, the field equations return the shape function already quoted in Eq. (3).

It helps to read the matter content straight off the geometry. In the Einstein frame the line element (2) solves $G_{\mu\nu} = T_{\mu\nu}^{\text{eff}}$ in the units $8\pi G = 1$ used here. A short calculation leaves a single non-vanishing mixed component,

$$G^t_t = \frac{f'(r)}{2r}, \quad G^r_r = G^\phi_\phi = 0, \quad (5)$$

so the effective source is an energy density with no radial or tangential pressure,

$$\rho = -\frac{f'(r)}{2r} = -\frac{b_0}{2r^3} + \frac{Q^2 \ell^4}{4r^4}, \quad p_r = p_\phi = 0. \quad (6)$$

Because r_0 is a simple (non-extremal) throat, $f(r_0) = 0$ with $f'(r_0) > 0$, and hence $\rho(r_0) < 0$. The energy density turns negative near the throat. This is the expected signature of the null energy condition violation that keeps the wormhole open, with the dilaton and NS matter of the action (4) supplying the exotic source. Here, α denotes the disclination parameter [84-86], which characterizes the angular deficit caused by topological defects in the space-time. The parameter ℓ represents the curvature radius, serving as a fundamental length scale in the geometry. The quantity Q corresponds to the NS (Neveu-Schwarz) charge, associated with the antisymmetric tensor field arising in the NS sector of string theory. Finally, b_0 is an integration constant, often related to the WH throat or initial geometric conditions. It is worth noting that the metric function $f(r) =$

$(1 - [b_0/r] + [Q^2 \ell^4/4r^2])$ satisfies $f(r) \rightarrow 1$ as $r \rightarrow \infty$, indicating that the space-time becomes asymptotically conical. This behavior, rather than asymptotic flatness, arises due to the presence of disclinations encoded by the parameter α .

The metric tensor $g_{\mu\nu}$ and its inverse $g^{\mu\nu}$ for the space-time (2) are given by

$$g_{\mu\nu} = \text{diag} \left(-1, \frac{1}{f(r)}, \alpha^2 r^2 \right), \quad (7)$$

$$g^{\mu\nu} = \text{diag} \left(-1, f(r), \frac{1}{\alpha^2 r^2} \right). \quad (8)$$

The throat radius of the WH is obtained by the following condition:

$$f(r = r_0) = 0. \quad (9)$$

Using the relation (3), we find the throat radius as,

$$r_0 = b_0/2 + \sqrt{b_0^2 - Q^2 \ell^4/2} \geq b_0/2, \quad (10)$$

provided the constraint on the parameters satisfied $b_0 \geq Q \ell^2$. The range of the NS charge is $Q \in (0, b_0/\ell^2]$.

TABLE I. Throat radius r_0 for various values of b_0 and Q with $\ell = 1$. The constraint $b_0 \geq Q \ell^2$ must be satisfied.

b_0	Q	r_0
1.0	0.2	0.989898
1.0	0.4	0.958258
1.0	0.6	0.900000
1.0	0.8	0.800000
1.0	1.0	0.500000
1.5	0.2	1.493303
1.5	0.4	1.472842
1.5	0.6	1.437386
1.5	0.8	1.384429
1.5	1.0	1.309017
2.0	0.2	1.994987
2.0	0.4	1.979796
2.0	0.6	1.953939
2.0	0.8	1.916515
2.0	1.0	1.866025
2.5	0.2	2.495994
2.5	0.4	2.483896
2.5	0.6	2.463466
2.5	0.8	2.434272
2.5	1.0	2.395644

The flare-out condition at the throat requires $b'(r_0) < 1$. From Eq. (3), we compute $b'(r) = Q^2 \ell^4/(4r^2)$, which gives

$$b'(r_0) = \frac{Q^2 \ell^4}{4r_0^2}. \quad (11)$$

Since $r_0 \geq b_0/2 \geq Q \ell^2/2$, we have $4r_0^2 \geq Q^2 \ell^4$, ensuring $b'(r_0) \leq 1$, with equality only in the extremal limit $b_0 = Q \ell^2$. Thus, the flare-out condition is satisfied for all non-extremal parameter choices.

As seen from the table, the throat radius r_0 decreases monotonically with increasing NS charge Q for fixed b_0 , and collapses to the extremal value $r_0 = b_0/2$ when $b_0 = Q \ell^2$.

3. Ray optics in BSCWH with disclinations

In this section, we analyze NG motion to determine the behavior of photon trajectories in a 3D BSCWH space-time, described by the line element (2). We show geometrical parameters including disclination alter these trajectories.

The NG motion can be studied using a well-known method called the Lagrangian formalism, where the Lagrangian density function is given by $\mathcal{L} = (1/2) g_{\mu\nu} \dot{x}^\mu \dot{x}^\nu$, with the dot denoting differentiation with respect to an affine parameter and $g_{\mu\nu}$ is the metric tensor for curved geometry.

For the metric given in Eq. (2), the Lagrangian density function is given by

$$\mathcal{L} = \frac{1}{2} \left[- \left(\frac{dt}{d\tau} \right)^2 + \frac{1}{f(r)} \left(\frac{dr}{d\tau} \right)^2 + \alpha^2 r^2 \left(\frac{d\phi}{d\tau} \right)^2 \right]. \quad (12)$$

From the above function, one can see that there exist two Killing vector fields, namely, $\xi_{(t)} \equiv \partial_t$ associated with temporal coordinate and $\xi_{(\phi)} \equiv \partial_\phi$ associated with the orbital coordinate. The conserved quantities are the energy E and the angular momentum L , fixed by $E = -g_{\mu\nu} \xi_{(t)}^\mu \dot{x}^\nu$ and $L = g_{\mu\nu} \xi_{(\phi)}^\mu \dot{x}^\nu$. Since $g_{tt} = -1$ and $g_{\phi\phi} = \alpha^2 r^2$, we find [87]:

$$E = \frac{dt}{d\tau}, \quad L = \alpha^2 r^2 \frac{d\phi}{d\tau}. \quad (13)$$

The factor α^2 follows directly from $g_{\phi\phi} = \alpha^2 r^2$, since L is the conserved charge of $\xi_{(\phi)} = \partial_\phi$, that is $L = g_{\phi\phi} \dot{\phi}$. With these, the non-radial NG paths for r coordinate from Eq. (12) simplify to:

$$\frac{1}{f(r)} \left(\frac{dr}{d\tau} \right)^2 = E^2 - \frac{L^2}{\alpha^2 r^2}. \quad (14)$$

The equation of orbit is therefore defined by

$$\left(\frac{1}{r^2} \frac{dr}{d\phi} \right)^2 = \alpha^2 f(r) \left(\frac{1}{\beta^2} - \frac{1}{r^2} \right), \quad (15)$$

where $\beta = L/(\alpha E)$ is the impact parameter for photon particles, so that the corrected definitions leave Eq. (15) and every expression derived from it unchanged.

3.1. Absence of photon sphere and critical impact parameter

A distinctive feature of the BSCWH geometry (2) is the trivial redshift function $\Phi(r) = 0$, which implies $g_{tt} = -1$. In standard BH spacetimes, the photon sphere (unstable circular photon orbit) arises from the competition between the gravitational redshift (encoded in g_{tt}) and the centrifugal barrier. The effective potential governing photon orbits takes the general form $V_{\text{eff}}^{\text{orb}}(r) = -g_{tt}(r)/r^2$, whose local maximum defines the photon sphere radius r_{ps} .

In the present BSCWH geometry, however, the NG condition (14) can be recast as

$$\dot{r}^2 = f(r) \left(E^2 - \frac{L^2}{\alpha^2 r^2} \right). \quad (16)$$

Defining the orbital effective potential $\mathcal{V}(r) \equiv 1/r^2$, the turning point condition $\dot{r} = 0$ (with $f(r) > 0$) yields

$$\frac{1}{\beta^2} = \frac{1}{r_{\text{tp}}^2} \implies r_{\text{tp}} = \beta. \quad (17)$$

Since $\mathcal{V}(r) = 1/r^2$ is a monotonically decreasing function with no local maximum for finite r , the BSCWH geometry admits *no photon sphere*. This is a direct consequence of $g_{tt} = -1$; in the absence of gravitational redshift, there is no competing radial force to create an unstable circular orbit.

Consequently, the photon dynamics are governed solely by the impact parameter β relative to the throat radius r_0 :

- If $\beta > r_0$: the photon reaches the turning point at $r_{\text{tp}} = \beta > r_0$, scatters, and returns to infinity. The deflection angle is finite and depends on the spacetime parameters.
- If $\beta = r_0$: the photon grazes the WH throat, defining the **critical impact parameter**

$$\beta_c = r_0 = \frac{b_0}{2} + \frac{\sqrt{b_0^2 - Q^2 \ell^4}}{2}. \quad (18)$$

- If $\beta < r_0$: the turning point lies at $r_{\text{tp}} = \beta < r_0$, which falls inside the throat region where $f(r) < 0$. The photon reaches the throat and traverses the WH to the other asymptotic region.

The critical impact parameter β_c thus plays the role analogous to the shadow radius in BH spacetimes, delineating scattered from captured (traversing) photon trajectories. Table II presents values of β_c for representative parameter combinations.

Transforming to a new variable via $r = 1/u$ in the above Eq. (15) yields:

$$\left(\frac{du}{d\phi} \right)^2 = \frac{\alpha^2}{\beta^2} f(u) - \alpha^2 u^2 f(u). \quad (19)$$

where $f(u)$ explicitly can be written as

$$f(u) = 1 - b_0 u + \frac{Q^2 \ell^4}{4} u^2. \quad (20)$$

TABLE II. Critical impact parameter $\beta_c = r_0$ and the flare-out derivative $b'(r_0) = Q^2 \ell^4 / (4 r_0^3)$ for various parameter values with $\ell = 1$.

b_0	Q	$\beta_c = r_0$	$b'(r_0)$
1.0	0.2	0.989898	0.010205
1.0	0.4	0.958258	0.043559
1.0	0.6	0.900000	0.111111
1.0	0.8	0.800000	0.250000
1.0	1.0	0.500000	1.000000
1.5	0.4	1.472842	0.018437
1.5	0.6	1.437386	0.043562
1.5	0.8	1.384429	0.083478
1.5	1.0	1.309017	0.145898
2.0	0.4	1.979796	0.010205
2.0	0.6	1.953939	0.023573
2.0	0.8	1.916515	0.043559
2.0	1.0	1.866025	0.071798

Differentiating both sides of Eq. (19) w. r. t. ϕ and after simplification results

$$\begin{aligned} \frac{d^2 u}{d\phi^2} + \alpha^2 \left(1 - \frac{Q^2 \ell^4}{4 \beta^2} \right) u &= -\frac{\alpha^2 b_0}{2 \beta^2} \\ &+ \frac{3 \alpha^2 b_0}{2} u^2 - \frac{\alpha^2 Q^2 \ell^4}{2} u^3. \end{aligned} \quad (21)$$

In the limit $Q = 0$ corresponding to the absence of NS charge, the above equation reduces as

$$\frac{d^2 u}{d\phi^2} + \alpha^2 u + \frac{\alpha^2 b_0}{2 \beta^2} = \frac{3}{2} \alpha^2 b_0 u^2. \quad (22)$$

Figures 1–2 and 3–4 present the parametric plots of photon trajectories $r(\phi) = 1/u(\phi)$ based on Eq. (21) for various values of the disclination parameter α and the NS charge Q . Figure 5 compares the photon trajectories with and without the influence of α and Q , highlighting the impact of these parameters on the photon's path. We set the initial boundary condition $u(0) = 0.001$ and $u'(0) = 0.01$.

Moreover, for radial NG, where the angular momentum vanishes, $L = 0$, the geodesic paths for t and r coordinates from Eqs. (13)–(14) reduces as,

$$\frac{dt}{d\tau} = E, \quad \frac{dr}{d\tau} = \pm E \sqrt{f(r)}. \quad (23)$$

From the above equation, we find the radial motion of photon particles in temporal coordinate as,

$$\frac{dr}{dt} = \pm \sqrt{f(r)}. \quad (24)$$

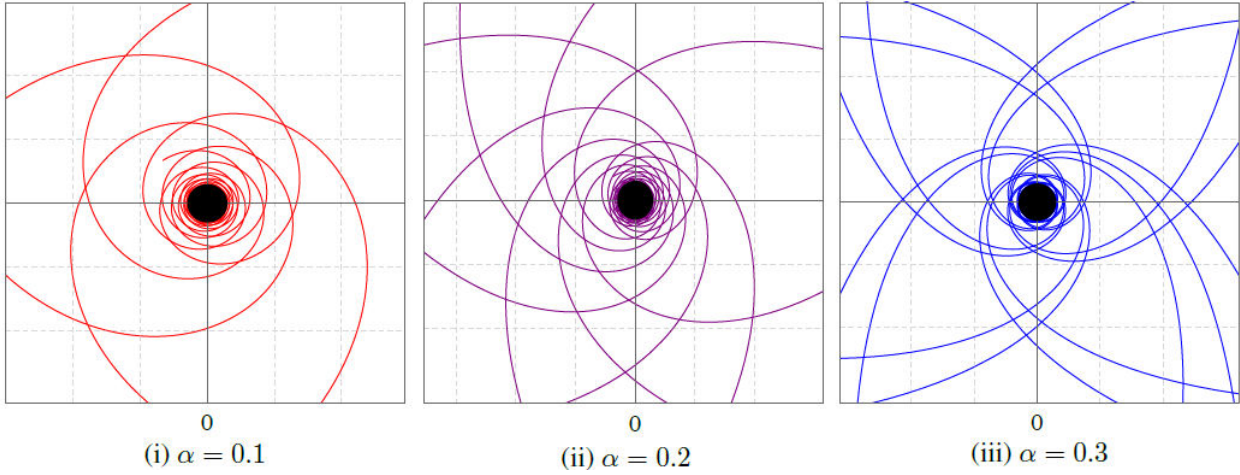


FIGURE 1. Parametric plot of the Photon trajectory for different values of the disclination parameter α , while keeping $\beta = 1.5$, $\mathcal{Q} = 1 = \ell = b_0$. The horizontal and vertical axes are the Cartesian coordinates $X = r \cos \phi$ and $Y = r \sin \phi$ (in units of b_0) built from the orbit $r(\phi) = 1/u(\phi)$ of Eq. (21); the central black disk marks the throat at $r = r_0$.

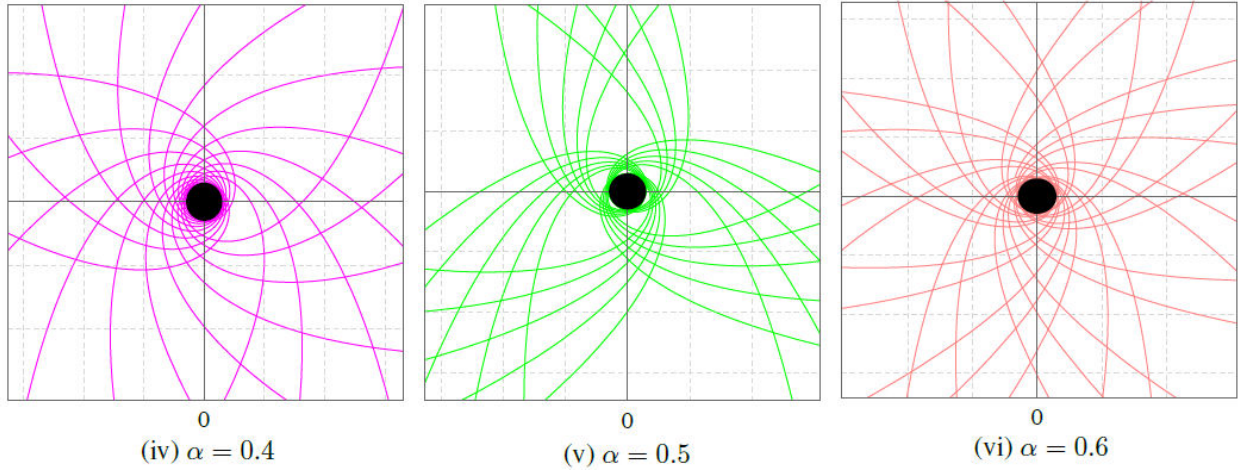


FIGURE 2. Parametric plot of the Photon trajectory for different values of the disclination parameter α , while keeping $\beta = 1.5$, $\mathcal{Q} = 1 = \ell = b_0$. The horizontal and vertical axes are the Cartesian coordinates $X = r \cos \phi$ and $Y = r \sin \phi$ (in units of b_0) built from the orbit $r(\phi) = 1/u(\phi)$ of Eq. (21); the central black disk marks the throat at $r = r_0$.

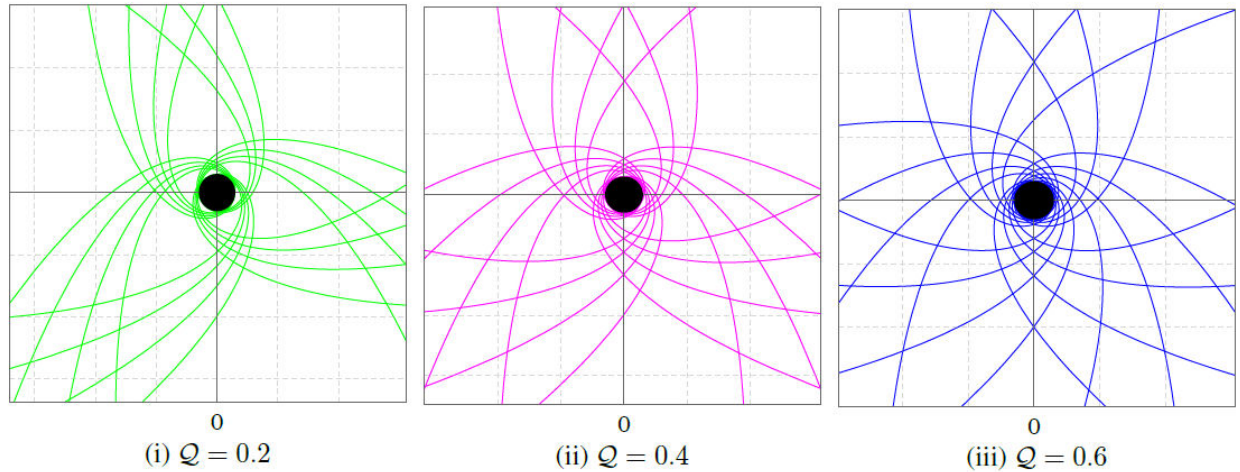


FIGURE 3. Parametric plot of the Photon trajectory for different values of NS charge $\mathcal{Q}$, while keeping $\beta = 1.5$, $\alpha = 0.5$, $\ell = 1 = b_0$. The axes are the Cartesian coordinates $X = r \cos \phi$ and $Y = r \sin \phi$ (in units of b_0) obtained from the orbit $r(\phi) = 1/u(\phi)$; the central black disk marks the throat at $r = r_0$.

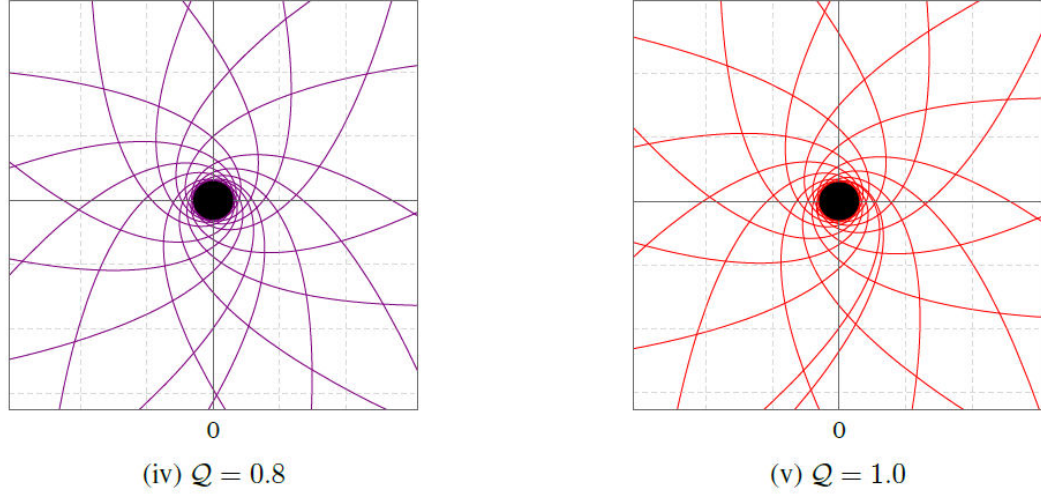


FIGURE 4. Parametric plot of the Photon trajectory for different values of NS charge Q , while keeping $\beta = 1.5$, $\alpha = 0.5$, $\ell = 1 = b_0$. The axes are the Cartesian coordinates $X = r \cos \phi$ and $Y = r \sin \phi$ (in units of b_0) obtained from the orbit $r(\phi) = 1/u(\phi)$; the central black disk marks the throat at $r = r_0$.

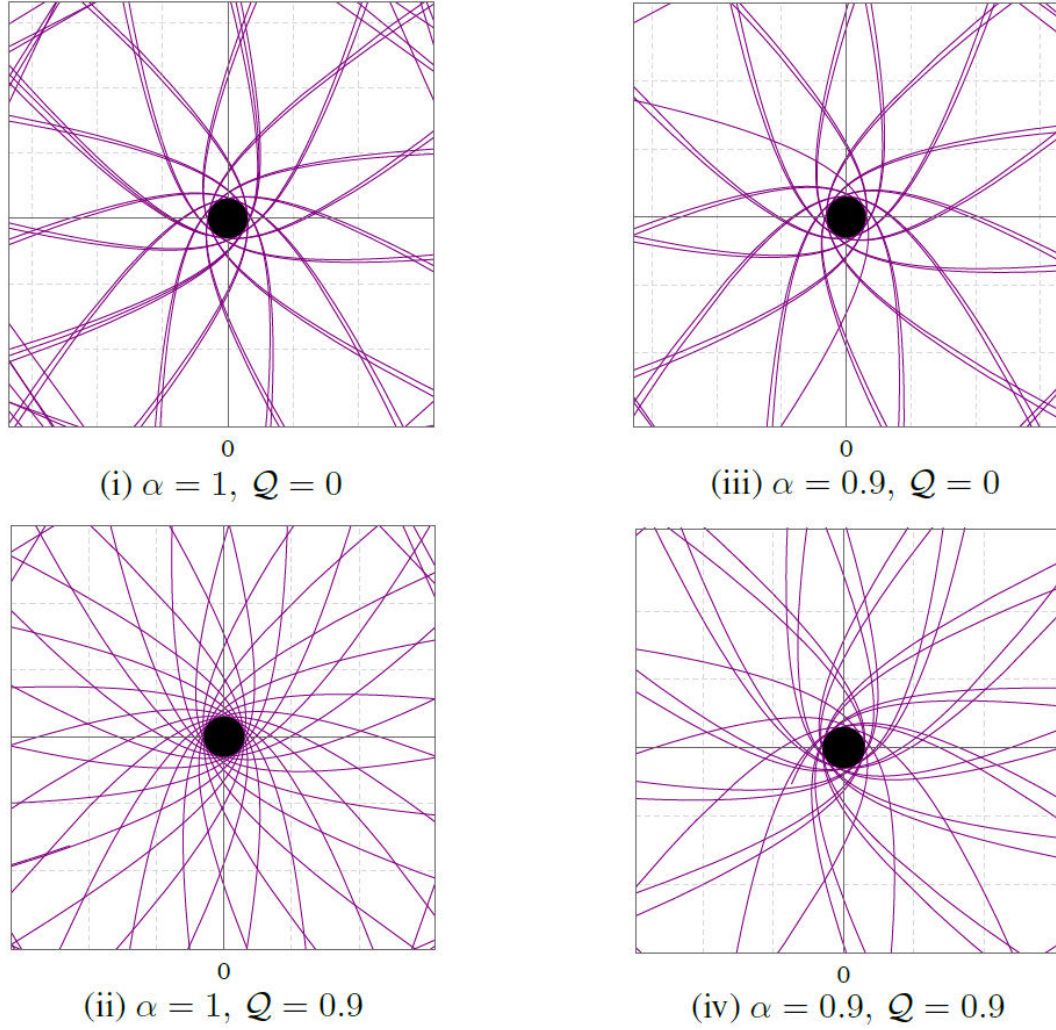


FIGURE 5. Parametric plot of the Photon trajectory $r(\phi) = 1/u(\phi)$ for different values of NS charge Q without and with disclination parameter α , while keeping $\beta = 1.5$, $\ell = 1 = b_0$. The axes are the Cartesian coordinates $X = r \cos \phi$ and $Y = r \sin \phi$ (in units of b_0); the central black disk marks the throat at $r = r_0$.

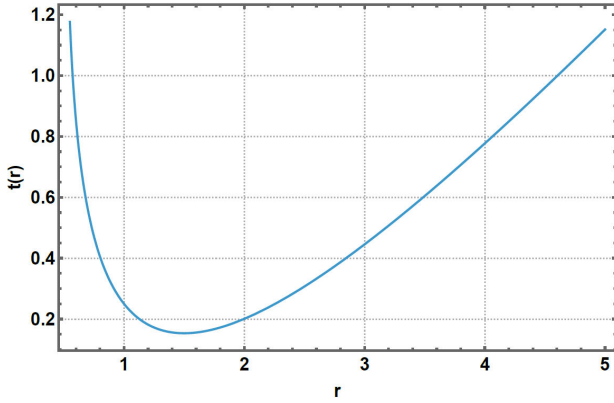


FIGURE 6. Variation of the temporal coordinate $t(r)$ as a function of r for the radial NG motion. Here, we set $\ell = 1$, $\mathcal{Q} = 1$, $b_0 = 1$, $C = 0$. The horizontal axis is the radial coordinate r and the vertical axis is the coordinate time $t(r)$, both in units of b_0 .

Therefore, the temporal coordinate $t(r)$ as

$$t(r) = \pm \int \frac{dr}{\sqrt{f(r)}} = \pm \frac{dr}{\sqrt{1 - \frac{b_0}{r} + \frac{\mathcal{Q}^2 \ell^4}{4r^2}}}. \quad (25)$$

Simplification of the above integral results

$$t(r) = \frac{1}{2} \sqrt{r^2 - b_0 r + \frac{\mathcal{Q}^2 \ell^4}{4}} - \frac{b_0}{2} \ln \left| r - \frac{b_0}{2} + \sqrt{r^2 - b_0 r + \frac{\mathcal{Q}^2 \ell^4}{4}} \right| + C, \quad (26)$$

where C is an integrating constant.

Figure 6 illustrates the evolution of the temporal coordinate $t(r)$ along a radial photon trajectory, plotted as a function of the axial coordinate r . This behavior is obtained by integrating the geodesic equation for radial null trajectories ($L = 0$). In this plot, the curvature radius is set to $\ell = 1$, the NS charge $\mathcal{Q} = 1$, the throat radius $b_0 = 1$, and the integration constant $C = 0$. The curve exhibits a monotonic increase in $t(r)$, with the steepness of the curve reflecting how the space-time geometry causes a delay in coordinate time as the photon approaches the WH throat. Notably, the presence of the charge parameter and the WH geometry both influence the shape of this function through the metric component $f(r)$, thereby affecting the effective gravitational time delay experienced by radially in-falling photons.

To obtain an expression of the deflection angle of photon particles, we can write Eq. (19) with the help of Eq. (20) as,

$$\frac{du}{d\phi} = \frac{\alpha}{\beta} \sqrt{\left(1 - b_0 u + \frac{\mathcal{Q}^2 \ell^4}{4} u^2\right) (1 - \beta^2 u^2)}. \quad (27)$$

The deflection angle is given by

$$\delta\phi = \frac{\beta}{\alpha} \Delta\phi - \pi, \quad (28)$$

where

$$\Delta\phi = \int_{u_0}^{\infty} \frac{du}{\sqrt{\left(1 - b_0 u + \frac{\mathcal{Q}^2 \ell^4}{4} u^2\right) (1 - \beta^2 u^2)}}. \quad (29)$$

Recall that $u_0 = 1/r_0$, where r_0 is defined in Eq. (10). Noting that for the special case $b_0 = \mathcal{Q} \ell^2$, we have $r_0 = b_0/2$, which implies $u_0 = 2/b_0$. Under this condition, the lower limit of the integral in Eq. (29) coincides with the point where the integrand becomes singular. As a result, the integral diverges at the lower limit. We therefore conclude that the deflection angle can be determined only when $b_0 \neq \mathcal{Q} \ell^2$.

The integral (29) after a few mathematical steps, we find (see notes at the end)

$$\begin{aligned} \Delta\phi &= \frac{1}{\sqrt{-\beta^2 + \frac{\mathcal{Q}^2 \ell^4}{4}}} [F(\pi/2, k) - F(\phi_0, k)] \\ &= \frac{1}{\sqrt{-\beta^2 + \frac{\mathcal{Q}^2 \ell^4}{4}}} [K(k) - F(\phi_0, k)], \end{aligned} \quad (30)$$

where we have defined the following:

$$\begin{aligned} k^2 &= \frac{-\beta^2 - \frac{\mathcal{Q}^2 \ell^4}{4} + \sqrt{\left(-\beta^2 - \frac{\mathcal{Q}^2 \ell^4}{4}\right)^2 + b_0^2 \beta^4}}{2 \left(-\beta^2 + \frac{\mathcal{Q}^2 \ell^4}{4}\right)}, \\ \phi_0 &= \arcsin \left(\sqrt{\frac{\left(-\beta^2 + \frac{\mathcal{Q}^2 \ell^4}{4}\right) (u_0 - \xi_1)}{\left(-\beta^2 - \frac{\mathcal{Q}^2 \ell^4}{4} + \Sigma\right) (u_0 - \xi_2)}} \right), \\ u_0 &= \frac{2}{b_0 + \sqrt{b_0^2 - \mathcal{Q}^2 \ell^4}}, \\ \xi_{1,2} &= \frac{b_0 \pm \sqrt{b_0^2 - \mathcal{Q}^2 \ell^4}}{\frac{1}{2} \mathcal{Q}^2 \ell^4}, \\ \Sigma &= \sqrt{\left(-\beta^2 - \frac{\mathcal{Q}^2 \ell^4}{4}\right)^2 + b_0^2 \beta^4}. \end{aligned} \quad (31)$$

Here, $K(k)$ and $F(\phi_0, k)$ denote the complete and incomplete elliptic integrals of the first kind, respectively [88,89].

We observe from the above analysis that the deflection angle of photon particles is influenced by geometrical parameters ($b_0, \mathcal{Q}, \ell$) and the disclinations parameter α .

3.2. Weak-field deflection angle

In the weak-field regime, corresponding to a large impact parameter $\beta \gg b_0$, we can derive a closed-form approximation for the deflection angle by expanding the orbit equation perturbatively. The total angular sweep of a photon traveling from infinity to the turning point $r_{\text{tp}} = \beta$ and back is

$$\phi_{\text{total}} = \frac{2}{\alpha} \int_0^{1/\beta} \frac{du}{\sqrt{f(u) (1/\beta^2 - u^2)}}. \quad (32)$$

Expanding $1/\sqrt{f(u)}$ for small u (i.e., large r),

$$\frac{1}{\sqrt{f(u)}} \approx 1 + \frac{b_0}{2} u + \left(\frac{3b_0^2}{8} - \frac{\mathcal{Q}^2 \ell^4}{8} \right) u^2 + \mathcal{O}(u^3), \quad (33)$$

TABLE III. Weak-field deflection angle $\delta\phi_{\text{weak}}$ (in radians) for $b_0 = 1$, $\ell = 1$, and selected values of α , $\mathcal{Q}$, and β .

α	$\mathcal{Q}$	β	$\delta\phi_{\text{weak}}$
0.7	0.0	5.0	1.665771
0.7	0.5	5.0	1.662966
0.7	1.0	5.0	1.654551
0.8	0.0	5.0	1.064851
0.8	0.5	5.0	1.062396
0.8	1.0	5.0	1.055033
0.9	0.0	5.0	0.597468
0.9	0.5	5.0	0.595286
0.9	1.0	5.0	0.588741
1.0	0.0	5.0	0.223562
1.0	0.5	5.0	0.221598
1.0	1.0	5.0	0.215708
1.0	0.0	10.0	0.105890
1.0	0.5	10.0	0.105400
1.0	1.0	10.0	0.103927
1.0	0.0	20.0	0.051473
1.0	0.5	20.0	0.051350
1.0	1.0	20.0	0.050982

and employing the standard integrals

$$\begin{aligned}
\int_0^{1/\beta} \frac{du}{\sqrt{1/\beta^2 - u^2}} &= \frac{\pi}{2}, \\
\int_0^{1/\beta} \frac{u du}{\sqrt{1/\beta^2 - u^2}} &= \frac{1}{\beta}, \\
\int_0^{1/\beta} \frac{u^2 du}{\sqrt{1/\beta^2 - u^2}} &= \frac{\pi}{4\beta^2},
\end{aligned} \quad (34)$$

we obtain

$$\phi_{\text{total}} = \frac{\pi}{\alpha} + \frac{b_0}{\alpha\beta} + \frac{\pi(3b_0^2 - \mathcal{Q}^2\ell^4)}{16\alpha\beta^2} + \mathcal{O}(\beta^{-3}). \quad (35)$$

The weak-field deflection angle is therefore

$$\begin{aligned}
\delta\phi_{\text{weak}} &= \frac{\pi(1-\alpha)}{\alpha} + \frac{b_0}{\alpha\beta} \\
&+ \frac{\pi(3b_0^2 - \mathcal{Q}^2\ell^4)}{16\alpha\beta^2} + \mathcal{O}(\beta^{-3}).
\end{aligned} \quad (36)$$

This expression admits a transparent physical interpretation:

1. The first term $\pi(1-\alpha)/\alpha$ represents the **topological deflection** due to the disclination-induced angular deficit. For $\alpha < 1$, this yields a positive deflection, focusing light toward the defect core, in complete analogy with cosmic string lensing [84].
2. The second term $b_0/(\alpha\beta)$ is the **leading gravitational deflection**, the $(2+1)$ -dimensional analogue of

the Schwarzschild result $4M/b$ in four dimensions. It is enhanced by the factor $1/\alpha$ due to the conical geometry.

3. The third term introduces **post-leading corrections** involving both the WH parameter b_0 and the NS charge $\mathcal{Q}$. Notably, the NS charge reduces the deflection angle, counteracting the gravitational bending.

In Table III, we present the weak-field deflection angle $\delta\phi_{\text{weak}}$ for representative parameter values, demonstrating the interplay between disclination, gravitational, and charge contributions.

As evident from the table, the disclination parameter α dominates the deflection for moderate impact parameters, while the NS charge provides a secondary correction that systematically reduces $\delta\phi$.

4. Wave optics in BSCWH with disclinations

In this section, we examine the dynamics of wave propagation within the effective geometry of a WH, focusing specifically on the corresponding electromagnetic wave modes. In free space, Maxwell's equations govern the behavior of electromagnetic fields. For a monochromatic wave with time dependence of the form $e^{-i\omega t}$, Maxwell's equations reduce to the Helmholtz equation: $\nabla^2\psi + k^2\psi = 0$, where $k = \omega/c$ is the wave number. This equation describes the spatial distribution of electromagnetic waves under time-harmonic conditions in a source-free region. The solutions to the Helmholtz equation correspond to the permitted electromagnetic modes in the frequency domain.

In the context of curved spacetime or effective geometries such as that of a WH as described by the line element (2), the Helmholtz wave equation can be expressed as [63,67,73-78,80,81]:

$$(\Delta_{\text{LB}} + k_g^2)\Psi = 0, \quad (37)$$

where Δ_{LB} represents the Laplace-Beltrami (LB) operator. The term k_g corresponds to the propagation constant associated with the wave frequency $k_g = \omega/c = \omega$, while Δ_{LB} shows the effects of curvature on wave propagation. Specifically, for a generic metric $ds^2 = -dt^2 + g_{ij} dx^i dx^j$, the LB operator takes the following form:

$$\Delta_{\text{LB}}\Psi = \frac{1}{\sqrt{g}} \partial_i (\sqrt{g} g^{ij} \partial_j \Psi), \quad (38)$$

where $g = \det(g_{ij})$ is the determinant of the spatial metric tensor g_{ij} , and the indices i, j correspond to the coordinates in the geometry, which in this case are r and ϕ . For the metric (2), the determinant of the spatial metric tensor g_{ij} is given by

$$g = \det(g_{ij}) = \frac{\alpha^2 r^2}{f(r)}. \quad (39)$$

In our case, we find

$$\Delta_{\text{LB}}\Psi = \frac{\sqrt{f(r)}}{r} \frac{\partial}{\partial r} \left(r \sqrt{f(r)} \frac{\partial}{\partial r} \right) + \frac{1}{\alpha^2 r^2} \frac{\partial^2}{\partial \phi^2}, \quad (40)$$

To proceed, we now express the Helmholtz equation in a form suitable for the specific geometry of the WH. According to the space-time (2), let us consider the wave function

$$\Psi = \exp(im\phi) \psi(r), \quad (41)$$

where m is the magnetic quantum number and $\psi(r)$ is the radial function.

Substituting Eq. (40) into Eq. (37) and using the wave function ansatz (41), we arrive at the following equation:

$$\frac{\sqrt{f(r)}}{r} \frac{\partial}{\partial r} \left(r \sqrt{f(r)} \frac{\partial \psi}{\partial r} \right) + \left(\omega^2 - \frac{m^2}{\alpha^2 r^2} \right) \psi(r) = 0. \quad (42)$$

Now, let us try to determine the effective potential acting on waves within the curved background. To do this, we remove the first-order derivative term appeared in the above differential equation. For that, we perform the following transformation:

$$\psi(r) = \frac{\chi(r)}{r^{1/2} f(r)^{1/4}}. \quad (43)$$

Substituting this transformation (43) into the Eq. (42) and after simplification results in the Schrödinger-like equation:

$$\chi''(r) + (\omega^2 - U(r)) \chi(r) = 0, \quad (44)$$

where

$$U(r) = \frac{f''(r)}{4f(r)} - \frac{3}{16} \left(\frac{f'(r)}{f(r)} \right)^2 + \frac{f'(r)}{4r f(r)} + \frac{m^2/\alpha^2 - 1/4}{r^2}. \quad (45)$$

Substituting function $f(r)$ and after simplification results the following expression for the effective potential governing the wave optics as,

$$U(r) = \frac{\mathcal{A}(r)}{\mathcal{D}(r)},$$

$$\mathcal{A}(r) = 2m^2 (4r^2 + \mathcal{Q}^2 \ell^4)^2 + (-8r^4 - 8\mathcal{Q}^2 r^2 \ell^4 + \mathcal{Q}^4 \ell^8) \alpha^2 + 2b_0^2 r^2 (16m^2 + \alpha^2) - 2b_0 r \{ 8m^2 (4r^2 + \mathcal{Q}^2 \ell^4) + (-8r^2 + \mathcal{Q}^2 \ell^4) \alpha^2 \},$$

$$\mathcal{D}(r) = 2r^2 (-4b_0 r + 4r^2 + \mathcal{Q}^2 \ell^4)^2 \alpha^2. \quad (46)$$

For the zero magnetic quantum number, $m = 0$, the effective potential reduces as,

$$U(r) = \frac{\mathcal{B}(r)}{\mathcal{D}(r)},$$

$$\mathcal{B}(r) = (-8r^4 - 8\mathcal{Q}^2 r^2 \ell^4 + \mathcal{Q}^4 \ell^8) \alpha^2 + 2b_0^2 r^2 \alpha^2 - 2b_0 r \alpha^2 (-8r^2 + \mathcal{Q}^2 \ell^4). \quad (47)$$

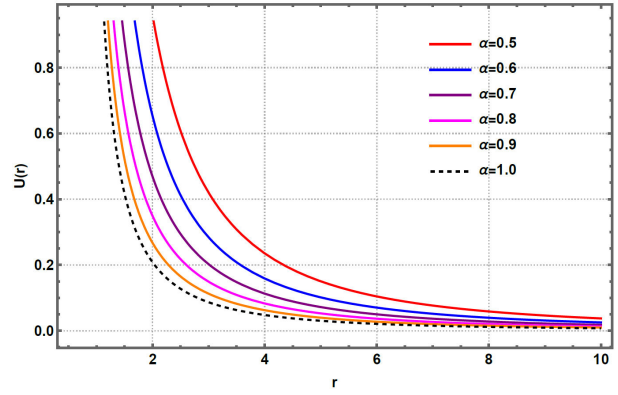


FIGURE 7. Graphical representation of the effective potential $U_{\text{eff}}(r)$ as a function of r for different values of the disclination parameter α . Here, we set $\ell = 1$, $\mathcal{Q} = 1$, $b_0 = 1$, $m = 1$.

The effective potential (46) plays a central role in understanding how wave propagation is influenced by the geometry of the WH. It depends on the radial coordinate r , the magnetic quantum number m , and several geometric parameters, including the throat size b_0 , the charge $\mathcal{Q}$, the curvature scale ℓ , and the disclination parameter α . Notably, the WH space-time induces a repulsive effective potential which acts as a barrier to incoming waves. The strength of this repulsive interaction decreases gradually as the radial distance r increases. As expected from the geometry, the potential diverges in the limit $r \rightarrow r_0$, reflecting the strongly repulsive nature near the WH throat for $m = 0$ or $m \neq 0$, and asymptotically vanishes as $r \rightarrow \infty$, indicating that spacetime becomes effectively locally flat at large distances.

Figure 7 illustrated the radial variation of the effective potential $U(r)$ for different values of the disclination parameter $\alpha = \{0.7, 0.8, 0.9, 1.0\}$. In this plot, the curvature radius is set to $\ell = 1$, the NS charge $\mathcal{Q} = 1$, the throat radius $b_0 = 1$, and the angular quantum number $m = 1$. As α decreases from unity (implying a stronger angular deficit), the effective potential increases, which physically corresponds to stronger scattering or trapping behavior for scalar waves. This provides us precise information about topological defects in modulating wave dynamics in the WH space-time.

Let us now derive the expression for the RI $n(r, \omega)$. In a spatially varying medium, the Helmholtz equation can be written as $\nabla^2 \varphi + k_{\text{eff}}^2(r) \varphi = 0$, where $k_{\text{eff}}(r)$ is the effective wave number that accounts for the influence of the medium on wave propagation. The RI $n(r)$ relates to this effective wave number by $k_{\text{eff}}(r) = (\omega/c)n(r)$. Substituting this relation into the Helmholtz equation yields $\nabla^2 \varphi + (\omega/c)^2 n^2(r) \varphi = 0$, which represents the general form of the wave equation in a medium with a spatially varying RI. Recognizing that the term $k^2 - U_{\text{eff}}(r)$ modifies the system's wave number, and comparing it with the wave equation in the RI medium, we identify $k_{\text{eff}}^2(r) = k^2 - U_{\text{eff}}(r)$. Using the relation $k = \omega/c = \omega$, we obtain $n^2(r) = 1 - [U_{\text{eff}}(r)/\omega^2]$. Therefore, the behavior of the effective potential $U_{\text{eff}}(r)$ directly influences the spatial profile of the RI, which is given by

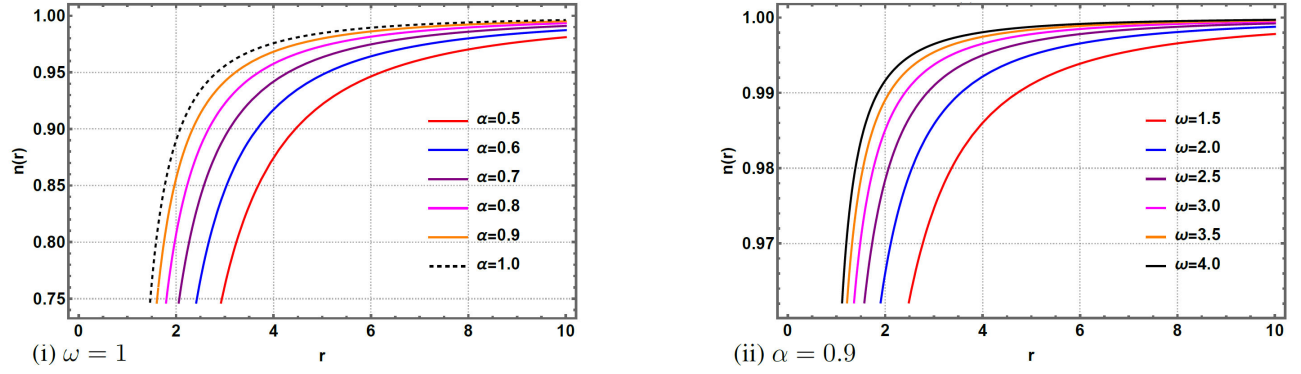


FIGURE 8. Graphical representation of the effective refractive index $n(r)$ as a function of r for different values of the disclination parameter α (left panel) and frequency ω (right panel). Here, we set $\ell = 1$, $\mathcal{Q} = 1$, $b_0 = 1$, $m = 1$.

$$n(r) = \sqrt{1 - \frac{\mathcal{A}(r)}{\omega^2 \mathcal{D}(r)}}. \quad (48)$$

For the zero magnetic quantum number, $m = 0$, the RI reduces as,

$$n(r) = \sqrt{1 - \frac{\mathcal{B}(r)}{\omega^2 \mathcal{D}(r)}}. \quad (49)$$

Figure 8 shows the behavior of the effective RI $n(r)$ as a function of the axial coordinate r , for different values of the disclination parameter α and the wave frequency ω . In the left panel, the frequency is fixed at $\omega = 1$, while in the right panel, the disclination parameter is fixed at $\alpha = 0.9$. Other parameters are held constant across both panels: the curvature radius $\ell = 1$, the NS charge $\mathcal{Q} = 1$, the throat radius $b_0 = 1$, and the angular quantum number $m = 1$. In the left panel, it is observed that as α approaches unity, the RI profile $n(r) < 1$ increases with r . In the right panel, the RI increases with rising wave frequency $\omega = \{1.5, 2.0, 2.5, 3.0\}$, for fixed $\alpha = 0.9$ again $n(r) < 1$. This illustrates a dispersive effect in the WH geometry: higher-frequency waves experience stronger refractive behavior and are more significantly influenced by the curvature and topological defects of the space-time.

A RI $n < 1$ implies that the phase velocity of light or waves in the medium exceeds the speed of light in vacuum, c . This property is characteristic of metamaterials—artificially engineered materials designed to exhibit unusual optical behaviors such as negative refraction, where light bends in the opposite direction compared to conventional materials. Metamaterials with $n < 1$ enable remarkable phenomena like superlensing, allowing imaging beyond the diffraction limit to achieve exceptionally high resolution. Importantly, although a RI below unity corresponds to superluminal phase velocities, this does not violate causality or special relativity, since the group velocity—which governs the actual transmission of information—remains limited by c .

4.1. Total reflection and scattering interpretation

The divergence of the effective potential $U(r)$ as $r \rightarrow r_0$ carries profound physical consequences for wave scattering. Near the throat, $f(r) \rightarrow 0$, and the dominant contribution to $U(r)$ arises from the terms proportional to $1/f(r)^2$ in the denominator of Eq. (46). This divergence creates an *infinite potential barrier* at the WH throat, which enforces total reflection of all incoming scalar wave modes, regardless of their frequency ω or angular quantum number m .

More precisely, defining the reflection coefficient $\mathcal{R}$ and transmission coefficient $\mathcal{T}$ for the Schrödinger-like problem (44), the infinite barrier height implies

$$|\mathcal{R}|^2 = 1, \quad |\mathcal{T}|^2 = 0, \quad (50)$$

for all modes. This result stands in sharp contrast to BH spacetimes, where the event horizon acts as a perfectly absorbing boundary ($|\mathcal{T}|^2 > 0$), giving rise to finite greybody factors. The BSCWH geometry thus provides a concrete example of a gravitational configuration that scatters waves elastically, with the throat functioning as a perfect mirror.

While no net absorption occurs, the scattered waves acquire frequency-dependent phase shifts $\delta_m(\omega)$ that encode the full structure of the effective potential. These phase shifts can in principle be extracted from the asymptotic behavior of the scattered wave:

$$\chi(r) \xrightarrow{r \rightarrow \infty} A e^{i\omega r} + B e^{-i\omega r},$$

with $\frac{B}{A} = e^{2i\delta_m(\omega)}.$ (51)

The phase shifts carry information about the WH throat geometry, the NS charge, and the disclination parameter, and could serve as observational discriminators between WH and BH spacetimes in the context of analogue gravity experiments.

The peak value $U_{\text{máx}}$ of the effective potential, attained at a radius $r_{\text{máx}}$ slightly above the throat, determines the characteristic frequency scale at which the transition from low-energy (strongly reflected) to high-energy (weakly perturbed) scattering occurs. In Table IV, we present $U_{\text{máx}}$ for various parameter combinations.

TABLE IV. Peak effective potential $U_{\text{máx}}$ and corresponding radius $r_{\text{máx}}$ for $b_0 = 1$, $\ell = 1$, and selected values of α , $\mathcal{Q}$, and m .

α	$\mathcal{Q}$	m	$r_{\text{máx}}$	$U_{\text{máx}}$
0.7	0.5	0	0.9830	112.5269
0.7	0.5	1	0.9830	114.6389
0.7	0.5	2	0.9830	120.9748
1.0	0.5	0	0.9830	112.5269
1.0	0.5	1	0.9830	113.5618
1.0	0.5	2	0.9830	116.6664
0.7	1.0	0	0.5500	247.1074
0.7	1.0	1	0.5500	253.8539
0.7	1.0	2	0.5500	274.0934
0.9	1.0	0	0.5500	247.1074
0.9	1.0	1	0.5500	251.1887
0.9	1.0	2	0.5500	263.4323
1.0	1.0	0	0.5500	247.1074
1.0	1.0	1	0.5500	250.4132
1.0	1.0	2	0.5500	260.3306

TABLE V. Effective RI $n(r)$ at selected radii for $b_0 = 1$, $\ell = 1$, $\mathcal{Q} = 1$, $m = 1$.

α	ω	$n(r=2)$	$n(r=3)$	$n(r=5)$	$n(r=10)$
0.7	1.5	0.889810	0.953983	0.983869	0.996008
0.7	2.0	0.939609	0.974383	0.990959	0.997756
0.7	3.0	0.973622	0.988697	0.995992	0.999003
0.8	1.5	0.919188	0.966283	0.988181	0.997074
0.8	2.0	0.955385	0.981177	0.993369	0.998355
0.8	3.0	0.980422	0.991678	0.997058	0.999269
0.9	1.5	0.938799	0.974627	0.991127	0.997805
0.9	2.0	0.966052	0.985808	0.995018	0.998766
0.9	3.0	0.985056	0.993718	0.997789	0.999452
1.0	1.5	0.952579	0.980552	0.993228	0.998327
1.0	2.0	0.973610	0.989107	0.996196	0.999059
1.0	3.0	0.988358	0.995174	0.998311	0.999582

As seen from the table, the potential peak increases sharply with $\mathcal{Q}$ (since larger charge shrinks the throat, concentrating curvature) and with m (reflecting the centrifugal barrier). Notably, for $m = 0$ the peak value $U_{\text{máx}}$ is *independent* of α , since the α^2 factors cancel identically in Eq. (47); the disclination affects only the m -dependent angular barrier contribution.

In Table V, we present numerical values of the effective RI at selected radial positions, quantifying the dispersive behavior.

The table confirms that $n(r) \rightarrow 1$ as $r \rightarrow \infty$ for all parameter combinations, and that the deviation from unity is most pronounced near the throat and for low frequencies, consis-

tent with the dispersive analogue-gravity interpretation.

5. Conclusions

This study examined the optical properties—both ray-like and wave-like—of a three-dimensional static charged BSCWH space-time incorporating topological disclinations. The objective was to understand how non-trivial geometric and topological features influenced the photon trajectories and scalar waves. The WH geometry was defined via a specific shape function $b(r)$, and the space-time incorporated a NS charge $\mathcal{Q}$ from string theory, along with a disclination parameter α that accounted for angular deficits due to topological defects. These components led to a non-asymptotically flat space-time exhibiting rich and complex optical behavior. The analysis of ray optics began with the study of NG motion. It was shown that both the disclination parameter α and the NS charge $\mathcal{Q}$ including the WH parameter b_0 significantly affected photon trajectories. The derived orbital equations and impact parameter relations, along with analytical expressions for the radial and angular evolution of light paths, show that photons experienced modified bending and shifting of trajectories, depending on the WH parameter b_0 , the curvature scale ℓ , and the disclination parameter α .

A key finding in the ray-optics sector is the identification of the critical impact parameter $\beta_c = r_0$, which delineates scattered from traversing photon trajectories. We demonstrated that the trivial redshift function ($\Phi = 0$) inherent to the BSCWH geometry precludes the existence of a photon sphere, in contrast to standard BH spacetimes. This absence is a direct consequence of the metric structure and provides a potential observational signature for distinguishing BSCWH geometries from BH spacetimes. Furthermore, we derived the closed-form weak-field deflection angle (Eq. 36), which transparently separates the topological contribution $\pi(1 - \alpha)/\alpha$ from the gravitational bending $b_0/(\alpha\beta)$ and the NS charge correction. This analytical result complements the exact elliptic integral expression and facilitates direct comparison with cosmic string lensing phenomenology [84].

The study then extended to wave optics by formulating the scalar Helmholtz equation in the curved space background and transforming it into a Schrödinger-like equation. This transformation allowed the identification of an effective potential $U(r)$, which depended on the disclination parameter, NS charge, and WH geometry. The resulting potential profiles showed that a decrease in α —indicating stronger topological defects—led to more localized and pronounced potentials. This suggested that disclinations enhanced wave localization and interference effects for scalar waves. Crucially, the divergence of $U(r)$ at the WH throat ($r \rightarrow r_0$) was shown to enforce total reflection of all scalar wave modes ($|\mathcal{R}|^2 = 1$), providing a clear wave-optics discriminator between WH and BH spacetimes: whereas BH horizons absorb incoming radiation (yielding finite greybody factors), the BSCWH throat acts as a perfect mirror, producing only frequency-dependent phase shifts (Table IV). In addi-

tion, we derived a frequency- and position-dependent effective RI $n(r)$ from the effective wave number $k_{\text{eff}}(r)$. The RI was found to depend not only on the radial coordinate r , but also on the wave frequency ω , the angular quantum number m , the curvature radius ℓ , the NS charge Q , and the WH parameter b_0 . This indicated a dispersive optical medium, wherein higher-frequency waves experienced stronger refractive effects, analogous to GL and optical phenomena in analogue gravity systems. Graphical analysis (see Figs. 7 to 8) and numerical tabulation (Tables V and IV) illustrated the behavior of the effective potential and RI under variations in α and ω , further confirming the influence of curvature and topological structure on wave propagation.

In summary, this investigation demonstrated the deep connection between spacetime geometry and the behavior of light in both classical and quantum regimes. It showed that topological features such as disclinations were not merely mathematical abstractions, but had measurable effects on wave and photon dynamics. These findings provided new insights into WH physics in lower-dimensional space-times and suggested potential applications in the design of analogue gravity systems and metamaterials, where engineered geometries could emulate such curved-space phenomena. In particular, the $n < 1$ RI profiles derived here share the characteristic features of metamaterial platforms studied in Refs. [69,70], while the disclination-induced lensing connects naturally to phonon transport in topological defect channels [68].

A natural direction for future work would be to extend the present analysis by considering more general classes of charged and rotating BSCWH geometries with topological defects, where the inclusion of angular momentum and higher-order curvature ($\mathcal{D}$) corrections could reveal richer optical behaviors. Also, test the influence of additional string-inspired fields, such as dilaton or Kalb-Ramond (KR) models, on photon trajectories and wave scattering, thereby connecting the optical properties of WHs with string theory frameworks. In this context, testing different types of perturbations, including electromagnetic and gravitational modes, could provide a broader illustration of how curvature (topological defect parameters) and disclinations affect wave propagation. Also, one could test the influence of the effective RI in GL models, especially its implications for distinguishing WH geometries from BH spacetimes. In this context, possible applications in analogue gravity platforms, such as metamaterials or optical lattices, may offer experimental realizations of the results, enabling the study of WH-inspired optics in controlled laboratory environments. Additionally, extending the wave-optics analysis to include quasinormal mode (QNM) calculations [17], electromagnetic perturbations, and the extraction of scattering phase shifts from the effective potential would provide a complete characterization of the BSCWH spectral fingerprint. The connection to holographic optics [90] and the recent developments in ray geodesics on curved surfaces [79] also merit further investigation.

Notes: Evaluation of the integral

We start with the integral

$$\Delta\phi = \int_{u_0}^{\infty} \frac{du}{\sqrt{(1 - b_0 u + \frac{Q^2 \ell^4}{4} u^2)(1 - \beta^2 u^2)}}.$$

Define the quadratic polynomials

$$P(u) = 1 - b_0 u + \frac{Q^2 \ell^4}{4} u^2,$$

and

$$Q(u) = 1 - \beta^2 u^2.$$

The integral becomes

$$\Delta\phi = \int_{u_0}^{\infty} \frac{du}{\sqrt{P(u)Q(u)}}.$$

$$u_0 = \frac{2}{b_0 + \sqrt{b_0^2 - Q^2 \ell^4}},$$

The polynomial $P(u)$ is quadratic in u . Its roots are

$$\xi_{1,2} = \frac{b_0 \pm \sqrt{b_0^2 - Q^2 \ell^4}}{\frac{1}{2} Q^2 \ell^4}.$$

We rewrite

$$P(u) = \frac{Q^2 \ell^4}{4} (u - \xi_1)(u - \xi_2).$$

To bring the integral into a standard elliptic form, perform the substitution

$$u = \frac{1}{\beta} \sin \theta,$$

Computing du ,

$$du = \frac{1}{\beta} \cos \theta d\theta.$$

The integrand denominator becomes

$$\begin{aligned} \sqrt{P(u)Q(u)} &= \sqrt{P\left(\frac{\sin \theta}{\beta}\right) \left(1 - \beta^2 \frac{\sin^2 \theta}{\beta^2}\right)} \\ &= \sqrt{P\left(\frac{\sin \theta}{\beta}\right)} \cos \theta. \end{aligned}$$

Thus the integral is

$$\int \frac{\frac{1}{\beta} \cos \theta d\theta}{\cos \theta \sqrt{P\left(\frac{\sin \theta}{\beta}\right)}} = \frac{1}{\beta} \int \frac{d\theta}{\sqrt{P\left(\frac{\sin \theta}{\beta}\right)}}.$$

Substitute,

$$P\left(\frac{\sin \theta}{\beta}\right) = 1 - \frac{b_0}{\beta} \sin \theta + \frac{Q^2 \ell^4}{4\beta^2} \sin^2 \theta.$$

Denote

$$A = 1, \quad B = -\frac{b_0}{\beta}, \quad C = \frac{Q^2 \ell^4}{4\beta^2}.$$

So,

$$\begin{aligned} P\left(\frac{\sin \theta}{\beta}\right) &= A + B \sin \theta + C \sin^2 \theta \\ &= C(\sin \theta - \beta \xi_1)(\sin \theta - \beta \xi_2). \end{aligned}$$

Rewrite the integral as

$$\begin{aligned} I &= \int \frac{d\theta}{\sqrt{A + B \sin \theta + C \sin^2 \theta}} \\ &= \int \frac{d\theta}{\sqrt{C(\sin \theta - \beta \xi_1)(\sin \theta - \beta \xi_2)}}. \end{aligned}$$

This integral can be transformed into standard elliptic integrals by completing the square or using substitution.

The integral becomes

$$\Delta\phi = \frac{1}{\sqrt{-\beta^2 + \frac{Q^2 \ell^4}{4}}} [K(k) - F(\phi_0, k)],$$

where $K(k) = F(\pi/2, k)$ is the complete elliptic integral of the first kind, and $F(\phi_0, k)$ is the incomplete elliptic integral of the first kind.

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Data availability statement

No data associated in the manuscript.

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A brief study concerning thermal transport properties of B-C-N monolayers and graphene/X nanoribbon heterojunctions: Influences of carbon concentration and mean temperature

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A wide variety of two-dimensional (2D) materials provides an optional route for manipulating heat fluxes at the nanoscale. Nowadays, 2D carbon-based materials have received important attention due to their adjustable transport properties by a controlled tuning of composition, junction, geometry, etc. In the present paper, we address the thermal transport properties of the B-C-N (Boron-Carbon-Nitride) monolayers and graphene/X (X=hBN, hSiC, and graphane) nanoribbon heterojunctions by performing non-equilibrium molecular dynamics simulations. Our results show that the carbon concentration modifies the thermal conductivity of B-C-N monolayers at a mean temperature of 300 K, producing values of 29.47, 28.94, and 16.58 W/m-K for concentrations of 90, 10, and 50 %, respectively. Nevertheless, no major effect of carbon concentration on the temperature profile of B-C-N monolayers is observed. On the other hand, the mean temperature influences the interface thermal resistance and thermal conductivity of coplanar graphene/X nanoribbon heterojunctions, these variations are observed for the forward direction of the heat flux, modulating the temperature drop at the interface. Besides, graphene/hBN and graphene/graphane heterojunctions show a pronounced thermal rectification at a mean temperature below 300 K, compared to graphene/hSiC heterojunction. In which the heat fluxes present an asymmetry in the $j - \Delta$ curve, highlighting that the heat flux in the backward direction preferentially flows from X (hBN and graphane) to graphene nanoribbons.

Keywords: B-C-N monolayers; graphene-based nanoribbon heterojunctions; thermal transport properties; NEMD simulations.

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1. Introduction

Since the discovery of graphene (2004), the family of two-dimensional (2D) honeycomb lattice materials has expanded rapidly. As a result several 2D materials have been fabricated and extensively studied, such as hexagonal boron nitride (hBN) [1], transition metal dichalcogenides (MoS₂ and WS₂) [2], transition metal carbides and nitrides (MXenes) [3], and a few others [4,5]. The significance of 2D materials is associated with their relevant and novel physicochemical properties that depend mainly on their structure, size, chirality, and composition. These aspects make them useful for the development of new technologies such as thermal-electronic devices, sensors, and energy storage, among other applications [1-5], unlike the zero band gap (Dirac cone) of graphene.

In order to address the next-generation thermal-management materials, it is important to explore novel 2D materials that are candidates to solve certain limitations of current technology. As is well known, the hBN and graphene are similar and comparable systems in some aspects (there are also many differences), *i.e.*, mechanical properties, thermal response, covalent bonds with sp^2 hybridization, low mass density, etc [6,7]. Currently, hexagonal boron carbon nitrides (hBCNs) are a new group of 2D structures consist-

ing mainly of complex materials including B-C, C-N, B-N, and C-C bonds [6,8,9]. The stoichiometry-dependent properties of hBCNs, as well as the difficult-to-control domain distribution (between B, N, and C atoms), create challenges for device fabrication with efficient and reproducible performance [10-12]. In addition, by exploring the B-C-N ternary phase diagram, it is possible to indicate stable phases, where some physical properties of different monolayers such as BCN, BC₂N, and BC₄N are being determined [6,13,14]. Likewise, these structures are being applied in a wide range of fields, including supercapacitors and lithium-ion batteries to electrocatalysts and sensors [6,15]. Therefore, constant monitoring of the chemical proportions in hBCNs is a challenge in relation to the final composition that can deviate from B/C/N=1:1:1 [8].

In the same line of research, other 2D material heterojunctions, such as thermal diodes, are promising candidates for future cooling technologies. The main application of heat sinks, as a type of thermal interface material, is passive cooling, which is particularly attractive when the size of the electronic device to be cooled is taken into account. In addition, this type of cooling is economical and does not require maintenance or consume additional energy [7]. In fact, the graphene-based heterojunctions consist of graphene and other 2D materials in vertical and horizontal coupling;

this additional diversity can enhance the thermal transport properties. For example, several 2D heterojunctions, such as graphene/ hBN [16-19], silicene [20,21], MoS₂ [16,22], graphane [23,24], and black phosphorene [25], have been studied in both simulation and experimental works. Besides, over the last two decades, emerging 2D materials have been explored to manipulate interfacial thermal conductance, thermal conductivity, and thermal rectification ratio [7,26,27].

In this article, we report the thermal transport properties of B-C-N monolayers and coplanar graphene/X (X=hBN, hSiC, and graphane) nanoribbon heterojunctions under the influence of carbon concentration and the effect of mean temperature. We have performed non-equilibrium molecular dynamics simulations for this study. In the next section, we describe simulation details and methods, and then proceed to discuss the results, which are divided into two subsections. Finally, in the last section, our conclusions are summarized.

2. Computational details and methodology

The simulations were carried out using the non-equilibrium molecular dynamics (NEMD) method implemented in the LAMMPS code [28]. The standard velocity Verlet algorithm was used to integrate Newton's equations of motion, and the molecular dynamic time step was set to 0.1 fs. Before the NEMD simulations, all investigated systems were initially relaxed using the conjugate method to optimize the structures (relaxation time equal to 0.1 ps). Then, for each mean temperature, T_0 , the equilibration runs for 5 ns considering an NVT ensemble (canonical ensemble) with a Nosé-Hoover thermostat. Once the temperature reached the required value, the thermostat was removed, and the NEMD simulations were carried out for 20 ns. Furthermore, the temperatures for left and right heat baths were defined as $T_L = (1 + \Delta)T_0$ and $T_R = (1 - \Delta)T_0$ (see Fig. 1), where heat flux flows left-to-right for the forward direction and right-to-left for the backward direction. Also, we considered a temperature bias of $\Gamma = |T_L - T_R| = 2\Delta T_0$ (Δ parameter varies from 0.01 to 0.5). Additionally, to avoid spurious effects associated with the specific choice of velocities (related to temperature), an average of five random choices of the initial velocity distribution was additionally performed.

As a matter of fact, the computational details mentioned are valid for the two graphitic systems studied: B-C-N monolayers and coplanar graphene/X (X=hBN, hSiC, and graphane) nanoribbon heterojunctions. It is worth mentioning that hSiC is a 2D silicon carbide with a hexagonal and planar structure [29]. On the one hand, the interactions among B, C, and N atoms for B-C-N monolayers were simulated by using an optimized Tersoff force field parametrized by Kinaci *et al.* [30], which has been widely used for the investigation of the physical properties of various BCN nanomaterials [17,19,31]. On the other hand, we have used three force fields for graphene/X nanoribbon heterojunctions as follows: X=hBN (hexagonal boron nitride), X=hSiC (siligraphene 1:1), and X=graphane (hydrogenated graphene)

were simulated using the optimized Tersoff potential by Kinaci *et al.* [30], the many-body potential proposed by Tersoff [32], and the adaptive intermolecular reactive bond order (AI-REBO) potential provided by Stuart *et al.* [33], respectively.

In order to quantify the thermal transport properties, the temperature profile was first computed by dividing the graphitic system into a certain number of slabs and using the relation [18,34]:

$$T_i = \frac{1}{3N_i k_B} \sum_{a=1}^{N_i} \langle m_a v_a^2 \rangle, \quad (1)$$

where N_i is the number of atoms in the i -th slab, and m_a and v_a correspond to the mass and velocity of atom- a . Moreover, the calculated temperature for each slab (T_i) was averaged over a time interval to obtain a smooth temperature profile. The next quantity calculated was the thermal conductivity, κ , which is the heat conduction ability along graphitic systems and for graphene/X heterojunctions can be calculated by a mixture rule-based expression, which has been successfully used to study hybrid monolayers [20]:

$$\kappa^{-1} = \frac{1}{2}\kappa_g^{-1} + \frac{1}{2}\kappa_X^{-1} + \frac{1}{L}G^{-1}, \quad (2)$$

where κ_g and κ_X are the thermal conductivities of graphene and X nanoribbons, respectively. The $\kappa_X = jL/A|T_L - T_R|$ (valid for B-C-N monolayers) comes from Fourier's law of heat conduction. The G is the thermal conductance, $G = R_K^{-1}$, which comes from calculating the interface thermal resistance (called Kapitza resistance) between graphene and X nanoribbons at the interface, $R_K = A\Delta T/j$. In addition, $A = W \times h$ ($h = 0.33$ nm) is the cross-sectional area that the heat flux passes through, and ΔT is the temperature drop across the interface.

Another important phenomenon is the thermal rectification, η , which appears when the heat flux is different in the reverse direction [17,19,26,35]. Therefore, the thermal rectification is defined as $\eta(\%) = |(j_+/j_-) - 1| \times 100$, where the heat fluxes $j_{+,-}$ indicate whether the graphene/X nanoribbon heterojunction is operated in the forward or backward direction. The $j_{+,-}$ induced by the temperature bias Γ are computed as $j_{+,-} = (\partial E_L^{+,-}/\partial t + \partial E_R^{+,-}/\partial t)/2$, where $E_L^{+,-}$ and $E_R^{+,-}$ are the total energies that have been added to/subtracted from the atoms in the hot/cold regions for temperature control, respectively.

3. Results and discussion

3.1. B-C-N monolayers: Influences of carbon concentration and mean temperature

We first analyzed the thermal transport properties of B-C-N monolayers using average quantities such as thermal conductivity and temperature profile, where we only focused on the forward direction of heat flux. Following the experimental

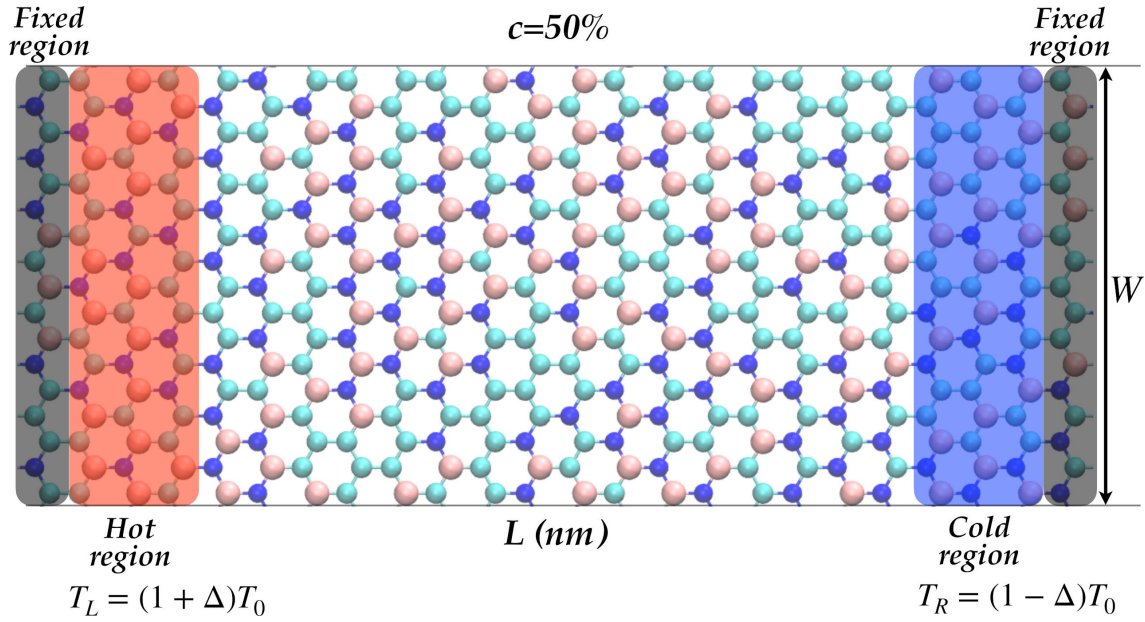


FIGURE 1. Schematic representation of thermal transport setup for B-C-N monolayer at 50 % of carbon concentration. For all concentrations, the dimensions are $L \approx 13 \text{ nm}$, $W \approx 7,3 \text{ nm}$, and the hot or cold region $\approx 3,3 \text{ nm}$. The pink, cyan, and blue balls correspond to the B, C, and N atoms, respectively.

study on h-BCN by Beniwal *et al.* [8] and theoretical works by Zhang *et al.* [31,36], we have considered a model based on a random carbon substitution in h-BN as an alternative proposal for a different atomic ratio of B/C/N. The carbon concentration was defined as $c = (N_C/N)100\%$, where N_C is the number of carbon atoms, and N is the total number of atoms, maintaining the same number of B and N atoms. For example, the atomic ratio with the concentration of 50 % is B/C/N=1:2:1. In Fig. 1, the illustrative model for NEMD of thermal transport at $c = 50\%$ is shown. We have fixed the ends in the X-direction (fixed region) to avoid global rotations of the system during the simulation. Also, we have considered periodic boundary conditions on the XY plane for all carbon concentrations of B-C-N monolayers.

The thermal conductivity of B-C-N monolayers as a function of carbon concentration is shown in Fig. 2a). The thermal conductivities present large values of 28.94 and 29.47 W/m-K for concentrations of 10 % and 90 %, respectively, and a small value of 16.58 W/m-K for the concentration around 50 %. The κ values are similar to h-BCN systems close in the atomic ratio [36], these values are very small compared to the pristine graphene and hBN systems. Meanwhile, the experimental thermal conductivity of the BCN nanosheets exhibited a relatively low value (0.58-1.86 W/mK) [10]; however, aligned carbon doping in hBCN thin films can improve heat transport ($836 \pm 312 \text{ W/mK}$) [37]. In our work it is clearly observed that the values of κ depend strongly on the heat flux [see inset of Fig. 2a)] that manages to pass through the monolayer with a certain carbon concentration. In the meantime, we can observe in Fig. 2b) that the temperature profile for the forward direction gradually decreases along the B-C-N monolayers (L). This decrease in temperature th-

roughout the transport device occurs for different carbon concentrations corresponding to a thermal bath of $T_L = 330 \text{ K}$ (the first three points on the left) and $T_R = 270 \text{ K}$ (the last three points on the right) with a temperature bias of $\Gamma = 60 \text{ K}$. The relationships between T and L are practically linear and quasi-independent of the carbon concentration. Furthermore, this trend is observed for other high values of mean temperature (data not shown), which suggests that these B-N-C monolayers can be used as thermal devices that operate at high temperatures without losing their sensitivity.

Likewise, the influence of mean temperature on the thermal conductivities and temperature profiles of B-C-N monolayers for a temperature bias of $0,2 \times T_0$ is shown in Fig. 3. The κ values of the three concentrations increase as the T_0 increases, the gradual increase being monotonic for any concentration, resulting in values of 23.89, 18.08, and 24.70 W/m-K at 700 K for 20, 50, and 80 %, respectively [see Fig. 3a)]. This marked dependence is mainly due to the significant increase in the heat flux provided by the thermal bath throughout the monolayer (see the inset box). For example, for $T_0 = 200, 400$, and 600 K , we have the temperature bias of 40, 80, and 120 K, respectively. Indeed, the value of heat fluxes is due to the majority or minority contribution of the B, N, and C atoms in the monolayer. However, for the 50 % concentration, it is observed that the values of κ are always lower than the rest of the concentrations (20 % and 80 %). This characteristic is consistent with the κ in graph Fig. 2a) for $c=50\%$. Consequently, in Fig. 3b), no significant influence of the T_0 on the temperature profile for the forward direction is observed, *i.e.*, all $T(K)$ show practically a linear and decreasing dependence along the B-C-N monolayer (L)

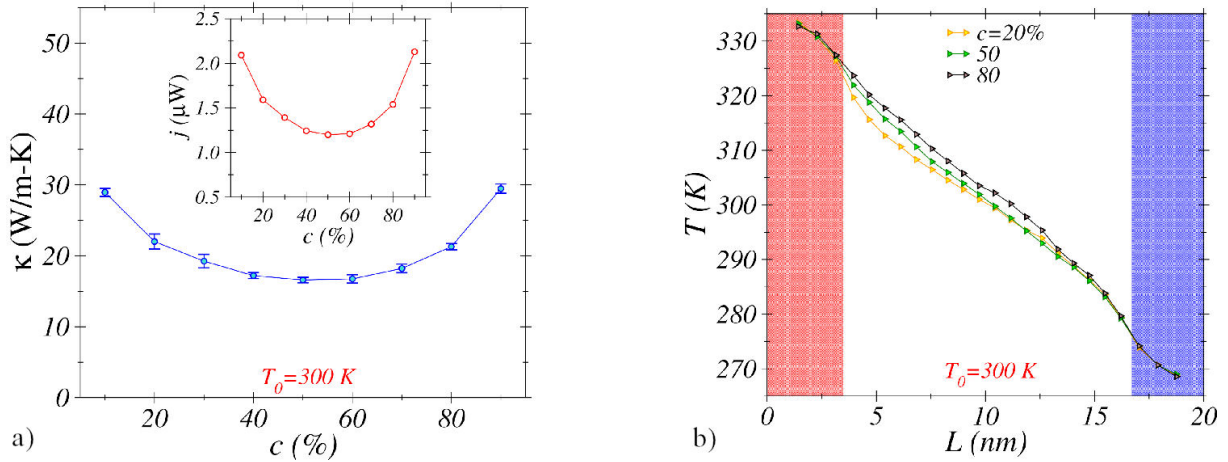


FIGURE 2. a) The thermal conductivity and the heat flux (inset box) of the B-C-N monolayer as a function of carbon concentration. b) Temperature profiles concerning the length of the system for carbon concentrations of 20 %, 50 %, and 80 %. Both graphs at a mean temperature of 300 K and for $\Delta = 0,1$.

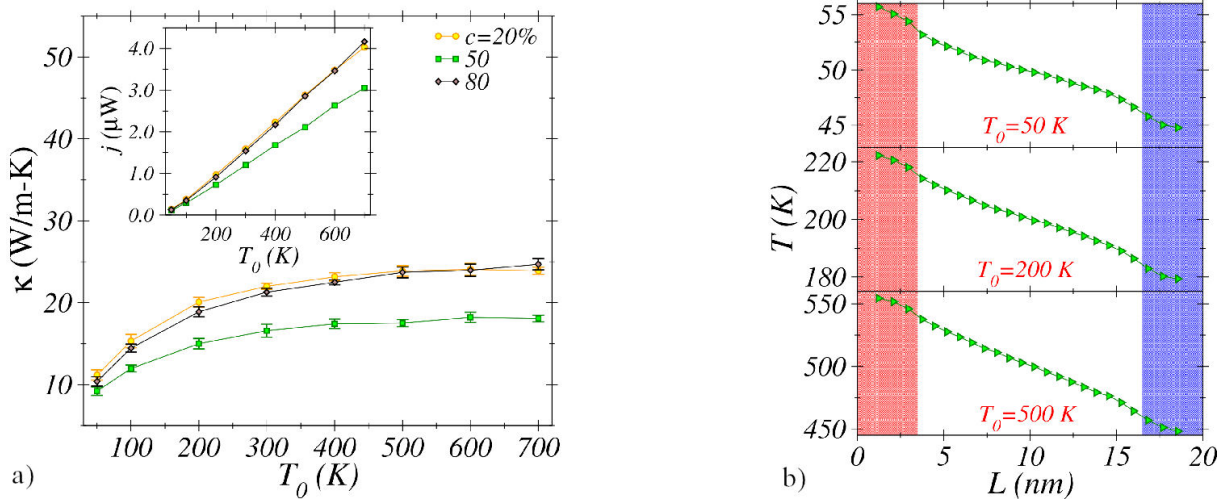


FIGURE 3. a) Thermal conductivities and heat fluxes (inset box) versus mean temperature of the B-C-N monolayers for carbon concentrations of 20 %, 50 %, and 80 %. b) Temperature profiles concerning the length of the system for three values of the mean temperature at 50 % of carbon concentration and for $\Delta = 0,1$.

for a fixed carbon concentration. This thermal response of the B-C-N monolayers is independent of the temperature bias of 10, 40, and 100 K, at $T_0 = 50$, 200, and 500 K, respectively.

3.2. Graphene/X nanoribbon heterojunctions: Effect of mean temperature

In this subsection, we proceed to study the dependence of mean temperature on the thermal transport properties of coplanar graphene/X ($X = \text{hBN}$, hSiC , and graphene) nanoribbon heterojunctions using the average quantities such as thermal conductivity, temperature profile, interface thermal resistance, thermal rectification, and $j - \Delta$ curve (corresponding to the $I - V$ curve for an electric rectifier). The setups of the thermal transport of graphene/X heterojunctions are shown in Fig. 4, where fixed regions, thermal baths, and the zig-zag interface are observed. At the interface, C-N, C-C, and

C-C bonds are formed for $X = \text{hBN}$, hSiC , and the graphene, respectively. After structural relaxation, the average bond lengths were 1.45 (B-N), 1.78 (Si-C), and 1.1 (C-H) Å, which are different from the bond length of graphene 1.42 Å. All simulations for free-standing heterojunctions have been done with free boundary conditions in all directions.

Once the graphene/X heterojunction reaches a thermal steady state, a heat flux is imposed along the entire device length ($L_G + L_X$), and the temperature profile is computed. Figure 5a) shows the temperature profile along the graphene to X nanoribbons (forward direction, j_+) at a mean temperature of 300 K and a temperature bias of 60 K. It is worth mentioning that in the NEMD simulation, the total energies of hot and cold regions are changing continuously, thus these regions are excluded from the thermal quantities calculations. The temperature variations in graphene/X hetero-

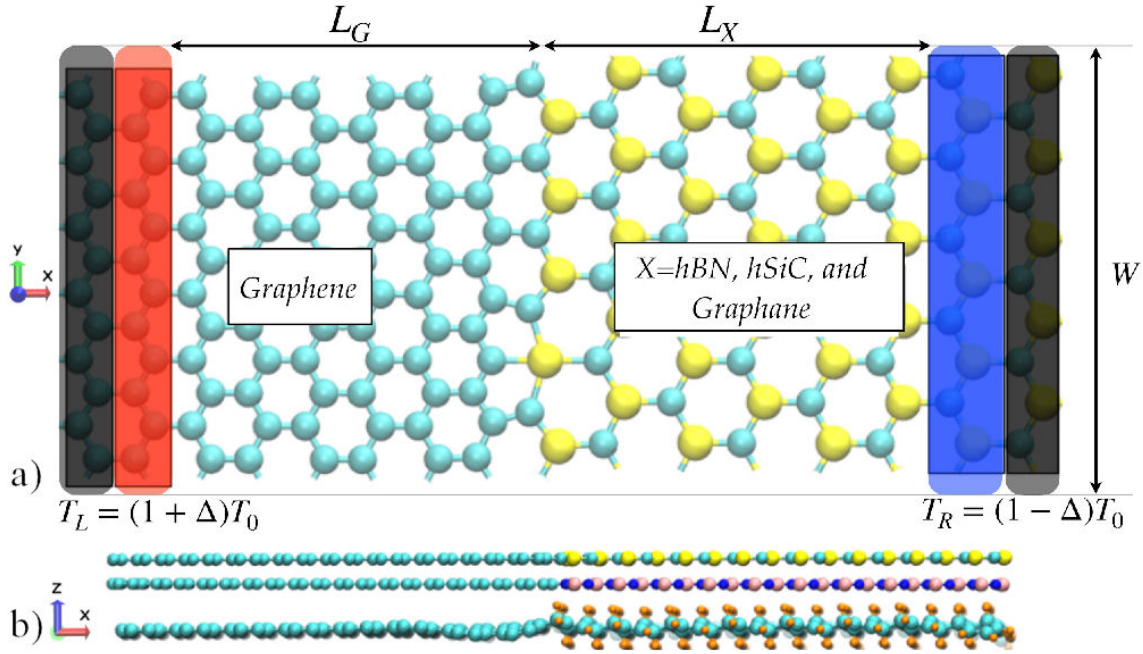


FIGURE 4. a) Schematic representation of thermal transport setup for the coplanar graphene/hSiC nanoribbon heterojunction from a top view. b) Atomic configuration of coplanar graphene/X ($X=\text{hSiC}$, hBN , and graphane) nanoribbon heterojunctions from a frontal view. For all heterojunctions, the dimensions are $L_G + L_X \approx 6$ nm, $W \approx 4.5$ nm, and the hot or cold region ≈ 1.5 nm. The cyan, yellow, pink, blue, and orange balls correspond to the C, Si, B, N, and H atoms, respectively.

junctions and the temperature drops at the interface are observed in these temperature profiles. This temperature drop (ΔT) is used to calculate the thermal resistance, indicating that the interface plays a crucial role in controlling or enhancing thermal transport in different heterojunctions. The noticeable change in temperature drop at the heat bath-device interface is $\Delta T \sim 24$ K (for $X=\text{hBN}$) compared to $\Delta T \sim 16$ K (for hSiC) or $\Delta T \sim 12$ K (for graphane).

For the forward direction, the interface thermal resistance, R_K , is reduced according to the mean temperature increase independently of material heterojunction [see Fig. 5b)]. To our knowledge, the R_K is usually lower as the temperature is higher [16,18]. Moreover, this decrease in the R_K values is directly associated with a small ΔT and big heat flux from the graphene to the other nanoribbon, *i.e.*, as the mean temperature increases, the heat flux passes through the device with a lower opposition at the interface. Various experimental techniques were used to measure the thermal contact resistance in different graphene-based nanomaterials; the works report higher orders of R_K [27,38]. Interestingly, our results are in contrast to those found for thermal conductivities, which gradually increase as a function of the mean temperature, reaching a maximum value of 106 W/m-K at 700 K for the graphene/hBN heterojunction compared to graphene/graphane heterojunction (61 W/m-K).

For the sake of clarity, we now focus on the forward and backward directions of the heat flux (j_+ and j_-) to analyze the thermal rectification, η . As seen in Fig. 6a), the η (%) displays a non-monotonous dependence with respect to the mean temperature, where for high T_0 a minimum at the cross-

ing point of the forward and backward heat fluxes is observed. The η can reach values up to $\sim 86\%$, 67% , and 27% when the mean temperature is 50 K for $X=\text{hBN}$, graphane , and hSiC , respectively. Furthermore, the gradual decrease of η is mainly because the forward and backward heat fluxes are similar. For the graphene/hBN heterojunction, the value $j_+ \equiv j_-$ is at temperatures greater than 400 K [see inset of Fig. 6a)]. The heat flux in the backward direction from hBN towards graphene nanoribbon heterojunction is always greater than in the forward direction ($j_- > j_+$), in which an asymmetry in the heat flux is predicted; the results for thermal rectification and heat flux are in agreement with previously published theoretical and experimental work [17,26,39].

In order to test the prediction above, we present the heat flux versus the Δ parameter at room temperature in Fig. 6b). In general, the relationship between j and Δ is indeed asymmetric with respect to $\Delta = 0$ for two graphene/X heterojunctions. We first analyze the graphene/hBN heterojunction, when $\Delta < 0$, the heat flux ($j_{\text{hBN} \rightarrow \text{G}}$) increases rapidly with Δ , meanwhile for $\Delta > 0$, the heat flux ($j_{\text{G} \rightarrow \text{hBN}}$) is much smaller and presents a negative differential thermal resistance (NDTR) at $\Delta = 0.5$, akin to that of other studies [17,40]. This effect on negative differential resistance was also observed in CNTs connected with BNNTs at high bias voltages [41]. Likewise, the graphene/graphane heterojunction also presents an asymmetry with respect to $\Delta = 0$, *i.e.*, the heat flux is greater/lesser for $\Delta < 0/\Delta > 0$. Obviously, this phenomenology is not clearly observed for the graphene/hSiC heterojunction. Therefore, the heat fluxes preferentially flow

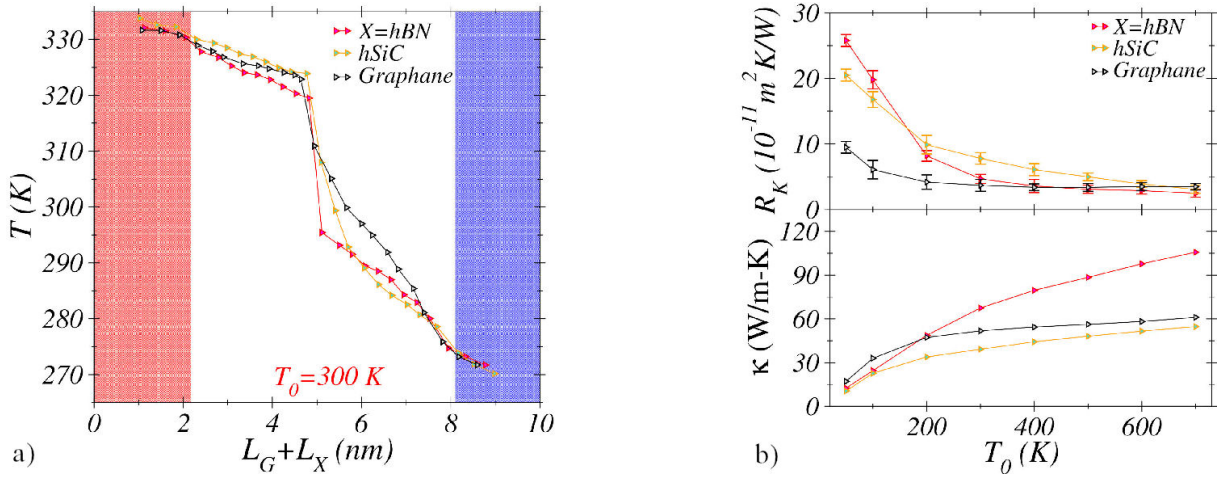


FIGURE 5. a) Temperature profiles concerning the device length for coplanar graphene/X nanoribbon heterojunctions. b) Interface thermal resistances and thermal conductivities as a function of the mean temperature of graphene/X nanoribbon heterojunctions. Both graphs are for the forward direction of the heat flux and $\Delta = 0.1$.

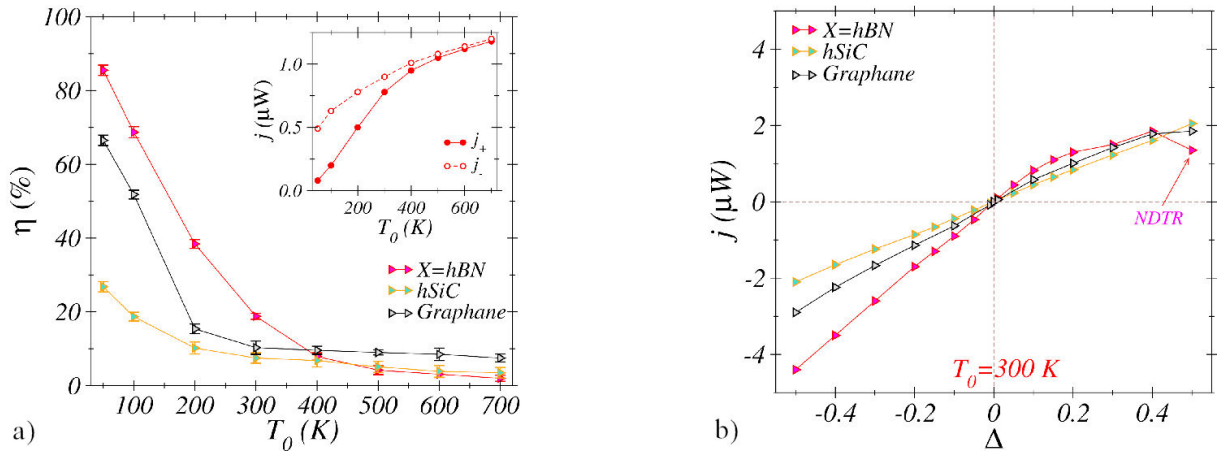


FIGURE 6. a) Thermal rectifications as a function of the mean temperature for graphene/X nanoribbon heterojunctions. Inset: heat fluxes in the forward and backward directions only for graphene/hBN heterojunction. b) The $j - \Delta$ curve (heat fluxes versus Δ parameter) for graphene/X nanoribbon heterojunctions at the mean temperature of 300 K.

from the X (hBN and graphane) to the graphene domain, which demonstrates a pronounced thermal rectification effect in these coplanar nanoribbon heterojunctions.

4. Conclusions

In this study, the influences of carbon concentration and mean temperature of B-C-N monolayers and coplanar graphene/X (X=hBN, hSiC, and graphane) nanoribbon heterojunctions were achieved by the use of molecular dynamics simulations. On the one hand, we have concluded that the carbon concentration modifies the thermal conductivity of B-C-N monolayers, generating various values at a mean temperature of 300 K, such as 29.47, 28.94, and 16.58 W/m-K for carbon concentrations of 90, 10, and 50 %, respectively. Otherwise, no major effect of the carbon concentration on the temperature profile of B-C-N monolayers is observed. Likewise, when considering the increase in mean temperature, the thermal conductivity increases similarly for any concentra-

tion (except to a lesser extent for the 50 %).

On the other hand, we also observed that the mean temperature influences the transport properties of coplanar graphene/X nanoribbon heterojunctions, namely, the interface thermal resistance decreases, and the thermal conductivity increases as the mean temperature increases for the forward direction of the heat flux. These variations were mainly due to the fact that the temperature drop (ΔT) observed in the temperature profile decreases, and the heat flux increases for increasingly larger thermal baths. Furthermore, the thermal rectification shows that graphene/hBN and graphene/graphane heterojunctions are good rectifiers at mean temperatures below 300 K, compared to graphene/hSiC heterojunction, because the rectification decreases as the mean temperature increases ($T_0 > 300$). This fact of pronounced rectification was corroborated in the $j - \Delta$ curve, in which there is an asymmetry in the heat flux with respect to $\Delta = 0$ for these two heterojunctions, indicating that the heat flux preferentially flows from X (hBN and graphane) to graphene nanoribbons in he-

terojunctions.

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Conflicts of interest

The authors declare that they have no conflicts of interest.

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Hot-rolled Zn₂₂Al₂Cu-NaCl composite with initial fine-grained and cast-metal matrix microstructures

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A composite of a Zn₂₂Al₂Cu matrix and NaCl particles was developed to establish whether this material could be hot-rolled and, if feasible, to determine the structural changes according to the initial matrix microstructure and percent section reduction achieved with this process. The composite was made by melting the alloy, adding the particles, molding, compressing the mixture of metal and particles, and air cooling, with an approximate (mass of particles)/(mass of alloy) ratio equal to 0.6. Plates of the composite with the initial cast-metal matrix microstructure and with a heat-treated initial fine-grained matrix microstructure were hot-rolled in two stages to approximately 80 % section reduction at 230°C. Plate samples that were not rolled, plates hot-rolled to approximately 50 % section reduction and plates hot-rolled to the maximum percent reduction were mirror-polished, and the matrix and NaCl-particle interfaces were analyzed and imaged with a scanning electron microscope. Vickers microhardness was measured in the matrix and in NaCl particles, and Rockwell hardness F of the nonrolled and hot-rolled composites was determined. The cast-metal matrix microstructure acquired shape texture without recrystallization, while the fine-grained matrix microstructure recrystallized with increasing rolling %. The NaCl particles deformed together with the matrix and hardened, with the hardening speed being greater when the matrix was fine-grained. The composite could be hot-rolled with either microstructure, with the cast-metal matrix microstructure being more favorable. The hot-rolling of this material allows the production of thin cellular sheets to be obtained.

Keywords: Hot-rolling; Zn₂₂Al₂Cu-NaCl composite; microstructure characterization; hardness.

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1. Introduction

The alloy of eutectoid composition Zn₂₂Al has been studied extensively. It has been known for a long time that this material is superplastic when it has a fine-grained microstructure of a phase rich in Al (α) and another phase rich in Zn (η) and deforms at a quasistatic deformation rate [1,2] at a temperature close to 0.5 T_f (the melting temperature of the alloy), plastically deforming several hundred percent before fracturing.

This microstructure is achieved, for example, by applying a heat treatment to this alloy, consisting of maintaining it at a temperature above 273°C for approximately 45 hours and subsequent tempering in a water or ice-water bath. This procedure has been used alone or in combination with other techniques to study different aspects of the superplastic behavior of this alloy [3–6].

The Zn₂₂Al alloy has been used as a base alloy for the manufacture of other alloys with different types and amounts of solutes, for example, the solutes Cu [7–10], Si [11], Ti [12] Ag [13], Ce [14] and Fe [15], to investigate superplas-

tic behavior, phase transformations, mechanical and physical properties, and evolution of the microstructure.

In addition, the Zn₂₂Al alloy has been used as the matrix of composites [16–18] and has been converted to a foam alloy [19,20] and composite foam [21,22] to investigate mechanical properties.

Among the various alloys derived from the Zn₂₂Al alloy with certain solutes is the Zn₂₂Al₂Cu alloy, which has been interesting to researchers and technologists. This alloy is reported to have higher corrosion resistance than galvanized products, can be hot-rolled [23] and is weldable [24]. A fine microstructure is obtained by performing the aforementioned procedure for the Zn₂₂Al alloy without Cu, and this alloy also has superplastic properties [25]. This alloy has been used as a matrix for composites with structural components of Al₂O₃, hydroxyapatite or graphite [26], ZnO [27], solid glass spheres [28,29], and SiC [30] to investigate the mechanical properties of these composites and has been obtained as a cellular alloy [31,32].

One way to make cellular metals is to use particles as space maintainers or NaCl preforms that can be, for exam-

ple, infiltrated by the alloy in the liquid state [33], and the resulting composite in the solid state is immersed in boiling water for a certain amount of time to dissolve NaCl. This cellular alloy has, similar to all materials of its kind, multiple properties and applications [34]. The same cellular alloy can serve as a vibration damper, a support for catalysis, a heat exchanger, a filter, and a protective wrap for fragile objects, with the advantage of having twice the mechanical strength of aluminum foams.

In a related co-authored work involving the authors of this study, concerning the Zn22Al2Cu-NaCl composite with six different densities, two NaCl grain textures, and matrix microstructures similar to those used in this work, tested under compression at room temperature, it was established that the NaCl particles do not reinforce the matrix; rather, they deform along with it, especially when the composite has the lowest density, a cast matrix microstructure, and smoothed NaCl grains [35].

NaCl is an ionic solid with a face-center cubic crystallographic structure. NaCl monocrystals exhibit a stress-strain curve similar to that of metals with the same crystallographic structure [36]. NaCl polycrystals are brittle at room temperature but ductile at temperatures above 200°C [37].

Therefore, the Zn22Al2Cu-NaCl composite is expected to be successfully formed above 200°C, as the superplastic behavior of the matrix alloy also occurs above 200°C for this purpose, sharp NaCl particles could potentially be used.

This work investigates whether the Zn22Al2Cu-NaCl composite can be hot-rolled using two different initial matrix microstructures: one obtained during material fabrication (cast-metal matrix microstructure) and another obtained by heat treatment (fine-grain matrix microstructure).

If hot rolling is possible, the changes in each initial matrix microstructure will be established as the percentage reduction in the composite's cross-section increases. The production of sheets of this composite is crucial, as they can be easily transformed into very thin cellular sheets for use as filters, heat sinks or composite sheets assembled into a stack within an insertable and replaceable cartridge in a water hydrolysis chamber for green hydrogen production. However, additional tests and measurements must be performed, such as, for example, determining the cell size, electrical conductivity, and corrosion resistance of the sheets that will integrate the cartridge.

2. Experimental procedure

2.1. Preparation of the matrix alloy

The Zn22Al2Cu alloy was produced by conventional casting at 700°C. Zn, Al and Cu ingots were used with purities of 99.99 %, 99.27 % and 99.999 %, respectively. A Velab VE-300 scale with a precision of 10^{-4} g was used to obtain the correct quantities of the elements. A zirconia-lined graphite crucible and a Lindberg 5189A muffle furnace were used

for the casting. The density of the alloy was obtained by the Archimedean method, resulting in a value of 5.4 g/cm³.

2.2. NaCl particles

The NaCl particles used had an irregular shape and an average size of 2.25 ± 0.25 mm. The particles were selected by sifting different-sized particles. The physical properties of the particles were an elastic modulus of approximately 40 GPa, a melting temperature of 816°C, and a density of 2.16 g/cm³.

2.3. Composite manufacturing

The composite was elaborated by remelting 800 g of the alloy at 700°C and preheating 480 g of NaCl particles, equivalent to 0.6 times the mass of the alloy, at 400°C. This ratio ensures the production of a low-density composite, which will have a greater plastic deformation under compression, as found in another research [35] co-led by the authors of this work. The hot NaCl particles were then submerged in the liquid alloy and pushed in with a piston to retain them while the mixture cooled in air until complete solidification.

The average density of the composite was determined by establishing the average value of the mass/volume ratios of several sections. An average density of 3.0835 g/cm³ was obtained.

Using the equation of the mixture rule [38] for the composite density, in terms of volume fractions and densities of NaCl and matrix alloy, 2.16 g/cm³ and 5.4 g/cm³, respectively, and the experimental value of the composite density, 3.0835 g/cm³, a volume percentage of NaCl 71.5 is obtained.

The composite obtained was cut into two equal parts, and one part was subjected to a heat treatment as described in section 2.4 to change the initial microstructure of the matrix. Subsequently, the two halves of material were cut into 8 mm-thick sections for hot-rolling.

2.4. Microstructures in the matrix

The initial matrix microstructures were obtained by casting and heat-treatment. The first microstructure was formed by air-cooling during the last stage of the composite manufacturing process; the other microstructure was obtained after the composite with cast metal microstructure was heated and maintained at 350°C for 45 hours and then tempered in acetone at 1°C.

Samples of the casting material with heat-treatment were finely ground and submerged in C₂H₆O at 1 % HNO₃ to reveal the microstructure. A JEOL JCM 600 portable scanning electron microscope and a JEOL JSM-7600F field emission electron microscope were used to characterize the microstructures. The compositions of the constituents in each initial matrix microstructure of the samples were determined by energy-dispersive X-ray spectroscopy (EDXS).

The microhardnesses (10 g test charge) of the constituents of each initial matrix microstructure and the embedded NaCl

particles and the Rockwell hardness F of the nonrolled composites were determined using a Micromet 2003 microdurometer and a Misawa Seiki Seisakusho durometer.

All measurements were made on both sides of the 0.8 cm thick plate of the composite with one and the other microstructure, performing approximately a similar number of measurements in regions from one end of the plate to the other to complete, according to the dispersion of the data, between 10 and 15 Vickers microhardness measurements on the matrix; 11, on NaCl grains, and between 10 and 27 Rockwell F hardness measurements.

2.5. Hot-rolling process

The alloy without NaCl grains was not hot rolled because this work was performed and reported by Negrete [23].

Plates approximately 8 mm thick with the cast-metal matrix microstructure and the fine-grained matrix microstructure obtained after heat-treatment were hot-rolled at an angular velocity of 10 revolutions/minute (4 mpm) and a temperature of 230°C using a FENN 5^a mill rolling (with rollers of 5" diameter) until a plate thickness reduction of approximately 80 % was achieved: the final thickness of the sheets obtained was approximately 1.6 mm. The temperature and angular velocity were chosen based on what has been reported about the rolling Zn22Al2Cu alloy [23].

The effects of rolling on the composite were evaluated with metallographic studies, making observations and taking images of different zones of the matrix and interfaces between constituents in plates with different microstructures and

with approximately 50 % and 80 % reductions in thickness using the electronic microscopes mentioned in Sec. 2.4.

The average Vickers microhardness of constituents in resulting microstructures and the medium Rockwell hardness F of the hot-rolled plates were determined by taking a similar measurements number on both sides of the sheets, as described in the previous section, after each percentage reduction in area. The compositions of different microstructural zones in the matrix were determined by EDXS. The samples used had been previously polished with a diamond suspension and then subjected to ultrasonic cleaning with acetone and drying with warm air.

3. Results

3.1. Microstructures in the matrix

3.1.1. Initial microstructures

The initial cast-metal matrix microstructure of the nonrolled composite is shown in Fig. 1a). The microstructure consisted of dendrites and an interdendritic component.

The compositions determined by EDXS in the different zones (dendrite center, dendrite edge, interdendritic contour and interdendritic zone) of the initial cast-metal matrix microstructure are presented on the left side of Table I. These data show that the Zn and Cu contents increased and the Al content decreased from the center of the dendrites to the interdendritic zone. The Cu content in the interdendritic contours did not follow this pattern, as the amount of Cu measured in this zone was less than the amount of Cu at the dendrite edge.

TABLE I. Composition of the constituents in the nonrolled initial cast-metal matrix microstructure and 47.6 % hot-rolled composite by EDXS.

Constituent or region	Not rolled			47 % hot-rolled		
	Zn(%p)	Al(%p)	Cu(%p)	Zn(%p)	Al(%p)	Cu(%p)
Dendritic center	52.70	46.29	0.40	61.07	38.93	0.00
Dendrite edge	63.42	34.04	2.54	71.59	28.41	0.00
Interdendritic contour	67.97	30.72	1.31	89.00	3.96	7.05
Interdendritic zone	93.14	2.22	4.64	91.36	2.51	6.13

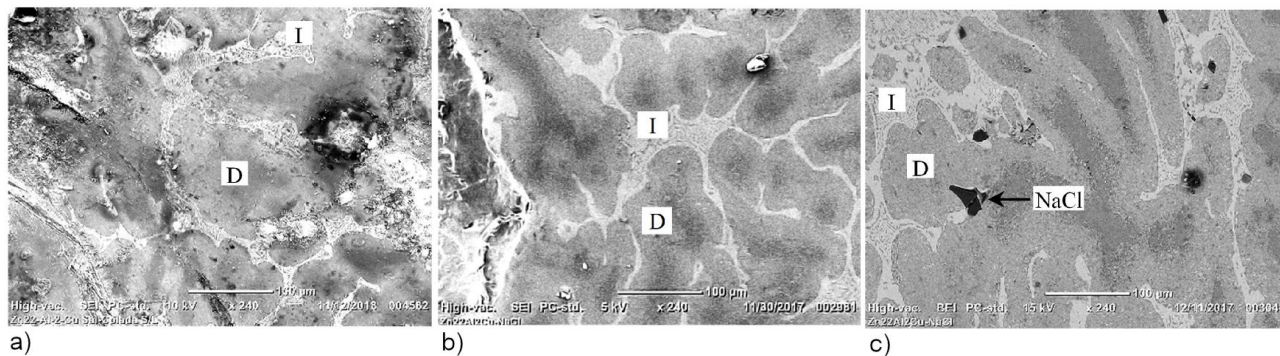


FIGURE 1. a) Initial cast-metal matrix microstructure and the resulting microstructures for b) 47.6 % and c) 82 % section reduced composites rolled at 230°C. D: dendrite, I: interdendritic zone.

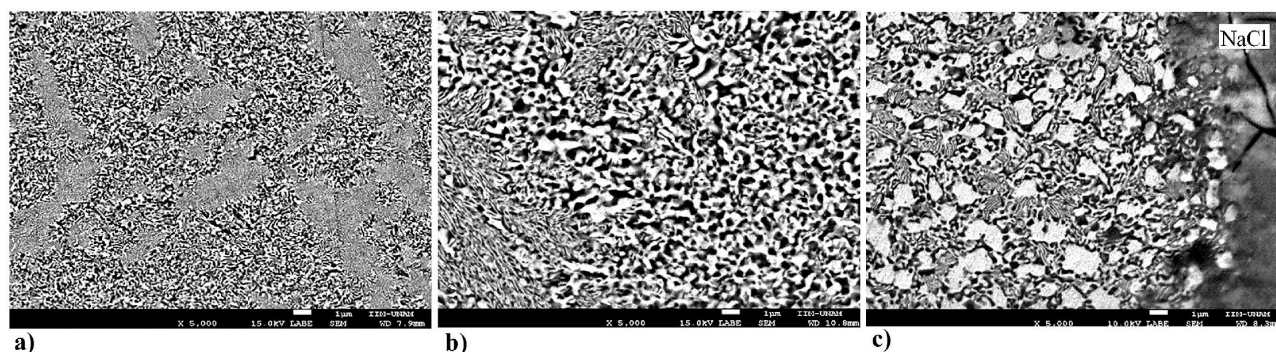


FIGURE 2. a) Initial fine-grained matrix microstructure and the resulting matrix microstructures for b) 58.33 % and c) 78 % section reduced composites hot-rolled at 230°C.

TABLE II. Composition of the nonrolled fine-grained matrix microstructure and constituents in the composite hot-rolled to 78 % as measured by EDXS.

Constituent or region	Not rolled			78 % hot-rolled		
	Zn(%p)	Al(%p)	Cu(%p)	Zn(%p)	Al(%p)	Cu(%p)
Dark embedded region [see Fig. 2c)]	*	*	*	63.91	34.24	1.85
Thin pearlite-type substructure (see Fig. 2c)]	*	*	*	70.82	27.26	1.92
Fine particles [see Fig. 2a)]	77	21	2	74.24	23.99	1.77
Light embedded islands [see Fig. 2c)]	*	*	*	84.70	12.20	3.10

The microstructure obtained in the matrix with the application of heat treatment is shown in Fig. 2a): the microstructure was composed of two types of alternating regions with fine constituents alternating between light (rich in Zn) and dark (rich in Al). One type of region had much finer constituents. This microstructure is hereafter called the fine-grained matrix microstructure.

The composition of the initial fine-grained matrix microstructure is shown on the left side of Table II, which was approximately the overall composition of the alloy matrix.

3.1.2. Microstructures produced by hot-rolling

The matrix microstructures of the initial cast-metal 47.6 % and 82 % hot-rolled composites are shown in Figs. 1b) and 1c), respectively. These figures show that the dendrites and interdendritic components became increasingly deformed as the rolling percentage increased.

The compositions established by EDXS in different zones (dendrite center, dendrite edge, interdendritic contour and interdendritic zone) of the microstructures obtained in the initial cast-metal 47.6 % hot-rolled composite are presented on the right side of Table I.

These data show that the content of Zn goes from lowest

to highest and that of Al from highest to lowest from the center of the dendrites to the interdendritic zone, as established in the initial cast-metal microstructure. The Cu content was null in the dendrite center and edge and was higher in the interdendritic contour than in the interdendritic zone. In addition, the contents of all the detected elements were higher in all the zones of this matrix microstructure compared with those established in each similar zone in the microstructure of the nonrolled cast-metal matrix composite.

Figure 3 shows micrographs at higher magnification of the microstructures obtained after 47.6 % and 82 % hot-rolling of the initial cast-metal matrix composite. The figures clearly show that an increase in the size of the components of the dendrite substructure occurred when the rolling percentage increased.

Figures 2b) and 2c) present the microstructures obtained after 58.33 % and 78 % hot-rolling at 230°C of the initial fine-grained matrix composite. The size of the constituents increased, and then, new light and dark islands were formed; the former were greater in quantity, evenly distributed, and surrounded by regions of fine pearlite and a fine-particle substructure, increasing with the section percentage reduction at 230°C of the initial fine-grained matrix composite.

The compositions of the dark islands, regions with a fi-

ne pearlite substructure, regions of fine particles and light islands in the microstructure of the 78 % hot-rolled composite with the initial fine-grained matrix microstructure are shown on the right side of Table II. All the alloying elements were present in these constituents.

The regions with Zn contents from lowest to highest and Al contents from highest to lowest were in the following or-

der: the dark islands, regions with a fine pearlite substructure, fine-particle regions, and light islands. The Cu content was approximately the same (between 1.77 % and 1.92 % by weight) in the first three constituents and slightly higher (by more than 1 %) in the light islands. The contents of Zn and Cu decreased slightly in the fine-grained regions with rolling.

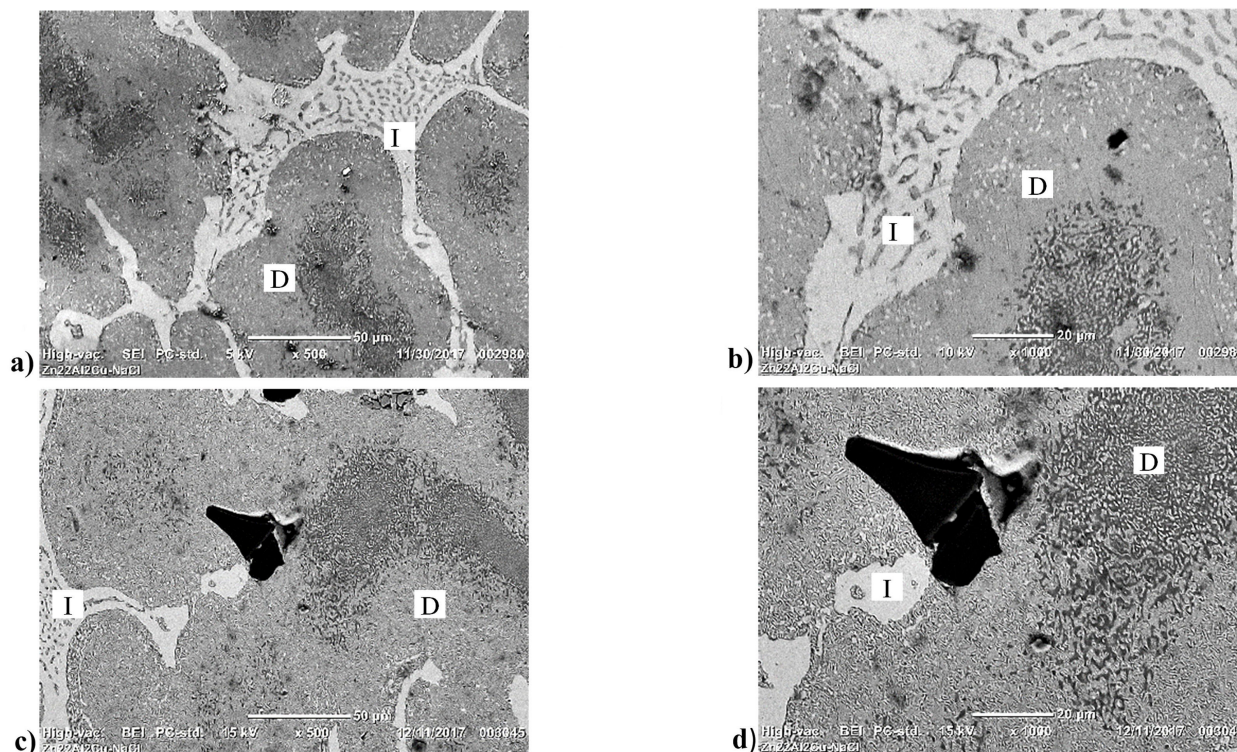


FIGURE 3. Higher magnification micrographs of the microstructures obtained for the initial cast-metal matrix composites with a) and b) 47.6 % and c) and d) 82 % section reduction at 230 °C. An increase in the size of the components of the dendrite substructure is observed when the % section reduction increases. D: dendrite, I: interdendritic zone.

3.2. Vickers microhardness and Rockwell hardness F

The variation of the Vickers microhardness at room temperature in the matrix and NaCl particles with section reduction of the composites with the two types of initial microstructures hot-rolled at 230 °C is shown in Fig. 4.

The initial fine-grained microstructure was harder than the initial cast-metal matrix microstructure, while the NaCl particles embedded in the fine-grained microstructure were softer than those in the cast-metal microstructure.

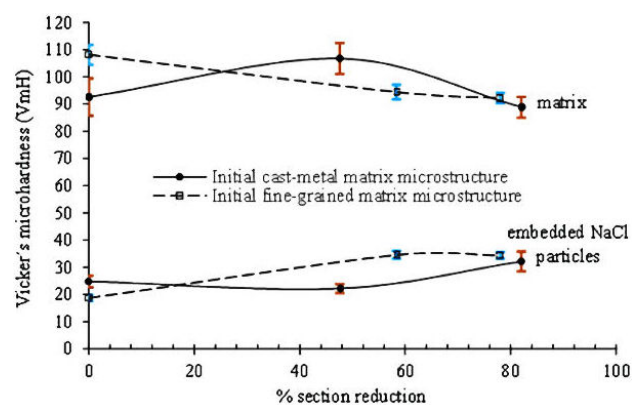


FIGURE 4. Variation of the Vickers microhardness established at room temperature in the matrix and NaCl particles with % section reduction of the initial cast-metal and fine-grained composites hot-rolled at 230 °C.

For the initial fine-grained composite, the matrix was fully softened from the first stage of rolling and remained soft after the maximum section reduction; for the initial cast-metal composite, the matrix first hardened and then signifi-

cantly softened with increasing section reduction.

In the fine-grained composite, the NaCl particles reached maximum hardness at the first stage of rolling, while for the cast-metal composite, the NaCl particles had almost constant hardness from the nonrolled state to the first stage of rolling and then acquired maximum hardness when the composite was hot-rolled to the maximum percentage.

The microhardness of the NaCl particles was considerably lower than the microhardness of the matrix for both types of microstructure before rolling and after each rolling step.

The variation of the Rockwell hardness F determined at room temperature in the two different composites with the section reduction at 230°C is shown in Fig. 5.

The hardness of the composites first increased and then substantially decreased with increasing section reduction regardless of the initial matrix microstructure, with the Rockwell hardness F being greater for the initial fine-grained composite.

4. Discussion

Images in Fig. 1 show that the components became increasingly elongated as the area reduction percentage of the com-

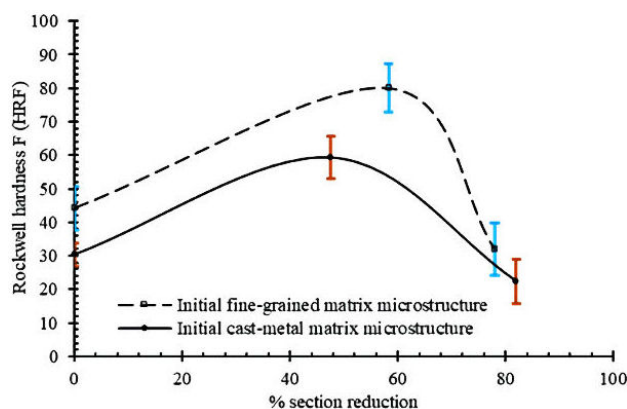


FIGURE 5. Variation of the Rockwell hardness F measured at room temperature with % section reduction of the initial cast-metal and fine-grained composites at 230°C.

posite increases. The cast-metal matrix microstructure then acquires the texture of the shape during the rolling process.

The initial fine-grained matrix microstructure undergoes constituent growth and the formation of new phases and constituents, as seen in Fig. 2 and Table II; that is, this microstructure recrystallizes as hot rolling progresses.

The thermal energy and the energy contributed by rolling the initial cast-metal composite increased the Zn content of most of the components except the interdendritic region. These energies caused the compositions of the centers and edges of dendrites to become uniform, resembling the eutectoid Zn22Al composition reported in the Al-Zn equilibrium diagram [39]. The compositions of the interdendritic

zone and the interdendritic contours approximated the eutectic Zn4.5Al composition, modified with Cu, of the same diagram. In addition, the Cu came out of the dendrites and entered the interdendritic zones and the interdendritic contours.

In the microstructure of the initial fine-grained composite rolled to a 78 % section reduction at 230°C, the fine particle and fine pearlite regions had approximately the eutectoid compositions Zn22Al and Zn30.5Al, respectively, of the Al-Zn equilibrium diagram [39], but they had Cu. The light and dark islands were both rich in Zn and low in Cu content, but the dark islands had approximately 2.8 times as much Al as the light islands. The latter were nonequilibrium phases with compositions that did not resemble the phases reported in the aforementioned Al-Zn equilibrium diagram.

The lower microhardness of the NaCl particles in the initial fine-grained matrix was probably due to the increase of NaCl particle crystal size when the composite was maintained at 350°C for 45 hours before being tempered to produce the fine-grained microstructure in matrix.

The deformation of the constituents in the initial cast-metal composite caused hardening of the matrix to approximately 47.6 % section reduction of the composite, while the increase in the size of the constituents and the appearance of new constituents due to increasing section reduction were associated with continuous softening of the initial fine-grained matrix, Fig. 4. Reportedly, the microstructure of fine particles softens when deformed [23,40].

The considerable softening of the matrix that occurred above the 47.6 % section reduction of the composite with the initial cast-metal matrix microstructure could be due to the increase in the size of the constituents that form the dendrite substructure, as seen in Fig. 3.

The NaCl particles were hardened by deformation with increasing section reduction regardless of the matrix microstructure of the composite, hardening faster when the particles were embedded in the initial fine-grained microstructure, as seen in the lower part of Fig. 4.

Gabriel *et al.* reported [24] that the constituents of the fine-grained microstructure of the Zn22Al2Cu alloy are dislocation free. Thus, in the composite studied here with this matrix microstructure, the stress applied during rolling was transferred from constituent to constituent in the matrix and then almost entirely to the NaCl particles. For the initial cast-metal composite, the stress applied during rolling caused deformation of the cast-metal matrix, attenuating the stress ultimately applied to the particles embedded in the matrix. For this reason, hardening by deformation was achieved more quickly for the NaCl particles embedded in the initial fine-grained microstructure.

As seen in Fig. 5, the Rockwell hardness F variations established for both types of composites indicate that the NaCl particles oppose the plastic deformation of the matrix, acting as structural reinforcement until the first stage of section reduction. This effect becomes more evident when the microstructure transfers more stress to the NaCl particles, such as with the fine-grained microstructure, as explained in the pre-

vious paragraph.

This opposition of the NaCl particles to the plastic deformation of the matrix was more significant for the initial fine-grained microstructure. This is inferred because the Rockwell hardness F established of the fine-grained composite increased until the first stage of rolling, as seen in Fig. 5, although the matrix was continuously softened, the NaCl particles hardened slightly with rolling, and the particles were softer than the matrix, as seen in Fig. 4.

The decrease in the Rockwell hardness F of both types of composites from the first section reduction to the last section reduction, as seen in Fig. 5, maybe is due to the existence

of more extensive areas of NaCl exposed on the surface of the plates, as seen in Figs. 7a) and 7b). Another factor causing this phenomenon could be the absence of a matrix below certain NaCl particles.

The Rockwell hardness F variation of the initial cast-metal matrix microstructure composite fully agreed with the microhardness variation of the matrix.

Figure 6 shows images of the initial cast-metal matrix microstructure composite for different percentages of section reduction. Through these images, deformation and thinning of the matrix and the embedded NaCl particles were observed as the percentage of section reduction increased.

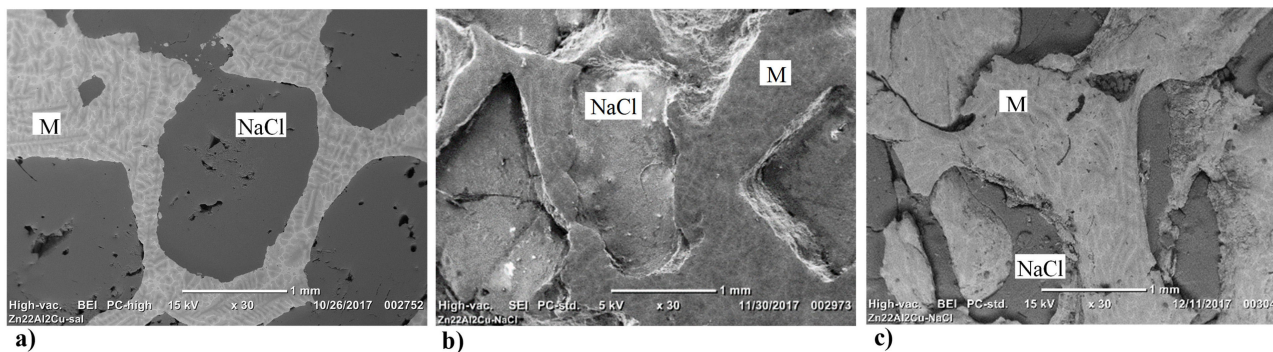


FIGURE 6. Micrographs of the initial cast-metal matrix microstructure composites a) not rolled and b) with 47.6 % and c) 82 % section reduction at 230°C. The increase in the deformation and thinning of the matrix and salt particles is observed with increasing section reduction. M: matrix.

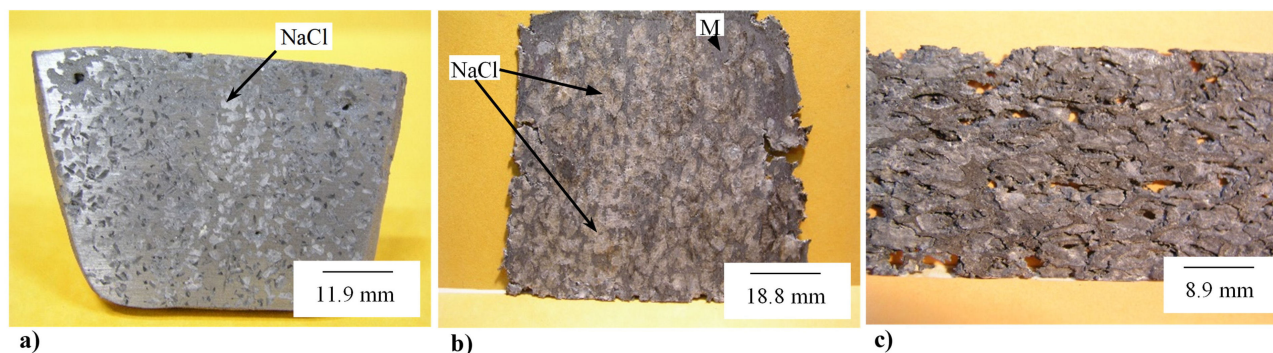


FIGURE 7. a) Nonrolled plate, b) sheet obtained with 82 % section reduction of the Zn22Al2Cu-NaCl composite, and c) cellular sheet obtained by dissolving the NaCl in a sheet with 82 % section reduction in boiling water. Initial cast-metal matrix microstructure. M: matrix.

The requirement of support of a greater percentage of stress imposed by the initial fine-grained microstructure on the NaCl particles results in increased brittleness in addition to the inherent brittleness of the salt, as NaCl is a solid formed by ionic bonds, which is associated with its hardening by deformation. This brittleness was evidenced by the presence of cracks in certain particles and by the separation or exfoliation of the NaCl particles of the composite hot-rolled at the maximum percentage when polishing or during ultrasonic cleaning of the samples, as seen on the right side of Fig. 2c).

Figure 7 shows a nonrolled plate, a piece of sheet of the initial cast-metal matrix microstructure composite with 82 % section reduction, and a piece of sheet with the same initial

microstructure and percent section reduction in which the NaCl was dissolved with boiling water, resulting in a cellular sheet of Zn22Al2Cu alloy.

A potential application of thin sheets of the Zn22Al2Cu-NaCl composite would be as an easily replaceable array of sheets in a receptacle that produces green hydrogen by splitting water molecules through alkaline hydrolysis: this method is considered one of the two main commercially available methods and is likely to become the dominant technology for green hydrogen production in the immediate future [41-44].

The metal in an array of sheets of this composite, forming a kind of cartridge, would be one of the electrodes immersed in the water to be hydrolyzed. After the NaCl dissolves in

the water, the multiple cells of the Zn22Al2Cu cellular alloy would have a larger surface area, as shown in Fig. 7c), which could improve the efficiency of H₂ production in the receptacle. Once the salt has dissolved and the function of these sheets is completed, the cartridge can be removed and each of its sheets can be reused in one or more of the multiple recognized applications for cellular materials [34].

The very thin composite sheets, converted into cellular sheets, could also be used, for example, as air filters or heat sinks.

The proposed applications require complementary studies and measures to verify their viability.

5. Conclusions

Zn22Al2Cu-NaCl composite can be hot-rolled at 230°C. By increasing the section reduction of the composite, the constituents of the initial cast-metal matrix microstructure mainly acquire shape texture, the sizes of the dendritic substructures slightly increase, and the constituents tend to be similar in composition. In contrast, for the initial fine-grained

microstructure, the constituents grow, and new constituents later appear. The NaCl particles are hardened by deformation with increasing section reduction of the composite, with the speed of hardening being greater when the matrix has an initial fine-grained microstructure. Hot-rolling to approximately 50 % section reduction produces plates of Zn22Al2Cu-NaCl composite with increased hardness and plastic deformation strength when the initial matrix microstructure is fine-grained or cast. Thin sheets of cellular alloy Zn22Al2Cu can be obtained with this process under the conditions used in this work and by dissolving the salt in boiling water. Both microstructure types of this composite can be hot-rolled, with the cast-metal microstructure being more suitable because the integrity of the composite is maintained.

Acknowledgments

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Influence of active layer thickness on the performance of P3HT: PC₆₁BM organic photovoltaic devices analyzed via $J-V$ characteristics

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Optimizing the thickness of the active layer is essential to improve the performance of organic solar cells. In this study, we examined how the thickness of the active layer, made of a P3HT:PC₆₁BM blend, influences the key electrical parameters of inverted organic solar cells. Four prepared photovoltaic cells were prepared using a typical device structure of ITO/ZnO/P3HT:PC₆₁BM/MoO₃/Ag. The active layer of P3HT:PC₆₁BM was deposited by spin coating with different thicknesses of 80, 150, 200, and 300 nm. We used the different $J-V$ characteristics to extract parameters such as the open-circuit voltage, short-circuit current density, series resistance, and shunt resistance. Based on these measurements, the results indicate that V_{oc} remains nearly stable between 80 nm and 200 nm, before dropping sharply at 300 nm due to recombination losses. Furthermore, J_{sc} increases with thickness and reaches its maximum at 300 nm, thanks to improved light absorption. The fill factor peaks ($\sim 50\%$) at a thickness of 150 nm, then decreases, reflecting an imbalance between charge collection and internal losses. To provide a deeper understanding of this behavior, we also analyzed the resistive parameters. The series resistance R_s increases from $27.11 \Omega \cdot m^2$ to $27.52 \Omega \cdot m^2$ when the thickness increases from 80 to 150 nm due to the increased defect density in the layer structure with additional layer stacking, then rises to $28.87\text{--}34.55 \Omega \cdot m^2$ for 200–300 nm, respectively, because of the longer charge transport path and increased recombination. Finally, the shunt resistance R_{sh} increases up to 150 nm, suggesting improved film uniformity and better surface coverage, thus minimizing shunt defects, before decreasing at 200 and 300 nm. This suggests that increasing the material volume statistically leads to a higher density of volumetric defects.

Keywords: Organic photovoltaic cells; active layer thickness; series resistance; shunt resistance; cell design parameters.

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1. Introduction

The transition to renewable energy sources has become essential in response to growing environmental concerns and the depletion of fossil fuel resources. Among emerging technologies, organic photovoltaics (OPV) have gained increasing attention due to their lightweight nature, mechanical flexibility, potential for low-cost production, and compatibility with large-scale printing processes [1-5]. Unlike traditional silicon-based solar cells, OPVs rely on organic materials, primarily conjugated polymers and small organic molecules to absorb light and generate electricity [6-13]. In recent decades, important advancements have been made in understanding the fundamental mechanisms of photovoltaic conversion in organic materials, as well as in optimizing device architectures. Nevertheless, OPVs still face challenges related to power conversion efficiency and operational stability when compared to their inorganic counterparts. Improving the performance of OPVs requires better control over the optoelectronic properties of the active materials and the optimization of each layer within the device, particularly the active layer and the charge transport layers.

The organic photovoltaic cell is characterized by several key parameters that determine its efficiency in converting light into electrical energy. The first of these parameters is the open-circuit voltage, noted V_{oc} , which represents the maximum voltage the cell can deliver when no current is flowing through the circuit. It is mainly determined by the energy

difference between the HOMO level of the donor material and the LUMO level of the acceptor material minus internal energy losses. The second parameter is the short-circuit current density, noted J_{sc} , which corresponds to the amount of current generated when the cell's terminals are directly connected. It depends on the absorption of light, the efficient separation of photogenerated electron-hole pairs, and their collection at the electrodes. Another important parameter is the fill factor (FF), which reflects the quality of the cell's current-voltage ($J-V$) curve. It is defined as the ratio of the maximum power actually delivered by the cell to the theoretical power given by the product $V_{oc} \times J_{sc}$. Finally, the power conversion efficiency, noted PCE, expresses the percentage of the incident light energy that is converted into electricity. In this context, the current work focuses on investigating the effect of the active layer thickness on key performance parameters namely the open-circuit voltage, short-circuit current density, and power conversion efficiency (PCE) of an organic photovoltaic cell based on the P3HT:PC₆₁BM blend. By analyzing the current-voltage ($J-V$) characteristics, the goal is to assess how variations in the active layer thickness influence charge generation, transport, and recombination processes. In addition to the conventional performance metrics, the study also examines the influence of thickness on series resistance (R_s), shunt resistance (R_{sh}). These additional parameters provide deeper insight into the internal physical mechanisms governing device behavior, and help identify the optimal active layer thickness for maximizing photovoltaic performance.

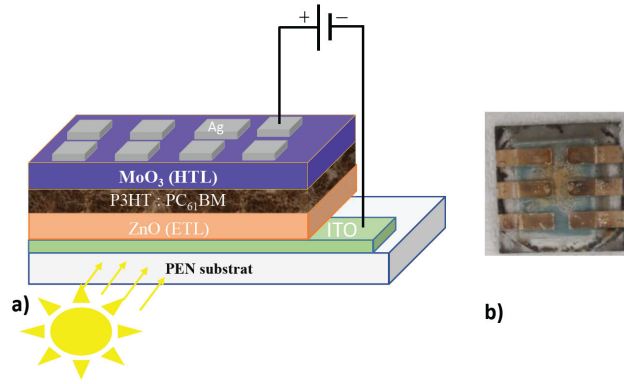


FIGURE 1. a) Schematic illustration of the fabricated OSC with the device architecture of ITO/ZnO/P3HT: PC₆₁BM/MoO₃/Ag, and b) photograph of the fabricated device.

2. Experimental details

Here, we describe the fabrication steps of organic solar cells (OSCs). Flexible PEN/ITO substrates ($2 \times 2 \text{ cm}^2$, $\leq 15 \text{ } \Omega/\text{sq.}$) were cleaned in an ultrasonic bath using detergent, acetone, isopropyl alcohol, and deionized water, followed by 30 minutes of UV ozone treatment. ZnO films were deposited by RF magnetron sputtering using a high-purity (99.999 %) ZnO target, under an argon atmosphere at a pressure of 10^{-2} mbar, with 100 W power and a substrate temperature of about 40°C , resulting in a thickness of $\sim 54 \text{ nm}$. Then, PEN/ITO/ZnO samples were annealed in oxygen at temperature 160°C for 1 hour. The active layer was spin-coated using a 1:1 (wt %) P3HT:PC₆₁BM solution in dichlorobenzene, with spin speeds of 3000, 2000, 1800, and 800 rpm to obtain thicknesses of 80, 150, 200, and 300 nm, respectively. The P3HT (98.5 % regioregular) and PC₆₁BM were used without further purification [14,15]. After deposition, the samples were annealed at 140°C for 15 minutes in a nitrogen-filled glove box. MoO₃ (5 nm) and Ag (120 nm) were then thermally evaporated under high vacuum (2×10^{-6} Torr) through a shadow mask. The complete device structure (as illustrated in Fig. 1) had an active area of about 9 mm^2 . For comparison, the same procedure was applied to rigid ITO-coated PEN substrates ($20 \times 20 \text{ mm}^2$, $\leq 20 \text{ } \Omega/\text{sq.}$).

In brief, the cell layers studied consist of the following constituents:

- **Substrate:** PEN (used as the supporting base for the device structure)
- **Transparent electrode (Anode):** ITO
- **Electron transport layer (ETL):** ZnO
- **Photoactive layer:** P3HT:PC₆₁BM blend (poly(3-hexylthiophene) and [6,6]-phenyl-C₆₁-butyric acid methyl ester)
- **Hole transport layer (HTL):** MoO₃

■ Cathode: Ag (silver)

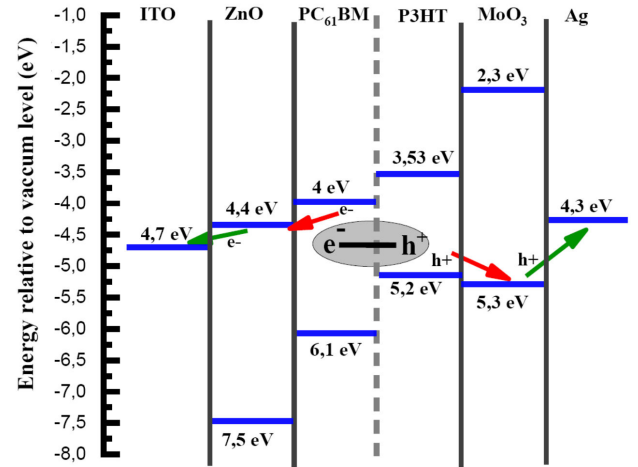


FIGURE 2. Energy levels and charge transport in the studied inverted organic photovoltaic cell.

The energy level diagram of the component materials of the studied inverted P3HT:PC₆₁BM organic solar cells (OSCs) is shown in Fig. 2 [16-20].

Light absorbed in the P3HT component of the P3HT:PC₆₁BM active layer generates excitons through a HOMO–LUMO electronic transition. Due to the strong Coulomb binding in organic semiconductors, these excitons diffuse toward the P3HT/PC₆₁BM interface, where their dissociation is driven by the energy offset between the LUMO levels of the donor and acceptor (Fig. 2). This process results in electron transfer to PCBM while holes remain in P3HT. The free charge carriers are subsequently injected into the charge transport layers, with electrons transported through ZnO and holes through MoO₃, and finally collected at the aluminum cathode and ITO anode to generate the photovoltaic current [14,21-23].

The $J-V$ curves representing current density as a function of voltage of the OSCs were measured using an HP Agilent source measurement unit under simulated illumination. A solar simulator operating under AM 1.5G conditions (Oriel Xenn 150W) was employed. The light intensity was calibrated using a standard silicon solar cell to achieve an illumination of $100 \text{ mW}/\text{cm}^2$. Device performance measurements were conducted under a nitrogen atmosphere.

3. Results and discussions

In this case, we execute the standard diode model as expressed in the following analytical Eq. (1) [24,25]:

$$J = J_0 \left[\exp \left(\frac{e(V - JR_s)}{nkT} \right) - 1 \right] + \frac{V - JR_s}{R_{sh}} - J_{ph}, \quad (1)$$

where J_0 and J_{ph} are the diode saturation current density and photocurrent density, R_s and R_{sh} are the series and shunt resistances, n an ideality factor close to 1 indicates bimolecular recombination, while a value near 2 suggests trap-assisted or

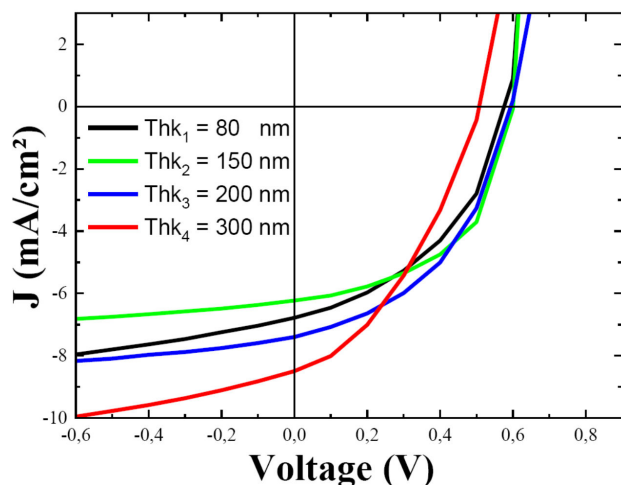


FIGURE 3. Current density-voltage response of P3HT:PC₆₁BM devices as a function of the active layer thickness.

interface recombination, e , k , and T represent the elementary charge, the Boltzmann constant, and the absolute temperature, respectively; and V the applied voltage. The $J-V$ curves of the organic solar cells (OSCs) with different active layer thicknesses were displayed in Fig. 3. The current-voltage ($J-V$) characteristics of organic solar cells (OSCs) were measured as a function of active layer thickness. The results show that thickness strongly affects device efficiency. An OSC with an 80 nm active layer exhibits a short-circuit current density (J_{sc}) of 6.8 mA/cm², an open-circuit voltage (V_{oc}) of 0.57 V, and an efficiency (η) of 1.7 %. Increasing the thickness to 150 nm slightly reduces J_{sc} to 6.3 mA/cm², while V_{oc} improves to 0.60 V, leading to the highest PCE of 1.9 %. Further increasing the thickness to 300 nm degrades V_{oc} and overall efficiency, despite a slight increase in J_{sc} .

The influence of the active layer thickness on the photovoltaic performance was investigated by analyzing the evolution of the open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), series resistance (R_s), shunt re-

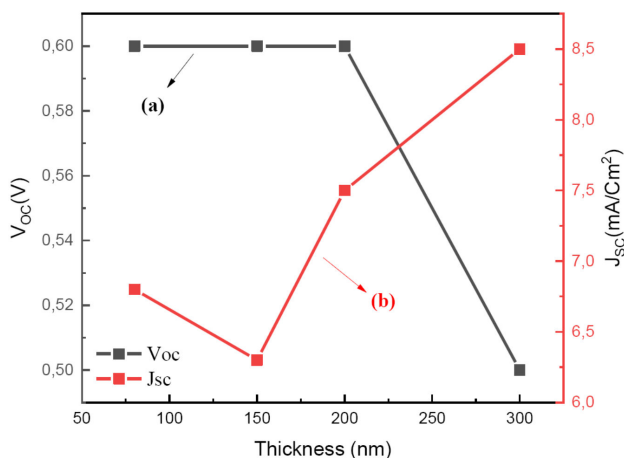


FIGURE 4. a) Open-circuit voltage (V_{oc}) and b) short-circuit current density (J_{sc}) of P3HT:PC₆₁BM solar cells versus active layer thickness.

sistance (R_{sh}), and efficiency (η) as a function of thickness.

The performance parameters of the devices corresponding to the $J-V$ curves are listed in Table I, in which it clearly appears that the active layer thickness has a significant impact on device efficiency.

As presented in Fig. 4a), the open-circuit voltage (V_{oc}) remains almost constant at around 0.60 V for active layer thicknesses ranging from 80 nm to 200 nm. However, a significant decrease is observed when the thickness reaches 300 nm. This reduction in V_{oc} at greater thickness leads to an increase in energy loss, defined as $E_{loss} = E_g - eV_{oc}$, where E_g is the optical band gap of P3HT:PC₆₁BM ($E_g = 1.9$ eV) [26]. For devices with active layers between 80 and 200 nm, V_{oc} was maintained at 0.6 V, corresponding to an energy loss of about 1.3 eV. When the thickness increases to 300 nm, E_{loss} rises to 1.4 eV. This increase in energy loss is attributed to enhanced non-radiative recombination, which reduces the open-circuit voltage and leads to higher energy dissipation, factors that directly influence V_{oc} , as described by Eq. (2) [21,27,28]:

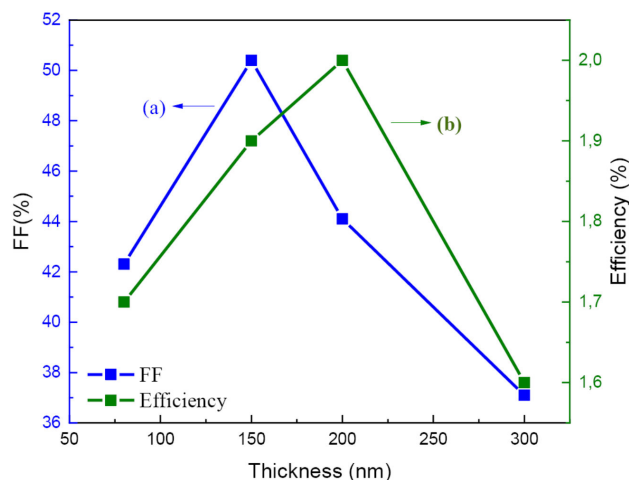
$$V_{oc} = \frac{E_g}{e} - \frac{kT}{e} \ln \left(\frac{(1-P)(B_L + B_{SRH})N_{CV}^2}{PG} \right), \quad (2)$$

where E_g denotes the effective bandgap of the active layer, P represents the exciton dissociation probability (exciton = (electron-hole) pairs), N_{CV} is the effective density of states, while G is the generation rate of excitons; B_L and B_{SRH} are the strengths of Langevin and Shockley-Read-Hall (SRH) recombination, respectively [29]. As described in Eq. (2), the increase in energy loss in thicker active layer devices is mainly due to higher charge recombination. When the thickness increases, charge carriers displace longer distances, which increases the probability of bimolecular (BL) and Shockley-Read-Hall (SRH) recombination before reaching the electrodes. This reduces the number of collected free charges and increases energy losses. In contrast, the short-circuit current density (J_{sc}) observed in Fig. 4b) increases steadily with increasing active layer thickness, reaching its maximum value at 300 nm. This trend is expected since thicker layers absorb more incident light, generating more charge carriers [27]. However, beyond a certain thickness, the recombination losses may offset the gain in light absorption. The fill factor (FF), shown in Fig. 5a), reaches its maximum ($\sim 50\%$) at around 150 nm, then decreases with further increases in thickness. This behavior suggests that an optimal thickness exists where the internal resistance is minimized and charge collection is most efficient. Thinner layers may suffer from insufficient absorption, while thicker layers may introduce transport limitations [21,27,30,31]. Studies have shown that the distribution of excitons affects charge transport and collection due to the mobility and transport distance of the carriers [32-34].

Generally, an active layer thickness around 150-200 nm appears to provide a good balance between light absorption and charge collection, leading to optimal device performance. At 300 nm, although J_{sc} is maximized, the simultaneous drop

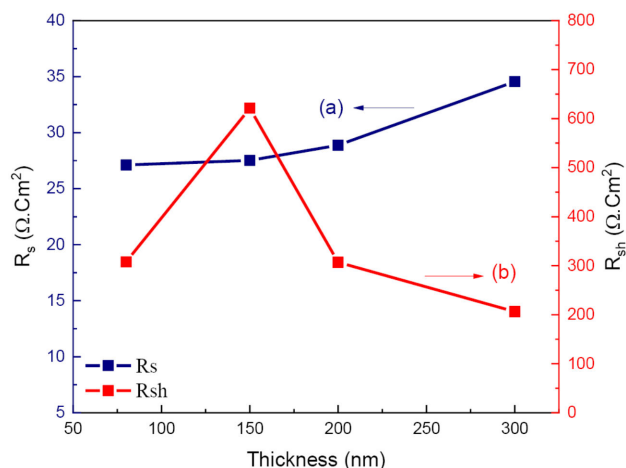
TABLE I. Photovoltaic parameters of P3HT: PC₆₁BM BHJ OSCs with different active layer thickness under AM 1.5 G solar illumination.

Active layer thickness	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	Efficiency (η %)	R_s ($\Omega \cdot \text{cm}^2$)	R_{sh} ($\Omega \cdot \text{cm}^2$)
80 nm	0.57	6.8	42.3	1.7	27.11	307.76
150 nm	0.60	6.3	50.4	1.9	27.52	621.38
200 nm	0.59	7.5	44.1	2.0	28.87	306.82
300 nm	0.50	8.5	37.1	1.6	34.55	206.23

FIGURE 5. a) Fill factor, b) Efficiency (%) of P3HT: PC₆₁BM solar cells as a function of the active layer thickness.

in V_{oc} and FF likely results in a reduced overall power conversion efficiency. The parasitic resistances are derived from the $J(V)$ curve: the series resistance R_s is the inverse of the slope near the V_{oc} point, while the shunt resistance R_{sh} is the inverse of the slope near the J_{sc} point [35]. These values are crucial for assessing performance losses, using linear fits the obtained values were displayed in Table I.

The series resistance R_s values are illustrated in Fig. 6a) (The obtained values are of the same order of magnitude as those reported by other researchers for organic photovoltaic cells [7,30]. We observed that the series resistance increases with thickness [see Fig. 6a)]. However, the main factors limiting the performance of devices with a thicker PC₆₁BM:P3HT active layer lie in the low electron mobility within the active layer, caused by the increased defect density in the material structure with additional layer stacking, as well as the reduced charge collection efficiency at the electrodes, since holes and electrons recombine before reaching the electrodes, rather than in the increase of R_s itself [21,27,30]. The values of R_{sh} were shown in Fig. 6b). The shunt resistance value was found to be 307.76 $\Omega \cdot \text{cm}^2$ for the 80 nm thickness and 621.38 $\Omega \cdot \text{cm}^2$ for the 150 nm thickness. The shunt resistance increases significantly. In this range, the initial increase in active layer thickness may lead to improved film uniformity and better surface coverage, thereby reducing the density of short-circuited regions and leakage paths (shunt defects) created during deposition. Then, the shunt resistance value decreases to 606.81 $\Omega \cdot \text{cm}^2$ at 200 nm and 206.23 $\Omega \cdot \text{cm}^2$ at 300 nm.

FIGURE 6. Variation of a) series resistance (R_s) and b) shunt resistance (R_{sh}) with active layer thickness in P3HT:PC₆₁BM solar cells.

When the active layer becomes excessively thick (beyond 150 nm), the number of bulk defects increases, the larger volume of material statistically increases the total number of defects (pores, agglomerates, and impurities) [30].

The optimal active layer thickness for the cell under study was found to be 150 nm. This choice represents the best compromise, as it allows the maximization of shunt resistance R_{sh} (which minimizes leakage current losses) while keeping the series resistance R_s at a low value, thus ensuring an optimized overall performance of the cell. For the efficiency η presented in Fig. 5b), we observe that when the thickness of the active layer in a photovoltaic cell increases, the ability to absorb light improves, which enhances the generation of electrical charges and thus the efficiency [36]. However, beyond a certain thickness (here 300 nm), negative effects start to dominate: the generated charges have more difficulty reaching the electrodes, which increases recombination because the charges neutralize before producing current. This reduces the overall efficiency of the cell.

4. Conclusions

In summary, we have explored how varying the active layer thickness affects the photovoltaic response of P3HT:PC₆₁BM polymer solar cells. The results show that V_{oc} remains almost constant between 80 nm and 200 nm, then drops significantly at 300 nm, indicating increased recombination losses. J_{sc} increases steadily with thickness, reaching a maximum at 300 nm due to improved light absorption. The

fill factor reaches its peak ($\sim 50\%$) at 150 nm and then decreases, reflecting a balance shift between charge collection and internal losses.

Our results show that the active layer thickness strongly affects R_s and R_{sh} : an optimal value around 150 nm minimizes defects, improves film quality, and enhances charge

transport, leading to better photovoltaic performance. These results demonstrate that the thickness of the active layer has a complex yet critical influence on the overall performance of organic solar cells, and that an optimal compromise must be found between light absorption, charge transport, and recombination.

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Synthesis and characterization of graphene oxide from tropical fruit peel waste using liquid phase exfoliation sonication and magnetite as catalyst

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Graphene oxide (GO) is a highly versatile nanomaterial with remarkable structural, electrical, and surface properties, making it useful for energy storage, catalysis, and biomedical applications. In this study, durian peel waste was used as a carbon-rich precursor for the synthesis of GO, offering a sustainable and cost-effective route to nanomaterials. The raw material was first subjected to pyrolysis at 400°C in a rocket stove reactor to produce biochar. The resulting carbon was processed using liquid-phase acid sonication (LAS) and ultrasonication to synthesize GO. The samples were characterized by X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM). The XRD patterns confirmed the presence of oxidized graphitic structures, Raman spectra revealed the characteristic D and G bands with an increased ID/IG ratio indicating the formation of structural defects, and SEM images showed wrinkled, layered morphologies typical of GO sheets. These results demonstrate that tropical fruit waste can be valorized into advanced nanomaterials through environmentally friendly processing, highlighting the dual benefits of waste reduction and material innovation.

Keywords: Graphene oxide; durian peel waste; pyrolysis; liquid-phase acid sonication; ultrasonication; XRD; Raman spectroscopy; SEM.

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1. Introduction

The conventional synthesis of graphene oxide (GO) remains largely dominated by graphite-based chemical approaches, such as the Hummers method and its subsequent modifications, which involve the use of strong oxidizing agents including KMnO_4 and concentrated H_2SO_4 [1,2,3]. Despite their effectiveness, these methods pose significant environmental and occupational safety concerns. Moreover, they rely heavily on commercially sourced graphite, which is relatively expensive and non-renewable. An alternative strategy that addresses several of these limitations is the liquid phase exfoliation (LPE) method. LPE mitigates the need for hazardous chemical oxidants by mechanically exfoliating graphite layers through physical forces, thereby offering a comparatively greener and safer approach [4,5]. Nevertheless, the synthesis of GO via LPE still predominantly depends on commercial graphite as the primary carbon source.

In recent years, there has been a growing shift toward the utilization of biomass, such as basil seeds, wheat straw, rice husks, peanut shells, and other agricultural residues as sustainable and renewable carbon precursors for the production of graphene-based materials [6,7,8]. The LPE technique has demonstrated its capability to convert biomass-derived precursors, for instance rice stem, into graphene-like materials, providing a viable alternative to conventional graphite feedstocks [9]. These developments highlight the necessity for further optimization and advancement of the LPE method to enhance its efficiency, scalability, and applicability in sustainable graphene production.

On the other hand, durian (*Durio zibethinus*), often referred to as the “king of fruits,” is one of the most popular tropical fruits in Southeast Asia, particularly in countries such as Indonesia, Malaysia, and Thailand. With the growing consumption and industrial-scale processing of durian, a substantial amount of durian peel waste is generated annually, accounting for approximately 60-70 % of the total fruit mass [10]. This organic residue is typically discarded in open areas or landfills, leading to environmental problems such as unpleasant odor, methane emission from anaerobic decomposition, and vector attraction [11].

The accumulation of durian peel waste has therefore become a pressing environmental concern in durian-producing regions of Southeast Asia, prompting efforts to valorize this biomass into high-value carbon-based materials. To address this issue, durian peel waste can be valorized through thermochemical conversion, one of which involves transforming it into biochar via controlled thermal treatment at specific temperatures. Previous studies have reported that durian peel waste can be successfully converted into biochar at relatively low temperatures, typically in the range of 300°C to 600°C [12,11]. Biochar derived from organic waste through thermal treatment within this temperature range exhibits significant potential as a sustainable alternative to commercial graphite in the synthesis of graphene oxide (GO) [7]. Its utilization not only reduces reliance on mined graphite but also promotes a more environmentally benign and circular approach to GO production.

To further improve the efficiency of the LPE process, recent studies have investigated the integration of Fe_3O_4 nano-

particles as a complementary exfoliation agent, working synergistically with linear alkylbenzene sulfonate (LAS) to enhance layer delamination and dispersion stability. The shear forces generated by the collision of Fe_3O_4 particles with graphite surfaces synergistically enhance the ultrasonication process and the surface tension reduction effect induced by LAS, promoting more effective exfoliation of graphite layers and leading to improved graphene yield [13,4]. The shear forces induced by Fe_3O_4 are not limited to the exfoliation of graphite layers but have also demonstrated the capability to delaminate other layered materials, such as boron nitride surfaces [14]. This versatility highlights the potential of Fe_3O_4 as an effective exfoliation agent in LPE, particularly in the context of GO synthesis.

Based on the identified research gaps and proposed solutions drawn from previous studies, this work aims to convert graphite derived from durian peel waste via low-temperature pyrolysis into graphene oxide (GO) using a modified liquid-phase exfoliation (LPE) method. The modification involves a synergistic combination of linear alkylbenzene sulfonate (LAS) and Fe_3O_4 to facilitate mechanical delamination of graphite layers under ultrasonic bath irradiation. The crystallinity, defect structure, and morphological characteristics of the synthesized GO will be systematically characterized using X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM).

2. Materials and methods

Durian peels were collected, cleaned, and dried before pyrolysis. The pyrolysis process using a rocket stove reactor was conducted for a total duration of approximately four hours. During the first 30 minutes, the temperature gradually increased from ambient temperature (around 30°C) to approximately 200°C . In the next 15 minutes (at around the 45th minute), the temperature rose further to about 300°C . After one hour of operation, the temperature reached the target 400°C and was maintained at this level. At around 1.5 hours into the process, the release of pyrolysis gas was observed, indicating the active decomposition of the durian peel biomass. The produced pyrolysis gas was self-combusted and used as a supplementary heat source, allowing the external burner to be turned off. The combustible gas continued to evolve for approximately one hour before gradually ceasing, during which the reactor temperature slowly decreased to around 300°C after about 2.5 to 3 hours of processing. Once the pyrolysis gas was depleted, the external burner was reignited and maintained for an additional hour to ensure the completion of the carbonization process, resulting in a total reaction time of around four hours. Similar pyrolysis-based strategies have been reported to yield biochar rich in aromatic domains that can serve as a precursor for further oxidation [15].

A total of 250 mL of distilled water was mixed with 1 mL of linear alkylbenzene sulfonate (LAS) by stirring for 5

minutes at room temperature. Then, 1 gram of durian peel-derived graphite powder was slowly added to the solution and stirred for 30 minutes at room temperature. The resulting mixture was sonicated for 2 hours at 10-minute intervals with 2-minute pauses between each cycle. After sonication, the solution was filtered to separate the precipitate from the liquid. Finally, the filtrate was microwaved until completely dried to obtain graphene oxide (GO) powder. This carbonized material was then subjected to liquid-phase acid treatment, where the introduction of oxygen-containing groups increased the interlayer spacing of the carbon matrix [16]. Subsequently, ultrasonication promoted mechanical exfoliation, separating stacked graphitic layers into nanosheets of GO [17].

Characterization was performed to confirm structural transformation. XRD analysis was employed to identify the emergence of oxidation-related peaks and increased d-spacing, which are typical signatures of GO [18] [10]. Raman spectroscopy was used to detect the D band associated with defects and the G band related to graphitic domains, with the ID/IG ratio serving as an indicator of disorder and successful oxidation [19]. SEM provided direct evidence of morphological transformation, allowing observation of surface wrinkling and layered sheet structures that are characteristic of GO [20].

3. Results and discussion

GO was synthesized from durian peel waste graphite using the LPE method through the synergistic effects of LAS surfactant, Fe_3O_4 , and cavitation. The pyrolysis of organic waste (in this study, durian peel waste pyrolyzed at 400°C) generally produces carbon with an amorphous or turbostratic nature (disordered graphitic structure), as low to intermediate temperature pyrolysis is insufficient to rearrange carbon atoms into a well-ordered crystalline graphite structure, resulting in amorphous carbon being the dominant structure in the initial pyrolysis product [21]. Thus, the incorporation



FIGURE 1. GO sample synthesized with Fe_3O_4 assistance.

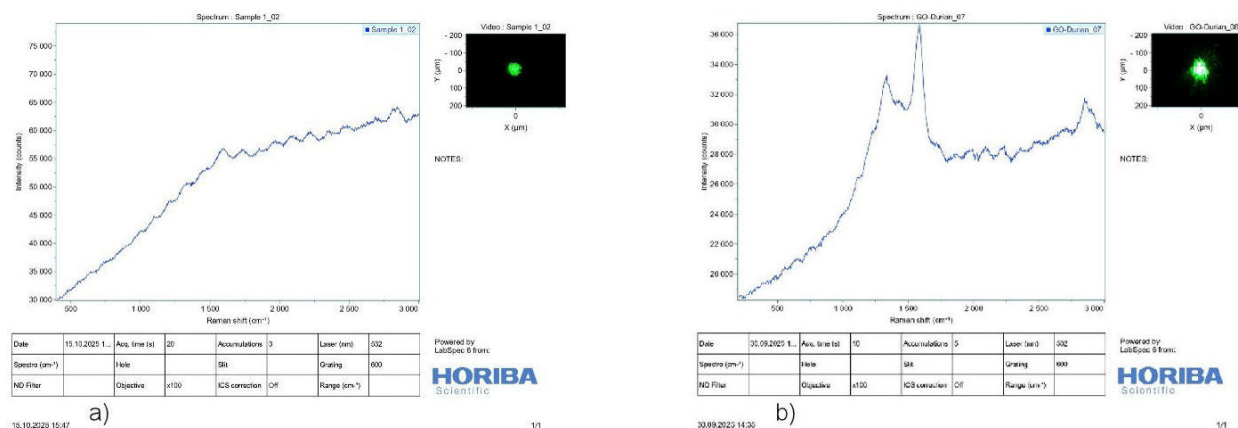


FIGURE 2. Raman spectra of GO: a) GO without Fe_3O_4 assistance and b) GO with Fe_3O_4 assistance.

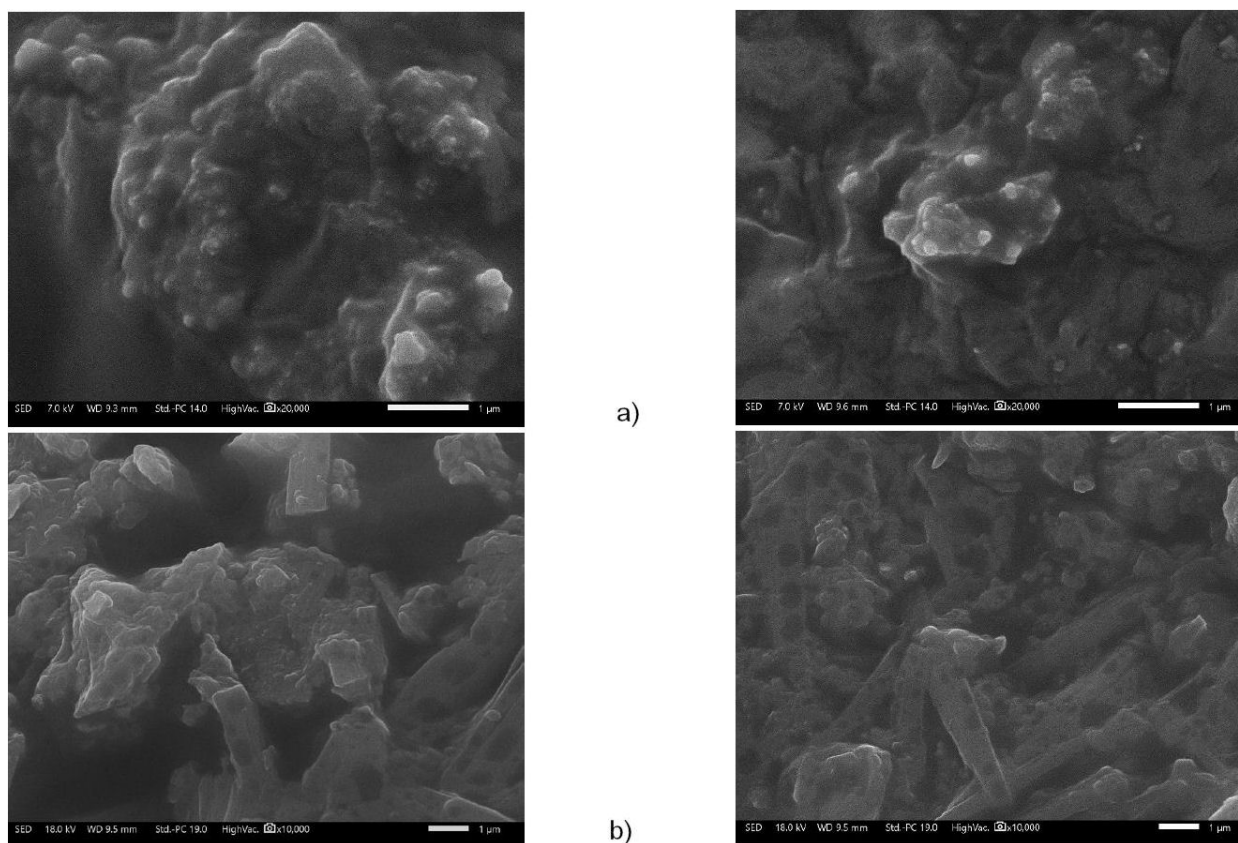


FIGURE 3. SEM images: a) GO without Fe_3O_4 assistance and b) GO with Fe_3O_4 assistance.

of Fe_3O_4 is necessary in the GO synthesis process using the LPE method.

LAS functions to reduce the interlayer tension of graphite, assisted by Fe_3O_4 , which enhances the active surface area and provides magnetic separation capability for individual graphite layers [22,23,24]. LAS interacts with the oxygen-functionalized graphene surface, thereby physically reducing the surface energy of the solution and weakening the van der Waals forces between graphite layers, which consequently lowers the external force required to separate the graphite

layers [22]. The cavitation effect generated by ultrasonication induces vibrations that mechanically separate the durian peel waste graphite layers previously weakened by LAS and Fe_3O_4 [25].

Ultrasonic cavitation originates from the formation of micro-vacuum bubbles within a liquid as a result of elastic pressure fluctuations induced by ultrasonic waves. Subsequently, these bubbles grow until they reach an unstable condition and then collapse implosively, generating high-pressure shock waves and microjets in their surrounding en-

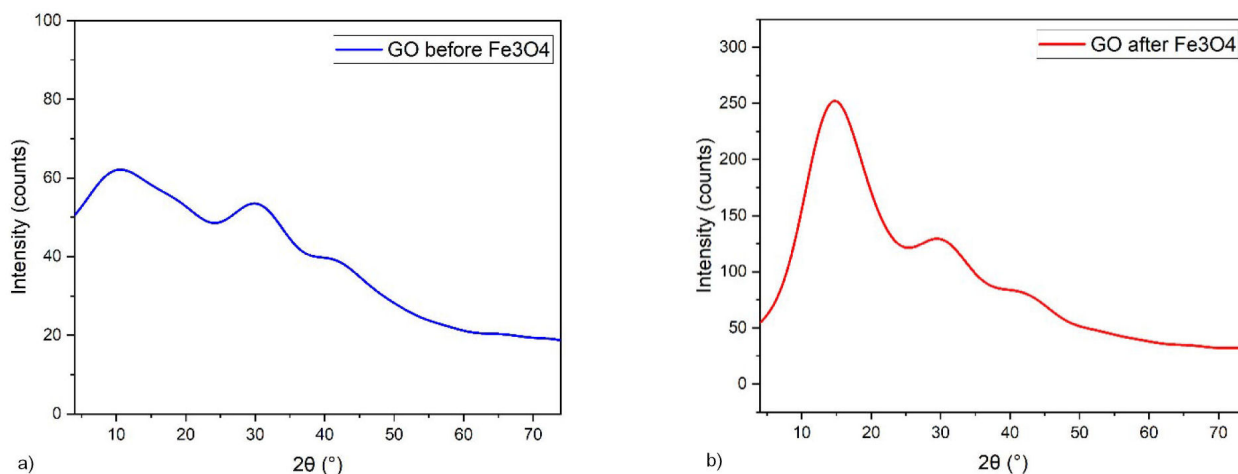


FIGURE 4. XRD diffractograms of GO: a) GO without Fe_3O_4 assistance and b) GO with Fe_3O_4 assistance.

vironment [26]. Importantly, the mechanical energy released during bubble collapse is substantially greater than the van der Waals forces, thereby overcoming the interlayer attractive forces of graphite and mechanically producing thin GO sheets [27].

Moreover, Fe_3O_4 is capable of reducing the surface tension of the solution by 42 % compared to pure water. This enables Fe_3O_4 to modify the local pressure distribution during sonication, such that the collapse of ultrasonically induced bubbles generates shock waves that more effectively disrupt the interlayer interactions of graphite [28]. Therefore, the combined effect of surface tension reduction through the adsorption of LAS and Fe_3O_4 particles, together with the intense mechanical forces generated by ultrasonic cavitation, creates an energetic environment that is physically capable of disrupting the interlayer forces of graphite and facilitating the formation of graphene oxide. Figure 1 presents the GO sample synthesized with the assistance of Fe_3O_4 .

Figure 2 shows the Raman spectra of the GO samples. GO synthesized without Fe_3O_4 assistance [Fig. 2a]) exhibits typical GO characteristics, as indicated by the presence of the D ($\sim 1350 \text{ cm}^{-1}$), G ($\sim 1580 \text{ cm}^{-1}$), and 2D ($\sim 2700 \text{ cm}^{-1}$) bands, with a relatively high $I(\text{D})/I(\text{G})$ ratio suggesting a high degree of oxidation [29]. However, in GO synthesized with Fe_3O_4 assistance [Fig. 2b)], these bands are not clearly observed. This phenomenon may be attributed to dominant Raman signals being masked by sample fluorescence or a high background signal [30].

SEM images (Fig. 3) reveal the morphology of graphite that has begun to exfoliate into GO sheets. A clear morphological difference is observed between GO synthesized without Fe_3O_4 assistance [Fig. 3a)] and GO synthesized with Fe_3O_4 assistance [Fig. 3b)]. The GO without Fe_3O_4 assistance shows initial exfoliation into sheets, but the extent is very limited, whereas the GO synthesized with Fe_3O_4 assistance exhibits more distinct sheet-like structures with relatively symmetrical, irregular rectangular shapes and the presence of several holes on the sheets.

In general, GO morphology is characterized by thin, sheet-like structures that are folded and wrinkled with a non-uniform surface, where wrinkles, folds, and visibly opened interlayer spacing reflect the presence of oxygen-containing functional groups and structural defects formed during the graphite oxidation process, resulting in a large surface area and a non-homogeneous two-dimensional structure [31,32,33,34]. Therefore, it can be concluded that GO synthesized with Fe_3O_4 assistance produces better-exfoliated GO sheets and exhibits a higher degree of oxidation compared to GO synthesized without Fe_3O_4 assistance.

The diffractogram presented in Fig. 4 indicates the absence of the characteristic sharp peak at $2\theta = 26^\circ$, which confirms that the graphite structure has been effectively exfoliated and oxidized to form GO [35]. However, a difference in peak sharpness is observed between the diffractograms in Figs. 4a) and 4b). GO synthesized with Fe_3O_4 exhibits a sharper diffraction peak compared to GO synthesized without Fe_3O_4 . This suggests that GO with Fe_3O_4 possesses a more ordered crystalline structure than GO without Fe_3O_4 [36]. Such peak sharpening occurs when a material consists of relatively large coherent diffraction domains (crystallites) with good lattice ordering, whereas peak broadening or flattening is associated with very small crystallite sizes and/or the presence of lattice strain and structural disorder, which lead to variations in the Bragg angle and broadening of the diffraction profile [37].

4. Conclusion

This study demonstrates that graphene oxide can be synthesized from durian peel waste through a combination of pyrolysis and LPE method. GO was successfully synthesized from durian peel waste graphite using the LPE method through the synergistic effects of LAS surfactant, Fe_3O_4 , and ultrasonic cavitation. Raman analysis confirmed the typical structural features of GO, while the absence of distinct Raman bands in Fe_3O_4 -assisted GO was attributed to fluores-

cence or high background interference. SEM observations revealed that Fe₃O₄ significantly enhanced the exfoliation process, producing more well-defined, sheet-like GO morphologies with characteristic wrinkles, folds, and defects associated with higher oxidation levels.

Furthermore, XRD results demonstrated the disappearance of the graphite peak at $2\theta = 26^\circ$, indicating successful oxidation and exfoliation, with sharper diffraction peaks in Fe₃O₄-assisted GO suggesting improved crystalline ordering. Overall, the incorporation of Fe₃O₄ during LPE effectively promotes graphite exfoliation and oxidation, resulting in GO with superior structural characteristics compared to GO synthesized without Fe₃O₄. The dual outcome of waste

valorization and material innovation makes this route highly promising for future applications in energy storage, catalysis, and environmental remediation.

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Simulation study of laser diode based GaInP/AlGaInP structure

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In this work, we investigate the energy levels and optimization of intrinsic parameters (such as number and width of wells, potential barrier width, refractive index, etc.) and extrinsic parameters (including temperature and pressure) in a laser diode based on the GaInP/AlGaInP structure. The computational techniques employed include the pseudo-empirical potential method to determine the electronic band structures and a graphical method for optimization. Our results are consistent with experimental and theoretical results.

Keywords: Laser diode; semi-conductor; GaInP/AlGaInP; pseudo-potential.

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1. Introduction

AlGaInP laser diodes (LDs) are used in a variety of digital equipment, such as MO/CD/DVD optical pickup units, laser printers and barcode scanners [1]. AlGaInP is a quaternary alloy and involves three binary compounds: GaP, InP and AlP.

The active material for visible light-emitting diodes (LEDs) has long been nitrogen-doped GaP. We shall only take into consideration GaP as the sole indirect-gap semiconductor (with X–L– Γ ordering of the conduction-band minima) that is devoid of Al.

Since it is the substrate for the majority of optoelectronic devices operating at the 1.55 μm communications wavelength, InP is a direct-gap semiconductor of significant technological importance. Among III–V compound semiconductors, AlP is undoubtedly the most “exotic” and least researched because of its large direct band gap.

Among non-nitride III–V semiconductors, the GaInP alloy exhibits some of the largest direct band gaps. Additionally, $\text{Ga}_{0.51}\text{In}_{0.49}\text{P}$ ($E_g = 1.9$ eV at 300 K) is lattice-matched to GaAs, making it a desirable material for wide-band-gap GaAs-based quantum-well devices such as red diode lasers [2].

Extensive studies have been performed on GaInP/AlGaInP structures, including semiconductor disk la-

sers (SDLs) [3], red lasers [4], microdisk lasers for biophotonics applications [5], red light-emitting diodes [6], and laser diodes [7], among others. In this paper, we report a study of the energy levels and the optimization of intrinsic and extrinsic parameters in a laser diode based on the GaInP/AlGaInP structure.

2. Results and Discussions

2.1. Adjustment of the Form Factors of the Three Binary Elements

The form factors (symmetrical and anti-symmetrical) of the various binary compounds (GaP, InP, and AlP) to which the quaternary compound AlGaInP refers are adjusted by the *Zajust* program, based on the nonlinear least-squares method. The injected parameters are iteratively optimized until the mean square root of the variation (RMS) is minimized. Table I illustrates the different types of parameters.

2.2. Electronic Band Structure of the Two Binary Compounds

The energy band structures in wave vector space (K), resulting from the data presented in Table II, for the three binary compounds GaP, InP and AlP are shown in Fig 1.

TABLE I. Form factors and lattice constants of the binary compounds.

Materials	Form Factors						Lattice constant A'	Lattice constant (u.a)
	$V^s(3)$	$V^s(8)$	$V^s(11)$	$V^a(3)$	$V^a(4)$	$V^a(11)$		
GaP	-0.211024	0.030000	0.072296	0.132573	0.070000	0.020000	5.451	10.30103
InP	-0.213877	0.000000	0.075010	0.088777	0.060000	0.030000	5.869	10.090953
AlP	-0.202663	0.040000	0.080000	0.133288	0.0880571	0.015000	5.450	10.3009

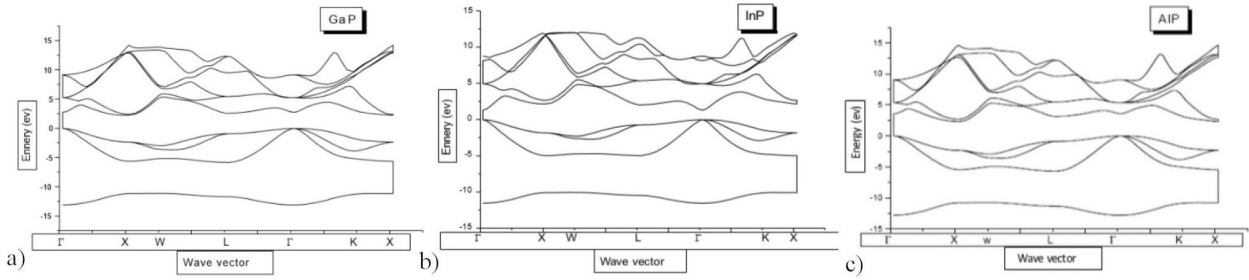
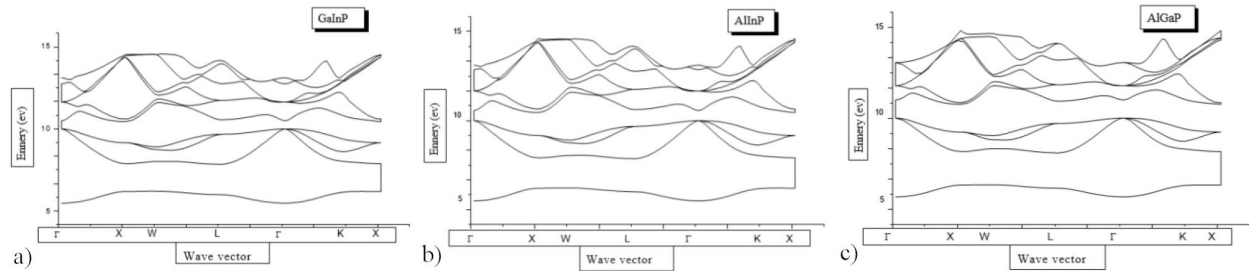


FIGURE 1. Structures of energy bands of GaP, InP and AlP.

TABLE II. Comparison of calculated and experimental energy gaps for the three binary compounds.

Materials	Energy Gaps (eV)					
	E_g^{Γ}		E_g^X		E_g^L	
	Exp, or other theoretical work	Our Simulation	Exp, or another work	Our Simulation	Exp, or another work	Our Simulation
GaP	2,79 ^{a)}	2.77968	2,27 ^{a)}	2.25924	2,70 ^{a)}	2.59957
InP	1,34 ^{b)}	1.34387	2,20 ^{b)}	2.19608	2,04 ^{b)}	2.04482
AlP	3,61 ^{c)}	3.57380	2,31 ^{c)}	2.3095	3,12 ^{c)}	3.12952

a) [5]. b) [9]. c) [10].

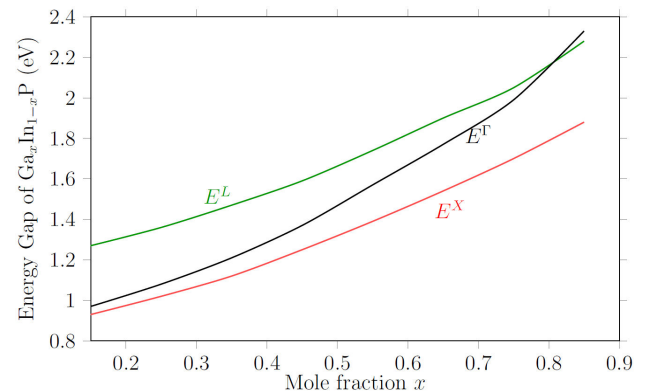
FIGURE 2. Structures of energy bands of Ga_{0,51}In_{0,49}P, Al_{0,51}In_{0,49}P, Al_{0,51}Ga_{0,49}P.

2.3. Electron band structure of the three ternary compounds with disorder

Figure 2 illustrates the energy band structures calculated using (EPM) of the three ternary compounds: Ga_xIn_{1-x}P, Al_xIn_{1-x}P and Al_xGa_{1-x}P, taking into account compositional disorder (but not volume disorder) for $x = 0,51$.

Figure 3 illustrates the variations in energy gaps $E_{\Gamma\Gamma}$, $E_{\Gamma X}$ and $E_{\Gamma L}$ for Ga_xIn_{1-x}P for different x concentration. In this context, where p is the tuning parameter that is deliberately varied, (while setting the composition x to a specific value each time), until the parameters of the Ga_xIn_{1-x}P ternary compound curve approximate experimental results and other theoretical calculations. Two values of the tuning parameter were considered:

- $p = 0$, corresponding to the traditional Virtual Crystal Approximation (VCA).
- $p = 0,65$, corresponding to the improved VCA model.

FIGURE 3. Gaps Ga_xIn_{1-x}P according to x .

The results the calculation oh the variation of the gap $E_{\Gamma\Gamma}$ according to the concentration x .

The calculations of the different energy gaps ($E_{\Gamma\Gamma}^{\Gamma}$, $E_{\Gamma\Gamma}^X$, and $E_{\Gamma\Gamma}^L$) by EPM (not taking into account the disorder ef-

TABLE III. Energy gaps E_g^Γ , E_g^X , E_g^L of $\text{Ga}_x\text{In}_{1-x}\text{P}$ with x ($0 < x < 1$).

Materials	Energy Gaps (eV)		
$\text{Ga}_x\text{In}_{1-x}\text{P}$	E_g^Γ	E_g^X	E_g^L
$x = 0,15$	0.97230	0.92587	1.27417
$x = 0,30$	1.15682	1.08416	1.42010
$x = 0,45$	1.39213	1.27360	1.60079
$x = 0,60$	1.66644	1.48400	1.80635
$x = 0,75$	1.98112	1.71778	2.03737
$x = 0,90$	2.35735	1.98351	2.30736

TABLE IV. Energy gaps E_g^Γ , E_g^X and E_g^L of $\text{Al}_x\text{In}_{1-x}\text{P}$ with x ($0 < x < 1$).

Materials	Energy Gaps (eV)		
$\text{Al}_x\text{In}_{1-x}\text{P}$	E_g^Γ	E_g^X	E_g^L
$x = 0,15$	0.949042	0.92831	1.25342
$x = 0,30$	1.21408	1.08594	1.47164
$x = 0,45$	1.55345	1.2798	1.74500
$x = 0,60$	1.94812	1.49742	2.06038
$x = 0,75$	2.39955	1.73705	2.41441
$x = 0,90$	2.93780	2.01676	2.82808

TABLE V. Energy gaps E_g^Γ , E_g^X and E_g^L of $\text{Al}_x\text{Ga}_{1-x}\text{P}$ with x ($0 < x < 1$).

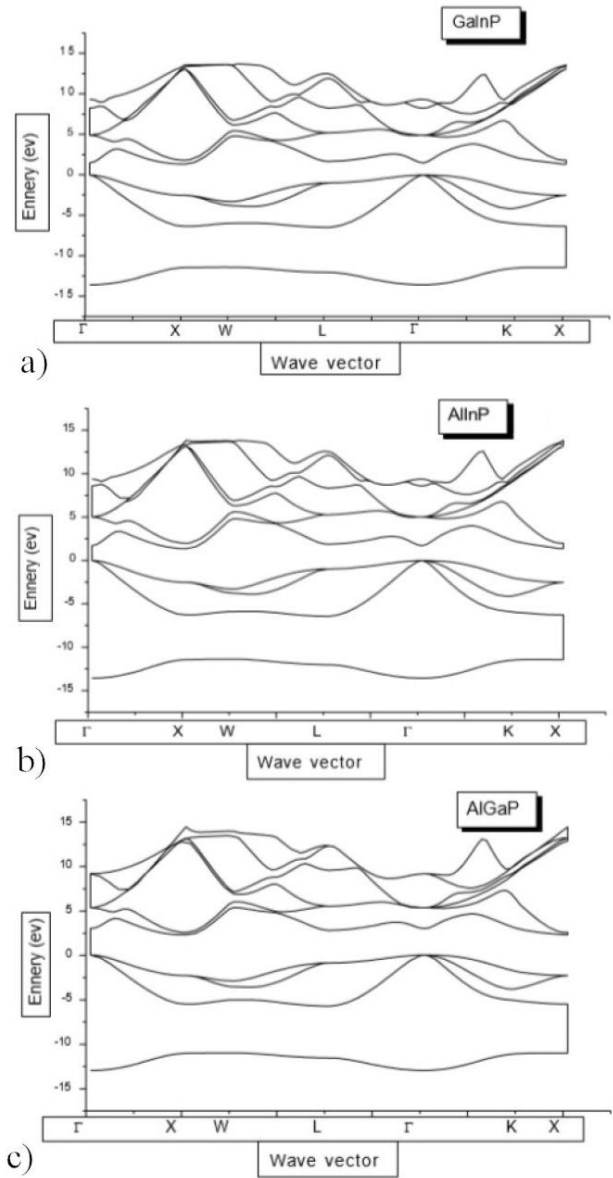
Materials	Energy Gaps (eV)		
$\text{Al}_x\text{Ga}_{1-x}\text{P}$	E_g^Γ	E_g^X	E_g^L
$x = 0,15$	2.75683	2.25742	2.57957
$x = 0,30$	2.83614	2.26369	2.64906
$x = 0,45$	2.93908	2.27138	2.73962
$x = 0,60$	3.05895	2.28026	2.84548
$x = 0,75$	3.19587	2.28865	2.96695
$x = 0,90$	3.35887	2.29798	3.11253

fect), for different gallium concentrations $0 \leq x \leq 1$ of the three ternary alloys: $\text{Ga}_x\text{In}_{1-x}\text{P}$, $\text{Al}_x\text{In}_{1-x}\text{P}$, and $\text{Al}_x\text{Ga}_{1-x}\text{P}$ are given in Tables III, IV and V.

2.4. Electronic Band Structure of the Three Ternaries with Disorder

Figure 4 illustrates the EPM energy band structures of the three ternaries : $\text{Ga}_x\text{In}_{1-x}\text{P}$, $\text{Al}_x\text{In}_{1-x}\text{P}$ and $\text{Al}_x\text{Ga}_{1-x}\text{P}$, taking into account compositional disorder (but not the bulk disorder) for $x = 0,51$.

In Fig. 4a) and 4b), the valence band maximum is the zero energy reference. These two figures show that the maximum

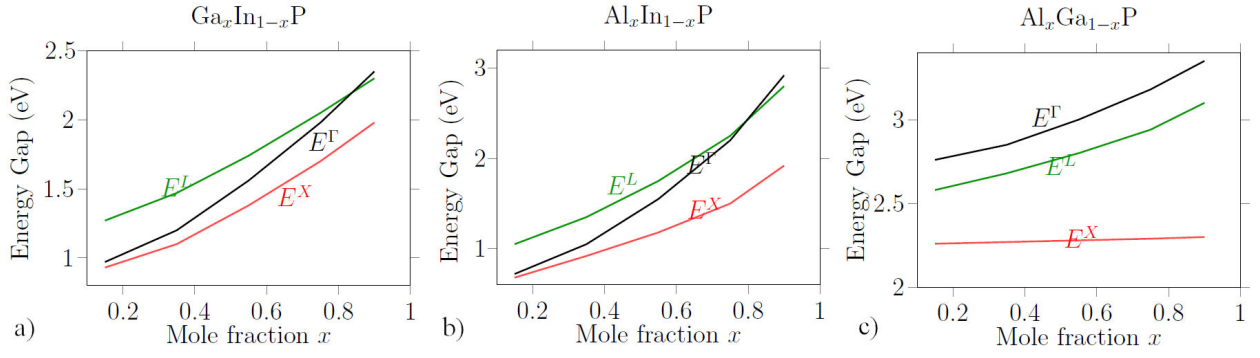
FIGURE 4. Energy band structures: $\text{Ga}_{0,51}\text{In}_{0,49}\text{P}$, $\text{Al}_{0,51}\text{In}_{0,49}\text{P}$ and $\text{Al}_{0,51}\text{Ga}_{0,49}\text{P}$.

of the valence band is at the point Γ that the conduction band minimum is also located at Γ . The ternary alloys $\text{Ga}_{0,51}\text{In}_{0,49}\text{P}$ and $\text{Al}_{0,51}\text{In}_{0,49}\text{P}$ are at direct gap, $E_{\Gamma\Gamma}$.

In Fig. 4c), where the valence band maximum is at point Γ and the conduction band minimum is at point L , the ternary $\text{Al}_x\text{Ga}_{1-x}\text{P}$ alloy is at indirect gap $E_{\Gamma L}$.

Figure 5 illustrates, respectively, the variations in the energy gaps E_g^Γ , E_g^X , and E_g^L for $\text{Ga}_x\text{In}_{1-x}\text{P}$, $\text{Al}_x\text{In}_{1-x}\text{P}$, and $\text{Al}_x\text{Ga}_{1-x}\text{P}$ for different x concentrations.

Polynomial interpolation of the curves representing variations in gaps as a function of concentration x , which gives rise to leading to Eqs. (1)–(9) below:

FIGURE 5. Gaps of $\text{Ga}_x\text{In}_{1-x}\text{P}$, $\text{Al}_x\text{In}_{1-x}\text{P}$ and $\text{Al}_x\text{Ga}_{1-x}\text{P}$ as a function of x .for $\text{Ga}_x\text{In}_{1-x}\text{P}$

$$E_g^\Gamma = 0,834 + 0,773x + 1,017x^2. \quad (1)$$

$$E_g^X(x) = 0,790 + 0,817x + 0,653x^2. \quad (2)$$

$$E_g^L(x) = 1,155 - 0,691x + 0,651x^2. \quad (3)$$

for $\text{Al}_x\text{In}_{1-x}\text{P}$

$$E_g^\Gamma = 0,746 + 1,134x + 1,440x^2. \quad (4)$$

$$E_g^X = 0,795 + 0,788x + 0,630x^2. \quad (5)$$

$$E_g^L = 1,076 + 1,018x + 1,028x^2. \quad (6)$$

for $\text{Al}_x\text{Ga}_{1-x}\text{P}$

$$E_g^\Gamma = 2,695 + 0,339x + 0,439x^2. \quad (7)$$

$$E_g^X = 2,250 + 0,03x + 0,014x^2. \quad (8)$$

$$E_g^L = 2,527 + 0,289x + 0,400x^2. \quad (9)$$

where p is the tuning parameter which is deliberately varied (each time setting the composition x to a precise value) until the curvature parameters of the $\text{Ga}_x\text{In}_{1-x}\text{P}$ sent ternary are

TABLE VI. Energy gap $E_{\Gamma\Gamma}$ as a function of x for classic VCA ($p = 0$): $\text{Ga}_x\text{In}_{1-x}\text{P}$.

x	0.31	0.49	0.52	0.68	0.76	0.91
$E_{\Gamma\Gamma}$	1.538	1.895	1.912	2.197	2.374	2.603

TABLE VII. Energy gap $E_{\Gamma\Gamma}$ as a function of x for improved VCA ($p = 0,65$): $\text{Ga}_x\text{In}_{1-x}\text{P}$.

x	0.31	0.49	0.52	0.68	0.76	0.91
$E_{\Gamma\Gamma}$	1.042	1.354	1.372	1.690	1.922	2.283

TABLE VIII. Energy gap $E_{\Gamma\Gamma}$ as a function of x for improved VCA ($p = 0,36$): $\text{Ga}_x\text{In}_{1-x}\text{P}$.

x	0.31	0.49	0.52	0.68	0.76	0.91
$E_{\Gamma\Gamma}$	1.265	1.597	1.612	1.916	2.125	2.425

close, with reference to experimental and other theoretical calculations. We have taken $p = 0$ (traditional VCA), and $p = 0,65$, $p = 0,36$ (improved VCA), the results of the calculation of the E_g^Γ gap variation with a concentration x are shown in Tables VI, VII and VIII.

The gap variations with a concentration x for the 2 types of VCA (conventional and improved), for $\text{Ga}_x\text{In}_{1-x}\text{P}$ without taking into account the volume effect.

After recording the $E_{\Gamma\Gamma}$ gap, we plotted its variation as a function of concentration x to determine its equation by polynomial interpolation, fit the curves, and thus deduce the curvature parameters c . Figure 6 shows the representative curves of $E_{\Gamma\Gamma}$ gap variation with x fraction for the 2 cases of VCA (conventional and improved) for $\text{Ga}_x\text{In}_{1-x}\text{P}$, polynomial interpolation of the representative curves of $E_{\Gamma\Gamma}$ gap variation with x gave the following polynomial equations:

For classic VCA ($p = 0$):

$$E_{\Gamma\Gamma} = 0,999 + 1,803x + 0,022x^2. \quad (10)$$

For the improved VCA ($p = 0,65$):

$$E_{\Gamma\Gamma} = 0,787 + 0,461x + 1,328x^2. \quad (11)$$

For the improved VCA ($p = 0,36$):

$$E_{\Gamma\Gamma} = 0,882 + 1,059x + 0,725x^2. \quad (12)$$

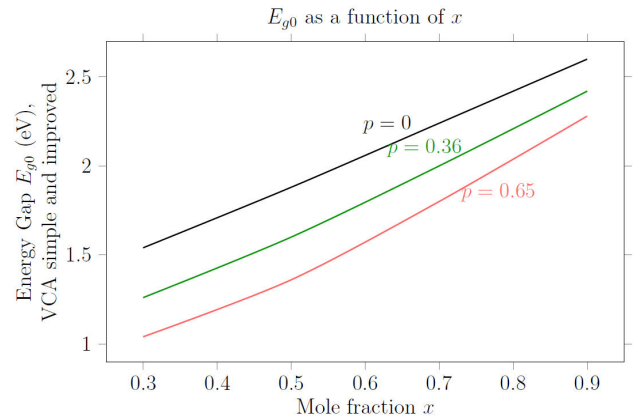
FIGURE 6. Gap versus x curves $E_{\Gamma\Gamma}$: conventional and improved VCA, for $\text{Ga}_x\text{In}_{1-x}\text{P}$.

TABLE XIX. Compares the calculated and measured $E_{\Gamma\Gamma}$ curvature parameters of $\text{Ga}_x\text{In}_{1-x}\text{P}$.

Our curvature parameter calculated by:	Result of other works
EPM and VCA classic ($p=0$) : -0,022	-0,07 ^d
EPM and VCA enhanced ($p=0,65$) : 1,328	-
EPM and VCA enhanced ($p=0,36$) : 0,725	0,72 ^d ($p=0,22$)

^d[11].

These $E(x)$ equations are of the form $a + bx + cx^2$, where c represents the curvature parameter of $\text{Ga}_x\text{In}_{1-x}\text{P}$. Table XIX compares the calculated and measured $E_{\Gamma\Gamma}$ curvature parameters of $\text{Ga}_x\text{In}_{1-x}\text{P}$, clearly showing that for $p = 0,36$ Eq. (12), the $\text{Ga}_x\text{In}_{1-x}\text{P}$ gap is one curvature parameter and close to the experimental.

2.5. Electronic band structure of $\text{Al}_x\text{Ga}_y\text{In}_{1-x-y}\text{P}$ without orders

Figure 7 illustrates the energy band structure by EPM of $\text{Al}_x\text{Ga}_y\text{In}_{1-x-y}\text{P}$ taking into account no compositional disorder (but not volume disorder) for $y = 0,3$.

Calculations of the different energy gaps (E_g^Γ , E_g^X , E_g^L) by EPM (not taking into account the disorder effect) for dif-

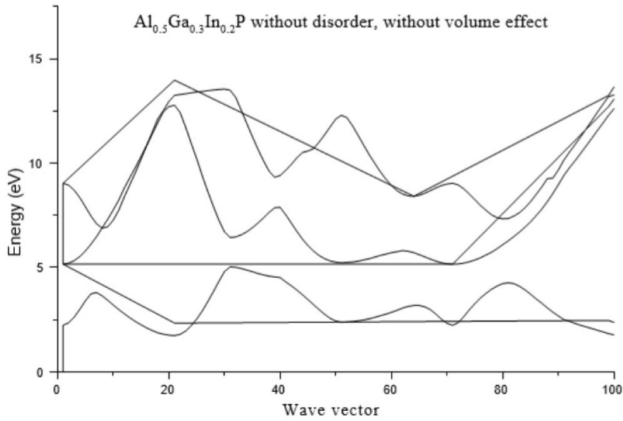


FIGURE 7. Energy band structures: $\text{Al}_{0,5}\text{Ga}_{0,3}\text{In}_{0,2}\text{P}$.

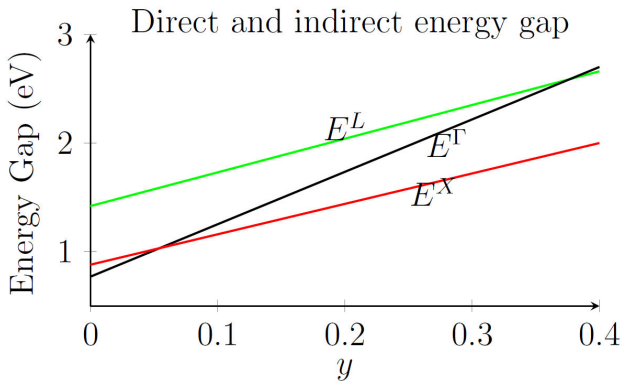


FIGURE 8. Gaps of $\text{Al}_{0,5}\text{Ga}_y\text{In}_{0,5-y}\text{P}$ as a function of y . Different concentrations $0 \leq y \leq 0,4$ of the quaternary alloys $\text{Al}_{0,5}\text{Ga}_y\text{In}_{0,5-y}\text{P}$ are given in Table X.

Figure 8 shows the respective variations in energy gaps for $\text{Al}_{0,5}\text{Ga}_y\text{In}_{0,5-y}\text{P}$, for different y concentrations.

Polynomial interpolation of the curves representing variations in gaps as a function of concentration y , which gives rise to the following equations,

$$E_g^\Gamma = 0,771 + 4,988y + 0,383y^2, \quad (13)$$

$$E_g^X = 0,879 + 2,945y + 0,383y^2, \quad (14)$$

$$E_g^L = 1,409 + 3,395y + 0,258y^2. \quad (15)$$

We conclude that the improved VCA used to calculate the gap curvature parameter of $\text{Ga}_x\text{In}_{1-x}\text{P}$ gives good results that are in almost total agreement with those obtained from experiment, which is not the case with the classical VCA, which does not faithfully reflect the results of these parameters.

Optimization of intrinsic and extrinsic physical parameters of structures $\text{Ga}_x\text{In}_{1-x}\text{P}/\text{AlGaInP}$.

2.6. Optimization using the graphical method

2.6.1. Mesh mismatches and well constraints

Based on the matching condition between the materials of the active layers in the $\text{Ga}_x\text{In}_{1-x}\text{P}$ quantum-well laser structure on the AlGaInP substrate, illustrated in Fig. 9, the evolution of $\Delta a/a_{\text{AlGaInP}}$ (quantifying the constraint in %) with the gallium (Ga) concentration for the $\text{Ga}_x\text{In}_{1-x}\text{P}$ structure is such that:

$$\frac{\Delta a}{a_{\text{AlGaInP}}} = \frac{-0,4182x + 0,243}{5,626}, \quad (16)$$

of $\text{Ga}_x\text{In}_{1-x}\text{P}/\text{Al}_{0,38}\text{Ga}_{0,21}\text{In}_{0,41}\text{P}$.

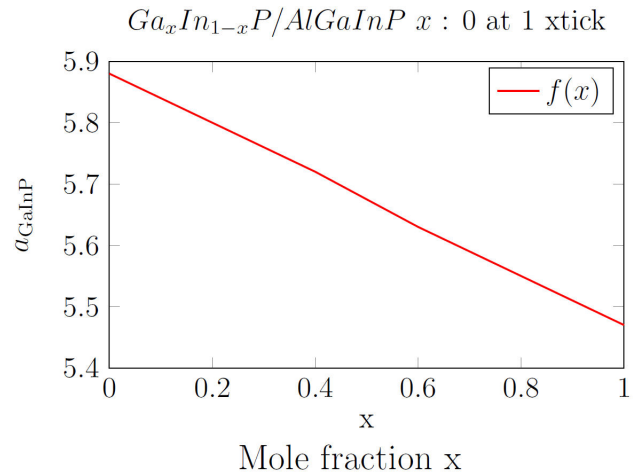
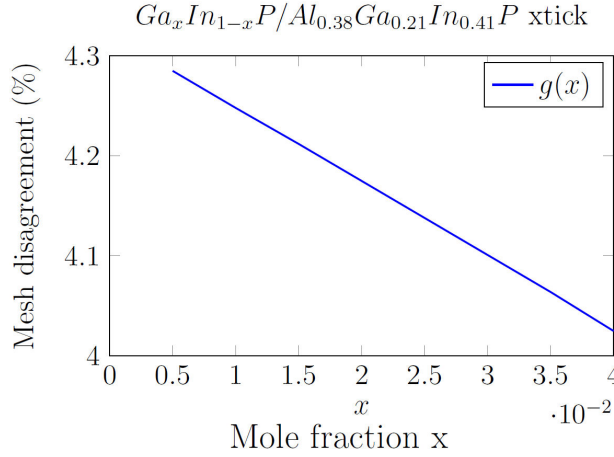


FIGURE 9. GaInP on AlGaInP matching condition.

TABLE X. Energy gaps E_g^{Γ} , E_g^X , E_g^L as a function of concentration y : $\text{Al}_{0.5}\text{Ga}_y\text{In}_{0.5-y}\text{P}$.

y	0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4
E_g^{Γ}	0.7723	1.0209	1.2676	1.5121	1.7548	1.9955	2.2344	2.4712	2.7062
E_g^X	0.8794	1.0261	1.1715	1.3156	1.4584	1.5999	1.7400	1.8788	2.0162
E_g^L	1.4103	1.5785	1.7435	1.9052	2.0636	2.2187	2.3704	2.5189	2.6640

FIGURE 10. $\Delta a/a_{\text{AlGaInP}}$ as a function of x ($\text{Ga}_x\text{In}_{1-x}\text{P}$).

2.6.2. Wave length

We will calculate the wavelength emitted by the diode using the ternary $\text{Ga}_x\text{In}_{1-x}\text{P}$ as an active layer (for $x = 0.5$), and the quaternary $\text{Al}_{0.31}\text{Ga}_{0.21}\text{In}_{0.48}\text{P}$ as a barrier. We also study the influence of temperature on the emission wavelength for a given well width.

a) Wavelength as a function of well width

A quantum-well laser is obtained when the active region has a dimension of less than 20 nm (the well width) [10].

We have the following equation, which gives the wavelength as a function of the quantum well width (L_z) [9]:

$$\lambda_n = \frac{1.24}{E_g + E_{cn} + E_{vn}} (\mu\text{m}), \quad (17)$$

E_{cn} and E_{vn} are given by the following approximate equations,

$$E_{cn} = (n+1) \frac{\Pi}{\sqrt{2m_c} L}, \quad (18)$$

$$E_{vn} = (n+1) \frac{\Pi}{\sqrt{2m_v} L}. \quad (19)$$

Figure 11 shows that the wavelength increases with the width of the well. This increase is very rapid at first, then becomes slower and slower, until it reaches zero. Thus, when the well width increases from 9 to 10 nm, the wavelength increases by only 0.25 %. So a well width of 9 nm can be used satisfactorily for a wavelength greater than 604 nm.

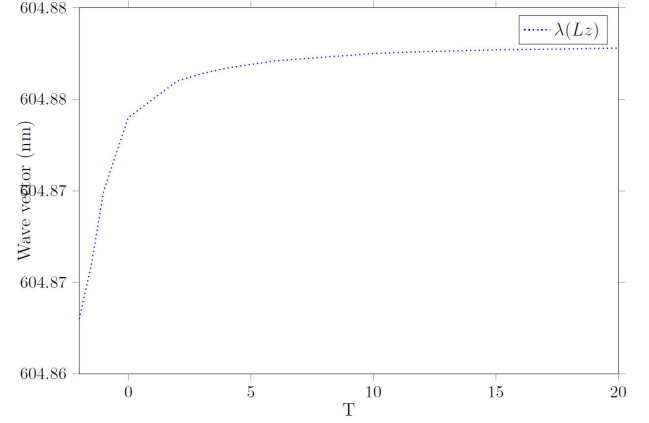


FIGURE 11. Wavelength variation as a function of well width for gallium concentrations in the active layer.

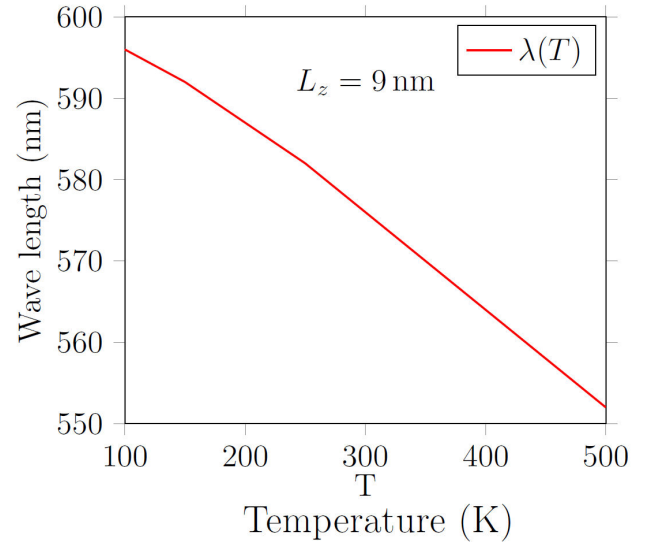


FIGURE 12. Wavelength variation as a function of temperature.

b) Wavelength as a function of temperature

Since temperature affects the energy gap, it also has an influence on wavelength. To study this influence, we use the VARSHNI model.

Figure 12 shows that wavelength decreases significantly with temperature. When the temperature rises from 100 to 400 K, the wavelength decreases by only 2.45 %, so the influence of temperature is remarkable.

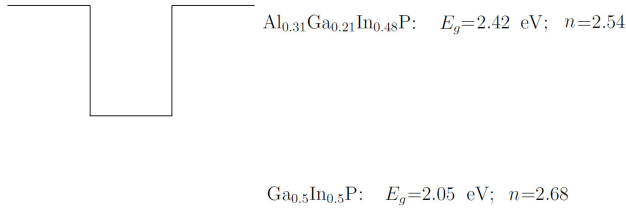


FIGURE 13. Represents the structure with their gap and refractive index.

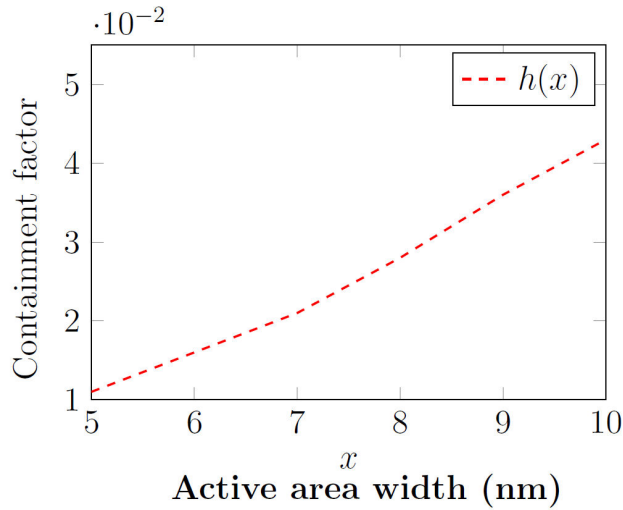


FIGURE 14. Change of the confinement factor as a function of the width of the active zone.

2.6.3. 2.6.3 Containment factor Γ

We will calculate the confinement factor for the quantum well structure. We will use the Ga_{0.5}In_{0.5}P ternary as an active layer and the Al_{0.31}Ga_{0.21}In_{0.48}P quaternary as a barrier for the following structure (Fig. 13).

a) Confinement factor as a function of well width

Figure 14 shows that the confinement factor of a quantum well threshold structure increases with the well width.

We also note a weak growth of the confinement factor with the aluminum content in the barrier. Note that all the values of the confinement factor are low (max 4 % for 10 nm).

2.6.4. Gain maximal

The maximum gain will be studied as a function of several parameters such as well width, carrier density, temperature, wavelength for the previous structure (Fig. 13).

a) Maximum gain with a carrier density

The gain increases with the carrier density (Fig. 15). Note that the gain becomes positive and increases from a density

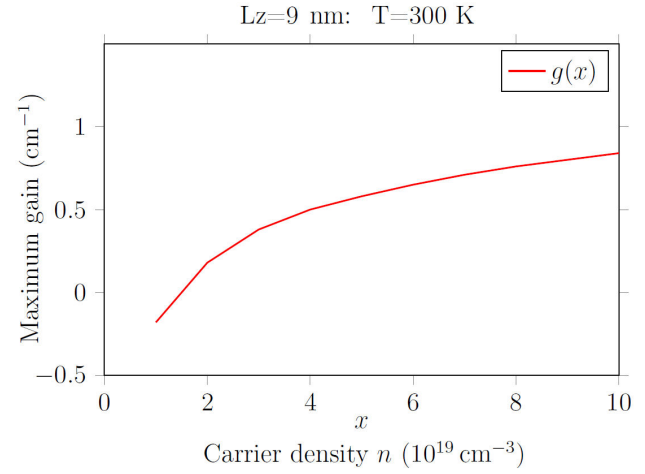


FIGURE 15. Change of maximum gain with an injection.

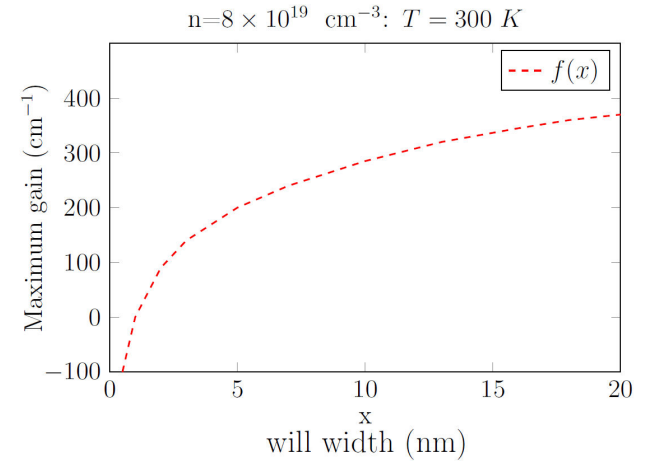


FIGURE 16. Change of maximum gain with a well width.

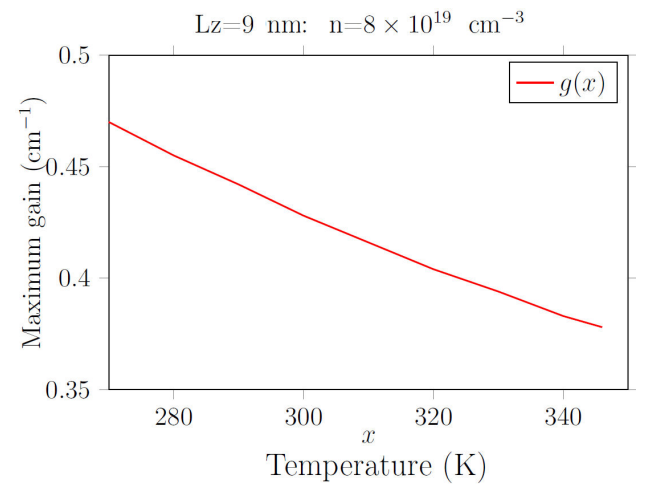


FIGURE 17. Change of maximum gain with a temperature.

equal to $2,858 \times 10^{18} \text{ cm}^{-3}$, which is the transparency density. Remember that transparency density corresponds to zero gain.

b) Maximum gain as a function of well width

Max gain increases with well width (Fig. 16). From a well width equal to 1 nm, this gain is positive.

c) Maximum gain as a function of temperature

Figure 17 shows that temperature has a slight but negative influence on the maximum gain. When the temperature increases from 200 to 300, the maximum gain increases by only 0.5 %, so the influence of temperature is negligible.

3. Conclusion

Using the empirical pseudo potential method (EPM) in conjunction with the virtual crystal approximation (VCA), we have examined the electrical characteristics of the $\text{Ga}_x\text{In}_{1-x}\text{P}$ alloy both with and without accounting for the effects of compositional disorder. Overall, there is good agreement between our findings and the experimental values. The studied material turns out to be a direct bandgap semiconductor for $x < 0,78$ and an indirect bandgap semiconductor for $x > 0,78$. We have calculated the confinement factor for a single quantum well structure. The values obtained are low, and the confinement factor increases with the well width. In

the study of the maximum gain, we have found the optimal values relating this maximum gain to the well width. We have also studied the change of the maximum gain with the current density. The maximum gain also depends on the temperature. Finally, this theoretical study allowed us to determine the optimal values for a GaInP/AlGaInP -based quantum well laser.

Declaration of competing interests:

No financial interests or personal relationships that may have influenced the work presented in this article.

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The data are available from the corresponding author.

Funding Declaration:

None

Research involving human and animal rights

The article adheres to the ethical principles of the journal and does not contain results of studies involving humans and/or animals.

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Electrical response of a soil microbial fuel cell under CoCl_2 -induced chemical perturbations

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Soil microbial fuel cells (SMFCs) are bioelectrochemical systems capable of generating electrical signals from microbially mediated oxidation processes occurring within the soil matrix. This study evaluates the electrical response of a soil microbial fuel cell (SMFC) subjected to controlled chemical perturbations induced by cobalt chloride (CoCl_2). SMFC microcosms were established under four treatments: control, low (50 mg), medium (100 mg), and high (200 mg) CoCl_2 , with four replicates per treatment. Soil physicochemical parameters, including pH, conductivity, moisture, and nutrient content, were monitored together with voltage and current outputs. CoCl_2 addition produced transient soil acidification and increased ionic strength. Current exhibited strong sensitivity to these changes, whereas voltage remained comparatively stable. Spearman correlation analysis revealed a consistent negative relationship between current and soil pH, identifying pH as the dominant controlling variable. A theoretical electrochemical framework confirmed that CoCl_2 acts as a chemical modulator rather than an electron source. These results highlight the potential of SMFCs as responsive bioelectrochemical indicators of soil chemical dynamics.

Keywords: Soil microbial fuel cells; electrochemical perturbation; cobalt chloride; soil pH dynamics; bioelectrochemical response.

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1. Introduction

Soil microbial fuel cells (SMFCs) are bioelectrochemical systems capable of converting part of the chemical energy stored in soil organic matter into electrical energy through the metabolic activity of soil microorganisms. In these systems, organic compounds naturally present in the soil matrix, including the partially decomposed organic matter, are oxidized by electroactive microorganisms in the anode zone. This process releases electrons that are transferred through an external circuit toward a cathodic electron acceptor, typically oxygen, enabling continuous electricity generation driven by microbial metabolism within the soil environment. Although early developments of microbial fuel cells were largely focused on plant-associated configurations, the fundamental electrochemical principles described in these studies are directly applicable to soil-based SMFC systems [1–3].

Unlike conventional microbial fuel cells operated with liquid electrolytes, SMFCs function within heterogeneous and dynamic soil environments, where physicochemical condi-

tions vary temporally and spatially. As a consequence, the electrical output of SMFCs is strongly influenced by soil properties such as pH, moisture, temperature, ionic conductivity, and nutrient availability. These variables affect microbial activity, proton transport, internal resistance, and extracellular electron transfer pathways, all of which are strongly governed by the structure and functional dynamics of the microbial community. Comprehensive reviews on plant microbial fuel cells have highlighted the central role of electroactive microorganisms and their interaction with environmental conditions in regulating system performance [4, 5]. Although PMFC configurations differ from soil-only systems, the underlying microbial electrogenic mechanisms are shared across bioelectrochemical platforms.

Among these factors, pH has been identified as a key parameter governing the performance of bioelectrochemical systems. Variations in pH influence microbial metabolism, proton accumulation near the anode, and electrochemical losses associated with polarization phenomena. Similarly, soil conductivity controls ionic transport between electrodes and

contributes to the overall ohmic resistance of the system. Consequently, changes in soil chemical conditions often lead to pronounced fluctuations in current, whereas voltage typically exhibits a more buffered response due to thermodynamic constraints imposed by electrode potentials [3].

Although the power density achieved by SMFCs remains low compared with conventional renewable technologies such as photovoltaic systems, their relevance lies in applications requiring ultra-low power levels. Recent studies have demonstrated the feasibility of coupling SMFCs with energy harvesting and power management circuits to operate autonomous sensors, positioning these systems as promising platforms for long-term, self-powered environmental monitoring [6, 7].

Beyond energy harvesting, SMFCs have been proposed as sensitive bioelectrochemical indicators of environmental disturbances. Chemical inputs, nutrient amendments, or ionic stressors can modify the structure of the microbial community and metabolic pathways, resulting in detectable changes in electrical signals. In particular, dissolved ions and metal species have been reported to influence extracellular electron transfer mechanisms and biofilm behavior in microbial electrochemical systems, even when these species do not participate directly in redox reactions [8, 9].

Cobalt chloride (CoCl_2) is a highly soluble salt that readily dissociates in aqueous environments into Co^{2+} and Cl^{1-} ions, producing transient changes in ionic strength and soil acidity. Although CoCl_2 is not an electron donor for microbial fuel cells, its addition can indirectly alter soil chemical conditions by modifying pH, ionic strength, and microbial stress responses. Such characteristics make CoCl_2 a useful agent for inducing controlled chemical perturbations in soil systems.

Despite growing interest in SMFCs, experimental studies quantifying the relationship between soil physicochemical parameters and electrical output under chemically perturbed conditions remain limited. In particular, the identification of the variables that most strongly govern current and voltage behavior under different levels of ionic stress is still poorly understood.

Therefore, the objective of this study is to evaluate the electrical response of a soil-based SMFC subjected to increasing concentrations of CoCl_2 , with particular emphasis on the temporal evolution of soil pH and its relationship with current and voltage generation. By combining continuous electrical measurements with physicochemical monitoring and correlation analysis, this work seeks to identify the main variables associated with SMFC performance under controlled chemical perturbation and to examine the differential sensitivity of current and voltage as indicators of bioelectrochemical activity.

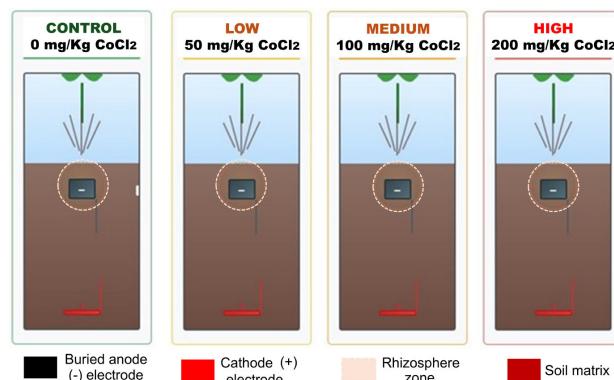


FIGURE 1. Schematic representation of the SMFC configuration used in this study, showing the soil matrix, buried anode, and cathode. CoCl_2 treatments (control, low, medium and high concentrations) were applied to induce controlled chemical perturbations of the soil environment.

2. Materials and methods

2.1. Experimental design and SMFC configuration

The experiment was conducted using SMFC established in individual pots under controlled laboratory conditions. Each SMFC is equipped with a pair of metallic electrodes acting as the anode and cathode. The anode was fabricated from a 3 m long copper wire arranged in a spiral configuration, covering an effective circular area of approximately $78,5 \text{ cm}^2$. The copper wire is inserted into a flexible plastic tube. The cathode consisted of a zinc electrode with an exposed surface area of 100 cm^2 . Both electrodes were embedded within the soil matrix and positioned at a fixed separation distance of 5 cm. Both electrodes were connected to allow periodic electrical measurements under open-circuit and short-circuit conditions. The SMFC configuration was identical for all treatments, ensuring that observed differences in electrical response were exclusively attributable to chemical perturbations rather than to geometric or material variability (Fig. 1).

2.2. CoCl_2 treatments and experimental conditions

Cobalt chloride ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, 98 % purity; Faglab) was selected as a highly soluble inorganic salt capable of inducing controlled, transient chemical perturbations in soil via ionic dissociation. Four experimental treatments were established: a control without CoCl_2 addition, a low-concentration treatment (50 mg CoCl_2), a medium-concentration treatment (100 mg CoCl_2), and a high-concentration treatment (200 mg CoCl_2) (as seen in Fig. 1). Reagent quantities were accurately weighed using an analytical balance (PA214C, OHAUS, Parsippany, NJ, USA). The external working humidity and temperature were 79 % and $T = 24\text{--}26^\circ\text{C}$, respectively. The sixteen SMFCs were the total result of each treatment being replicated four times.

Prior to application, CoCl_2 was dissolved in water and uniformly distributed within the soil of each pot to minimize

spatial heterogeneity. Upon dissolution, CoCl_2 dissociates into Co^{2+} and Cl^{1-} ions, increasing soil ionic strength and promoting transient acidification. All soil matrices were maintained under identical environmental conditions throughout the experiment. Soil was irrigated with 250 mL of water per pot on a weekly basis, for 4 months.

2.3. Physicochemical measurements

Soil physicochemical conditions were monitored continuously throughout the experimental period using *in situ* measurements. Data acquisition was performed with a portable multiparametric soil probe integrating simultaneous sensors for temperature, volumetric moisture content, electrical conductivity (EC), pH, and macronutrient availability (potassium (K), nitrogen (N), phosphorus (P)). The probe *portable 8-in-1 soil parameter detector (USB-C type, commercial device)* was interfaced with a mobile device, and measurements were recorded and visualized in real time via a dedicated smartphone application (*Soil Parameter Detector*), which stored the acquired data in comma-separated values (CSV) format for subsequent processing and analysis.

Soil pH was measured directly in the soil solution, as it constitutes a key variable influencing microbial metabolism and electrochemical behavior. Electrical conductivity was monitored to track changes in ionic strength associated with CoCl_2 dissociation. Nutrient concentrations were used to evaluate potential links between microbial activity and electrical output.

2.4. Electrical measurements

Voltage and current generated by each SMFC were measured once per day over a period of 106 consecutive days (approximately three months) using a calibrated digital multimeter (Fluke Corporation, USA). Open-circuit voltage (OCV) was measured directly across the electrodes. Short-circuit current (I_{SC}) was determined by directly connecting the electrodes through the ammeter function of the multimeter, effectively imposing negligible external resistance. Electrical measurements were systematically recorded and subsequently analyzed as time series to capture transient responses associated with chemically induced perturbations.

2.5. Data preprocessing and statistical analysis

Raw experimental data were organized by treatment, replicate, and time. To avoid pseudoreplication arising from high-frequency measurements, daily mean values were calculated for each replicate prior to statistical analysis.

Descriptive statistics, including mean and standard deviation, were computed to summarize temporal trends and treatment-level variability. Heatmaps were constructed to visualize heterogeneity among replicates and to identify periods of enhanced electrical activity.

Correlation analyses were performed using Spearman's rank correlation coefficient (ρ), selected due to the non-

normal distribution of several variables and the monotonic relationships expected between physicochemical parameters and electrical outputs. Correlations were evaluated independently for each treatment, and statistical significance was assessed using a threshold of $p < 0,05$. All data processing, statistical analyses, and graphical representations were conducted using MATLAB (MathWorks, USA), ensuring full reproducibility of the analytical workflow.

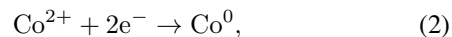
2.6. Theoretical electrochemical framework associated with CoCl_2 addition

To contextualize the magnitude of the electrical response observed in the SMFC system, a theoretical electrochemical framework was considered based on the amount of CoCl_2 added to the soil. This analysis does not imply that cobalt chloride acts as an electron donor within the SMFC; instead, it provides an upper theoretical limit for the charge that could be associated with the applied compound under hypothetical electrochemical conditions [10].

Cobalt chloride readily dissociates in aqueous environments according to:



Under soil conditions, neither Co^{2+} nor Cl^{1-} are expected to undergo spontaneous redox reactions that directly release electrons. However, assuming a hypothetical complete electrochemical reduction of cobalt ions,



each mole of CoCl_2 would correspond to a maximum of two moles of electrons. The total theoretical charge Q can thus be estimated as:

$$Q = n_e F, \quad (3)$$

where n_e is the number of moles of electrons and F is Faraday's constant (96485 C mol^{-1}).

This framework provides an upper bound that contextualizes the order of magnitude of the measured currents and reinforces the interpretation of CoCl_2 as a chemical modulator rather than an electrochemical fuel.

3. Results

3.1. Chemical perturbation induced by CoCl_2 addition

The addition of cobalt chloride generated clear and reproducible chemical perturbations in the soil system. Temporal monitoring of soil pH and electrical conductivity revealed an immediate response following CoCl_2 application, characterized by transient acidification and increased ionic strength (Fig. 2).

All treatments receiving CoCl_2 exhibited a marked decrease in pH during the initial experimental phase, whereas the control treatment remained comparatively stable. This

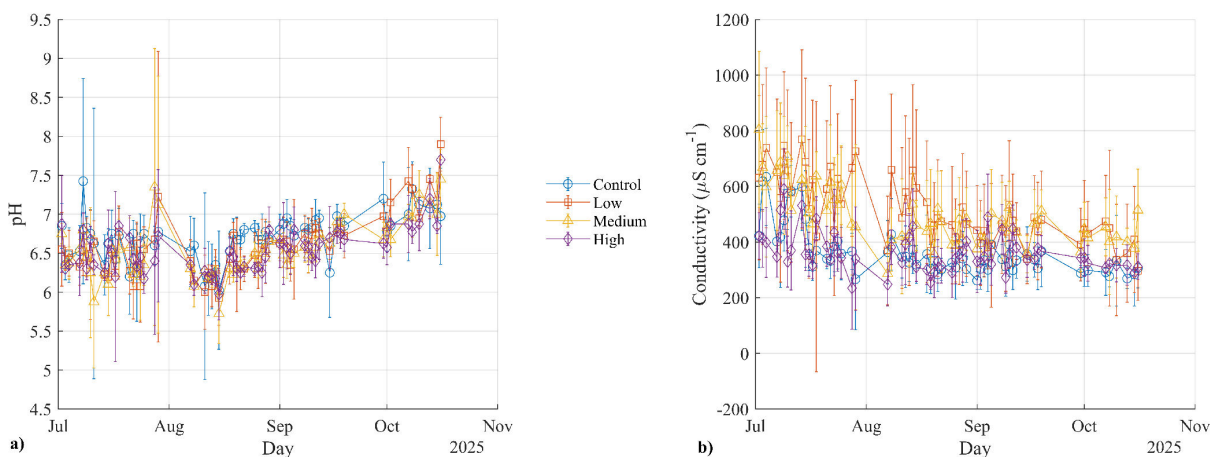


FIGURE 2. Temporal evolution of soil a) pH and b) electrical conductivity for the different CoCl_2 treatments.

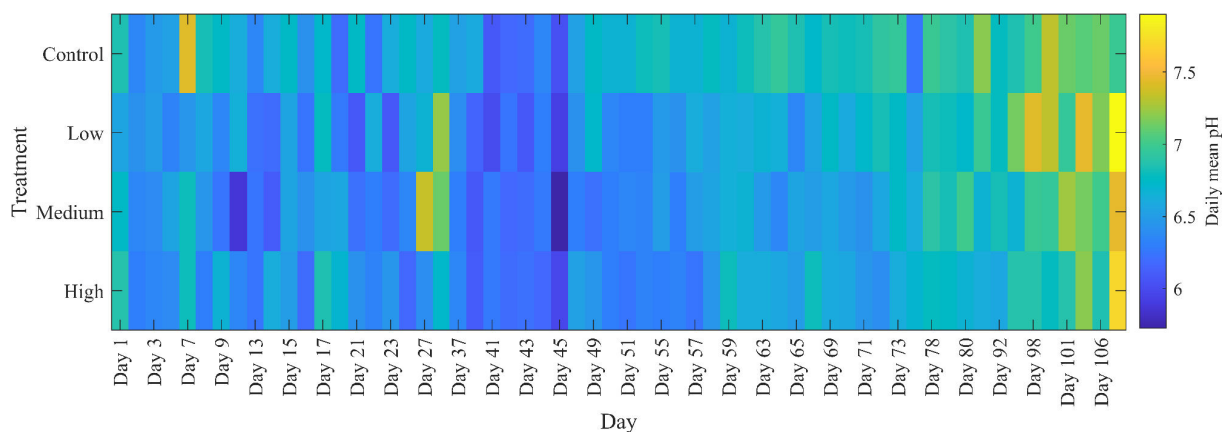


FIGURE 3. Heatmap showing temporal variability across replicates for soil pH under different CoCl_2 treatments. Color intensity reflects normalized values.

acidification was transient, with pH values progressively recovering toward near-neutral conditions within several days. The temporal behavior was consistent among replicates, as evidenced by the pH heatmap (Fig. 3), indicating that the chemical response was primarily driven by the applied salt rather than stochastic variability.

Soil electrical conductivity increased proportionally with CoCl_2 concentration, with the highest values observed under the high-dose treatment. Conductivity fluctuations were most pronounced during the early stage of the experiment and subsequently stabilized, suggesting the establishment of a new ionic equilibrium within the soil matrix. Together, these results confirm that CoCl_2 addition induces a short-term but measurable modification of soil chemical conditions, providing the initial perturbation to which the SMFC system responds.

3.2. Electrical response of the SMFC system to chemical perturbation

The chemical perturbations described above were translated into a measurable electrical response of the SMFC system. Temporal profiles of current and voltage are shown in Fig. 4.

I_{SC} exhibited pronounced variability during the early experimental phase, particularly in treatments containing low and medium CoCl_2 concentrations. Periods of elevated current coincided temporally with the phase of reduced pH and increased conductivity. In contrast, the control treatment showed comparatively stable current levels throughout the monitoring period.

Voltage displayed a distinct behavior. Although slight temporal fluctuations were observed, voltage values remained within a narrower range compared with current, indicating a more buffered electrical response. The heterogeneity of current generation across time and replicates is further illustrated in the current heatmap (Fig. 5), where localized periods of enhanced electrical activity were observed, particularly under chemically perturbed conditions. These patterns confirm that the SMFC system responds dynamically to changes in soil chemistry rather than maintaining a constant electrical output.

3.3. Distribution of electrical outputs among treatments

The distribution of daily mean current and voltage values across treatments is summarized in Fig. 6. Current distribu-

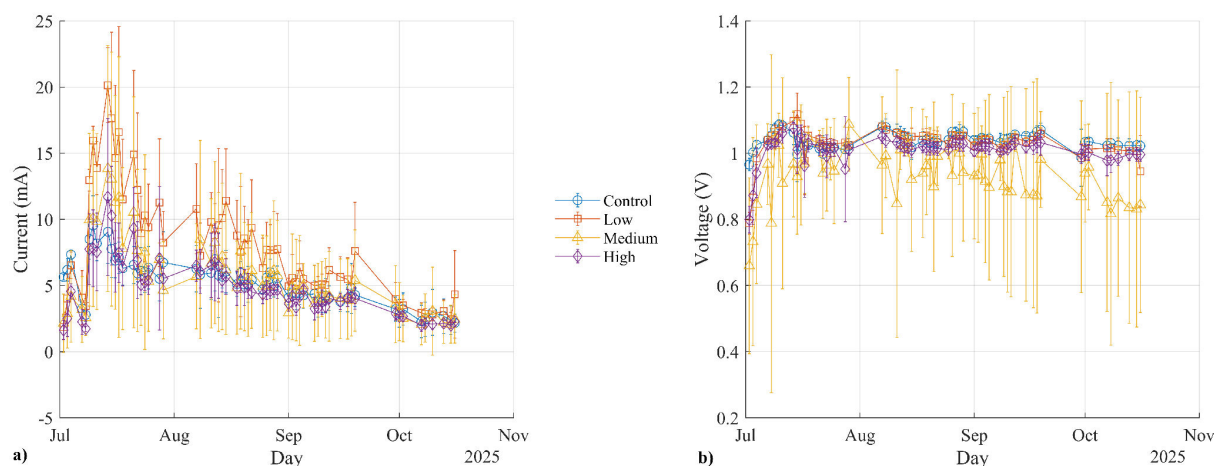


FIGURE 4. Temporal evolution of a) current, and b) voltage for the different CoCl_2 treatments. Shaded areas indicate the initial perturbation phase following salt addition.

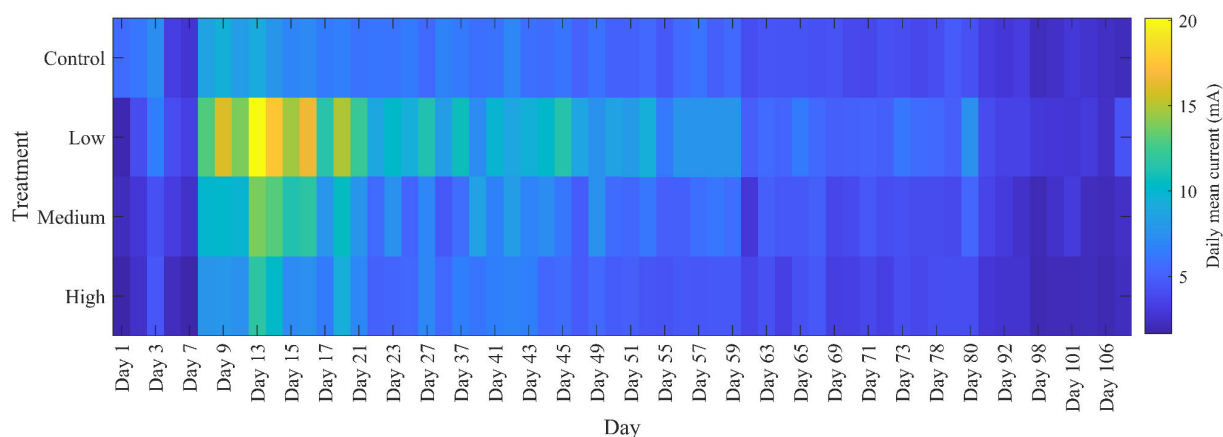


FIGURE 5. Heatmap showing temporal variability across replicates for current generation under different CoCl_2 treatments. Color intensity reflects normalized values.

tions differed among treatments, with broader interquartile ranges observed under low and medium CoCl_2 concentrations. These distributions indicate higher variability in current generation when the system was exposed to moderate chemical perturbation.

In contrast, the high-concentration treatment exhibited a narrower current distribution, suggesting a constrained electrical response at elevated CoCl_2 levels. Voltage distributions were comparatively more uniform across treatments, with substantial overlap observed among all conditions. This reinforces the observation that voltage is less sensitive to changes in soil chemical conditions than current.

Overall, these results indicate that current constitutes the primary responsive electrical variable in the SMFC system, whereas voltage behaves as a more stable parameter under chemical perturbation.

3.4. Differential sensitivity of current and voltage

A direct comparison of current and voltage responses reveals a clear difference in environmental sensitivity. While current responded strongly to temporal changes in soil che-

mistry, voltage exhibited weaker associations and reduced variability.

This differential sensitivity is reflected in the correlation analyses, where current displayed significant relationships with several soil physicochemical parameters, whereas voltage correlations were generally weaker or non-significant. These contrasting behaviors indicate that current more directly reflects variations in bioelectrochemical activity, while voltage is constrained by system-level electrochemical potentials.

Accordingly, current was selected as the principal indicator for identifying the variables controlling SMFC electrical performance.

3.5. Identification of controlling variables for current generation

The relationships between current and soil physicochemical parameters are presented in Fig. 7. Spearman rank correlations calculated from daily mean values revealed a strong and

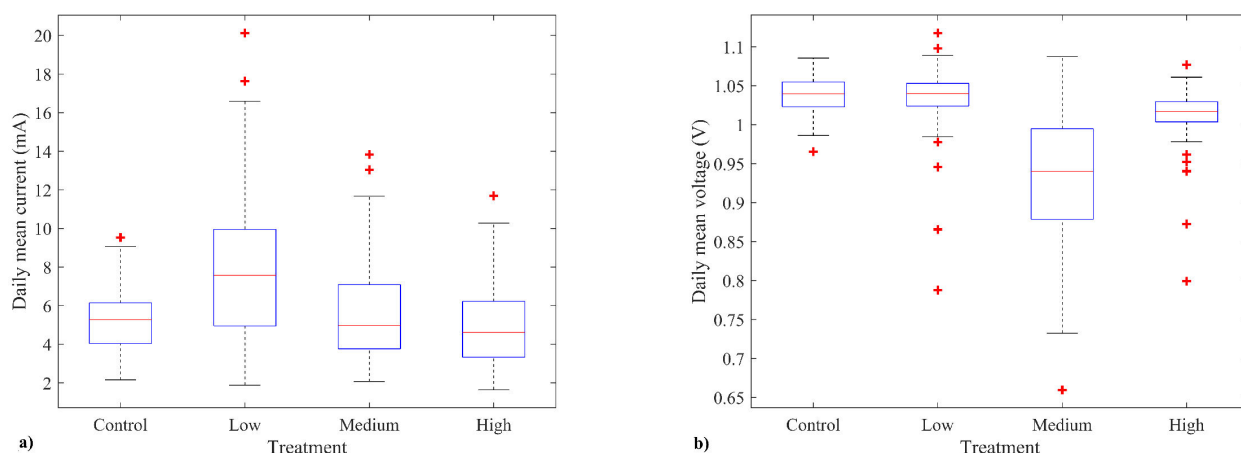


FIGURE 6. Distribution of daily mean a) current and b) voltage values across experimental treatments. Boxes represent interquartile ranges, horizontal lines denote medians, and whiskers indicate data dispersion.

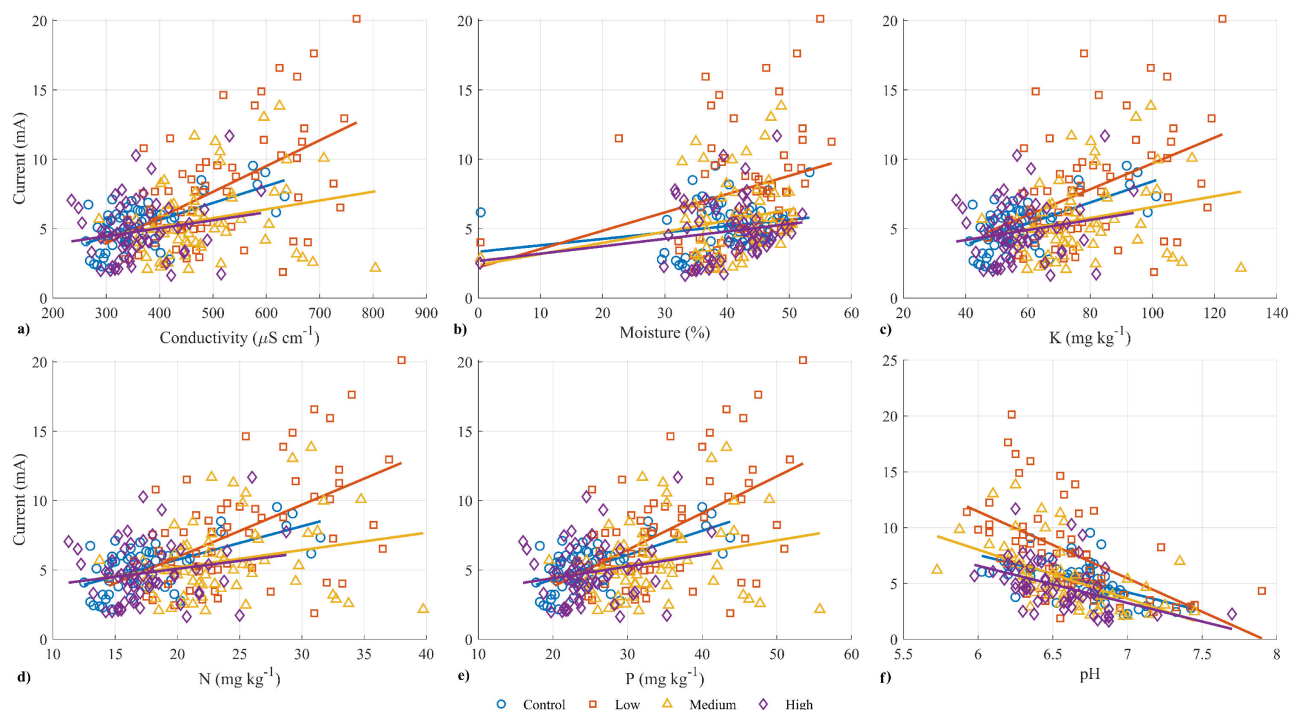


FIGURE 7. Relationships between current generation and soil physicochemical parameters under different CoCl_2 treatments: a) electrical conductivity, b) soil moisture, c) potassium concentration, d) nitrogen concentration, e) phosphorus concentration, and f) soil pH. Symbols represent individual daily mean values for each treatment (control, low, medium, and high CoCl_2), and solid lines correspond to linear fits shown for visual guidance.

consistent negative relationship between current and soil pH across all treatments [Fig. 7a)].

Lower pH values were systematically associated with higher current generation, with statistically significant correlation coefficients observed regardless of CoCl_2 concentration. This relationship emerged as the dominant control on current variability.

In addition to pH, current exhibited moderate positive correlations with nitrogen and phosphorus concentrations [Fig. 7c)–7d)], particularly under control and low CoCl_2

treatments. These associations weakened at higher salt concentrations, suggesting that nutrient-driven enhancement of current becomes less effective under stronger chemical perturbation.

Correlations between current and potassium content, moisture, and conductivity were generally weaker and more treatment-dependent [Fig. 7b), 7e)–7f)], indicating secondary or indirect influences. Overall, within the experimental conditions evaluated in this study, pH emerged as the primary controlling variable for current generation, while nutrients

TABLE I. Spearman rank correlation coefficients (ρ) between daily mean current and soil physicochemical parameters under different CoCl_2 treatments ($n = 60$ per treatment). Statistically significant correlations ($p < 0,05$) are indicated with an asterisk (*).

Variable	Control	Low	Medium	High
Conductivity ($\mu\text{S cm}^{-1}$)	0.534*	0.477*	0.256*	0.113
Moisture (%)	0.246	0.329*	0.245	0.118
K (mg kg^{-1})	0.533*	0.399*	0.252	0.119
N (mg kg^{-1})	0.523*	0.475*	0.244	0.108
P (mg kg^{-1})	0.538*	0.472*	0.242	0.109
pH	-0.677*	-0.626*	-0.678*	-0.539*

modulated the magnitude of the response under less chemically stressed conditions. The quantitative results of the Spearman correlation analysis are summarized in Table ???. Current exhibited statistically significant positive correlations with soil conductivity, potassium, nitrogen, and phosphorus under control and low CoCl_2 treatments. These associations weakened under medium concentrations and became non-significant under high CoCl_2 conditions.

In contrast, soil pH showed a strong and statistically significant negative correlation with current across all treatments, with the highest magnitude observed under control and medium conditions ($\rho \approx -0,68$). This pattern indicates a consistent inverse relationship between soil acidity and current generation, independent of cobalt concentration.

3.6. Modulation of system sensitivity by CoCl_2 concentration

The magnitude and structure of current–soil relationships varied with CoCl_2 concentration. Under low and medium treatments, correlations between current and multiple soil variables were stronger and more consistent. In contrast, the high-concentration treatment exhibited reduced correlation strength and lower variability.

This pattern indicates that increasing chemical perturbation alters the sensitivity of the SMFC system, potentially shifting it from a metabolically responsive regime toward a more constrained state. These results highlight the importance of considering concentration-dependent effects when evaluating chemical inputs in SMFC systems.

4. Discussion

The present study demonstrates that transient chemical perturbations induced by CoCl_2 addition produce measurable and reproducible modifications in the electrical response of the SMFC system. Although conceived as a preliminary assessment, the experimental results reveal consistent relationships between soil physicochemical variables and electrical output that can be interpreted within a general electrochemical framework governing bioelectrochemical systems [5, 11].

The most robust outcome of this work is the strong and persistent negative correlation between current and soil pH across all treatments. Independent of cobalt concentration, lower pH values were systematically associated with higher current generation. From an electrochemical standpoint, variations in pH modify proton activity within the soil electrolyte and can influence proton-coupled redox processes occurring at the anode. Because current under short-circuit conditions reflects the combined influence of reaction kinetics and internal transport limitations, changes in proton availability are expected to affect measurable current more strongly than equilibrium voltage.

Although interfacial resistances and polarization components were not independently quantified in this study, the observed correlations are consistent with pH-dependent modulation of electrochemical kinetics. Similar pH-related effects have been reported in other microbial fuel cell configurations, where enhanced proton transport is associated with increased current densities [11, 12]. While those studies were conducted in liquid-phase systems, the underlying principles of proton-coupled electron transfer are applicable to soil-based SMFCs [2, 3]. Nevertheless, the present results establish correlation rather than direct mechanistic quantification.

In contrast to current, voltage exhibited comparatively limited variability and weaker correlations with soil parameters. This divergence reflects fundamental electrochemical considerations: cell voltage is largely determined by the difference between anodic and cathodic equilibrium potentials, whereas current depends on kinetic and transport factors. Consequently, moderate physicochemical perturbations may significantly alter current without proportionally modifying voltage. The relative stability of voltage observed here is consistent with previous SMFC studies in which current density variations exceed voltage fluctuations [5].

The transient increase in soil electrical conductivity following CoCl_2 addition indicates enhanced ionic strength in the soil matrix. Increased ionic concentration may influence ionic transport properties and potentially reduce the ohmic component of internal resistance. However, because resistance contributions were not directly resolved, this interpretation remains qualitative. The moderate positive correlations bet-

ween current and conductivity under control and low treatments are consistent with improved charge transport under increased ionic availability, but these associations weakened at higher CoCl_2 concentrations.

Positive correlations between current and nutrient concentrations (N and P) were observed primarily under control and low treatments and diminished as cobalt concentration increased. Rather than attributing this attenuation exclusively to microbial stress, the data may indicate a shift in dominant limiting factors controlling current generation. Under mild perturbation, nutrient availability may indirectly influence electron production rates, whereas under stronger ionic modification, electrochemical constraints appear to play a comparatively larger role in determining system behavior.

The concentration-dependent reduction in correlation strength under high CoCl_2 treatment suggests that excessive ionic perturbation modifies the sensitivity of the SMFC system. Although cobalt ions do not function as electron donors, their addition alters soil acidity and ionic composition, which in turn modulates electrochemical conditions at the electrode-soil interface. Similar concentration-dependent effects of metal ions on bioelectrochemical performance have been described in related systems [8]. Within the experimental range evaluated here, the persistence of the pH-current relationship across all treatments indicates that proton dynamics constitute the most stable predictor of current variability.

Overall, the results indicate that current acts as the primary responsive electrical variable under chemically perturbed conditions, while voltage behaves as a comparatively buffered parameter. Within the limits of the present experimental design, soil pH emerged as the dominant controlling factor for current generation. Although microbial community composition and internal resistance components were not independently resolved, the observed patterns are consistent with established electrochemical principles governing low-power bioelectrochemical systems.

Future investigations incorporating electrochemical impedance spectroscopy, polarization analysis, and microbial community characterization would enable quantitative separation of ohmic, activation, and mass transport contributions and provide deeper mechanistic resolution of SMFC operation under chemical perturbation [11].

5. Conclusions

This study demonstrates that the electrical behavior of a soil microbial fuel cell (SMFC) is strongly influenced by transient chemical perturbations of the soil environment induced by cobalt chloride (CoCl_2) addition. Among the monitored physicochemical variables, soil pH emerged as the dominant factor controlling current variability, with lower pH values consistently associated with enhanced current generation across all treatments.

In contrast, voltage exhibited comparatively limited variation in response to changes in soil chemical conditions, highlighting a clear differential sensitivity between the two electrical outputs. Moderate positive associations between current and soil nutrient availability, particularly nitrogen and phosphorus, were observed under control and low CoCl_2 concentrations, whereas increasing ionic stress at higher CoCl_2 levels reduced the strength and consistency of these relationships.

The theoretical electrochemical framework confirms that CoCl_2 does not function as an electron source within the SMFC system but instead acts as a chemical modulator that alters soil conditions governing microbial metabolism and extracellular electron transfer. The concentration-dependent response observed in this work suggests the existence of a threshold beyond which chemical perturbation constrains, rather than enhances, bioelectrochemical activity.

Overall, the results indicate that SMFC electrical signals—particularly current—respond reproducibly to short-term chemical perturbations and can serve as sensitive indicators of soil bioelectrochemical dynamics. These findings support the potential application of SMFCs not only as ultra-low-power energy harvesting devices but also as self-powered sensors for investigating soil chemical and microbial processes under controlled environmental modifications.

Acknowledgements

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High-frequency effective dynamical parameters for a viscoelastic layered medium modeling soft tissue

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Shear wave propagation in a layered medium made of Voigt viscoelastic layers is studied. It is argued that it is possible to obtain closed-form analytical approximate expressions for the effective dynamical parameters of the layered medium in the high-frequency regime. The multiple-scale method is applied to obtain the frequency-dependent effective dynamical parameters. Lower-order analytical solution approximations for harmonic steady-state were obtained. Numerical comparison against precise numerical solutions via the transfer matrix method was carried out. This could contribute to the model design of tissue-like phantom materials for ultrasound devices calibration as well as in the processing of signals from shear wave elastography.

Keywords: Multiple scales, effective parameters, shear wave elastography, high-frequency ultrasound.

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1. Introduction

Ultrasound devices play an important role in present-day medical practice and research. The correct functioning of such devices depends, on the one hand, on the manufacturer and, on the other hand, on the final users (medical and technical staffs), the maintenance staff and the conditions of each device. When it comes to maintenance, it is necessary that the device be properly calibrated (several calibration techniques are summarized in Refs. [1,2]). Some calibration techniques are based on the use of phantoms, which mainly consist of a contact or propagation medium that is required to have dynamical parameters similar to those of the soft tissue to be analyzed, such as the average speed of sound, the acoustic impedance and the attenuation parameter (for the relevance of these quantities in the design of materials with specific dynamical parameters, see [3]). These parameters can be approximated using various materials and configurations. Typical materials include agar, gelatin and polyvinyl-alcohol solutions [4], whereas common configurations are cubes with embedded spheres or rods [5-7]. New phantom designs are frequently produced and evaluated [8-10]. In addition to practical experimental intuition, development of new phantoms can be guided by theoretical models based on the particularities of employed materials and configurations [11-14]. For instance, mathematical models would contribute not only to the rapid evaluation of these materials, but also to their design based on their geometry and frequency response. Therefore, understanding the propagation mechanisms in these materials

would further the development of better design tools, which is the general objective of the present work. In particular, this contribution focuses on the mathematical modeling of the waves produced by medical ultrasound imaging devices. Such devices are considered here in the simplest conceptual form, that is, capable of producing ultrasonic waves through soft tissues and collecting the corresponding dispersion response signals for later processing [16,15].

We want to model soft tissue as simply as possible that lets us arrive at explicit parameter expressions as functions of frequency in the case of shear wave propagation. Speed propagation and attenuation of the wave are the goal parameters, whose expressions are expected to be of help as theoretical guide in some phantom design process. Soft tissue is an extremely complex medium composed by enormous number of diverse elements. Generally speaking, most models in literature assumed it to be a type of solid or fluid in which infinitesimal or finite, elastic or plastic strain relations govern [17-22]. Geometry composition is a major aspect here. Particularly a laminated model will be employed because of both its simplicity and resemblance to the structure of skin, as it is composed of layers of different tissues (epithelium, membranes, parenchyma thickness, etc.). In fact, the use of layered structural designs is recurrent to achieve specific functional parameters of materials for technological application, as a phantom propagation medium itself could be (see [23-27] among many others).

Each layer will be considered as a solid viscoelastic material [28], with Voigt constitutive relation. The simplicity

and linearity of the Voigt constitutive relation are the first attributes that were considered for choosing it. Both Maxwell and Voigt models are very useful for simply modeling the viscosity of a medium (a good review can be seen in Ref. [29]). In particular, a good summary of the most common models of tissue mechanics and their limitations can be found in Ref. [30]. Particularly for the case of skin you can also consult [31]. Some authors have already pointed out that the best description of soft biological tissues is achieved with Voigt constitutive relation or some variation of this under the appropriate frequency ranges. Among the works in this regard you can see [32,33] where tissue substitute materials are treated.

To deal forward with the complexity of tissue layers we will take advantage from multiple scales homogenization method to obtain effective parameters [34,35] representing global behavior. The notion of effective parameter guiding us here is an abstract concept based on the black box model as follows: given two systems, S_1 and S_2 , subject to the same boundary conditions, if the values of the response variables observed for system S_2 are sufficiently close to those obtained for system S_1 , then system S_2 can be considered to be equivalent to (or a substitute for) system S_1 . Thus, if the tissue substitute is a homogeneous material, then the constant parameters characterizing it are the so-called effective parameters of the substituted real tissue. Note that such a definition of effectiveness is pragmatic in nature [36], which differs from the ones based on the asymptotic homogenization methods [35] or averaging methods [37,38].

Section 2 presents the original continuum mechanics model of one-dimensional shear wave propagation in a non-homogeneous medium. Then, Sec. 3 states the perturbative model to be solved derived from the original one. Section 4 displays the solution process in detail to get the effective parameters. In Sec. 5 the approximated solution to the perturbative problem (based on effective parameters) and numerical solution to the original problem with transfer matrix method are compared for non-homogeneous media taken as random laminated ones.

2. The model

The linear problem to be treated is as follows:

$$\begin{cases} \hat{\rho} \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left(\hat{G} \frac{\partial u}{\partial x} + \hat{\eta} \frac{\partial^2 u}{\partial t \partial x} \right), & a \leq x, \quad 0 \leq t, \\ u|_{x=a} = u_a \cos(\omega t), \\ \sigma|_{x=a} = \sigma_a \cos(\omega t + \theta_a). \end{cases} \quad (1)$$

Function $u(x, t)$ represents the displacement field of a transversal wave motion on a semi-infinite medium that extends over $[a, \infty) \ni x$ as shown in Fig. 1a). Constant parameters u_a , σ_a , θ_a and ω mean displacement amplitude, shear stress, response phase delay and harmonic frequency,

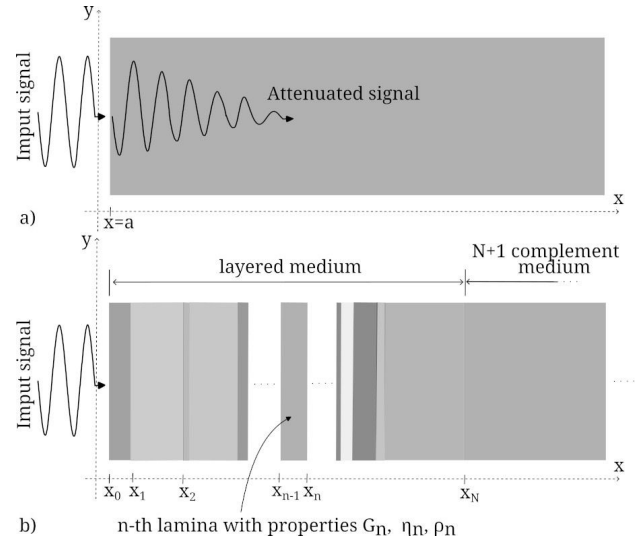


FIGURE 1. a) An imposed or entering signal and the corresponding propagated signal through a viscoelastic medium. b) Composite of N lamina, where x_n is the position of interfaces. The left boundary is at $x = x_0 = a$ and the right one is at $x = x_N$. In addition the wave is attenuated as $x \rightarrow \infty$.

respectively. Physically, the problem can be associated with a transversal plane wave induced in a pure normal way on the boundary $x = a$ of the medium. In addition, the medium is assumed to be layered [Fig. 1b)] as such non-homogeneity resembles many biological tissues. This continuum mechanical linear model is obtained from approximate Euler's motion equation $\partial_x \sigma = \rho \partial_{tt} u$ and Voigt's model $\sigma = \hat{G} \varepsilon + \hat{\eta} \partial_t \varepsilon$, where σ is the stress and $\varepsilon = \partial_x u$ is the strain. Parameters $\hat{G}$, $\hat{\eta}$ and $\hat{\rho}$ are the shear modulus, dynamical viscosity and density, respectively, that in general depends on x for a non-homogeneous medium. By the third Newton's law we expect that translational force density $\hat{\rho} \partial_{tt} u$ must be continuous throughout the whole domain in position x and time t , so the smoothness of u must be at least C^2 in t and C^0 in x , which implies that stress $\sigma = \hat{G} \partial_x u + \hat{\eta} \partial_{tx} u$ is at least C^1 in x , which means that $\hat{G} \partial_x u + \hat{\eta} \partial_{tx} u$ is C^1 but not necessarily each term and factor by itself. From the same Newton's law the deformative stress must be continuous too in x and t , so σ must be continuous. Thus, in case $\hat{G}$, $\hat{\eta}$ or $\hat{\rho}$ are piecewise continuous, these conditions must be satisfied in each boundary. On the other hand, there is a third condition that states the signal attenuation as it propagates to the right along the x -axis (which is a consequence of viscosity of the medium), i.e.

$$\lim_{x \rightarrow \infty} u(x, t) = 0, \quad (2)$$

which has the effect of relating the two boundary conditions.

A problem more suitable for computation associated with

problem (1) can be stated in terms of complex functions as

$$\left\{ \begin{array}{l} \frac{d}{dx} \left(G^* \frac{d\hat{w}}{dx} \right) + \omega^2 \hat{\rho} \hat{w} = 0, \quad a \leq x, \\ \hat{w}|_{x=a} = \hat{w}_a, \\ G^* \frac{d\hat{w}}{dx} \Big|_{x=a} = \hat{s}_a. \end{array} \right. \quad (3)$$

Problem (3) is obtained by changing to a problem where u is the real part of a complex function $W = u + iv$ with v its imaginary part and supposing $W = \hat{w}(x) \exp(-i\omega t)$ with function $\hat{w}$ carrying the spatial dependency. $\hat{w}_a$ and $\hat{s}_a$ are the corresponding boundary values of complex displacement $\hat{w}$ and complex stress $\hat{s} = G^*(d\hat{w}/dx)$ at $x = a$. $G^*(x, \omega) = \hat{G}(x) - i\omega\hat{\eta}(x)$ is the so-called complex or dynamical modulus. Also, note that the parametric description in terms of frequency ω (instead of wave number) is adopted for attaining spatial attenuation rather than a temporal one [39].

Given Boltzmann's superposition principle for the constitutive relation of a viscoelastic material, $\sigma(x, t) = \int_0^t G(x, t - t') \partial_{t'} \varepsilon(x, t') dt'$ considering no σ and ε for $t < 0$ [29], its form in the frequency domain is $\sigma(x, \omega) = G^*(x, \omega) \varepsilon(x, \omega)$, where the function $G^*(x, \omega)$ is recognized as the complex modulus in its most general form. The material's properties are encapsulated in $G^*(x, \omega)$, so its behavior can be capricious, although subject to specific qualitative conditions at frequency limits close to zero or tending to infinity [40]. In a neighborhood of a frequency ω_0 , a linear approximation $G^*(x, \omega) \approx G^*(x, \omega_0) + \partial_\omega G^*(x, \omega_0)(\omega - \omega_0)$ can be useful, which would have the form derived from Voigt model $G^*(x, \omega) \approx \hat{G}(x) - i\hat{\eta}(x)\omega$. It is in this sense that the Voigt model will be used, where the determination of the values of $\hat{G}$ and $\hat{\eta}$ is done experimentally in the frequency range to be treated.

3. Perturbative problem

The multiple scales method is applied here to problem (3) in order to find an asymptotic approximation of its solution. The multiple scales method is a perturbation method that considers a formal power series expansion of the solution of a problem depending on a small parameter [34,41]. The method requires, in addition to the expansion parameter, the definition of two or more hierarchical scale variables which in this case are space variables ranked according to the powers of the expansion parameter.

3.1. Dimensionless formulation

We want to explore the asymptotic behavior in the high-frequency regime. On the other hand, higher frequency im-

plies shorter wavelength, so the microstructural details of the propagation medium of characteristic length smaller than this wavelength remain undetected by the wave, as they appear as homogeneous regions at its resolution scale. Then, the wavelength is taken as the scale of observation, that is, the unit length from which the medium is seen as a nested hierarchy of homogeneous blocks that extend longitudinally in powers of such a unit. In particular, if the medium is overdamped, the wave attenuates before propagating more than one wavelength so, in this case, the mean attenuation length can also serve as an observation scale.

An appropriate choice of the small expansion parameter allows, in addition to a good approximation, simplification in solving the problem. We are interested in exploring the frequency domain as $\omega \rightarrow +\infty$, hence a small parameter inverse to the frequency makes sense. The following dimensionless variables are proposed: $x = l\xi$, $w(\xi) = \hat{w}(l\xi)/l$, $\xi_a = a/l$, $w_a = \hat{w}_a/l$, $G(\xi) = \hat{G}(l\xi)/\tilde{G}$, $\eta(\xi) = \hat{\eta}(l\xi)/\tilde{\eta}$, $\rho(\xi) = \hat{\rho}(l\xi)/\tilde{\rho}$, $s_a = \hat{s}_a/\omega\tilde{\eta}$, $\epsilon = \tilde{G}/(\omega\tilde{\eta})$ y $l = \sqrt{\tilde{G}/(\omega^2\tilde{\rho})}$, with which problem (3) becomes

$$\left\{ \begin{array}{l} \frac{d}{d\xi} \left((\epsilon G - i\eta) \frac{dw}{d\xi} \right) + \epsilon \rho w = 0, \quad \xi_a \leq \xi, \\ w(\xi)|_{\xi=\xi_a} = w_a, \\ (\epsilon G - i\eta) \frac{dw}{d\xi} \Big|_{\xi=\xi_a} = s_a. \end{array} \right. \quad (4)$$

$\tilde{G}$, $\tilde{\eta}$ and $\tilde{\rho}$ are suitable constant values, for example, their corresponding maximum or mean values through the layered medium could work.

3.2. The expansion parameter

The value of parameter ϵ for tissue and ultrasonic scanning frequency is of order $\mathcal{O}(10^{-6})$, which is coherent with the fact that $\omega\hat{\eta} \gg \hat{G}$ for high frequency values, so ϵ is a good candidate for expansion parameter. As choosing adequate expansion parameter and parametrization strategy is crucial [42,43], it proves useful to take the expansion parameter $\nu = \sqrt{\epsilon}$ to avoid fractional powers of ϵ , although working with fractional power expansions is possible [44]. Thus, the problem to be solved is

$$\left\{ \begin{array}{l} \frac{d}{d\xi} \left((\nu^2 G - i\eta) \frac{dw}{d\xi} \right) + \nu^2 \rho w = 0, \quad \xi_a \leq \xi, \\ w(\xi)|_{\xi=\xi_a} = w_a(\nu), \\ (\nu^2 G - i\eta) \frac{dw}{d\xi} \Big|_{\xi=\xi_a} = s_a(\nu). \end{array} \right. \quad (5)$$

Following [45], the solution to problem (5) is sought via the asymptotic expansions

$$\begin{aligned} w(\xi) &= w_0(\xi_0, \xi_1, \xi_2, \dots) + \nu w_1(\xi_0, \xi_1, \xi_2, \dots) + \nu^2 w_2(\xi_0, \xi_1, \xi_2, \dots) + \dots, \\ \frac{d}{d\xi} &= \frac{df_0}{d\xi} \frac{\partial}{\partial \xi_0} + \nu \frac{df_1}{d\xi} \frac{\partial}{\partial \xi_1} + \nu^2 \frac{df_2}{d\xi} \frac{\partial}{\partial \xi_2} + \dots \\ w_a &= w_{a0} + \nu w_{a1} + \nu^2 w_{a2} + \dots, \\ s_a &= s_{a0} + \nu s_{a1} + \nu^2 s_{a2} + \dots, \end{aligned} \quad (6)$$

where $\xi_m = \nu^m f_m(\xi)$, $m = 0, 1, 2, \dots$, are the rescaling variables, f_m are functions to be determined, and ξ_0 is the reference or original variable, that is, $f_0(\xi) = \xi$ and therefore, $\xi_0 = \xi$, then $\xi_m = \nu^m f_m(\xi_0)$. So, variables ξ_m will be treated as independent of each other except for ξ_0 . The w_m (with $m = 0, 1, 2, \dots$) is the m -th coefficient of the formal series of w in powers of ν , and is expected behave asymptotically at least like w_{m-1} to ensure term $\nu^m w_m$ has a contribution of order $\mathcal{O}(\nu^m)$ to the solution w . Coefficients $f'_m d/d\xi_m$ of differential operator should be understood in the same way. Expansions for boundary values were proposed because it is expected they depend on frequency, at the same time expansion parameter is expected to be related inversely with frequency that is supposed to be high enough. So, coefficients w_{am} and s_{am} could be understood as expansion coefficients in the sense of Taylor's series.

By substituting (6) into the differential equation of problem (5), followed by some manipulations and grouping by powers of ν , the asymptotically zero expression is obtained which, to be satisfied, the coefficients powers of ν must be zero, that is,

$$\sum_{l+m+n=\tilde{n}} f'_l \frac{\partial}{\partial \xi_l} \left(\eta f'_m \frac{\partial w_n}{\partial \xi_m} \right) + i \sum_{l+m+n=\tilde{n}-2} f'_l \frac{\partial}{\partial \xi_l} \left(G f'_m \frac{\partial w_n}{\partial \xi_m} \right) + i \rho w_{\tilde{n}-2} = 0, \quad l, m, n, \tilde{n} \in \{0, 1, 2, \dots\}. \quad (7)$$

The sum subject to condition $l + m + n = \tilde{n}$ means that if $\tilde{n} = 0$ then $(l, m, n) = (0, 0, 0)$ and the sum has a single term; if $\tilde{n} = 1$ then the sum has three terms for $(l, m, n) = (1, 0, 0)$, $(l, m, n) = (0, 1, 0)$ and $(l, m, n) = (0, 0, 1)$; and so on for $\tilde{n} \geq 2$. It is agreed that $f'_m = 0$ and $w_m = 0$ in case $m < 0$. The boundary and attenuation conditions are also expanded, which yields

$$\begin{cases} w_n|_{\xi=\xi_a} = w_{an}, \\ s_{an} = \left(G \sum_{l+m=n-2} f'_l \frac{\partial w_m}{\partial \xi_l} - i \eta \sum_{l+m=n} f'_l \frac{\partial w_m}{\partial \xi_l} \right) \Big|_{\xi=\xi_a}, \\ \lim_{\xi \rightarrow \infty} w_m = 0, \quad l, m, n \in \{0, 1, 2, \dots\}, \end{cases} \quad (8)$$

where the rules just described for indices are the same here. The last condition is the already stated attenuation condition expected for each w_m .

4. Effective parameters

First, take $\tilde{n} = 0$ in Eq. (7) and $n = 0$ (8), so the zeroth-order problem is

$$\nu^0 : \begin{cases} f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_0 \frac{\partial w_0}{\partial \xi_0} \right) = 0, \\ w_0|_{\xi=\xi_a} = w_{a0}, \\ -i \eta f'_0 \frac{\partial w_0}{\partial \xi_0} \Big|_{\xi=\xi_a} = s_{a0}, \\ \lim_{\xi_0 \rightarrow \infty} w_0 = 0. \end{cases} \quad (9)$$

whose differential equation is easily integrated to obtain the general solution

$$\begin{aligned} w_0 &= A_0(\xi_1, \xi_2, \dots) \int_{\xi_a}^{\xi_0} \frac{1}{\eta(\mu) f'_0(\mu)} d\mu \\ &+ B_0(\xi_1, \xi_2, \dots), \end{aligned} \quad (10)$$

where A_0 and B_0 are the integration constants with respect to the integration variable ξ_0 , and $f'_0 \equiv 1$. Note that A_0 and B_0 do not depend explicitly on ξ_0 but through the other ξ_m ($m = 1, 2, \dots$). However, expresion (10) doesn't met the attenuation condition in general for a $\eta(\xi)$ strictly positive function, for example, a piecewise constant function which is the case for layered medium has an integral would grows unboundedly when $\xi_0 \rightarrow \infty$. As a consequence A_0 must be identically zero, implying too the zero first contribution to the response signal, $s_{a0} = 0$. Thus, the information gathered from the zeroth-order problem is

$$\left. \begin{aligned} -i A_0|_{\xi=\xi_a} &= s_{a0}, \\ B_0|_{\xi=\xi_a} &= w_{a0}, \\ A_0 &= 0, \\ s_{a0} &= 0, \\ w_0 &= B_0(\xi_1, \xi_2, \dots), \\ \frac{\partial w_0}{\partial \xi_0} &= 0. \end{aligned} \right\} : \nu^0 \quad (11)$$

Now, take $\tilde{n} = 1$ in (7) and $n = 1$ in (8), so the first-order

problem is

$$\nu^1 : \begin{cases} f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_0 \frac{\partial w_1}{\partial \xi_0} \right) = -f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_1 \frac{\partial w_0}{\partial \xi_1} \right) \\ - f'_1 \frac{\partial}{\partial \xi_1} \left(\eta f'_0 \frac{\partial w_0}{\partial \xi_0} \right), \\ w_1|_{\xi=\xi_a} = w_{a1}, \\ -i\eta \left(f'_0 \frac{\partial w_1}{\partial \xi_0} + f'_1 \frac{\partial w_0}{\partial \xi_1} \right) \Big|_{\xi=\xi_a} = s_{a1}, \\ \lim_{\xi_0 \rightarrow \infty} w_1 = 0, \end{cases} \quad (12)$$

where terms containing $\partial w_0 / \partial \xi_0 = 0$ can be eliminated. Then, direct integration provides the general solution as

$$w_1 = -\frac{\partial B_0}{\partial \xi_1} \int \left\{ \frac{f'_1}{f'_0} \right\} + A_1 \int \left\{ \frac{1}{\eta f'_0} \right\} + B_1, \quad (13)$$

where the limits $\xi_a = a/l$ (lower), ξ_0 (upper) and the integration variable ξ_0 have been omitted for the sake of brevity and their respective integrands were embraced, which will be done from now on unless otherwise indicated. The dependencies of each variable were also omitted, A_1 and B_1 being the integration constants with respect to ξ_0 . As before, A_1 and $\partial B_0 / \partial \xi_1$ must be restricted to satisfy the attenuation condition. Lighthill anti-secularism criterion [46] in its relaxed form

$$\frac{w_{n+1}}{w_n} \sim \text{const.}, \forall \xi_m \rightarrow \infty, \quad m, n \in \{0, 1, 2, \dots\}, \quad (14)$$

provides a way to proceed. Here, it means that the contribution w_1 behaves as w_0 as $\xi_0 \rightarrow \infty$. Since w_0 is constant with respect to ξ_0 , then w_1 should also be constant at least in the limit. Then, the Lighthill criterion becomes

$$-\frac{\partial B_0}{\partial \xi_1} \int \left\{ \frac{f'_1}{f'_0} \right\} + A_1 \int \left\{ \frac{1}{\eta f'_0} \right\} \sim \text{const.}, \quad \text{as } \xi_0 \rightarrow \infty, \quad (15)$$

The constant in the right-hand side of (15) is zero because the left-hand side expression is zero in $\xi_0 = \xi_a$ and, also, because the attenuation condition requires it. Then, we have

$$\begin{aligned} \lim_{\xi_0 \rightarrow \infty} \left(-\frac{\partial B_0}{\partial \xi_1} \int \left\{ \frac{f'_1}{f'_0} \right\} + A_1 \int \left\{ \frac{1}{\eta f'_0} \right\} \right) &= 0, \\ \Rightarrow \frac{A_1}{\frac{\partial B_0}{\partial \xi_1}} &= \lim_{\xi_0 \rightarrow \infty} \frac{\int \left\{ \frac{f'_1}{f'_0} \right\}}{\int \left\{ \frac{1}{\eta f'_0} \right\}} = \text{const.}, \quad \frac{\partial B_0}{\partial \xi_1} \neq 0, \end{aligned}$$

Hence, with constant α_{01} ,

$$A_1 = \alpha_{01} \frac{\partial B_0}{\partial \xi_1} \quad (16)$$

and, therefore,

$$\alpha_{01} = \lim_{\xi_0 \rightarrow \infty} \frac{\int \left\{ \frac{f'_1}{f'_0} \right\}}{\int \left\{ \frac{1}{\eta f'_0} \right\}}. \quad (17)$$

Condition (17) on f_1 indicates that this function must be $\mathcal{O}(\int \eta^{-1})$ provided there is a solution. This condition is similar to the one used in Ref. [47] in the discussion of the multiple scales method for homogenization.

By putting the definition

$$g_{01}(\xi_0) = \alpha_{01} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_1}{f'_0} \right\}, \quad (18)$$

into (13) with (16), w_1 is written as $w_1 = g_{01} \partial B_0 / \partial \xi_1 + B_1$. Such a consideration, together with (11) in the first-order problem (12), leads to $B_1|_{\xi=\xi_a} = w_{a1}$ and $-i\alpha_{01}(\partial B_0 / \partial \xi_1)|_{\xi=\xi_a} = s_{a1}$, so the first-order information is

$$\left. \begin{aligned} s_{a0} &= 0, \\ w_0 &= B_0(\xi_1, \xi_2, \dots), \\ B_0|_{\xi=\xi_a} &= w_{a0}, \\ -i\alpha_{01} \frac{\partial B_0}{\partial \xi_1} \Big|_{\xi=\xi_a} &= s_{a1}, \\ w_1 &= g_{01}(\xi) \frac{\partial B_0}{\partial \xi_1}(\xi_1, \xi_2, \dots) \\ &\quad + B_1(\xi_1, \xi_2, \dots), \\ B_1|_{\xi=\xi_a} &= w_{a1}. \end{aligned} \right\} : \nu^1 \quad (19)$$

Next, take $\tilde{n} = 2$ in (7) and $n = 2$ in (8), so the second-order problem is

$$\nu^2 : \begin{cases} f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_0 \frac{\partial w_2}{\partial \xi_0} \right) = -f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_1 \frac{\partial w_1}{\partial \xi_1} \right) \\ - f'_1 \frac{\partial}{\partial \xi_1} \left(\eta f'_0 \frac{\partial w_1}{\partial \xi_0} \right) - f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_2 \frac{\partial w_0}{\partial \xi_2} \right) \\ - f'_1 \frac{\partial}{\partial \xi_1} \left(\eta f'_1 \frac{\partial w_0}{\partial \xi_1} \right) - f'_2 \frac{\partial}{\partial \xi_2} \left(\eta f'_0 \frac{\partial w_0}{\partial \xi_0} \right) \\ - i f'_0 \frac{\partial}{\partial \xi_0} \left(G f'_0 \frac{\partial w_0}{\partial \xi_0} \right) - i \rho w_0, \\ w_2|_{\xi=\xi_a} = w_{a2}, \\ s_{a2} = G f'_0 \frac{\partial w_0}{\partial \xi_0} \Big|_{\xi=\xi_a} \\ - i \eta \left(f'_0 \frac{\partial w_2}{\partial \xi_0} + f'_1 \frac{\partial w_1}{\partial \xi_1} + f'_2 \frac{\partial w_0}{\partial \xi_2} \right) \Big|_{\xi=\xi_a}, \\ \lim_{\xi_0 \rightarrow \infty} w_2 = 0, \end{cases} \quad (20)$$

which, by using the information in (19), produces the general solution

$$w_2 = - \left(\alpha_{01} \left(\int \left\{ \frac{f'_1}{f'_0} \int \frac{1}{\eta f'_0} \right\} + \int \left\{ \frac{1}{\eta f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \right. \\ \left. - \int \left\{ \frac{f'_1}{f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \frac{\partial^2 B_0}{\partial \xi_1^2} - \mathbf{i} \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\} B_0 \\ - \int \left\{ \frac{f'_1}{f'_0} \right\} \frac{\partial B_1}{\partial \xi_1} - \int \left\{ \frac{f'_2}{f'_0} \right\} \frac{\partial B_0}{\partial \xi_2} + \int \left\{ \frac{1}{\eta f'_0} \right\} A_2 \\ + B_2,$$

where braces delimiting integrand of inner integrals were omitted because the scopes of these integrals are deduced from the outer ones. A_2 and B_2 are the integration constants that depend on ξ_n , $n > 0$. In this case, the Lighthill criterion (14) involves all terms but B_2 , since the same reasons given to eliminate first term of expression (10) apply here too. Then, the criterion becomes

$$- \left(\alpha_{01} \left(\int \left\{ \frac{f'_1}{f'_0} \int \frac{1}{\eta f'_0} \right\} + \int \left\{ \frac{1}{\eta f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \right. \\ \left. - \int \left\{ \frac{f'_1}{f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \frac{\partial^2 B_0}{\partial \xi_1^2} - \mathbf{i} \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\} B_0 \quad (21) \\ - \int \left\{ \frac{f'_1}{f'_0} \right\} \frac{\partial B_1}{\partial \xi_1} - \int \left\{ \frac{f'_2}{f'_0} \right\} \frac{\partial B_0}{\partial \xi_2} + \int \left\{ \frac{1}{\eta f'_0} \right\} A_2 \\ \sim \text{const.}, \quad \text{as } \xi_0 \rightarrow \infty.$$

In this case, as we are looking for a wave-type solution, the terms of $\partial^2 B_0 / \partial \xi_1^2$ and B_0 could form a wave equation, whereas, analogously to the previous first-order case, the remaining terms can be related to a suitable form of A_2 . This approach is reinforced by the fact that the coefficients in these term association proposals are of the same integration order. So, it is more natural to establish a proportionality relation between, for example, the coefficients of $\partial B_1 / \partial \xi_1$ and A_2 than between the coefficients of B_0 and $\partial B_0 / \partial \xi_2$. Of course, one must keep in mind that f_1 behaves asymptotically as the first-order integral of η^{-1} , so its participation would count as an order of integration. With such considerations, criterion (21) is decomposed into two parts as

$$- \left(\alpha_{01} \left(\int \left\{ \frac{f'_1}{f'_0} \int \frac{1}{\eta f'_0} \right\} + \int \left\{ \frac{1}{\eta f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \right. \\ \left. - \int \left\{ \frac{f'_1}{f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \frac{\partial^2 B_0}{\partial \xi_1^2} - \mathbf{i} \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\} B_0 \sim \text{const.}, \\ - \int \left\{ \frac{f'_1}{f'_0} \right\} \frac{\partial B_1}{\partial \xi_1} - \int \left\{ \frac{f'_2}{f'_0} \right\} \frac{\partial B_0}{\partial \xi_2} \\ + \int \left\{ \frac{1}{\eta f'_0} \right\} A_2 \sim \text{const.}, \quad \text{as } \xi_0 \rightarrow \infty. \quad (22)$$

Now, reasoning as in the first-order case, we propose

$$\frac{\partial^2 B_0}{\partial \xi_1^2} = -\kappa_{01}^2 B_0, \quad (23) \\ A_2 = \alpha_{11} \frac{\partial B_1}{\partial \xi_1} + \alpha_{02} \frac{\partial B_0}{\partial \xi_2},$$

from which the following conditions are obtained:

$$\lim_{\xi_0 \rightarrow \infty} \left(\left(\alpha_{01} \left(\int \left\{ \frac{f'_1}{f'_0} \int \frac{1}{\eta f'_0} \right\} + \int \left\{ \frac{1}{\eta f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \right. \right. \right. \\ \left. \left. - \int \left\{ \frac{f'_1}{f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \kappa_{01}^2 - \mathbf{i} \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\} \right) = 0, \quad (24)$$

$$\lim_{\xi_0 \rightarrow \infty} \left(\alpha_{11} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_1}{f'_0} \right\} \right) = 0, \quad (25)$$

$$\lim_{\xi_0 \rightarrow \infty} \left(\alpha_{02} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_2}{f'_0} \right\} \right) = 0, \quad (26)$$

where κ_{01} , α_{11} and α_{02} are suitable constants. Condition (25) for f_1 is the same as (17) provided that $\alpha_{11} = \alpha_{01}$, which is assumed to avoid contradiction. Also, condition (26) for f_2 is analogous to that for f_1 with its corresponding asymptotic proportionality constant α_{02} . As for condition (24), it can be reduced to see that it is indeed consistent with the proposals made, so κ_{01} can be obtained.

Consider the definition

$$g_2(\xi_0) = \left(\alpha_{01} \left(\int \left\{ \frac{f'_1}{f'_0} \int \frac{1}{\eta f'_0} \right\} + \int \left\{ \frac{1}{\eta f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \right. \\ \left. - \int \left\{ \frac{f'_1}{f'_0} \int \frac{f'_1}{f'_0} \right\} \right) \kappa_{01}^2 - \mathbf{i} \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\}, \quad (27)$$

recall that $f'_0 = 1$, and impose $f_1(\xi_0)|_{\xi=\xi_0} = 0$ since it is a perturbation to ξ_0 as [41]

$$\xi \sim \xi_0 + \xi_1 + \xi_2 + \dots \\ = \xi_0 + \nu f_1(\xi_0) + \nu^2 f_2(\xi_0) + \dots \quad (28)$$

Then, (27) becomes

$$g_2(\xi_0) = \frac{1}{2} f_1 \left(\alpha_{01} \int \left\{ \frac{1}{\eta} \right\} + \left(\alpha_{01} \int \left\{ \frac{1}{\eta} \right\} - f_1 \right) \right) \kappa_{01}^2 \\ - \mathbf{i} \int \left\{ \frac{1}{\eta} \int \rho \right\},$$

where expression inside inner parentheses is just (18), which tends to zero when $\xi_0 \rightarrow \infty$ due to condition (17). Taking the limit $\xi_0 \rightarrow \infty$ for (27) also becomes zero implying

$$\kappa_{01}^2 = 2\mathbf{i} \lim_{\xi_0 \rightarrow \infty} \frac{\int \left\{ \frac{1}{\eta} \int \rho \right\}}{\left(\alpha_{01} \int \left\{ \frac{1}{\eta} \right\} \right)^2}, \quad (29)$$

Formula (29) is the definition of κ_{01} or, more precisely, its shape. At the same time, it is a condition on the parameters of the medium, that is, in order for κ_{01} to be finite, it is necessary that the second-order integral in the numerator grows asymptotically at the same rate as the square of the first-order

integral in the denominator, which restricts the choice of parameters ρ and η . For instance, if we consider the case of a homogeneous medium (with constant parameters), both numerator and denominator are polynomials of degree two, so they have the same asymptotic behavior. Also, for a layered medium composed of homogeneous layers whose parameter values oscillate around their constant effective values, this assumption seems to be sensible as well.

By taking κ_{01} as the principal square root of (29), the general solution of (23) is $B_0 = C_0(\xi_2, \dots) \exp(i\kappa_{01}\xi_1(\xi_0)) + D_0(\xi_2, \dots) \exp(-i\kappa_{01}\xi_1(\xi_0))$, from which the contributions of right- and left-traveling waves are evident. By using the boundary conditions in (19), it follows that $C_0|_{\xi=\xi_a} = (\alpha_{01}\kappa_{01})^{-1}(\alpha_{01}\kappa_{01}w_{a0} + s_{a1})$ and $D_0|_{\xi=\xi_a} = (\alpha_{01}\kappa_{01})^{-1}(\alpha_{01}\kappa_{01}w_{a0} - s_{a1})$, where $\xi_1|_{\xi=\xi_a} = 0$ because $f_1|_{\xi=\xi_a} = 0$. As the real and imaginary parts of κ_{01} are positive, the second term diverges as $\xi_0 \rightarrow \infty$, so the attenuation condition implies $D_0 = 0$, leading to the first contribution to the response signal $s_{a1} = \alpha_{01}\kappa_{01}w_{a0}$, which produces $B_0 = C_0(\xi_2, \dots) \exp(i\kappa_{01}\xi_1(\xi_0))$ with $C_0|_{\xi=\xi_a} = w_{a0}$.

In order to know the behavior of w_0 , it is still necessary to find f_1 , which in turn requires the analysis of the following order ($\tilde{n} = 3$ in (7) and $n = 3$ in (8)). Define

$$g_{11}(\xi_0) = \alpha_{11} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_1}{f'_0} \right\} \quad (30)$$

and

$$g_{02}(\xi_0) = \alpha_{02} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_2}{f'_0} \right\}, \quad (31)$$

so the second-order information is

$$\left. \begin{aligned} B_0 &= C_0(\xi_2, \dots) \exp(i\kappa_{01}\xi_1(\xi_0)), \\ C_0|_{\xi=\xi_a} &= w_{a0}, \\ w_0 &= B_0, \\ s_{a0} &= 0, \\ w_1 &= i\kappa_{01}g_{01}B_0 + B_1, \\ B_1|_{\xi=\xi_a} &= w_{a1}, \\ s_{a1} &= \alpha_{01}\kappa_{01}w_{a0}, \\ w_2 &= g_2B_0 + g_{11}\frac{\partial B_1}{\partial \xi_1} + g_{02}\frac{\partial B_0}{\partial \xi_2} + B_2, \\ B_2|_{\xi=\xi_a} &= w_{a2}, \\ -i\left(\alpha_{11}\frac{\partial B_1}{\partial \xi_1} + \alpha_{02}\frac{\partial B_0}{\partial \xi_2}\right)\Big|_{\xi=\xi_a} &= s_{a2}. \end{aligned} \right\} : \nu^2 \quad (32)$$

Next, take $\tilde{n} = 3$ in (7) and $n = 3$ in (8), so the third-order

problem is

$$\nu^3 : \left\{ \begin{aligned} f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_0 \frac{\partial w_3}{\partial \xi_0} \right) &= -f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_1 \frac{\partial w_2}{\partial \xi_1} \right) \\ &- f'_1 \frac{\partial}{\partial \xi_1} \left(\eta f'_0 \frac{\partial w_2}{\partial \xi_0} \right) - f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_2 \frac{\partial w_1}{\partial \xi_2} \right) \\ &- f'_1 \frac{\partial}{\partial \xi_1} \left(\eta f'_1 \frac{\partial w_1}{\partial \xi_1} \right) - f'_2 \frac{\partial}{\partial \xi_2} \left(\eta f'_0 \frac{\partial w_1}{\partial \xi_0} \right) \\ &- f'_0 \frac{\partial}{\partial \xi_0} \left(\eta f'_3 \frac{\partial w_0}{\partial \xi_3} \right) - f'_1 \frac{\partial}{\partial \xi_1} \left(\eta f'_2 \frac{\partial w_0}{\partial \xi_2} \right) \\ &- f'_2 \frac{\partial}{\partial \xi_2} \left(\eta f'_1 \frac{\partial w_0}{\partial \xi_1} \right) - f'_3 \frac{\partial}{\partial \xi_3} \left(\eta f'_0 \frac{\partial w_0}{\partial \xi_0} \right) \\ &- i f'_0 \frac{\partial}{\partial \xi_0} \left(G f'_0 \frac{\partial w_1}{\partial \xi_0} \right) - i f'_0 \frac{\partial}{\partial \xi_0} \left(G f'_1 \frac{\partial w_0}{\partial \xi_1} \right) \\ &- i f'_1 \frac{\partial}{\partial \xi_1} \left(G f'_0 \frac{\partial w_0}{\partial \xi_0} \right) - i \rho w_1, \\ w_3|_{\xi=\xi_a} &= w_{a3}, \\ s_{a3} &= G \left(f'_0 \frac{\partial w_1}{\partial \xi_0} + f'_1 \frac{\partial w_0}{\partial \xi_1} \right) \Big|_{\xi=\xi_a} \\ &- i \eta \left(f'_0 \frac{\partial w_3}{\partial \xi_0} + f'_1 \frac{\partial w_2}{\partial \xi_1} + f'_2 \frac{\partial w_1}{\partial \xi_2} + f'_3 \frac{\partial w_0}{\partial \xi_3} \right) \Big|_{\xi=\xi_a}, \\ \lim_{\xi_0 \rightarrow \infty} w_3 &= 0. \end{aligned} \right. \quad (33)$$

By substituting w_0 , w_1 and w_2 from (32) into the differential equation in (33), we find that

$$\begin{aligned} w_3 &= - \int \left\{ \frac{1}{\eta f'_0} \left(\kappa_{01} \eta f'_1 g_2 + i \kappa_{01} \int \{ \eta f'_1 g'_2 \} \right. \right. \\ &\quad \left. \left. - i \kappa_{01}^3 \int \left\{ \frac{\eta (f'_1)^2}{f'_0} g_{01} \right\} - \kappa_{01} \int \left\{ \frac{\rho}{f'_0} g_{01} \right\} \right) \right\} B_0 \\ &\quad \left(\int \left\{ \kappa_{01} \frac{G}{\eta f'_0} (f'_0 g'_{01} + f'_1) \right\} \right) B_0 \\ &\quad - \int \left\{ \frac{1}{\eta f'_0} \left(i \kappa_{01} \eta f'_1 g'_{02} + i \kappa_{01} \int \{ \eta f'_1 g'_{02} \} + i \kappa_{01} \eta f'_2 g_{01} \right. \right. \\ &\quad \left. \left. + i \kappa_{01} \int \{ \eta f'_2 g'_{01} \} + 2i \kappa_{01} \int \left\{ \frac{\eta f'_2 f'_1}{f'_0} \right\} \right) \right\} \frac{\partial B_0}{\partial \xi_2} \\ &\quad - \int \left\{ \frac{1}{\eta f'_0} \left(\eta f'_1 g_{11} + \int \{ \eta f'_1 g'_{11} \} + \int \left\{ \frac{\eta (f'_1)^2}{f'_0} \right\} \right) \right\} \frac{\partial^2 B_1}{\partial \xi_1^2} \\ &\quad - i \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\} B_1 \\ &\quad - \int \left\{ \frac{f'_1}{f'_0} \right\} \frac{\partial B_2}{\partial \xi_1} - \int \left\{ \frac{f'_2}{f'_0} \right\} \frac{\partial B_1}{\partial \xi_2} \\ &\quad - \int \left\{ \frac{f'_3}{f'_0} \right\} \frac{\partial B_0}{\partial \xi_3} + \int \left\{ \frac{1}{\eta f'_0} \right\} A_3 + B_3, \end{aligned}$$

where all terms but B_3 diverge as $\xi_0 \rightarrow \infty$ for the same

reasons exposed for first term of expression (10). There are signs of similarity with the structure of w_2 in the previous case. It is immediately obvious that A_3 can be related to the terms with first-order integral coefficients, that is, those of $\partial B_2/\partial \xi_1$, $\partial B_1/\partial \xi_2$ and $\partial B_0/\partial \xi_3$. Also, substitution of g_{11} into the coefficient of $\partial^2 B_1/\partial \xi_1^2$ reveals that it is exactly the same as that of $\partial^2 B_0/\partial \xi_1^2$ of w_2 and, together with the term in B_1 , the same differential equation is formed as for B_0 with respect to the same variable ξ_1 . It only remains to be seen how the terms of B_0 and $\partial B_0/\partial \xi_2$ would cancel out in the limit. Regarding this, one option is that they cancel each other by establishing a proportionality relation between B_0 and $\partial B_0/\partial \xi_2$, and the other option is that they cancel separately. The first option leads to an inconsistency in which f_2 would not behave asymptotically as required by (24). On the other hand, for the second option, it can immediately be seen that if the B_0 term must be zero at least in the limit, it would imply a condition on f_1 and the parameters of the medium. However, such a condition restricts the material parameters in a very capricious way. So, in order to maintain the maximum possible generality, the alternative is to take f_1 as the solution of the equation resulting from equating the coefficient of B_0 to zero. In addition, the term of $\partial B_0/\partial \xi_2$ must also become zero, for which there are three possibilities: the first one is that the coefficient cancels out in the limit, the second one is that it cancels out identically, and the third one is that $\partial B_0/\partial \xi_2 = 0$. In fact, the first two possibilities are inconsistent with the conditions for f_1 and f_2 in (24), leaving the third one as the only possibility. With such considerations, we have

$$\frac{\partial^2 B_1}{\partial \xi_1^2} = -\kappa_{11}^2 B_1, \quad (34)$$

$$A_3 = \alpha_{21} \frac{\partial B_2}{\partial \xi_1} + \alpha_{12} \frac{\partial B_1}{\partial \xi_2} + \alpha_{03} \frac{\partial B_0}{\partial \xi_3}, \quad (35)$$

$$\begin{aligned} & \int \left\{ \frac{1}{\eta f'_0} \left(\kappa_{01} \eta f'_1 g_2 + \kappa_{01} \int \eta f'_1 g'_2 \right. \right. \\ & \quad \left. \left. - \kappa_{01}^3 \int \frac{\eta (f'_1)^2}{f'_0} g_{01} - \kappa_{01} \int \frac{\rho}{f'_0} g_{01} \right) \right\} \\ & - \int \left\{ \kappa_{01} \frac{G}{\eta f'_0} (f'_0 g'_{01} + f'_1) \right\} = 0, \end{aligned} \quad (36)$$

$$\frac{\partial B_0}{\partial \xi_2} = 0. \quad (37)$$

Now, define

$$\begin{aligned} g_3 &= \int \left\{ \frac{1}{\eta f'_0} \left(\eta f'_1 g_{11} + \int \eta f'_1 g'_{11} + \int \frac{\eta (f'_1)^2}{f'_0} \right) \right\} \kappa_{11}^2 \\ & - \kappa_{01} \int \left\{ \frac{1}{\eta f'_0} \int \frac{\rho}{f'_0} \right\}, \end{aligned}$$

$$\begin{aligned} g_{21} &= \alpha_{21} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_1}{f'_0} \right\}, \\ g_{12} &= \alpha_{12} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_2}{f'_0} \right\}, \\ g_{03} &= \alpha_{03} \int \left\{ \frac{1}{\eta f'_0} \right\} - \int \left\{ \frac{f'_3}{f'_0} \right\}, \end{aligned} \quad (38)$$

so $g_3 = g_2$ and $g_{21} = g_{11} = g_{01}$ for $\alpha_{21} = \alpha_{11} = \alpha_{01}$, and $g_{12} = g_{02}$ for $\alpha_{12} = \alpha_{02}$. Then, we write $w_3 = g_3 B_1 + g_{21} \partial B_2/\partial \xi_1 + g_{12} \partial B_1/\partial \xi_2 + g_{03} \partial B_0/\partial \xi_3 + B_3$. The wave equation of B_1 with respect to ξ_1 results in $\kappa_{11} = \kappa_{01}$. At this point we can already observe the recursiveness in the decision-making of the integration constant A_n and the dependence of each contribution w_n with respect to ξ_1 . From this, it could even be deduced that most likely no other contribution w_n depends on ξ_2 , something that in any case remains to be proven elsewhere. On the other hand, we have finally arrived at the equation that defines f_1 : manipulating (36), it can be rewritten as

$$\begin{aligned} & \left(-\frac{\varsigma}{6} \right) \left(\frac{f_1}{\alpha_{01}} \right)^3 + \left(\frac{\varsigma}{2} \int \left\{ \frac{1}{\eta} \right\} \right) \left(\frac{f_1}{\alpha_{01}} \right)^2 \\ & + \left(- \int \left\{ \frac{1}{\eta} \int \rho \right\} \right) \left(\frac{f_1}{\alpha_{01}} \right) \\ & + \left(\int \left\{ \frac{1}{\eta} \int \left\{ \rho \int \frac{1}{\eta} \right\} \right\} + \int \left\{ \frac{G}{\eta^2} \right\} \right) = 0, \end{aligned} \quad (39)$$

where $\varsigma = -\kappa_{01}^2 \kappa_{01}^2$. This cubic equation has analytical solutions given by [48]

$$\left(\frac{f_1}{\alpha_{01}} \right)_n = -\frac{1}{3a} \left(b + \left(\sqrt[3]{\Delta_1} \right)^n C_{\pm} + \frac{\Delta_0}{\left(\sqrt[3]{\Delta_1} \right)^n C_{\pm}} \right), \quad (40)$$

with $n \in \{0, 1, 2\}$, where $\Delta_0 = b^2 - 3ac$, $\Delta_1 = 2b^3 - 9abc + 27a^2d$ and $C_{\pm} = \sqrt[3]{(\Delta_1 \pm \sqrt{\Delta_1^2 - 4\Delta_0^3})/2}$, being a, b, c, d the coefficients of the powers of f_1/α_{01} in equation (39) and $\sqrt[3]{\Delta_1} = (-1 + i\sqrt{3})/2$.

It is necessary to verify that f_1/α_{01} satisfies condition (17). For this, rewrite Δ_0 and Δ_1 as

$$\begin{aligned} \Delta_0 &= \left(\frac{\varsigma}{2} \int \left\{ \frac{1}{\eta} \right\} \right)^2 \left(1 - \frac{\delta_1}{\varsigma} \right), \\ \Delta_1 &= \left(\frac{\varsigma}{2} \int \left\{ \frac{1}{\eta} \right\} \right)^3 \left(2 - 3 \frac{\delta_1}{\varsigma} + \frac{\delta_2}{\varsigma} \right), \end{aligned}$$

where

$$\begin{aligned} \delta_1(\xi_0) &= \frac{\int \left\{ \frac{1}{\eta} \int \rho \right\}}{\int \left\{ \frac{1}{\eta} \int \frac{1}{\eta} \right\}}, \\ \delta_2(\xi_0) &= \frac{\int \left\{ \frac{1}{\eta} \int \left\{ \rho \int \frac{1}{\eta} \right\} \right\} + \int \left\{ \frac{G}{\eta^2} \right\}}{\int \left\{ \frac{1}{\eta} \int \left\{ \frac{1}{\eta} \int \frac{1}{\eta} \right\} \right\}}, \end{aligned} \quad (41)$$

considering relations $(\int \{1/\eta\})^2 = 2 \int \{1/\eta \int \{1/\eta\}\}$ and $(\int \{1/\eta\})^3 = 6 \int \{1/\eta \int \{1/\eta \int \{1/\eta\}\}\}$ that can be verify directly. It follows that

$$C_{\pm} = \frac{\varsigma}{2} \int \left\{ \frac{1}{\eta} \right\} \delta_3^{\pm},$$

with

$$\delta_3^{\pm}(\xi_0) = \left(\left(2 - 3\frac{\delta_1}{\varsigma} + \frac{\delta_2}{\varsigma} \right) \pm \sqrt{\left(2 - 3\frac{\delta_1}{\varsigma} + \frac{\delta_2}{\varsigma} \right)^2 - 4 \left(1 - \frac{\delta_1}{\varsigma} \right)^3} \right)^{1/3}, \quad (42)$$

which, by substitution into (40), produces

$$\left(\frac{f_1}{\alpha_{01}} \right)_n = \int \left\{ \frac{1}{\eta} \right\} \left(1 + (\sqrt[3]{i})^n \delta_3^{\pm} + \frac{1 - \frac{\delta_1}{\varsigma}}{(\sqrt[3]{i})^n \delta_3^{\pm}} \right), \quad (43)$$

with $n \in \{0, 1, 2\}$. Provided that δ_1 and δ_2 are finite for $\xi_0 \rightarrow \infty$, then $(f_1/\alpha_{01})_n$ would behave as desired, that is, they would be $\mathcal{O}(\int 1/\eta)$. Earlier we discussed the finitude of δ_1 in terms of the consistency of κ_{01} , but now it is necessary to assume that δ_2 is also finite, which seems sensible under the same arguments that the orders of integration of the parameters in the numerator and denominator are equal. That is, the obtained form of f_1/α_{01} is consistent with the requirement of its asymptotic behavior. Note that α_{01} serves as an indeterminate parameter, generally complex, whose determination from the data will be addressed in the validation section 5.

Now, we refocus on the objective of obtaining effective parameters. From (23) and (19), the homogenized problem is stated as

$$\left\{ \begin{array}{l} \frac{\partial^2 B_0}{\partial \xi_1^2} + \kappa_{01}^2 B_0 = 0, \\ B_0|_{\xi=\xi_a} = w_{a0}, \\ s_{a1} = -i\alpha_{01} \frac{\partial B_0}{\partial \xi_1} \Big|_{\xi=\xi_a}, \\ \lim_{\xi_0 \rightarrow \infty} w_0 = 0, \end{array} \right. \quad (44)$$

where κ_{01} is the effective wave number, specific for this first approximate description version of the original problem in terms of the variable ξ_1 . Apparently, there are three conditions, but it must be taken into account that response s_{a1} is considered unknown. The solution to problem (44) is

$$\begin{aligned} w_0(\xi_1) &= w_{a0} \exp(i\kappa_{01}\xi_1), \\ \alpha_{01}^2 \kappa_{01}^2 &= i \lim_{\xi_0 \rightarrow \infty} \frac{\int \left\{ \frac{1}{\eta} \int \rho \right\}}{\int \left\{ \frac{1}{\eta} \int \frac{1}{\eta} \right\}}, \\ s_{a1} &= \alpha_{01} \kappa_{01} w_{a0} \end{aligned} \quad (45)$$

with $\eta_a = \eta(\xi_0)|_{\xi=\xi_a}$. Referring to C_0 in (32) and the fact that B_0 does not depend on ξ_2 , it was used that $C_0(\xi_3 \dots) \approx w_{a0}$ when $\dots \xi_4 \ll \xi_3 \ll \xi_1$ due to boundary conditions. Recall that s_{an} depends on w_{an} due to the attenuation condition. From the physical point of view, we would say that the displacement w is the variable given or imposed as excitation to the system, whereas the strain $\partial_{\xi} w$ is the response variable, and $\xi = \xi_a$ is simultaneously the point of both application of the excitation and collection of the response.

The behavior of the contribution w_0 is obtained with $\xi_1 = \nu f_1(\xi_0)$. Since f_1 is not a linear function of ξ_0 , the behavior of w_0 as a function of the variable ξ_0 is not necessarily simply harmonic. Since the shape of w_0 is not harmonic and it is not an explicit function of the original spatial variable ξ_0 , κ_{01} is not the effective complex wave number as we need. In an effort to find a definition of such an effective parameter, the reasoning is as follows. If it is admitted that the limit

$$\langle \eta^{-1} \rangle = \lim_{\xi_0 \rightarrow \infty} \frac{1}{\xi_0 - \xi_a} \int_{\xi_a}^{\xi_0} \frac{1}{\eta(\mu)} d\mu, \quad (46)$$

exists, which defines the average of the reciprocal of the viscosity, in turn it is possible to define a local wave number

$$\kappa_{loc}(x) = l^{-1} \kappa_{01} \nu f_1'(x/l), \quad (47)$$

recalling that $\xi_0 = x/l$ and that x is the original space variable, in such a way that the average

$$\kappa_{cum}(x) = \frac{1}{x-a} \int_a^x \kappa_{loc}(\mu) d\mu, \quad (48)$$

has a well-defined limit when $x \rightarrow \infty$ as a result of (46) and (17). This average is obtained naturally from multiplying and dividing the exponential argument in (45) by $x-a$, then associating $\kappa_{01}\xi_1/(x-a)$ to resemble the wave number of a harmonic behavior.

In other words, the lowest-order non-zero solution (45) takes the form

$$w_0 = w_{a0} \exp(i\kappa_{cum}(x)(x-a)). \quad (49)$$

At the same time, as it is needed that effective wave number be a constant that enclosed the global behavior of the layered medium, global average of κ_{loc} just lets us induce a definition of effective wave number as:

$$\kappa_{eff} = \lim_{x \rightarrow \infty} \kappa_{cum}(x) = \lim_{x \rightarrow \infty} \frac{1}{x-a} \int_a^x \kappa_{loc}(\mu) d\mu. \quad (50)$$

Substituting (47) into (50) and calculating the integral taking into account that $f_1(a/l) = 0$, we have that

$$\kappa_{eff} = \lim_{x \rightarrow \infty} \frac{\kappa_{01} \nu f_1(x/l)}{x-a},$$

which requires that, for the limit to exist, the asymptotic behavior of f_1 at infinity must be linear in x . It is known from Eq. (43) that the asymptotic behavior at infinity of f_1

is $\int \eta^{-1}$, provided that δ_1 and δ_2 are finite, as already mentioned. To guarantee this, it is sufficient that the functions G , η , and ρ be bounded throughout their domain; that is, that there exists an upper bound for the values of each of them. For example, if H_1 is a constant such that $|\eta^{-1}(\xi_0)| \leq H_1$ for all $\xi_0 \in [a/l, \infty)$, then $\int \eta^{-1} \leq H_1(\xi_0 - \xi_a) \sim H_1 \xi_0$. Following a similar line of reasoning, one could arrive at $\int \{\eta^{-1} \int \eta^{-1}\} \leq H_2 \xi_0^2$ and so on if more integrals are nested. The same applies to the G and ρ , resulting in similar inequalities for nested integrations of their combinations as well. Thus, in the case of δ_1 in Eq. (41), the numerator would be ξ_0^2 as well as the denominator, whereas in the case of δ_2 , the numerator and denominator would be cubic powers. Requiring that the physical properties of shear modulus G , viscosity η , and mass density ρ be bounded is a natural and prudent requirement in this case. Thus, f_1 would be expected to behave asymptotically as $\xi_0 = x/l$ ensuring that the limit of κ_{eff} exists.

It is now convenient to express effective wave number as a function of the frequency ω for later use. To this end, we use (17) and (46) in (50) to get

$$\kappa_{eff} = l^{-1} \nu \langle \eta^{-1} \rangle \sqrt{i\zeta},$$

from which, by substituting $l^{-1} = \omega \sqrt{\tilde{\rho}/\tilde{G}}$ and $\nu = \sqrt{\tilde{G}}/\sqrt{\omega\tilde{\eta}}$, we get

$$\kappa_{eff} = \sqrt{\frac{\omega \tilde{\rho}}{\tilde{\eta}}} \langle \eta^{-1} \rangle \sqrt{i\zeta}, \quad (51)$$

which is the sought dependency because neither $\langle \eta^{-1} \rangle$ nor $\zeta = -i\alpha_{01}^2 \kappa_{01}^2$ depend on ω . Parameter α_{01} has been associated with f_1 to obtain the average value of $1/\eta$. Once the effective complex wave number is obtained, propagation speed and attenuation are immediate to find because by writing the body of the harmonic wave as $e^{i((\kappa_R + i\kappa_I)x - \omega t)}$, where $\kappa_{eff} = \kappa_R + i\kappa_I$, we have

$$\kappa_R = \frac{\omega}{v_{eff}}, \quad (52)$$

$$\kappa_I = \alpha_{eff}, \quad (53)$$

with v_{eff} the effective propagation speed and α_{eff} the effective attenuation.

Notably, this is to say that negative imaginary part $-\kappa_I$ becomes Floquet-Bloch's exponent when G , η and ρ are periodic functions [49,50]. Floquet-Bloch theory tells us that a solution of a differential equation like Eq. (5) with periodic coefficients sharing same period can be written as $e^{-kx} \psi(x)$ where ψ is a periodic function with period equal to that of the coefficients, e^{-kx} is the Floquet-Bloch factor and $-k$ is the Floquet-Bloch exponent or index. To see that $-\kappa_I$ is a Floquet-Bloch exponent we take solution (45) to its limit form when $\xi_0 \rightarrow \infty$. From Eq. (43), f_1 is dominated by the behavior of $\int \eta^{-1}$ in such a limit. Since η is periodic, say b -periodic, it is possible to write $\int \eta^{-1} = m_\eta(\xi_0 - \xi_a) + p_\eta(\xi_0)$

with $m_\eta = b^{-1} \int_{\xi_a}^{\xi_a+b} \eta^{-1}$ the mean value of η^{-1} over a period and $p_\eta(\xi_0)$ a suitable b -periodic function. Note that this linear growth is consistent with requirement of being η^{-1} bounded. Then, after some rearrangement, solution (45) is

$$\begin{aligned} \exp(i\kappa_{01}\xi_1) &= \exp\left(i\sqrt{i\zeta}\nu \frac{f_1(\xi_0)}{\alpha_{01}}\right) \xrightarrow{\xi_0 \rightarrow \infty} \\ &\exp\left(-\sqrt{\frac{\zeta}{2}}\nu m_\eta(\xi_0 - \xi_a)\right) \exp\left(-\sqrt{\frac{\zeta}{2}}\nu p_\eta(\xi_0)\right) \times \\ &\exp\left(i\sqrt{\frac{\zeta}{2}}\nu (m_\eta(\xi_0 - \xi_a) + p_\eta(\xi_0))\right), \end{aligned} \quad (54)$$

from which it is clear that as the last two exponential functions enclose exclusively periodic contributions, the first exponential function coincides with Floquet-Bloch factor and, therefore, $k = \sqrt{(\zeta/2)}\nu m_\eta l^{-1}$ is the negative Floquet-Bloch exponent. Moreover, when η is periodic, it follows that $\langle \eta^{-1} \rangle = m_\eta$ and $\kappa_I = k$, so effective wave number definition is in accordance with what is expected from Floquet-Bloch theory. This shows that the results for periodic properties are recovered as a special case since no prior restriction has been assumed regarding the arrangement of the layers, which can even be arranged randomly.

The approximate solution u of the original problem (1) is found from the real part of (49). Section 5 presents some numerical solutions.

5. Validation

Now problem (3) will be solved numerically with the transfer matrix method [51,52], and compared with approximate solution (49).

Restricting problem (3) to each layer of the medium (see Fig. 1) we get

$$\begin{cases} \frac{d^2 \hat{w}_n}{dx^2} + \kappa_n^2 \hat{w}_n(x) = 0, & x \in [x_n, x_{n+1}], \\ \hat{w}_n(x)|_{x=x_n} = \hat{w}_{n+1}(x)|_{x=x_n}, \\ G_n^* \frac{d\hat{w}_n}{dx} \Big|_{x=x_n} = G_{n+1}^* \frac{d\hat{w}_{n+1}}{dx} \Big|_{x=x_n}, \end{cases} \quad (55)$$

with $n = 1, \dots, N$; $\hat{w}_n$ is the complex displacement field solution in the n -th layer, and $\kappa_n = \sqrt{\omega^2 \hat{\rho}_n / G_n^*}$ with $\hat{\rho}_n$ and G_n^* the constant approximations of $\hat{\rho}(x)$ and $G^*(x, \omega)$ in the n -th layer. Note that $\hat{w}_n$ is not the n -th approximation order contribution w_n in the asymptotic expansion (6). In addition, the boundary and attenuation conditions are

$$\begin{cases} \hat{w}_1(x)|_{x=x_0} = \hat{w}_0, \\ G_1^* \frac{d\hat{w}_1}{dx} \Big|_{x=x_0} = \hat{s}_0, \\ \lim_{x \rightarrow \infty} \hat{w}_{N+1}(x) = 0, \end{cases} \quad (56)$$

where $\hat{w}_0 = \hat{w}_a$ and $\hat{s}_0 = \hat{s}_a$ are the constant complex boundary values in $x = x_0 = a$.

The solution of problem (55) on the n -th layer is

$$\hat{w}_n(x) = A_n e^{i\kappa_n x} + B_n e^{-i\kappa_n x}, \quad (57)$$

where A_n and B_n are the integration constants. Taking into account that the stress in the n -th layer is $\hat{s}_n(x) = G_n^* d\hat{w}_n/dx$, we can write

$$\begin{bmatrix} \hat{w}_n(x) \\ \hat{s}_n(x) \end{bmatrix} = M_n(x) \begin{bmatrix} A_n \\ B_n \end{bmatrix}, \quad (58)$$

with

$$M_n(x) = \begin{bmatrix} e^{i\kappa_n x} & e^{-i\kappa_n x} \\ i\kappa_n G_n^* e^{i\kappa_n x} & -i\kappa_n G_n^* e^{-i\kappa_n x} \end{bmatrix}. \quad (59)$$

Since matrix $M_n(x)$ is non-singular, we have

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = M_n^{-1}(x) \begin{bmatrix} \hat{w}_n(x) \\ \hat{s}_n(x) \end{bmatrix}, \quad (60)$$

where

$$M_n^{-1}(x) = \frac{1}{2i\kappa_n G_n^*} \begin{bmatrix} i\kappa_n G_n^* e^{-i\kappa_n x} & e^{-i\kappa_n x} \\ i\kappa_n G_n^* e^{i\kappa_n x} & -e^{i\kappa_n x} \end{bmatrix}. \quad (61)$$

The continuity conditions in (55) can be written as

$$\begin{bmatrix} \hat{w}_{n+1}(x_n) \\ \hat{s}_{n+1}(x_n) \end{bmatrix} = \begin{bmatrix} \hat{w}_n(x_n) \\ \hat{s}_n(x_n) \end{bmatrix}, \quad n = 1, 2, \dots, N, \quad (62)$$

from which it follows that

$$\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix} = M_{n+1}^{-1}(x_n) M_n(x_n) \begin{bmatrix} A_n \\ B_n \end{bmatrix}, \quad (63)$$

where (58) was used. This formula expresses the coefficients of the solution in the $(n+1)$ -th layer as a function of those in the n -th. Then, the iterative application of formula (63) starting from $N+1$ produces

$$\begin{bmatrix} A_{N+1} \\ B_{N+1} \end{bmatrix} = M_{N+1}^{-1}(x_N) M_N(x_N) \cdots M_{n+1}^{-1}(x_n) \quad (64)$$

$$\times M_n(x_n) M_{n-1}^{-1}(x_{n-1}) M_{n-1}(x_{n-1}) \cdots \quad (65)$$

$$\times M_2^{-1}(x_1) M_1(x_1) \begin{bmatrix} A_1 \\ B_1 \end{bmatrix}. \quad (66)$$

By left-multiplying (66) by matrix $M_{N+1}(x_N)$, then using (58) in $x = x_N$ to replace the product on the left-hand side, and using (60) to replace the column vector of layer $n = 1$ on the right-hand side, we obtain

$$\begin{bmatrix} \hat{w}_N \\ \hat{s}_N \end{bmatrix} = M_N(x_N) \cdots M_{n+1}^{-1}(x_n) M_n(x_n) M_{n+1}^{-1}(x_{n-1}) \quad (67)$$

$$\times M_{n-1}(x_{n-1}) \cdots M_1^{-1}(x_0) \begin{bmatrix} \hat{w}_0 \\ \hat{s}_0 \end{bmatrix}, \quad (68)$$

where $\hat{w}_N = \hat{w}_{N+1}(x_N) = \hat{w}_N(x_N)$ and $\hat{s}_N = \hat{s}_{N+1}(x_N) = \hat{s}_N(x_N)$. Define $T_n = M_n(x_n) M_{n+1}^{-1}(x_{n-1})$, so (68) can be rewritten as

$$\begin{bmatrix} \hat{w}_N \\ \hat{s}_N \end{bmatrix} = T \begin{bmatrix} \hat{w}_0 \\ \hat{s}_0 \end{bmatrix}, \quad (69)$$

where $T = T_N \cdots T_n \cdots T_1$, with

$$T_n = M_n(x_n) M_{n+1}^{-1}(x_{n-1}) = \begin{bmatrix} \cos(\kappa_n l_n) & \left(\frac{1}{\kappa_n G_n^*}\right) \sin(\kappa_n l_n) \\ -(\kappa_n G_n^*) \sin(\kappa_n l_n) & \cos(\kappa_n l_n) \end{bmatrix}, \quad (70)$$

and $l_n = x_n - x_{n-1}$ the thickness of the n -th layer, $n = 1, 2, \dots, N$. The elementary case of (69) for a single layer allows observing that T_n connects the values at one end of the n th layer with the values at its other end, that is,

$$\begin{bmatrix} \hat{w}_n(x_n) \\ \hat{s}_n(x_n) \end{bmatrix} = T_n \begin{bmatrix} \hat{w}_n(x_{n-1}) \\ \hat{s}_n(x_{n-1}) \end{bmatrix}, \quad n = 1, 2, \dots, N, \quad (71)$$

which means that if the values of displacement and stress on a boundary are known, then the corresponding values on the rest of the boundaries can be determined thanks to the continuity boundary conditions, and even the value at each point of the domain, as long as the parameters of each layer are known, namely, the thickness, the shear modulus of elasticity, the dynamical viscosity and the mass density. The first two boundary conditions of the relations (56) provide this information in principle, however, provided that the third of them is valid, which is the attenuation condition, one of the first two, displacement or stress, must remain unknown, that is, one of them would correspond to the imposed signal and the other to the response. In order to determine the response, it should be noted that the attenuation condition implies that the shape of the displacement in the $(N+1)$ -th medium (x_N, ∞) is $\hat{w}_{N+1}(x) = A_{N+1} e^{i\kappa_{N+1} x} + B_{N+1} e^{-i\kappa_{N+1} x}$, where the first term corresponds to the plane wave traveling to the right [see Fig. 1b)], whereas the second term corresponds to a wave traveling to the left. Since the standing wave is imposed from the left on the $x = x_0$ boundary, it is expected to propagate to the right through each layer, generating transmission and reflection at each interface until reaching the $(N+1)$ -th medium, where there would no longer be reflection but only propagation to the right. Hence, the coefficient of the leftward wave must be $B_{N+1} = 0$. From (60) we can see that $B_{N+1} = (i\kappa_{N+1} G_{N+1}^* e^{i\kappa_{N+1} x_N} \hat{w}_N - e^{i\kappa_{N+1} x_N} \hat{s}_N) / (i2\kappa_{N+1} G_{N+1}^*) = 0$, which implies that

$$i\kappa_{N+1} G_{N+1}^* \hat{w}_N - \hat{s}_N = 0. \quad (72)$$

Note now that this new condition deduced from the wave attenuation condition requires knowledge of parameters κ_{N+1} and G_{N+1}^* . On the one hand, the wave is expected to be almost completely attenuated by the time it reaches the $N+1$ st medium. This means that the contribution of these parameters is significantly reduced, but so is their inherent error, allowing for some freedom in their selection. In other words, the propagation involves only a few layers beyond which no information is available, so their parameters can be chosen conveniently. On the other hand, it is best if no further unknowns are introduced. Ideally, κ_{N+1} and G_{N+1}^* should be expressed

in terms of the already known parameters of the other layers. One possibility is to use the same parameters as the last layer; another is to take the average parameters from the set of properties of the first few layers. The parameters used will be the equivalent parameters of the laminated medium. An equivalent medium is understood here as one whose parameters κ and G^* relate the displacements and stresses at the boundaries of the laminate through a relation similar to (71), that is,

$$\begin{bmatrix} \hat{w}_{N+1} \\ \hat{s}_{N+1} \end{bmatrix} = \begin{bmatrix} \cos(\kappa L) & (\frac{1}{\kappa G^*}) \sin(\kappa L) \\ -(\kappa G^*) \sin(\kappa L) & \cos(\kappa L) \end{bmatrix} \times \begin{bmatrix} \hat{w}_0 \\ \hat{s}_0 \end{bmatrix}, \quad (73)$$

where $L = l_1 + l_2 + \dots + l_N = x_N - x_0$ is the total length of the composite medium. It should be noted that this idea of effectiveness is similar to the one proposed in Ref. [36] and explained as the black box idea in the introduction section. These parameters have been chosen because of their simple relationship with known parameters and because they encompass the entire laminated medium.

Equations (69), (72), (73) together with the imposed boundary condition, for example, $\hat{w}_0 = \text{const.}$, represent a system of six equations with six unknowns, namely, $\hat{w}_0$, $\hat{s}_0$, $\hat{w}_N$, $\hat{s}_N$, κ and G^* , but it must be kept in mind that $\kappa_{N+1} = \kappa$ y $G_{N+1}^* = G^*$, because of the construction of the effective medium.

It follows from (73) that

$$\cos(\kappa L) = \frac{\hat{w}_N \hat{s}_N + \hat{w}_0 \hat{s}_0}{\hat{w}_N \hat{s}_0 + \hat{w}_0 \hat{s}_N}, \quad (74)$$

$$(\kappa G^*)^2 = \frac{\hat{s}_0^2 - \hat{s}_N^2}{\hat{w}_N^2 - \hat{w}_0^2}. \quad (75)$$

Then, from (71), (72) and (75), we have

$$(r_{12}^2) (\mathbf{i} \kappa G^*)^4 + (2r_{11}r_{12}) (\mathbf{i} \kappa G^*)^3 + (r_{11}^2 - r_{22}^2) (\mathbf{i} \kappa G^*)^2 + (-2r_{21}r_{22}) (\mathbf{i} \kappa G^*) + (-r_{21}^2) = 0, \quad (76)$$

where r_{ij} are the components of matrix $R = T^{-1}$. Solving (76) for $\mathbf{i} \kappa G^*$, and then using (74) allows determining κ and G^* , which in turn reveals the relation between $\hat{w}_N$ and $\hat{s}_N$. With this relation, (72) and (69), it is possible to determine the two remaining unknowns having substituted the value imposed at the boundary. Regarding the four possible solutions of (76), only one has a consistent physical meaning.

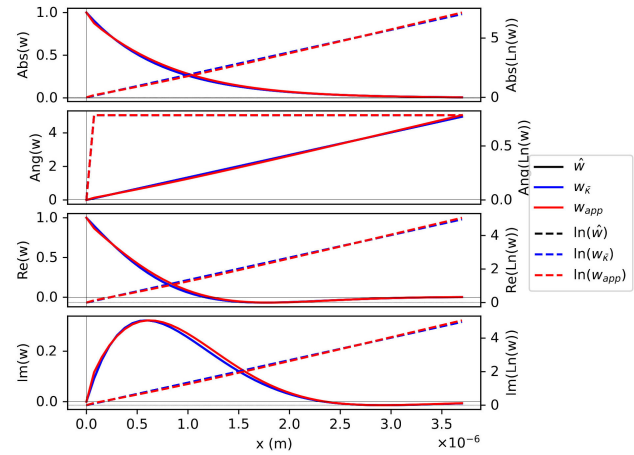


FIGURE 2. Comparison of solutions $\hat{w}$, $w_{\tilde{\kappa}}$ and w_{app} for frequency $\omega/2\pi = 10$ MHz and 1 layer. Vertical axes are dimensionless but the angle one is in rads. Right vertical axes in log scale apply for dashed lines.

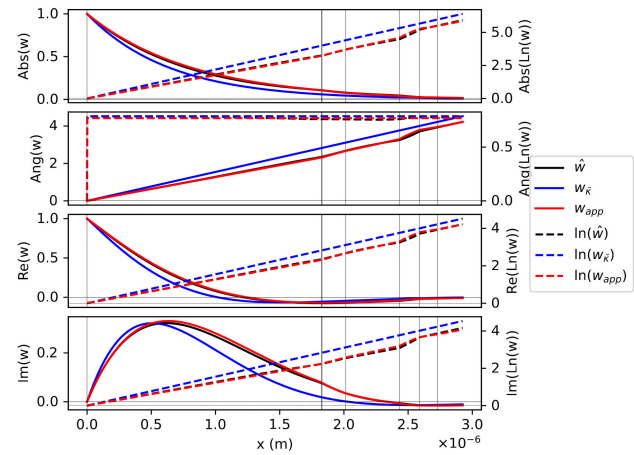


FIGURE 3. Same settings as in Fig. 2 but with 10 layers.

Figures 2-5 show the numerical solutions with the transfer matrix method denoted by $\hat{w}$ (black curves), the analytical solutions of lower order approximation (49) denoted by w_{app} (red curves) and, for comparison, the solutions when the parameter of the average complex wave number is used, weighted according to the width of the layers, denoted by $w_{\tilde{\kappa}}$ (blue curves), obtained via the formulas

$$w_{\tilde{\kappa}}(x) = w_a \exp(\mathbf{i} \tilde{\kappa}(x - x_0)), \quad (77)$$

$$\tilde{\kappa} = \frac{1}{L} \sum_{n=1}^N l_n \sqrt{\frac{\omega^2 \hat{\rho}_n}{\hat{G}_n - \mathbf{i} \omega \hat{\eta}_n}}. \quad (78)$$

Vertical lines in gray indicate the interfaces, showing only those inside the attenuation range of the wave. In each figure, the top four subfigures show the real and imaginary parts of solutions $\hat{w}$, $w_{\tilde{\kappa}}$ and w_{app} , as well as their absolute values and angles (left vertical axis and continuous curves), whereas the

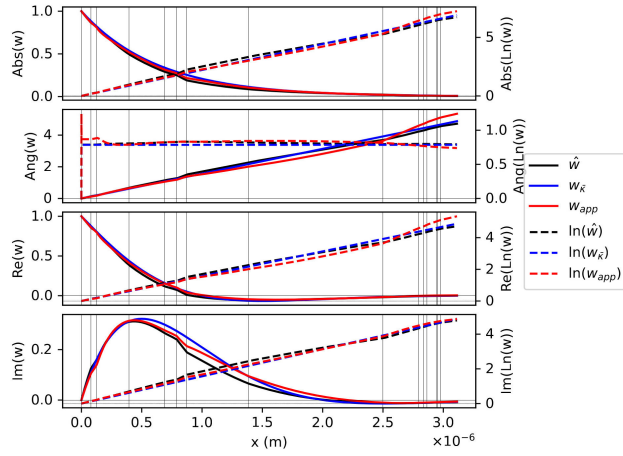


FIGURE 4. Same settings as in Fig. 2 but with 30 layers.

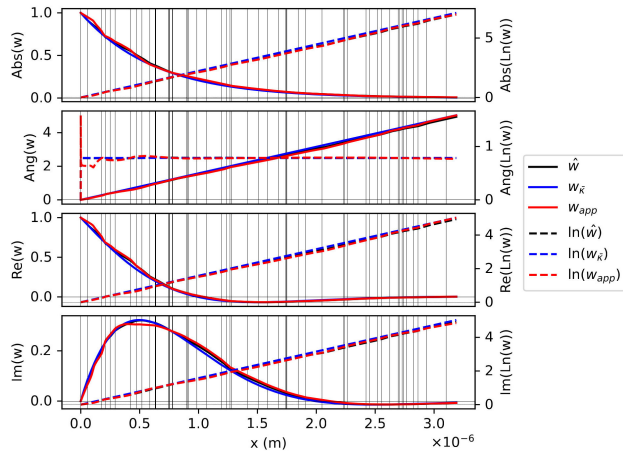
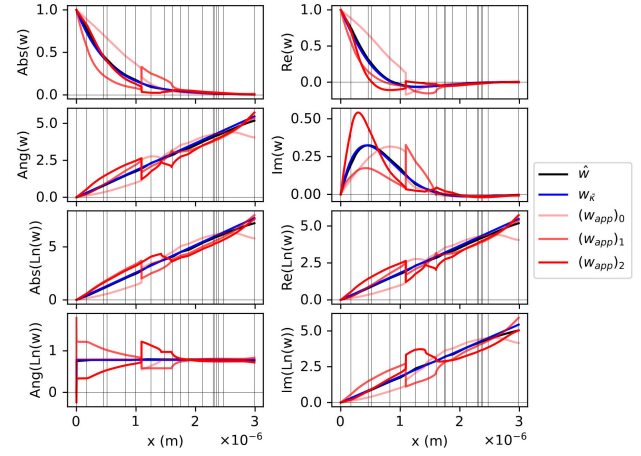


FIGURE 5. Same settings as in Fig. 2 but 100 layers.

right vertical axis is for natural logarithms of these quantities (dotted curves). Figures 2-5 correspond to 1, 10, 30 and 100 layers, respectively. The data sets of elasticity modulus, viscosity and density were generated randomly with standard distributions with average values from the data reported in Ref. [53] for bovine muscle tissue, therefore values $\tilde{G}$, $\tilde{\eta}$ and $\tilde{\rho}$ were taken as these average values as follows: $\tilde{G} = 0$, $\tilde{\eta} = 0,014$ Pa·s and $\tilde{\rho} = 1,080$ kg/m³, and their standard deviations as $\sigma_G = 6,250$ Pa, $\sigma_\eta = 0,0035$ Pa·s and $\sigma_\rho = 0$, that is, constant density. The choice of these values comes from the fact that, around $G = 0$, the $\tilde{G}/\omega\tilde{\eta} \ll 1$ approximation is the best, on which the definition of the small expansion parameter is based. Frequency is set at $\omega = 10$ MHz, which is approximately where the curve of the elasticity modulus crosses the horizontal axis, that is, where it changes sign.

For soft tissue such as skeletal muscle, $\tilde{G}$ values close to zero and $\tilde{\eta} \sim 0,01$ Pa·s can be found according to [54] at frequencies ~ 15 MHz, whereas for hydrogel (a soft tissue substitute) the values are approximately $\tilde{G} \sim 100$ kPa and $\tilde{\eta} \sim 0,1$ Pa·s at frequencies ~ 100 MHz according to [55]. Unfortunately, the response of this type of material reported in literature at frequencies of MHz is scarce, largely because

FIGURE 6. Comparison of solutions $\hat{w}$, $w_{\tilde{\kappa}}$ and the three possible solutions for w_{app} . Frequency $\omega/2\pi = 10$ MHz and 30 layers.

shear waves attenuate very quickly, as [53] points out, which makes the applicability of the results obtained here for these substitutes invalid, which is why no graphics have been presented for these materials. On the other hand, an encouraging aspect is that the trend shown by [55] themselves for higher frequencies seems to indicate that the dominant viscosity regime would be reached for a frequency on the order of ~ 10 MHz fulfilling the assumption $\sqrt{\tilde{G}/\omega\tilde{\eta}} \ll 1$.

In general, at first glance, $w_{\tilde{\kappa}}$ and w_{app} behave very similarly. However, tests with different groups of random data show that the w_{app} solution decreases in stability for increasing absolute value or dispersion of the elastic modulus data G and with increasing number of layers, which is expected in the first case, but not obvious in the second one. In fact, the greater the number of layers, the more frequently one can find behaviors like the one shown in Fig. 6, where jumps appear related to divisions by zero or changes of sign in the discriminant $\Delta_1^2 - 4\Delta_0^3$ associated with (39) in the numerical calculations. The yellow curves correspond to the different solution branches of w_{app} originating from the different solutions of f_1 (39). After testing with different data, we speculate that divisions by zero and sign changes of the discriminant seem to indicate opportunities to jump between the different solution branches, which could be tested in a future work. On the other hand, it should be noted that w_{app} seems to be effectively better than $w_{\tilde{\kappa}}$ in those cases in which the distribution of layers is not uniform, which is better observed in the case of a low number of layers as in Fig. 3. Moreover, w_{app} accompanies the numerical solution $\hat{w}$ in its breaks or non-smooth changes at the interfaces, whereas $w_{\tilde{\kappa}}$ does not due to its average nature. Also, the difference between the effective complex wave number (51) to (78) is less than 5%. Finally, it is important to take into account, from a methodological point of view, that the constant α_{01} was absorbed in the definition of f_1 . This constant was optimally chosen to fit the numerical solution w , that is, to select the best approximate solution as the one with the best least-squares fit.

6. Conclusions

Seeking to build models for biomaterials, this work addressed the problem of shear-type waves emitted at the boundary of a laminated medium with layers made of homogeneous Voigt-type viscoelastic materials. The focus was placed on what happens in the immediate environment of the ray of incidence, with propagation perpendicular to the interfaces, so plane waves do not disperse in longitudinal waves or by changes of direction. The model was transformed into a perturbation problem and studied via the multiple scales method, from which the lowest nonzero order approximate solution was obtained with respect to the expansion parameter $\sqrt{\tilde{G}/\omega\tilde{\eta}} \ll 1$, which can be interpreted as the viscous relaxation being much smaller than the propagation period of the harmonic plane wave. The thermal effects derived from local friction were neglected, which means that the alterations in the parameters due to temperature changes caused by the mechanical propagation are not taken into account. The layers were taken to have random parameters close to the values for bovine muscle tissue reported in Ref. [53] in the frequency range of 10 MHz for which the elastic modulus G approaches zero and the viscosity is relatively constant.

The results obtained via the multiple scales method are applicable to situations where the excitation frequency is moderately high, so the effects of nonlinear responses can be neglected. It can be noted that the use of information from the medium and the excitation signal to define the appropriate expansion parameter is crucial, resulting in important simplifications of analysis.

Unlike classical homogenization (*e.g.*, [56]), this formulation is applicable to non-periodic structures. It allows for obtaining analytical expressions, in contrast to the numerical solution approach, and opens new avenues of connection with other problems. For example, the coefficients of the differential equation (G , η , and ρ) can be not only piecewise constant functions but also continuous, like a sinusoidal periodic function as in the Mathieu equation [57]. Furthermore, it focuses on the dependence of the material's response on the strain rate (frequency), making it clear that the interpretation of the constitutive parameters of the Voigt model must be done in terms of a frequency range.

Comparison was made to the results of the transfer matrix method, which is easily generalizable to any number of layers

without making the expressions and computation more complex, with little loss of accuracy. Such expressions are useful for approximating the behavior of non-homogeneous media with piecewise continuous parameters, which allows the direct numerical treatment of the integrals. In fact, they are useful for media with random parameters of constant mean. Although further tests are needed in addition to numerical ones, such as dimensionless analysis, the variation with respect to the length fraction parameters l_n or others, as well as a more formal determination of the error, the results obtained so far are of practical value with relative low complexity.

Regarding the accuracy of the analytical expressions of lower order approximation (49) in comparison to the weighted wave number solution, it was observed that, in general, the former is not better than the latter. However, the lower order approximation solution has the virtue of reproducing the variations due to the structure of the medium, that is, to the value changes in the parameters of the propagation medium, which has the potential to transport information from the medium to the response signal and to decode it.

As future work, we can mention the application of these ideas to the design of agar-based phantoms with parameters guided via concentration, which would allow, from a theoretical point of view, the analysis of a greater number of configurations to evaluate their feasibility of implementation. In addition, the formulation will be generalized to more dimensions, considering the possibility of more elaborate geometries. In fact, these results would be part of a broader numerical simulation study, which in turn shortens the path for parameter estimation in situations of varying complexity. On the other hand, attenuation models in terms of conduction and internal friction could be incorporated to describe the dependence on the structure of the medium which, in turn, would lead to the proposal of possibly more appropriate constitutive models.

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A method for analyzing physiological data with multiple non-independent observations

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Physiological studies often involve recording multiple observations (*e.g.*, repeated muscle contractions or cardiac cycles) from the same subject. To compare groups of subjects, observations from one subject are then sometimes pooled with observations from other subjects in the same group, and analyses are performed on these pooled data. This approach presents a number of potential problems, including over- or under-representing certain subjects in the sample and non-independence of measurements. There are statistical methods available to deal with repeated measures, but many make assumptions about the distribution and completeness of data. Instead, we developed a method to deal with multiple observations from physiological data that ensures that each subject is represented only once in the analysis (*i.e.* it avoids pseudoreplication), and makes no assumptions about the distribution of the data. We demonstrate this method using two different physiological datasets: (1) muscle recordings taken from *Drosophila melanogaster* larvae during fictive crawling, and (2) electrocardiogram recordings taken from human volunteers before, during, and after exercise. Our results show the broad applicability and validity of this method.

Keywords: Analysis; data science; electrophysiology; physiology.

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1. Introduction

The study of physiological processes, like motor control or heart rate variability, often requires taking multiple observations from the same subject. For example, studying fictive crawling in *Drosophila melanogaster* larvae involves intracellular or extracellular recording of multiple muscle contraction cycles [1,2]. This spontaneous activity can last from seconds to minutes, representing tens of cycles recorded from the same animal. However, the variability across subjects can be substantial, depending on both the frequency of activity and its overall duration. Similarly, heart rate variability in human subjects is studied by recording multiple cardiac cycles using electrocardiography (ECG) and monitoring changes in the time between cycles (RR intervals) [3]. The number of RR intervals recorded from a single subject can be in the tens to thousands, varying widely depending on both heart rate and the total duration of the experimental protocol.

Such physiological studies share several challenges, including that there are multiple observations recorded from a single subject and that not all subjects have the same number of observations (*i.e.*, an unbalanced design). In some studies, data from subjects in a given group are pooled and the group sample size is taken as the total number of observations. This is problematic for two reasons. First, if there are a different number of observations for each subject, this means that subjects will be weighted differently in the pooled sample. If there are subjects that present different behaviors but have a

large number of observations, the pooled sample could skew towards these subjects. The issue becomes more serious if some of the variability between subjects in terms of the number of observations depends on one of the factors under study. For example, in studies of exercise, the number of cardiac cycles in a subject will depend on their heart rate. If observations are pooled, the distribution could skew towards those subjects with higher heart rates. Statistically, the group sample size should be the number of subjects, with each subject represented only once. This brings us to a second problem, namely that many statistical tests used to compare groups assume that the data points are independent of one another. However, multiple observations from the same subject are usually not independent, and treating them as such constitutes pseudoreplication [4].

Though the importance of pseudoreplication continues to be debated [5], it does appear to be prevalent in some disciplines (*e.g.*, 12-36 % in neuroscientific studies [6]) and can lead to erroneous positive results in physiological studies [7]. Analysis strategies and statistical tests exist to handle repeated measures, but are not ideal for the types of data discussed here. For example, one could take a single measure (*e.g.* the median RR interval) for each subject, and then work with a distribution of medians for the group – a method known as aggregation [8]. This addresses the pseudoreplication problem, but involves losing a lot of the richness in the data, among other issues [8]. Statistical tests like repeated measu-

res ANOVA are not suitable, since these have assumptions, *e.g.*, about sphericity and completeness of data [9], which are often not met.

To address these issues, we have developed a method designed to preserve the spread of the data from each subject, construct a representation of the group distribution using the distributions from its individuals, and still guarantee that each subject is represented only once in the analysis. Importantly, this method does not require the data to be approximately normally distributed, or that the range for the data points is restricted to any domain. We illustrate this method by using it to analyze two physiological datasets. The first consists of intramuscular recordings taken from *Drosophila* larvae during fictive crawling. These data were obtained by one of the present authors (ECM) and have been described previously [2]. The second dataset consists of ECG recordings from volunteer human subjects taken before, during, and after exercise. These recordings were obtained by two of the present authors (HA and AT) and have not been reported previously. We share all the data and code used to implement these analyses. Our results show the simplicity and broad applicability of this method, and we hope it will provide a viable alternative to pooling for researchers analyzing similar physiological data.

2. Methods

2.1. Physiological data

2.1.1. *Drosophila* muscle recordings

The fly lines, rearing conditions, dissection method, and electrophysiological recording technique have all been described in detail previously [2]. Briefly, larvae were dissected to expose the body wall muscles, and flexible sharp glass electrodes were inserted into muscle 1 (M1) [10] to record intracellularly from neighboring abdominal segments. In this way, spontaneous bouts of peristaltic muscle activity (fictive crawling) can be recorded as waves of contraction that advance from the posterior to anterior body segments. This activity is registered as regular bursts of action potentials. While several measures can be obtained from these data, we focus on the cycle duration, which is the time elapsed from the start of one burst to the start of the next. We compared the cycle durations of two groups: (1) wildtype (WT) larvae ($n = 21$), and (2) larvae expressing the *slo*¹ mutation ($n = 10$; Bloomington *Drosophila* Stock Center No. 4587; RRID BDSC_4587). Again, effects of this mutation on bursting activity have been reported previously in Ref. [2].

2.1.2. Human ECG recordings

Subjects were student volunteers between 18 and 24 years of age recruited within the School of Sciences at the National Autonomous University of Mexico (UNAM) between May and September of 2019. Volunteers were informed of

the study procedures, signed a letter of consent to participate, and were ensured that any identifying data would be kept confidential. ECGs were recorded using a Zephyr BioHarness before, during, and after exercise on a stationary bicycle (Pro-Form 325 CSX). Subjects were asked to remain at rest for the first 7 minutes of the recording, then begin cycling, gradually increasing intensity during minutes 7-9. At the 9-minute mark, subjects were asked to further increase their exercise to achieve a pre-specified intensity level (*e.g.* 60 watts, as indicated on the bicycle interface), and then maintain that intensity until minute 20. A recovery period followed until around the 30-minute mark, when the recording ended. The time elapsed between successive cardiac cycles was measured as the RR interval. We compared the RR intervals of two groups: (1) volunteers classified as physically fit, or active ($n = 11$), and (2) volunteers classified as less physically fit, or sedentary ($n = 10$). Classification was based on exercise tolerance: subjects who reached a heart rate of 150 beats per minute (BPM) at the 60-watt exercise intensity level were classified as less fit (group 2) than subjects whose heart rate did not reach 150 BPM until the 75-watt level (group 1). Based on our protocol, subjects did not proceed to the next watt-level once reaching 150 BPM. Therefore, for this study, we compared recordings at the maximum watt-level achieved by all subjects, *i.e.* 60 watts. To also minimize variability, we compared subjects' RR intervals during the period of exercise that was most stable, *i.e.* minutes 17-20. (Changes in RR intervals during the other protocol time periods will be explored in a future paper). All ECG data were collected by authors HA and AT. Authors ECM and MAHV were not involved in the original study but were given access to the anonymized ECG data for analysis in February of 2024. The Academic Ethics and Scientific Responsibility Committee of UNAM's School of Sciences (CEARC) reviewed the project methodology in August 2025, and concluded that the study complied with bioethical guidelines.

2.2. Data analysis

Let X represent a continuous random variable of interest (*e.g.* RR interval).

Empirical distributions

Consider a sample $S = (x_1, \dots, x_n)$ and assume, without loss of generality, that $x_i \leq x_{i+1}$ for all $i \in \{1, \dots, n-1\}$. Assuming the random variable X is continuous, the empirical distribution function (EDF, [11,12]) for the sample can be defined as

$$J(x) = \begin{cases} 0, & x < x_1, \\ i/n & x \in [x_i, x_{i+1}), \quad i \in \{1, \dots, n\} \\ 1 & x_n \leq x. \end{cases} \quad (1)$$

If the sample is unbiased and contains enough data points, the function $J(x)$ can serve as an approximation for the distribution function of the variable represented by the points in S [12].

2.2.1. Group samples

Assume that two groups of samples $C = \{C_1, \dots, C_M\}$ and $D = \{D_1, \dots, D_N\}$ of X values are collected, and let $F_1, \dots, F_M$ and $G_1, \dots, G_N$ respectively represent the EDFs from the samples of the two groups. The point-wise averages of the EDFs for the two groups can then be calculated by letting

$$F(x) = M^{-1} \sum_{i=1}^M F_i(x), \quad (2)$$

and

$$G(x) = N^{-1} \sum_{j=1}^N G_j(x). \quad (3)$$

These point-wise average functions F and G can be thought of as representative EDFs for the groups C and D , respectively. For the cycle durations (CDs) obtained from *Drosophila* muscle recordings, the sample EDFs from the two groups of subjects will be denoted as F_{CD} (WT) and G_{CD} (Slo), respectively. Similarly, for the RR intervals obtained from human subjects, the two groups will be respectively labeled F_{RR} (active) and G_{RR} (sedentary).

For the two groups in our case, the whole range for the variable X can be defined as

$$R_X = (\cup_{i=1}^M C_i) \cup (\cup_{j=1}^N D_j). \quad (4)$$

The interval $[a, b]$ with $a = \min\{x \in R_X\}$ and $b = \max\{x \in R_X\}$ serves as an extended range for values of X as extracted from the two groups. From there, it is possible to evaluate the average EDF for each group using $[a, b]$ as a common interval.

2.2.2. Sampling

Kolmogorov's theorem [13] can be used to obtain values representative of a random variable X . If F is the distribution function of X , and $p \in [0, 1]$, then $q = F^{-1}(p)$ is a value that represents X so that $P(X \leq q)$. Therefore, any ordered sample $\alpha_1, \dots, \alpha_n$ uniformly drawn from the interval $[0, 1]$ can be used to sample n values for X . Explicitly, the sample would be $x_1 = F^{-1}(\alpha_1), \dots, x_n = F^{-1}(\alpha_n)$. For instance, the set $\{0, 0.25, 0.5, 0.75, 1\}$ yields the group minimum, maximum, and the quartiles for X as described by F . This procedure can then be applied using a large enough number of points uniformly sampled from the interval $[0, 1]$ to obtain representative samples of the two groups from the two average EDFs in Eqs. (2)-(3).

2.2.3. Histograms

To visually explore how the data are distributed and any potential shifts between groups, we construct histograms using samples drawn from each group EDF. For any given number of bins n , it is then possible to create a uniform partition $a = p_0, \dots, p_n = b$ of the interval of $[a, b]$, with each

subinterval having length $(b - a)n^{-1}$. The size of the subintervals can be selected according to physiological or experimental criteria. Histograms are only used herein for illustrative purposes and not for any statistical testing. As such, the chosen bin size will not affect the results.

2.2.4. Statistical testing and sensitivity analysis

Group distributions can be overlaid to visually demonstrate shifts in the observed values as a result of certain group characteristics or treatments. However, statistical testing is needed to determine whether these shifts are significant relative to a predetermined margin of error. We elected to use the Mann-Whitney U test (also known as the rank sum test) due to its lack of assumptions about the distribution of the data and its ability to test for "distributional differences", including changes in shape and spread [14]. (Note that the non-parametric Kruskal Wallis test – an extension of the two-group Mann-Whitney U test – could be used, if the comparison involves three or more groups [15]). The alpha value for the test was set at 0.05. We test the null hypothesis that the X -values from the two groups come from the same distribution.

The values entered into the rank sum test were calculated from the group EDFs using the sampling method described above, *i.e.* by evaluating the EDFs for each of the groups at n uniformly chosen values between 0 and 1. To determine the effect of selecting a specific n , we performed a sensitivity analysis. First, two groups were selected for comparison (*Drosophila* WT vs Slo, or human active vs. sedentary). Then, we evaluated the EDFs for each group using an n that corresponded to theoretical sample sizes of between 5 and 40 values with the aid of a random number generator. Finally, a rank sum test was performed to compare the two reconstructed samples, and the resulting p-value recorded. This process was repeated ten times for each theoretical sample size, so that p-values could be compared to determine the consistency of the results.

2.2.5. Analysis software

Burst times were extracted manually from *Drosophila* muscle recordings using Spike2 software and exported to csv files, as explained in Ref. [2]. RR intervals were extracted from human ECG recordings using the Zephyr BioHarness software (v.1.0.24.0) and exported to txt files. Code to analyze csv or txt data was written in Python 3.13.3 using functions from NumPy [16] and SciPy [17]. Figures were produced with matplotlib [18] and seaborn [19]. Additional Python modules used include csv, math, os, pyabf, pylab, stats, and sys.

2.3. Resource availability

Resources generated by this study are available via GitHub github.com/emckiernan/physioanalysis and archived with a DOI via Zenodo

doi.org/10.5281/zenodo.15740855. To facilitate reuse, re-

sources are shared under open licenses (see

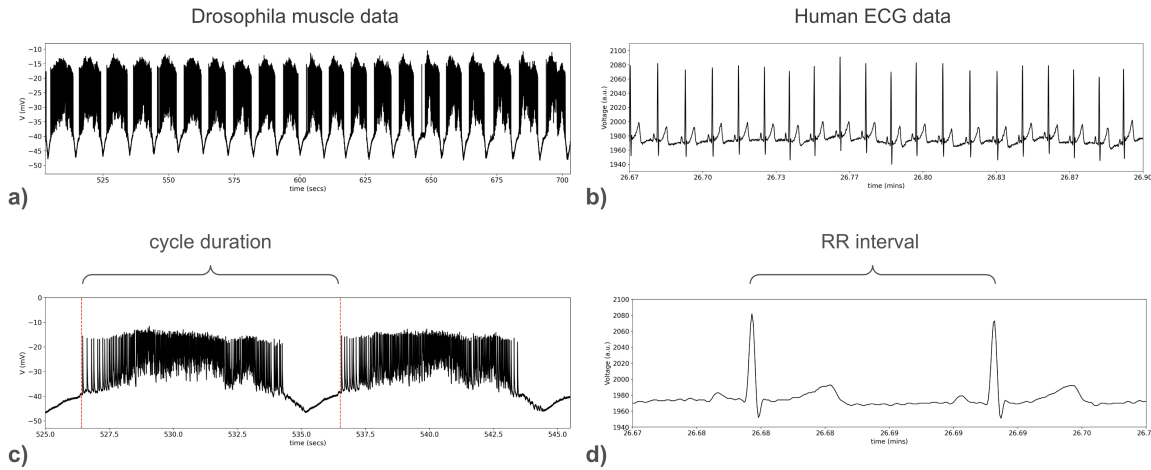


FIGURE 1. **Physiological data.** a) Intracellular muscle recording from a WT *Drosophila* larva. Activity was recorded during posterior to anterior contractile waves in muscle 1. Data from ECM [2]. b) ECG recording from a human volunteer. Original data from authors HA and AT. c) Zoom-in of data in A showing how cycle duration is calculated. d) Zoom-in of data in B showing how RR interval is calculated.

LICENSE.md in our repository). To promote reproducibility, Python code is embedded in Jupyter notebooks [20] that explain the code, how to use it, and how to generate figures.

3. Results and Discussion

3.1. Similarities between the datasets

Visual exploration shows that the two datasets share several characteristics important for their analysis (Fig. 1). First, both are continuous time series representing rhythmic physiological processes where the measure of interest repeats at regular intervals (Fig. 1a, 1b). Second, the measure of interest calculated from each time series (CD or RR interval) captures the length of a single cycle (Fig. 1c, 1d). Third, because we are measuring cycle length and the cycle repeats, the total number of observations from a single subject in both datasets will depend on two factors: (1) the frequency of activity (*i.e.* how many cycles occur per unit time), and (2) the total time of recording. Even when we can control the second factor by setting a fixed recording time, we will still have different numbers of observations across subjects due to variability in the first factor. Finally, because of these factors, subjects may have widely varying numbers of observations, with subjects generating higher-frequency activity necessarily having larger numbers.

3.2. Problems with pooling

Also in both datasets, we end up with repeated observations from a single subject that are not independent of one another. Many studies of such physiological processes ignore this issue, and pool observations for all subjects belonging to a given group (*e.g.* all CDs for WT subjects, or all RRs

for active subjects). To understand why this could be problematic, we look at the distributions for each subject in our samples to see their relative contributions. We do this by plotting their kernel density estimate (KDE), which is essentially a smoothed version of the histogram [21] for each subject that makes comparison visually easier (Fig. 2a, 2b). For both datasets, the subject KDEs show variability in their amplitude, shape, and spread. In other words, individual subjects may contribute very different sets of values to a pooled distribution. For example, the data from the WT *Drosophila* larvae show that two subjects have larger and more left-shifted KDEs than the rest of the subjects in the sample (see arrows in Fig. 2a). These are the two subjects with the largest numbers of observations (49 and 62 bursts). If we pool the data, these two subjects will be over-represented and could pull the group distribution to the left. We see something similar in the RR data from the active group (Fig. 2b). There is one subject whose values fall far to the right of the other subjects (see arrow), and could pull the distribution in that direction.

How much could these subjects affect a pooled distribution? To determine this, we took the same groups (WT *Drosophila* or active human volunteers), pooled subjects' observations within those groups, and plotted the respective histograms (referred to as the 'full' samples). We then removed the subjects of interest (those marked with arrows in Fig. 2a, 2b), and compared the histograms with these subjects removed ('restricted' samples). The results are similar for the two datasets (Fig. 2c, 2d). For the WT *Drosophila* larvae, removing the two subjects caused the three left-most bars in the histogram to either disappear or greatly diminish. In fact, this removed an entire peak which made the distribution (at least at this bin width) look bimodal. For the active volunteers, removing the one subject eliminated or reduced a large chunk (8 bars at this bin width) of the right side of the histogram.

These are well-known effects of what might be considered outliers, but we include them as visual confirmation of how

individual (or few) subjects can shift a pooled distribution, especially when samples are small.

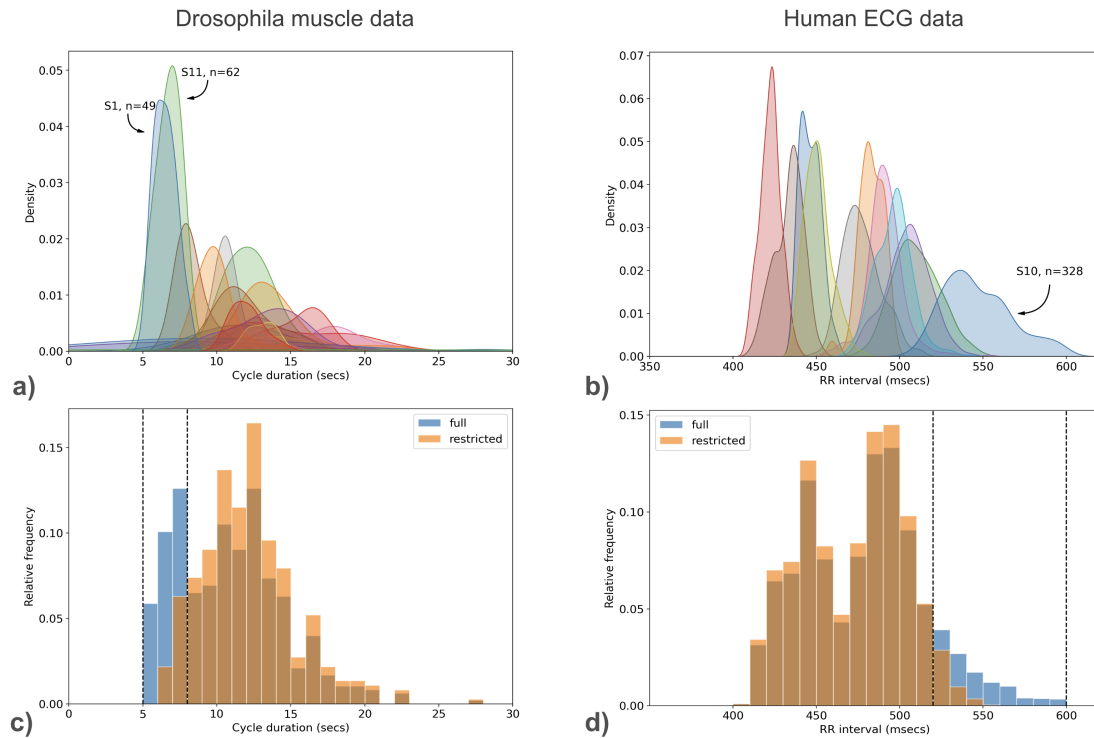


FIGURE 2. **Effects of pooling data.** a) KDEs for each subject in the WT *Drosophila* sample. Arrows mark two subjects with left-shifted peaks. b) KDEs for each subject in the active volunteer group. Arrow marks the right-shifted subject. c) Histograms of *Drosophila* data in a, comparing the full pooled sample (blue) to the restricted sample with two subjects removed (orange). d) Histograms of the active volunteer data in b, comparing the full pooled sample (blue) to the restricted sample with one subject removed (orange). Darker brownish areas in c and d show overlap between the blue and orange bars. Dashed lines in c and d delineate areas of difference between the full and restricted histograms.

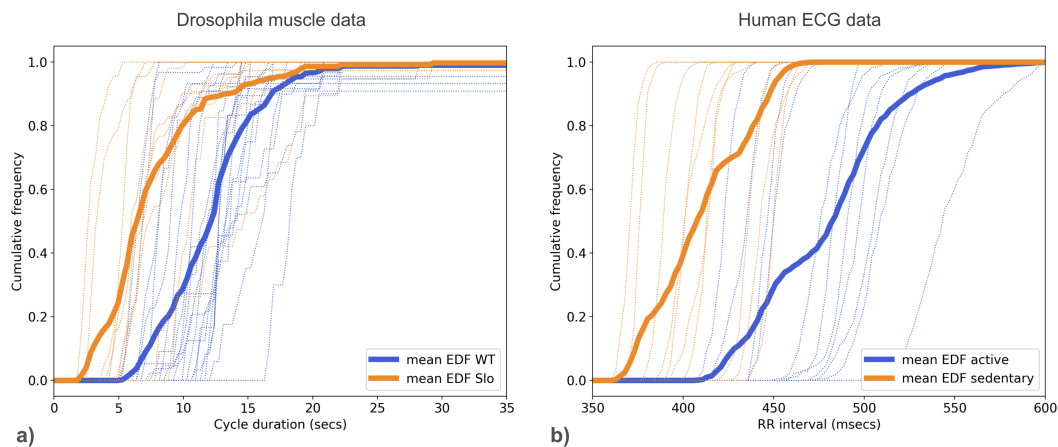


FIGURE 3. **Single-subject and group EDFs.** a) Single-subject (thin dashed lines) and averaged group (thick solid lines) EDFs for WT (blue) and Slo (orange) larvae. b) Single-subject (thin dashed lines) and averaged group (thick solid lines) EDFs for active (blue) and sedentary (orange) human volunteers.

3.3. Technique based on EDFs

Having established that pooling observations at best violates the assumption of independence and at worst leads to

skewed distributions, we need a better way to deal with such data. As described in the Methods, we did this by first calculating the empirical distribution function (EDF) of the CD or the RR values for a single subject, and then calculating

the point-wise average over all subjects in a given group to calculate the group EDF (Fig. 3). In this way, we do not lose the richness of the data – each subject is represented by their EDF, which captures the full range of values in their observations, rather than a single value like a mean or median. At the same time, taking a point-wise average of the EDFs means that at each point, each subject is represented only once. The subject EDFs are all independent of one another, and therefore, the resulting averaged group EDF is made up of independent ‘observations’ (subject EDFs), thereby avoiding pseudoreplication. In other words, each subject now contributes equally to the group, regardless of their initial number of observations. Importantly, while outliers could still skew a group distribution, using this averaged approach means no one subject is more able than any other to pull the distribution solely based on their number of observations. In both datasets, we can see that there is a clear separation between

the group EDFs (Fig. 3) that we should be able to test for statistical significance.

To test for statistical significance, we used the Mann-Whitney or rank sum test with a reference value for significance of 0.05 (standard for physiological studies). As described in the Methods, subsections ‘Samples’ and ‘Statistical testing and sensitivity analysis’, our technique relies on extracting values from the group EDFs for testing. We therefore ran a sensitivity analysis to see how the number of extracted values affects the results. To do this, we first set the theoretical sample size (the number of extracted values) between 5 and 40 values, and then used a random number generator to extract that number of values at different points along the averaged group EDFs. We run the statistical test on these extracted samples, and repeat the process 10 times for each sample size. Graphing the results shows how many of

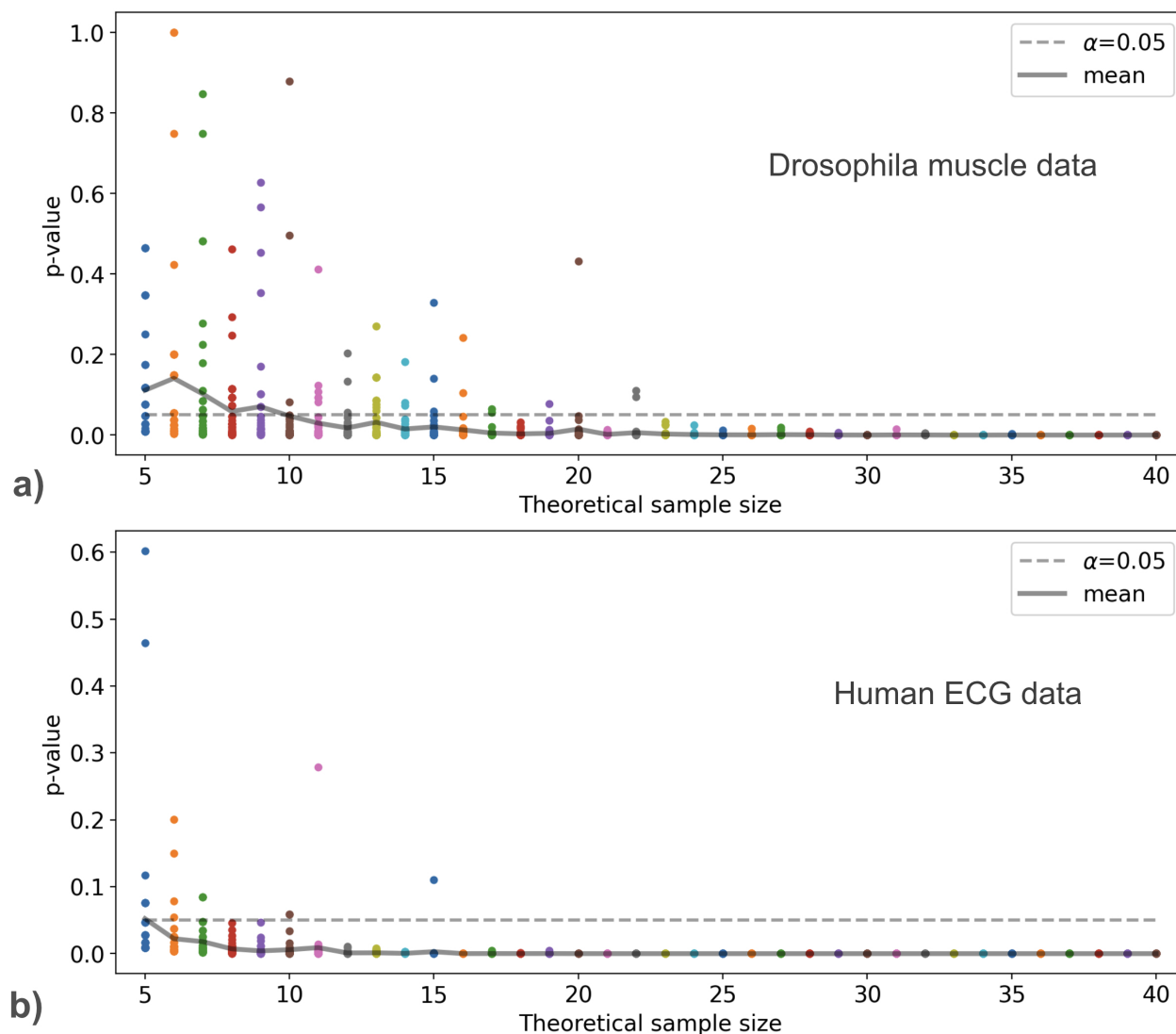


FIGURE 4. **Sensitivity analysis.** Statistical testing run 10 times for each theoretical sample size of 5 to 40 values extracted at random points along the group EDFs for *Drosophila* a) and human b) data. Note that not all points corresponding to each run are visible for all sample sizes due to overlap. Dashed line marks a cutoff for significance at 0.05. Solid line indicates the mean p-value over 10 runs at a given sample size.

these test-runs hit below the established alpha value of 0.05 for a given sample size (Fig. 4). For the *Drosophila* data, there is a large fluctuation in p-values at the lowest theoretical sample sizes of 5-10 (Fig. 4a). Between 10 and 20, there is still some fluctuation, though steadily decreasing as the sample size increases. Finally, most if not all test runs are below 0.05 as the sample size goes above 20. Similarly, for the human ECG data, there is some variability in p-values when the sample size is between 5 and 10, although this variability is smaller than that observed for the *Drosophila* data. For sample sizes greater than 10, most, if not all, runs yield p-values well below 0.05 (Fig. 4b). All our real samples include at least 10 and as many as 21 subjects in each group. Therefore, extracting 10-20 values from the group EDFs for statistical testing appears to be both reasonable and conservative.

The results from the sensitivity analysis (Fig. 4) may seem trivial, given it is well known that p-values decrease with sample size, but they are important in this specific context for two reasons. First, if the sensitivity analysis showed that it was necessary to extract a much larger number of values from the EDFs to reach significance than the number of subjects in the original samples, then the validity of the method could be in question. The quick decay in the p-values as a function of the theoretical sample sizes (Fig. 4) demonstrates that this was not the case. However, the reasonable range of values to extract will depend on the dataset, and should be evaluated on a case-by-case basis, which leads to the second point. This result represents a methodological recommendation for anyone using our technique: researchers should run a similar sensitivity analysis on their own data to determine the reasonable number of extracted values to use for statistical testing.

4. Conclusions

Proper data analysis, including ensuring we meet the assumptions of any statistical tests used, is crucial for the validity of study results and conclusions. We introduce an approach that allows researchers to analyze physiological datasets which present three common yet non-trivial issues: i)

non-Gaussian distributions, (ii) groups of unequal sizes, and (iii) repeated measurements from the same subject. While the individual mathematical techniques we use are not new, the novelty of our approach is in using the existing techniques in combination to address all three issues.

No one of these techniques is sufficient to address the various problems on its own. Using non-parametric statistical tests, such as Mann-Whitney or Kruskal-Wallis, only addresses issue (i), that the distributions are non-Gaussian. However, both tests still assume independence of observations [14,15], and cannot be applied until issue (iii) is dealt with. There are techniques designed to deal with repeated measures. However, as briefly reviewed in the Introduction, these either involve losing the original richness of the data (aggregation [8]), or involve assumptions about the distribution and completeness of data (e.g. repeated measures ANOVA [9]) that are violated by issues (i) and/or (ii). The same is true for issue (ii), where groups are of unequal size, or the experimental design is unbalanced. Many of the existing options are parametric in nature, and may involve a loss of data if observations have to be removed to achieve balance across groups [22]. The non-parametric options (like Mann-Whitney) again require independent observations.

Our technique has advantages over pooling data, including maintaining independence of measurements used for testing and avoiding pseudoreplication. It also represents advantages over techniques like aggregation in that the original richness of the data is preserved and considered. We show that this technique can be applied to different datasets, ranging from insect muscle to human heart recordings, demonstrating its generalizability. All our analysis code is publicly available so that it can be reused by other researchers and modified to fit their needs.

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Reuse of waste glass addition with industrial wastes and tungsten as new radiation shields: Spectroscopic and computational analysis

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The economic and environmental problems regarding waste encourage the researchers to reuse the waste and produce new materials. Waste glass, as a form of industrial waste, has gained growing attention in recent years. The objective of conducting this study is to evaluate the waste glasses obtained from our daily routines and to ascertain the radiation shielding capabilities of the waste materials obtained by adding other industrial wastes. With this purpose, three samples including both waste glass and industrial wastes (Bayburt stone dust and Oltu stone dust) were produced by mixing in different ratios. Also, tungsten was added to the samples in order to improve the protection ability. The Phy-X/PSD code was used to determine the radiation protection parameters. In addition to the shielding investigation, structural properties were characterized using EPR, XRD, and SEM-EDS spectroscopic techniques. It is obtained that the shielding performance of the sample including Bayburt stone dust and marble waste with tungsten addition is the highest. The lowest shielding performance is observed for the sample including Oltu stone dust and marble dust with tungsten addition. Neutron shielding capabilities are also found to be the same as photon shielding. It can be concluded that the newly prepared samples consisting of waste glass in order to support reusing and recycling have good protective features and the usage of the samples can be recommended.

Keywords: Waste glass; Industrial waste; Phy-X/PSD; Radiation shielding capability.

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1. Introduction

Waste glass (WG) is a kind of industrial waste that has become a bigger problem with the increasing population all over the world due to the increase in consumption. Increasing technologies for recycling and reusing waste has become important to focus on. Despite the use of recycling technologies, a large amount of waste glass is still waiting to be evaluated. It can be advantageous to use the waste glass as an alternative to concrete with the properties of being abundant, economical, optically transparent and non-toxic. Soda-lime-silica (SLS) glass is an alternative SiO₂ source generally seen in glass containers or window glass such as bottles and jars. Glass can be evaluated as radiation shield material due to its ease of manufacturing, low cost, physical and chemical properties. Radiation protection efficiencies can be changed and developed by addition of different materials. Industrial waste materials such as Bayburt stone dust, marble dust and Oltu stone dust with good refractory properties containing high amounts of silica and calcium, can be also reused to save the environment and contribute to the economy as building materials. Also, waste samples are supported by adding heavy elements such as tungsten (W) to improve shielding ability against harms of radiation [1–3]. W has non-toxicity property, and special features such as a high melting point, low neutron activation, high thermal conductivity, etc. among the high-Z elements.

Oltu stone (OS) with the other names as Black Amber, Erzurum stone or Carbon black, found in Oltu (Erzurum) in Turkey, has a matte and black appearance, after being po-

lished it gains an attractive black shine [4, 5]. Oltu stone is a dense mineral-like substance that resembles coal, but in appearance it is similar to obsidian [6]. Its most striking feature is that it is very soft when carved and maintains its softness even if it is not cut. It hardens when it comes into contact with air. Oltu stone is involved in Erzurum's economy with various aspects such as mining, stone processing, handicraft workshops, sales and trade. Oltu stone waste (OSW) is obtained either from mines or workshops after processing the stone [4]. Marble waste (MW) is generated when cutting marble to produce regular geometric shapes. Due to the growth in the construction industry, the use of marble has increased and therefore MW has increased. MW consisting of dust, stones of irregular shapes and sizes thrown into open fields and roadsides causes environmental and health problems [7]. Bayburt stone (BS) is a natural stone named after the Bayburt province in Turkey. BS have potential use due to their high pozzolanic activity and are ground into powder to be used as a material to replace the binder [8]. Bayburt stone waste (BSW) is formed during the cutting processing of stones in quarries. These wastes are very cheap, easy to find, economical, effective and suitable for different applications.

Radiation, whose benefits cannot be ignored in many fields such as industry, science, agriculture, energy, radiology and medicine, causes serious health problems in the long and short term due to exposure to radiation in everyone working or receiving services in these sectors. Consequently, in recent years, researchers have focused on the development of protective materials with higher radiation absorption abilities by different material types such as composites, glasses, alloys,

rocks, polymers, concretes etc. which are novel, non-toxic, cost-effective [1, 9–15]. In addition to these studies, waste materials were also studied widely [7, 10, 14, 16, 17]. The common features make the produced materials attractive are being effective for protection, being eco-friendly, and being designed to minimize environmental pollution.

The target of the study is to produce materials with good attenuation potentials based on waste glass and industrial wastes obtained from some industries. In this context, the shielding parameters; exposure and energy absorption build-up factors (EBF and EABF), mass attenuation coefficients (MAC), linear attenuation coefficients (LAC), effective atomic number (Z_{eff}), half-value layer (HVL), mean free path (MFP), fast neutron removal cross-section (FNRCs) of the samples, have been calculated by the code Phy-X/PSD [18] in this work.

The structural properties were also provided by spectroscopic methods as well as the shielding performances. Electron paramagnetic resonance (EPR) is used for the magnetic features of the systems in the external magnetic field by the microwave frequency. The identification of crystalline phases or amorphous structure of the samples is made by X-ray diffraction (XRD). Scanning electron microscopy (SEM) is used for surface structure and energy dispersive spectroscopy (EDS) is for obtaining the compositional content. The study will show that the wastes and industrial materials can be evaluated in different ways than their current usage areas.

2. Materials and methods

2.1. Sample preparation

Three samples were prepared and named as W1, W2, W3 including waste glass (WG), Oltu stone waste (OSW), Bayburt stone waste (BSW), Marble waste (MW) with addition of tungsten (W). The ratios of the ingredients of the prepared samples are given in Table I. Firstly, glass waste and other wastes were powdered, prepared in certain quantities and placed in porcelain crucibles. Secondly, the mixed materials were melted in the oven at 1100°C for 2 hours. The process continued in the oven at 500°C for 3 hours. Finally, the oven was turned off and the glass samples were allowed to cool until the temperature dropped to room temperature. The obtained glass samples were crushed and made ready for spectroscopic experiments.

2.2. Experimental techniques

Room temperature EPR spectra of the samples were taken by X-band JEOL JESFA300 EPR spectrometer with ≈ 9.2 GHz frequency and 100 kHz (0.0002-2mT) magnetic field modulation amplitude. Samples with 4 mm sizes were prepared and put in diamagnetic tubes for EPR experiment. XRD patterns were taken by BRUKER D8 ADVANCE XRD. X-ray diffractograms of the samples were recorded with a 2.5°/min (40 kV and 40 mA) scanning speed in the range of $2\theta \approx 10^\circ - 90^\circ$ by Cu-K α ($\lambda = 1.54060 \text{ \AA}$). SEM images were recorded by ZEISS EVO LS10. EDS results were taken by JEOL JSM-6610 spectrometer.

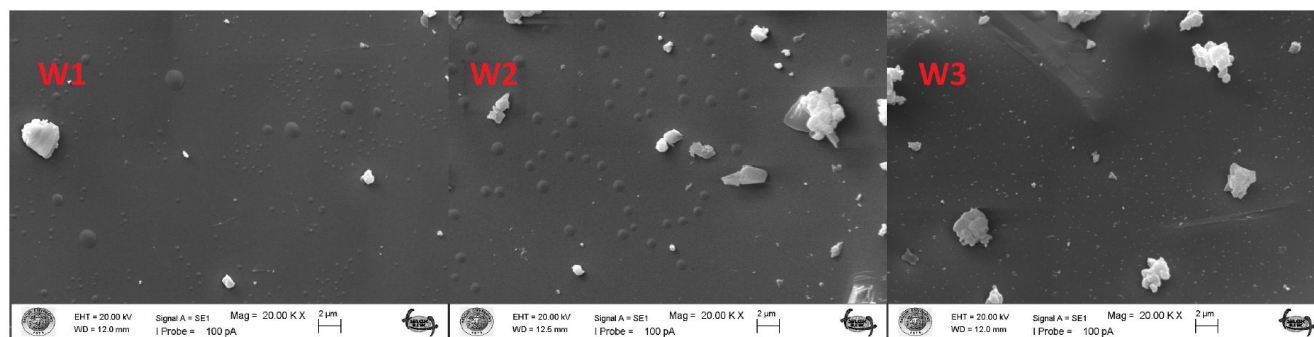


FIGURE 1. SEM images of the samples.

TABLE I. Compositional rate and ingredients of the prepared samples.

W1	Waste Glass (%)	Oltu Stone Waste (%)	Bayburt Stone Waste (%)	W (Tungsten) (%)
	90	2.5	5	2.5
W2	Waste Glass (%)	Oltu Stone Waste (%)	Marble Waste (%)	W (Tungsten) (%)
	90	2.5	5	2.5
W3	Waste Glass (%)	Bayburt Stone Waste (%)	Marble Waste (%)	W (Tungsten) (%)
	90	2.5	5	2.5

TABLE II. Knowledge of the parameters used in the study.

Parameter	Definition	Formula	Unit	Description
ρ_{mix}	The mass per unit volume	$\frac{\sum_{i=1}^n c_i A_i}{\sum_{i=1}^n (c_i A_i / \rho_i)}$	g/cm^3	c_i : atomic fraction A_i : atomic weight ρ_i : density of element ith [19]
$MAC(\mu_m)$	The attenuation of the radiation per unit mass	$\frac{\mu}{\rho} = \frac{\ln(I_0/I)}{t_m}$ or $\frac{\mu}{\rho} = \sum_i w_i (\frac{\mu}{\rho})_i$	cm^2/g	I_0 and I : incident and attenuated photon intensities $\rho(\text{g/cm}^3)$: density of material $t_m(\text{g/cm}^2)$: mass per unit area t (cm): thickness w_i : weight fraction $(\mu/\rho)_i$: mass attenuation coefficient of the ith constituent element [20]
$LAC(\mu)$	The fraction of attenuated incident radiation per unit thickness of a material	$\rho\mu_m$	$\mu(\text{cm}^{-1})$	μ_m : the mass attenuation coefficient $\rho(\text{g/cm}^3)$: density of material
HVL	The thickness of a shield that half the incident radiation	$\frac{\ln(2)}{\mu}$		μ : the linear attenuation coefficient
MFP	The average distance over which a photon travels before substantially changing its direction or energy	$\frac{1}{\mu}$		μ : the linear attenuation coefficient
$ACS(\sigma_a)$	Interaction probability per atom in a unit volume of any material	$\frac{N}{N_A} (\frac{\mu}{\rho})$	cm^2/g	N_A : Avogadro's number N : atomic mass of materials
$ECS(\sigma_e)$	Interaction probability per electron in a unit volume of any material	$\frac{\sigma_a}{Z_{\text{eff}}}$	cm^2/g	σ_a : the atomic cross section Z_{eff} : the effective atomic number
Z_{eff}	Average atomic number of the compound including more than one element	$\frac{\sigma_a}{\sigma_e}$		Z_{eff} : the effective atomic number σ_a : the atomic cross section σ_e : the electronic cross section
FNRCS ($\sum R$)	The probability of a fast neutron undergoing the first collision that will remove it from the environment penetrating group of uncollided neutrons	$\sum_i \rho_i (\frac{\sum R}{\rho})_i$	cm^{-1}	$(\frac{\sum R}{\rho})_i$: mass removal cross-section of the ith constituent element ρ_i : the partial density of the material [18]
Z_{eq}		$\frac{Z_1(\log R_2 - \log R) + Z_2(\log R - \log R_1)}{\log R_2 - \log R_1}$		$R : (\mu\text{m})_{\text{Compton}} / (\mu\text{m})_{\text{total}}$ for the material at a specific energy R_1, R_2 : values indicate $(\mu\text{m})_{\text{Compton}} / (\mu\text{m})_{\text{total}}$ ratios of two adjacent elements, with Z_1 and Z_2 atomic numbers

G-P fitting parameters	$\frac{F_1(\log Z_2 - \log Z_{eq}) + F_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1}$	F1, F2: values of G-P fitting parameters identical with the Z_1 and Z_2 atomic numbers at a certain energy [21]
EBF and EABF	$B(E, x) = 1 + \frac{(b-1)(K^x-1)}{(K-1)} \quad \text{for } K \neq 1$ $B(E, x) = 1 + (b-1)x \quad \text{for } K = 1$ $K(E, x) = cx^a + d \frac{\tanh(\frac{x}{X_K}-2) - \tanh(-2)}{1 - \tanh(-2)}$ for $x \leq 40mfp$	E: primary photon energy x: penetration depth a, b, c, d, X_K coefficients of the material [22,23]

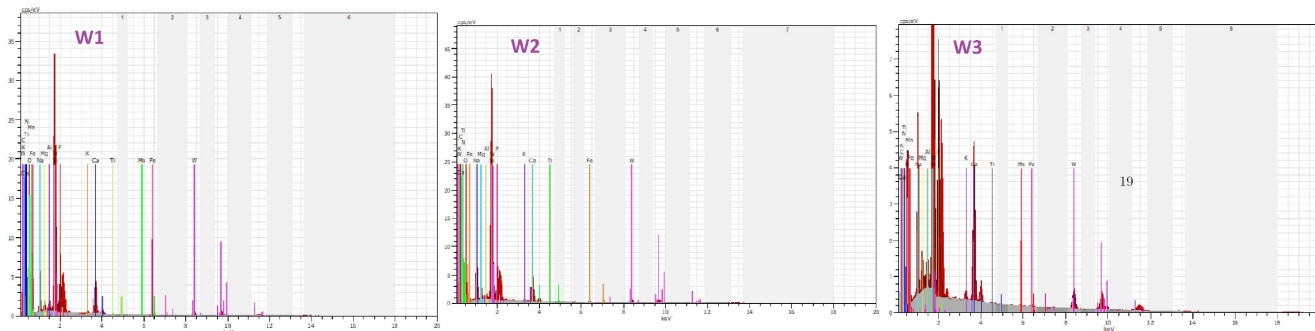


FIGURE 2. EDS results of the samples.

TABLE III.

Samples	O	C	Ca	K	Si	Na	Fe	Ti	Mg	P	Al	Mn	N	W	Density (g/cm ³)
W1	28.07	1.56	9.44	0.52	24.32	7.47	0.37	0.15	1.48	11.16	1.28	0.20	0.03	13.94	3.05
W2	32.82	1.21	7.97	0.45	23.08	10.20	0.33	0.08	2.02	9.06	1.48	-	0.02	11.28	2.73
W3	30.55	1.66	9.89	0.51	22.31	7.11	0.32	0.10	1.33	10.47	1.16	0.13	0.02	14.64	3.10

2.3. Theoretical process

For calculating the parameters by Phy-X/PSD code the composition of the material is entered in two ways such as mole fraction and weight fraction. The knowledge of density (g/cm³) of the material is also necessary for obtaining the attenuation parameters. The acquired results are supplied in a MS Excel. The information about the parameters investigated in the study is given in Table II.

3. Results and discussion

3.1. SEM and EDS analysis

SEM images and EDS spectra of the samples are given in Figs. 1-2. If the micrographs obtained from the surfaces of the samples are studied, smooth surfaces with some microcrystallites are seen. The weight % ratios of the elements obtained from these spectra are given in Table III. It is understood from the SEM images given in Fig. 1 that all the samples have smooth structures. Air bubbles are observed which were also stated before by Aygun [24]. EDS analysis results were found to be consistent except for W amount. The melting

temperature of W is higher than those of the others, so the EDS results give acceptable values different from the casting rates due to the problems that may arise from the incomplete dissolution of the samples for the element of W.

3.2. XRD analysis

XRD patterns recorded at room temperature are given in Fig. 3. The diffraction peaks were examined by the literature [1, 25, 26]. X-ray analysis of the samples shows similar results and the existence of calcite and SiO₂ phase peaks. The samples produced by W addition give α -W main phase. It is observed that the samples show more amorphous structure with some crystalline features in XRD patterns.

The crystallite size is calculated by the diffraction pattern depending on the full width half height (FWHM) and the Debye-Scherrer equation [27]. β the FWHM in radians; K the Scherrer's constant and in the order of $\cong 0.9$; λ the X-ray wavelength, d the average size of the crystalline, and θ the Bragg angle in degrees [1]:

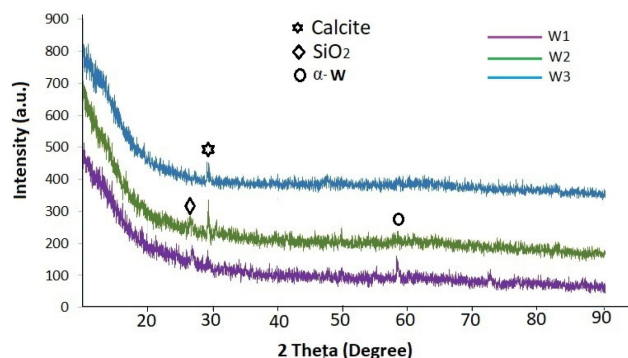


FIGURE 3. XRD patterns of the samples.

$$d = \frac{K\lambda}{\beta \cos \theta}. \quad (1)$$

The presence of the α -W main phase at $\approx 58^\circ$ has the crystallite size as 50.75 nm. The crystallite size of other main phase at $\approx 29^\circ$ assigned to calcite is ≈ 68 nm.

3.3. EPR study

EPR is a useful magnetic resonance technique which causes determination of the local chemical environment of magnetically active nuclei ($I \neq 0$), radicals or paramagnetic centers that have one or more unpaired electrons in their structure. The EPR effect is defined by the observation of transitions in the spin of electrons between energy states in the presence of an external magnetic field; these transitions are known as 'degenerate' when the magnetic field is absent [28, 29]. EPR is based on the measurement of the absorption of electromagnetic radiation in the microwave frequency region by a paramagnetic sample positioned within a magnetic field. It is important to note that these absorptions are observed at specific frequencies and magnetic field combinations, which are known to vary according to the type of paramagnetic species present and its characteristics. Consequently, the lines produced at distinct regions of the scanned magnetic field will vary significantly depending on the type of radical or metal ion under investigation [30]. The EPR lines are identified by g -values and the equation $h\nu = g\beta H$ with β the Bohr magneton, H the magnetic field, h the Planck constant, and ν the microwave frequency is used for the determination of the values. The paramagnetic center by the effect of local magnetic fields on unpaired electrons can be characterized by the g -factor. Therefore, the nature of the EPR signal can be ascribed to a paramagnetic center. EPR spectra of the samples taken at room temperature are given in Fig. 4. Fe^{+3} ions or high-spin isolated Fe^{+3} center is observed with g value of ≈ 4.21 for the samples [28]. A broad EPR signal with g -value of ≈ 1.98 which can be ascribed to Mn^{+2} ($I=5/2$) is detected. In general, it is expected to observe six hyperfine lines of Mn^{+2} but as a result of the random and close localization of Mn ions and their dipole-dipole or exchange interaction a broad signal can be seen [31].

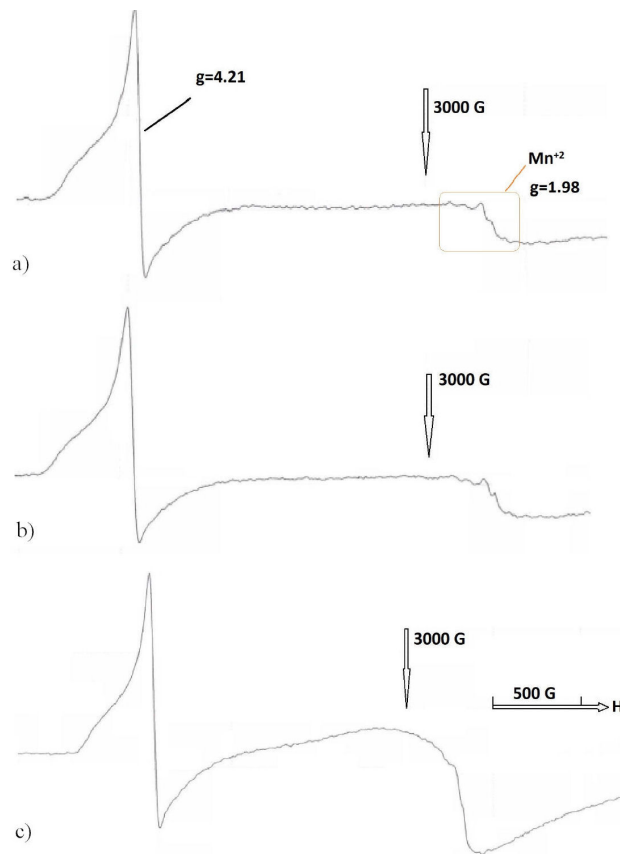


FIGURE 4. EPR spectra of the samples W1 a) W2 b) and W3 c).

3.4. Radiation protection analysis

Phy-X/PSD code was used to calculate radiation attenuation parameters with the chemical compositions (w %) of the samples determined by EDS (Table II). The MAC values changed with incident energies (1 keV-100 GeV) are shown in Fig. 5a). The changes in MAC results are affected by the processes at low (0.001-0.1 MeV), mid (0.1-5 MeV) and high energies (>5 MeV) correspond to photoelectric effect (PE), Compton scattering (CS) and pair production (PP), respectively. The LAC values varied with photon energies as seen in Fig. 5b). MAC values and material's density are the factors affect LAC parameter. Additionally, the MAC results of the samples are compared with previously reported ordinary concrete (OC) [32] and cement [33] [Fig. 5c)]. The MAC values and so the shielding efficiencies of the samples can be ordered as $W3 > W1 > W2 > \text{Cement} > \text{OC}$. Among the samples, W3 has the highest shielding ability, while W2 has the least. According to the results obtained at all energies, the common feature is that all samples have better protection potential than OC.

The MFP and HVL values changed with photon energies are given in Fig. 6. If the material has higher values of HVL and MFP, it is known as the worst shield. The highest values of HVL and MFP and so the lowest shielding performance is found for W2, whereas the highest one is obtained for W3.

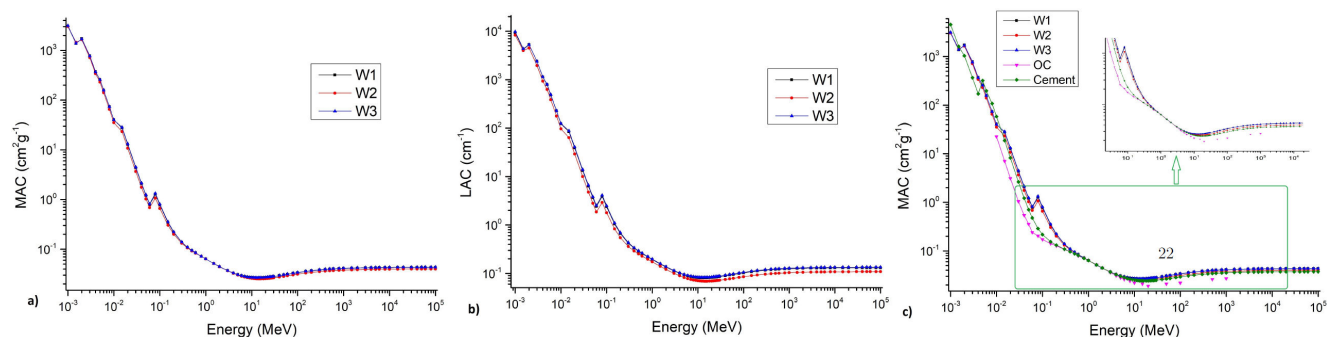


FIGURE 5. The variations of MAC a) LAC b) and the comparison of MAC values with OC and cement c) versus photon energies.

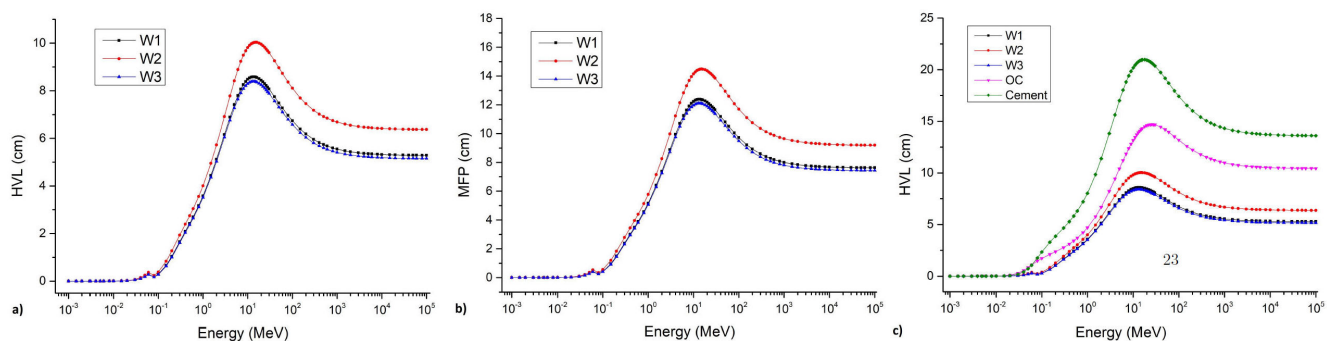


FIGURE 6. The variations of HVL a) MFP b) and the comparison of HVL values with OC and cement c) versus photon energies.

The radiation shielding capability (RSC) of the samples are compared by OC and cement [Fig. 6c]. It is concluded that the HVL values of the samples are lower than those of OC and cement.

The Z_{eff} values changed with photon energy is demonstrated in Fig. 7. In the low energy region (0.001-0.1 MeV), the PE cross-section (Z^{4-5}); in the mid-energy region (0.1-5 MeV), CS cross-section (E^{-1}) and in the high energy region (>5 MeV), PP cross-section (Z^2) are effective and therefore Z_{eff} values increase, decrease and are stable, respectively. Z_{eff} values can be influenced due to the elements with distinct

atomic numbers in the material. As, Z_{eff} is the atomic number of a material containing more than one element, structure with large atomic number differences cause fluctuations. The samples with W content have the highest Z_{eff} values and this kind of fluctuations. Thus, W3 has the highest shielding performance depending on Z_{eff} values.

The EBF and EABF varied with photon energies are given in Figs. 8-9. In the low, mid and high energy regions, EBF and EABF are lower, higher and again lower based on the PE, CS and PP effects, respectively. According to the obtained EBF and EABF values, the photons cluster more for W3 among the samples. So, it is seen that W3 shows the CS process is effective.

Attenuation of fast neutron of the samples was also achieved by the code and the cross sections are given as 0.092, 0.085 and 0.094 for W1, W2 and W3, respectively. The highest neutron attenuation is found for W3, the lowest one is for W2 like photon shielding. It can be also concluded that FNRCS values of W3 are better than those of the previously studied OC (0.093).

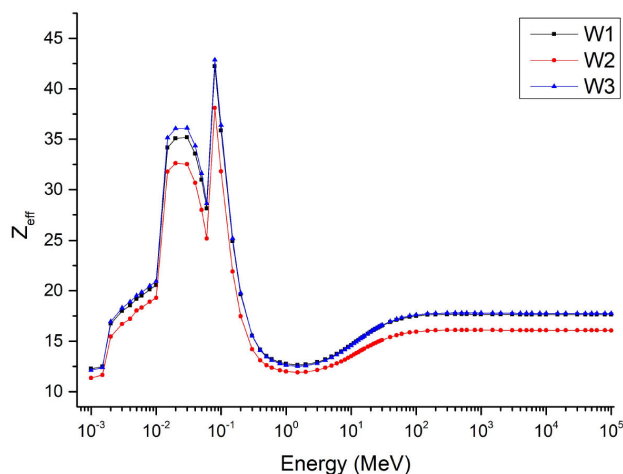


FIGURE 7. The variations of Z_{eff} versus photon energies.

4. Conclusions

The goal of the study was to develop alternative materials based on reusing of wastes for obtaining higher shielding features. To this end, RSC and spectroscopic details of the waste samples were determined by Phy-X/PSD code and the techniques. EPR spectra of the samples give an EPR signal with

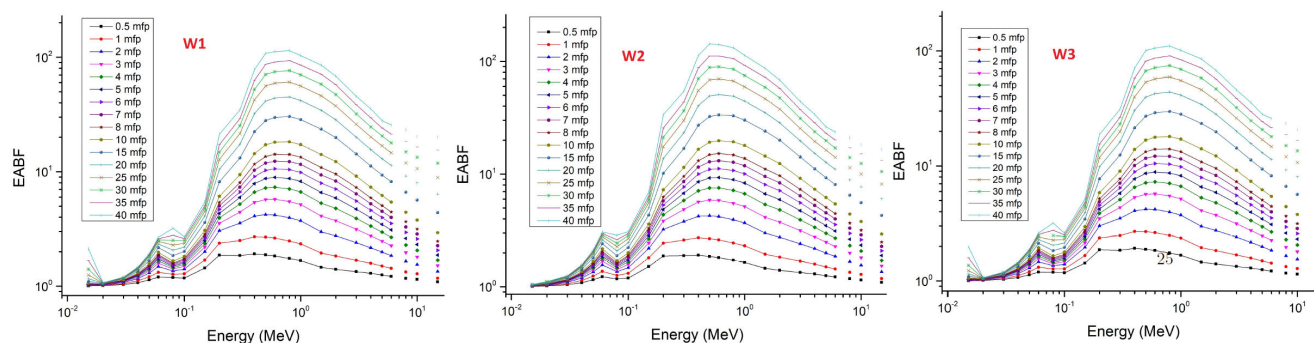


FIGURE 8. The changes of EABF values of the samples versus photon energies.

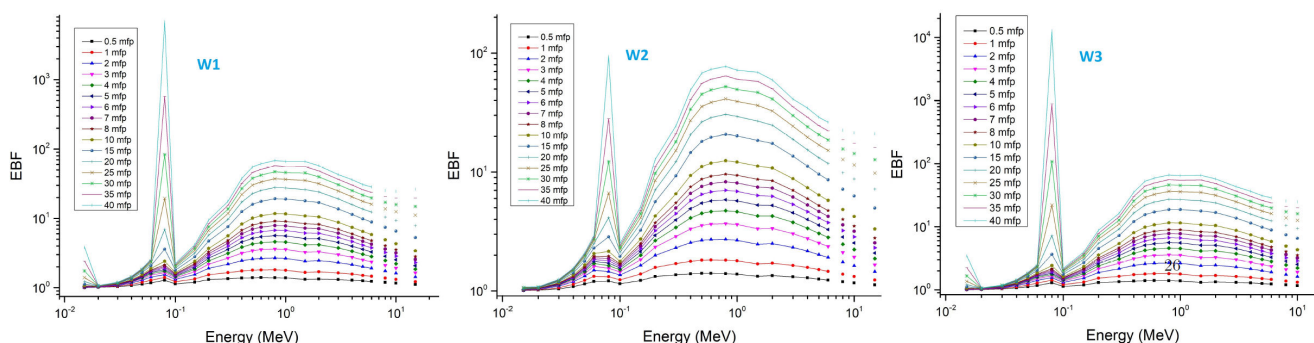


FIGURE 9. The changes of EBF values versus photon energies.

g value of 4.21 which is attributed to ferric center and signal with g value of 1.98 corresponds to Mn^{+2} . The XRD spectra show the amorphous structure with some crystallites. Computational results of radiation attenuation parameters, it would be useful to point out that the existence of heavy metal W content with higher atomic number in the sample improves the protection performance. In addition, it can be noted that the neutron attenuation capacity of W3 is the highest, similar to the photon attenuation property. As a result, all of the designed waste samples based on waste glass can be recommended as new protective materials. With this study, we wanted to show that these types of materials, which are used as ornaments or commercially and whose waste is abandoned in empty lands, can be used more functionally and for different purposes.

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Statements and declarations

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethics approval

Not applicable

Consent to participate

Not applicable

Consent for publication

Not applicable

Author contributions

All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by Zeynep AYGUN and Murat AYGUN. The first draft of the manuscript was written by Zeynep AYGUN and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Availability of data and materials

Data of this study are available from the corresponding author on responsible request.

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Fractional scale transform and fractional Mellin transform for scale, rotation, and translation invariant pattern recognition to discriminate between 30 phytoplankton species

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The fractional scale transform is introduced and studied to develop a new pattern recognition system invariant to scale, translation, and rotation. This system was also implemented with the fractional Mellin transform, and the results were compared with those obtained with the fractional scale transform. The analysis was performed to classify 30 phytoplankton species. For both transformations, optimal orders were found for each species. This study implemented nonlinear correlation and adaptive nonlinear correlation for the classification stage. The system achieved a mean accuracy of 0.998 with nonlinear correlation and 0.999 with adaptive nonlinear correlation.

Keywords: Computer vision; fractional Mellin transform; fractional scale transform; pattern recognition; phytoplankton.

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1. Introduction

The fractional Fourier transform (FrFT), as a generalization of the conventional Fourier Transform (FT), has found applications in different areas where the FT has been used, with the potential to obtain better results [1]. Image correlation using FrFT or fractional correlation has been used for object recognition [2], showing a less noisy response than conventional correlation. Likewise, for identifying 30 phytoplankton species, a pattern recognition methodology invariant to translation and rotation was developed based on one-dimensional signatures obtained with binary masks generated from the FrFT, which were classified using nonlinear correlation [3]. In this methodology, FrFT orders were found for each species, which improved discrimination capacity compared to the case in which the FT is used for mask generation.

In addition to the FrFT, the concept of fractional orders has been extended to other transforms, including the Mellin transform (MT), giving rise to the fractional Mellin transform (FrMT) [4]. Butzer *et al.* (2002) conducted an extensive study of fractional Mellin analysis, using the so-called Hadamard integrals [5–7]. The MT can be implemented via the FT, also known as the Fourier-Mellin transform [8,9]. However, by working with the FrFT, the FrMT can be obtained, also called the fractional Fourier-Mellin transform. Sazbon *et al.* (2002) implemented optical correlators based on the fractional Fourier-Mellin transform for navigation tasks to detect and control specific ranges of object motion [10]. In 2011, Sharma showed how the fractional Fourier-Mellin transform is a generalization of the conventional Fourier-Mellin transform [11]. Zuo and Zhou (2011) performed spectrum analysis with the MT and FrMT, finding that the fractional version preserves the scale-invariance property [12]. Zhou *et al.* (2012) applied the MT to develop a reality-preserving color encryption algorithm [13]. Vashisth *et al.* (2014) implemen-

ted a phase mask for encryption, based on the fractional Mellin transform [14]. In 2015, Sharma and Deshmukh proved the analyticity of the FrMT [15]. Baloch *et al.* (2019) established the relationship that the FrMT also has with the fractional Laplace transform [16]. Wang *et al.* (2020) presented an encryption scheme based on the reality-preserving FrMT with Gaussian opening [17].

Furthermore, Cohen proposed the concept of scale transform (ST) in 1993. In this transformation, the main magnitude to be represented is, as its name indicates, the scale, since scale can be considered as a physical attribute of a signal [18]. Like the MT, this transform has the property that its modulus is invariant to changes in scale, in the same way that the modulus of the FT is invariant to translation. Also, like the MT, this transformation can be implemented digitally, through the FT using a logarithmic mapping [19].

To enhance discriminative capabilities in image classification problems regardless of scale, rotation, and translation changes, this work proposes the fractional scale transform (FrST) by extending the concept of fractional orders to the ST. To achieve this, the FrFT is employed. In addition to the FrST, the FrMT was also implemented for classification using nonlinear and adaptive nonlinear correlations.

The rest of the article is organized as follows. In Sec. 2, the mathematical theory behind this work is presented. The methodology is described in Sec. 3. Section 4 presents the analysis and results, and finally, in Sec. 5, the conclusion is given.

2. Mathematical bases

2.1. The MT

The MT is an integral transform strongly related to the FT. The MT of a function is defined as

$$M(s) = \int_0^\infty f(x)x^{s-1}dx, \quad (1)$$

where, $s = jc + \beta$ and c is the scale variable. Equation (1) defines the β -Mellin transform family. If $\beta = 0$ we obtain a compression/expansion invariant transform [20], in this case

$$M(c) = \mathcal{M}\{f(x)\} = \int_0^\infty f(x)x^{-jc-1}dx. \quad (2)$$

The most useful property of the MT with $\beta = 0$ is that any change in scale in the spatial domain translates to a change only in phase in the Mellin domain, while its modulus remains invariant to those changes in scale. For the case of an image, the two-dimensional MT is used, which is given by [21]

$$\mathcal{M}\{f(x, y)\} = \int_0^\infty \int_0^\infty f(x, y)x^{-ju-1}y^{-jv-1}dxdy. \quad (3)$$

2.2. The scale transform

The scale transform (ST) is a special case of the MT with $\beta = 1/2$. The ST is given by [18]

$$D(c) = \mathcal{D}\{f(x)\} = \frac{1}{\sqrt{2\pi}} \int_0^\infty f(x) \frac{e^{-jc \ln x}}{\sqrt{x}} dx. \quad (4)$$

Equation (4) can also be written as

$$\mathcal{D}\{f(x)\} = \frac{1}{\sqrt{2\pi}} \int_0^\infty f(x)x^{-jc-\frac{1}{2}}dx, \quad (5)$$

which is equivalent to the MT with complex argument $s = -jc + 1/2$. In two dimensions, the scale transform is given by [22]

$$\begin{aligned} \mathcal{D}\{f(x, y)\} &= \frac{1}{\sqrt{2\pi}} \int_0^\infty \int_0^\infty f(x, y) \\ &\times \frac{e^{-jc_x \ln x - jc_y \ln y}}{\sqrt{xy}} dxdy. \end{aligned} \quad (6)$$

2.3. Relationship between the MT and the ST

The MT in Eq. (2) can also be written as

$$\mathcal{M}\{f(x)\} = \int_0^\infty \frac{f(x)x^{-jc}}{x} dx, \quad (7)$$

while the ST in Eq. (4) can be expressed as

$$\mathcal{D}\{f(x)\} = \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{f(x)x^{-jc}}{\sqrt{x}} dx. \quad (8)$$

Therefore, discarding the constant $1/\sqrt{2\pi}$, which is only for normalization purposes, there is a relationship between the MT and the ST, given by [23]

$$\mathcal{M}\{\sqrt{x}f(x)\} = \mathcal{D}\{f(x)\}. \quad (9)$$

2.4. FrMT and FrST

The FrMT is a generalization of the MT as the FrFT is to the FT. The two-dimensional FrMT of the order p of the function $f(x, y)$ is defined by [24]

$$\begin{aligned} \mathcal{M}^p\{f(x, y)\} &= \mathcal{M}_\alpha\{f(x, y)\} = \int_0^\infty \int_0^\infty f(x, y) \\ &\times K_\alpha(x, y, u, v) dxdy, \end{aligned} \quad (10)$$

where the kernel $K_\alpha(x, y, u, v)$ is defined by

$$\begin{aligned} K_\alpha(x, y, u, v) &= x^{\frac{2\pi u j}{\sin \alpha} - 1} y^{\frac{2\pi v j}{\sin \alpha} - 1} \\ &\times e^{\frac{\pi j}{\tan \alpha} [u^2 + v^2 + \ln x^2 + \ln y^2]}, \end{aligned} \quad (11)$$

for $0 < \alpha \leq \pi/2$, and the fractional order is $p = \alpha/(\pi/2)$.

The MT can be implemented via the FT [20] using logarithmic mapping. However, as the FrFT is a generalization of the FT, the fractional concept was also extended to the MT [4]. Therefore, the FrMT can be obtained by implementing the FrFT after the logarithmic mapping [10]. And based on the relationship between the MT and the ST given in Eq. (9), the fractional scale transform can be obtained by multiplying the input by the factor $\sqrt{xy}$ as

$$\mathcal{D}^p\{f(x, y)\} = \mathcal{M}^p\{\sqrt{xy}f(x, y)\}. \quad (12)$$

3. Methodology

In this work, two position, rotation and scale methodologies are presented. In the first method, the FrST is used. The fractional version of the scale transform is implemented using the FrFT. Then, the FrMT is also implemented to compare with the results obtained with the FrST.

3.1. Position, rotation and scale invariant correlation methodology based on the FrST

The system implementing the FrST is shown in the diagram of Fig. 1. It is based on the methodology used to obtain the ST [19], but now using the FrFT instead of the FT to implement the FrST. First, step (1) presents a target image to the system. In step (2), the modulus of the FT, named as the spectral image, is calculated, thus introducing translation invariance. After that, the factor $\sqrt{xy}$ that differentiates the FrST from the FrMT is introduced in step (3). Then, in step (4), the Cartesian coordinates are mapped to polar coordinates, thus obtaining rotation invariance [9,25]. In step (5), a logarithmic mapping is performed. In step (6), the FrST of order p of the target image is obtained by applying the FrFT to the logarithmically scaled data. Then, to get scale invariance, the modulus of the FrST of the target image is calculated in step (7). In step (8), a problem image $g(x, y)$ is introduced to the system, and from step (9) to step (14), the modulus of the FrST of the problem image is calculated. Finally, in step (15), the correlation of the modulus of the FrFTs of the target and problem images is performed to classify the images.

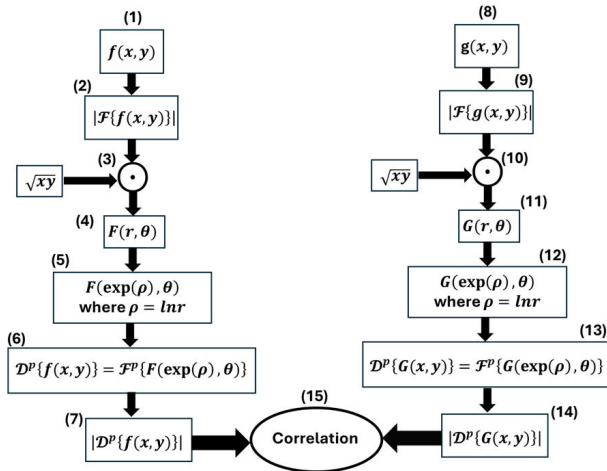


FIGURE 1. Block diagram of the position, rotation, and scale correlation methodology based on the FrST.

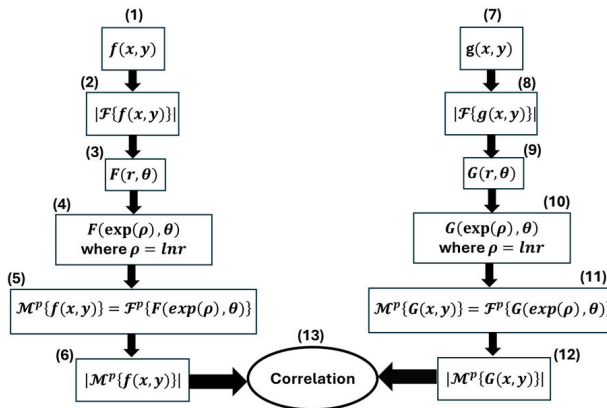


FIGURE 2. Block diagram of the position, rotation, and scale correlation methodology based on the FrMT.

3.2. Position, rotation and scale invariant correlation methodology based on the FrMT

Now, Fig. 2 shows the system implementing the FrMT. In step (1), a target image $f(x, y)$ is presented. In step (2), the spectral image is calculated. Then, in step (3), the Cartesian coordinates are mapped to polar coordinates. In step (4), a logarithmic mapping is performed. In step (5), the FrMT of the order p of the target image is obtained, and its modulus is calculated in step (6). Then, in step (7), a problem image is introduced. From step (8) to step (12), the modulus of the FrMT of the problem image is obtained. Finally, in step (13), the correlation of the modulus of the FrMTs of the target and problem images is calculated.

3.3. Correlation

In the classification stage, using the FrST or the FrMT, nonlinear and adaptative nonlinear correlations are used. The nonlinear correlation or k -law correlation is defined as [26]

$$C_{NL} = \mathcal{F}^{-1} \{ |\mathcal{F}\{P_{FR}\}|^k e^{i\phi_{P_{FR}}} |\mathcal{F}\{T_{FR}\}|^k e^{-i\phi_{T_{FR}}} \}, \quad (13)$$

where, for this work $\phi_{P_{FR}}$ and $\phi_{T_{FR}}$ are the phases of the FT of the fractional transformations of the problem image and target image, respectively, and $0 < k < 1$ is the nonlinearity factor. For this work, $k = 0.3$. The adaptative nonlinear correlation is a variation of the nonlinear correlation that gives better classification performance, and is defined as [27]

$$C_{NL} = \mathcal{F}^{-1} \{ |\mathcal{F}\{P_{FR}\}|^{k \cdot R} \times e^{i\phi_{P_{FR}}} |\mathcal{F}\{T_{FR}\}|^k e^{-i\phi_{T_{FR}}} \}, \quad (14)$$

where R is the factor that modifies the nonlinearity of the modulus of the FT of the fractional transformation of the problem image. For this work, the R factor is defined as

$$R = \begin{cases} \frac{\sigma(x, y)_{PI}}{\sigma(x, y)_{TI}}, & \sigma(x, y)_{PI} \leq \sigma(x, y)_{TI}, \\ \frac{\sigma(x, y)_{TI}}{\sigma(x, y)_{PI}}, & \sigma(x, y)_{PI} > \sigma(x, y)_{TI}, \end{cases} \quad (15)$$

where $\sigma(x, y)_{PI}$ is the standard deviation of the spectral image of the problem image, and $\sigma(x, y)_{TI}$ is the standard deviation of the spectral image of the target image. Calculating an autocorrelation makes $R = 1$, which turns the adaptative nonlinear correlation into a nonlinear correlation.

4. Analysis and results

This work discriminates between the 30 phytoplankton species in Fig. 3. The classification is made by implementing the FrST or the FrMT with an optimal order.

4.1. Obtaining the optimal order

As stated earlier, the parameter α can have values between 0 and $\pi/2$. Thus, the order p can have values between 0 and 1.

Therefore, it is necessary to determine the optimal value of p to use in the process.

A non-normalized autocorrelation is performed for a particular order p , and the peak value is extracted. This is done for different orders. In this way, each order will give its respective autocorrelation value. Finally, the order with the highest correlation value is considered the optimal order [3]. This is done for the FrST and the FrMT for all 30 species. The optimal order is searched by changing p from 0.01 to 1 with steps of 0.01. In this way, planes other than the ST and MT are selected, which are special cases of their fractional versions when $p = 1$. Table I shows the optimal order of each species obtained for the FrST and the FrMT. It can be observed that there is no single optimal order for all species, and in some cases, the optimal order of a species differs for each transformation. Also, for both transforms, no species has an optimal order equal to 1. This means that the species identified themselves better in both cases when working with fractional orders.

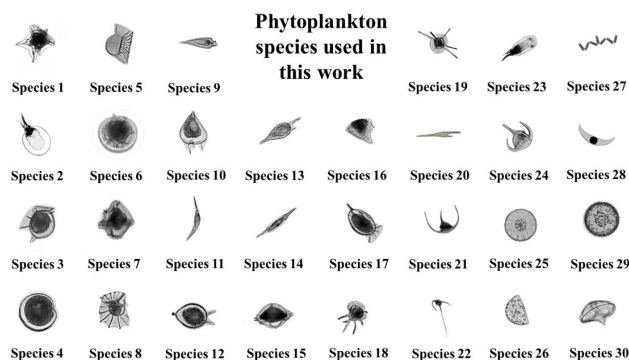


FIGURE 3. Images of the 30 phytoplankton species used in this work. Species 1: *Acanthogonyaulax spinifera*. Species 2: *Ceratium gravidum* Gourret. Species 3: *Dinophysis hastata*. Species 4: *Diplosalopsis orbicularis*. Species 5: *Histioneis*. Species 6: *Lingulodinium polyedrum*. Species 7: *Ornithocercu armata*. Species 8: *Ornithocercus magnificus*. Species 9: *Oxytoxum scolopax*. Species 10: *Podolampas bipes*. Species 11: *Podolampas spinifer*. Species 12: *Podolampas bipes*. Species 13: *Podolampas palmipes*. Species 14: *Podolampa spinifer*. Species 15: *Protoperidinium*. Species 16: *Dinophysis rapa*. Species 17: *Dinophysis hastate*. Species 18: *Ceratocorys horrida*. Species 19: *Ceratocorys horrida*. Species 20: *Ceratium furca*. Species 21: *Ceratium lunula*. Species 22: *Ceratium hexacanthum*. Species 23: *Ceratium praelongum*. Species 24: *Ceratium breve*. Species 25: *Asterolampira marylandica*. Species 26: *Hemidiscus cuneiformis*. Species 27: *Thalassionema nitzschioides*. Species 28: *Pyrocystis*. Species 29: *Hemidiscus*. Species 30: *Dinoflagellata*.

4.2. Classification

Thirty species of phytoplankton were used to analyze the performance of the two correlation methodologies invariant to position, rotation and scale presented in this work. The images are grayscale with a 307×307 size. Each of the 30

species was scaled $\pm 10\%$ in steps of 1% . Thus, the scale ranges from 90% to 110% of the original image (100% scale); this range is typical of this species type, which is why the range was selected. Therefore, considering the original image, 21 scaled versions were produced for each species. Then, the original image of each species was selected as the target and compared with all scaled versions of itself and all scaled versions of the other species. The comparison was made by following the transformation methodologies described in Secs. 3.1 and 3.2. The order used in each comparison was that of the target species, depending on the transformation used, as shown in Table I. This process was performed using non-linear correlation and adaptative non-linear correlation for both transformations. Figures 4 and 5 show the results obtained with the FrST and the FrMT when species 4 is the target. The box plots show the mean, ± 1 standard deviation, and the maximum and minimum values obtained from all the performed correlations.

Figure 4a) shows the results of the nonlinear correlation with the FrST. Considering the maximum and minimum values in the box plots, there is some overlap with species 25 only. Figure 4b) shows the results for the same transformation but using adaptive nonlinear correlation, with no overlaps. The results for the FrMT transform using nonlinear correlation are shown in Fig. 5a), and those with adaptive nonlinear correlation are shown in Fig. 5b), with no overlap in either case. To evaluate the performance with each species as the target, four metrics were used:

$$\text{accuracy}(S_n) = \frac{TP_n + TN_n}{TP_n + TN_n + FP_n + FN_n}, \quad (16)$$

$$\text{sensitivity}(S_n) = \frac{TP_n}{TP_n + FN_n}, \quad (17)$$

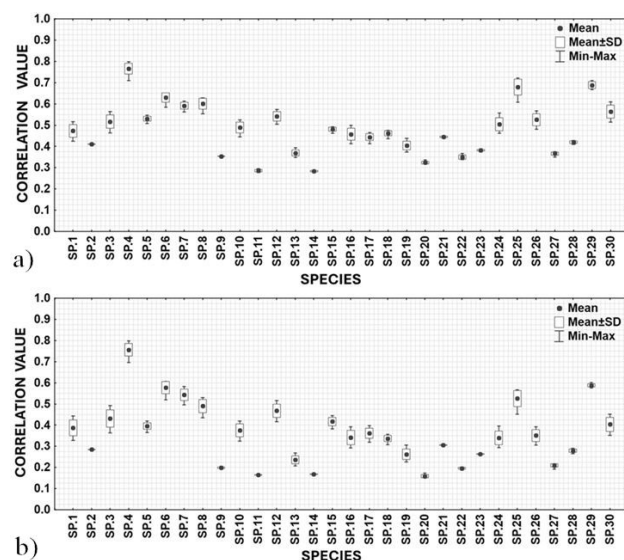


FIGURE 4. Results obtained by implementing the FrST using species four as the target. a) Nonlinear correlation. b) Adaptive nonlinear correlation.

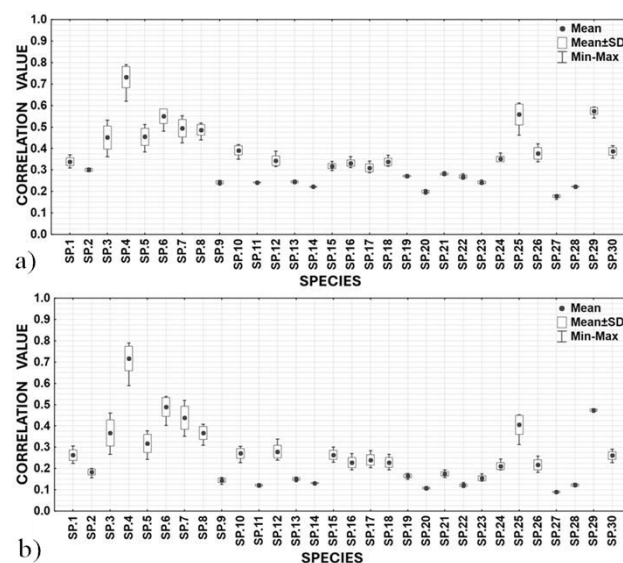


FIGURE 5. Results obtained by implementing the FrMT using species four as the target. a) Nonlinear correlation. b) Adaptive nonlinear correlation.

TABLE I. Optimal order for each phytoplankton species. Column 1 shows results obtained with FrST. Column 2 shows results obtained with FrMT.

Species	FrST optimal orders	FrMT optimal orders
1	0.986	0.986
2	0.991	0.991
3	0.978	0.978
4	0.978	0.953
5	0.979	0.986
6	0.978	0.978
7	0.978	0.952
8	0.979	0.979
9	0.986	0.986
10	0.986	0.986
11	0.993	0.992
12	0.978	0.978
13	0.984	0.984
14	0.974	0.974
15	0.985	0.985
16	0.985	0.978
17	0.978	0.978
18	0.986	0.986
19	0.986	0.986
20	0.977	0.978
21	0.978	0.978
22	0.985	0.985
23	0.983	0.984
24	0.978	0.978
25	0.978	0.978
26	0.985	0.979
27	0.978	0.978
28	0.978	0.978
29	0.978	0.978
30	0.979	0.978

TABLE II. Results of the FrST with nonlinear correlation.

Species	Accuracy	Sensitivity	Specificity	Precision
1	1	1	1	1
2	1	1	1	1
3	1	1	1	1
4	0.995	0.905	0.998	0.950
5	1	1	1	1
6	0.995	0.857	1	1
7	1	1	1	1
8	1	1	1	1
9	1	1	1	1
10	1	1	1	1
11	1	1	1	1
12	1	1	1	1
13	1	1	1	1
14	1	1	1	1
15	1	1	1	1
16	1	1	1	1
17	1	1	1	1
18	1	1	1	1
19	1	1	1	1
20	1	1	1	1
21	1	1	1	1
22	1	1	1	1
23	1	1	1	1
24	1	1	1	1
25	0.976	0.571	0.990	0.667
26	1	1	1	1
27	1	1	1	1
28	1	1	1	1
29	0.982	0.905	0.985	0.679
30	1	1	1	1
AVERAGE	0.998	0.974	0.999	0.976

Confusion Matrix																															
Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
1	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	0	0	0	19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	
5	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
6	0	0	0	1	0	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	
7	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
8	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
9	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
10	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
11	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
12	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
13	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
14	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	9	0	0	
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	19	0	
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	

FIGURE 6. Confusion matrix obtained with the FrST using nonlinear correlation. Rows represent true classes, while columns represent the predicted classes.

Confusion Matrix																															
Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
1	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
5	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
6	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
7	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
8	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
9	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
10	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
11	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
12	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
13	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
14	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	1	0	
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	

FIGURE 7. Confusion matrix obtained with the FrST using adaptive nonlinear correlation. Rows represent true classes, while columns represent the predicted classes.

TABLE III. Results of the FrST with adaptive nonlinear correlation.

Species	Accuracy	Sensitivity	Specificity	Precision
1	1	1	1	1
2	1	1	1	1
3	1	1	1	1
4	1	1	1	1
5	1	1	1	1
6	1	1	1	1
7	1	1	1	1
8	1	1	1	1
9	1	1	1	1
10	1	1	1	1
11	1	1	1	1
12	1	1	1	1
13	1	1	1	1
14	1	1	1	1
15	1	1	1	1
16	1	1	1	1
17	1	1	1	1
18	1	1	1	1
19	1	1	1	1
20	1	1	1	1
21	1	1	1	1
22	1	1	1	1
23	1	1	1	1
24	1	1	1	1
25	0.998	0.952	1	1
26	1	1	1	1
27	1	1	1	1
28	1	1	1	1
29	0.998	1	0.998	0.955
30	1	1	1	1
AVERAGE	0.999	0.998	0.999	0.998

TABLE IV. Results of the FrMT with nonlinear correlation.

Species	Accuracy	Sensitivity	Specificity	Precision
1	1	1	1	1
2	1	1	1	1
3	1	1	1	1
4	0.998	1	0.998	0.955
5	1	1	1	1
6	0.997	0.905	1	1
7	1	1	1	1
8	1	1	1	1
9	1	1	1	1
10	1	1	1	1
11	1	1	1	1
12	1	1	1	1
13	1	1	1	1
14	1	1	1	1
15	1	1	1	1
16	1	1	1	1
17	1	1	1	1
18	1	1	1	1
19	1	1	1	1
20	1	1	1	1
21	1	1	1	1
22	1	1	1	1
23	1	1	1	1
24	1	1	1	1
25	0.979	0.571	0.993	0.750
26	1	1	1	1
27	1	1	1	1
28	1	1	1	1
29	0.980	0.857	0.985	0.667
30	1	1	1	1
AVERAGE	0.998	0.977	0.999	0.979

TABLE V. Results of the FrMT with adaptive nonlinear correlation.

Species	Accuracy	Sensitivity	Specificity	Precision
1	1	1	1	1
2	1	1	1	1
3	1	1	1	1
4	1	1	1	1
5	1	1	1	1
6	1	1	1	1
7	1	1	1	1
8	1	1	1	1
9	1	1	1	1
10	1	1	1	1
11	1	1	1	1
12	1	1	1	1
13	1	1	1	1
14	1	1	1	1
15	1	1	1	1
16	1	1	1	1
17	1	1	1	1
18	1	1	1	1
19	1	1	1	1
20	1	1	1	1
21	1	1	1	1
22	1	1	1	1
23	1	1	1	1
24	1	1	1	1
25	0.998	0.952	1	1
26	1	1	1	1
27	1	1	1	1
28	1	1	1	1
29	0.998	1	0.998	0.955
30	1	1	1	1
AVERAGE	0.999	0.998	0.999	0.998

$$\text{specificity}(S_n) = \frac{TN_n}{TN_n + FP_n}, \quad (18)$$

$$\text{precision}(S_n) = \frac{TP_n}{TP_n + FP_n}, \quad (19)$$

where TP_n are true positives for the n species, TN_n , are true negatives for the n species, FP_n are false positives for n species, and FN_n are the false negatives for n species.

Tables II and III show the results obtained for the FrST with nonlinear and adaptative nonlinear correlations, respectively. The tables show the accuracy, sensitivity, specificity, and precision obtained with each species. The last row shows the averages of the four metrics. The results show a value of one for the four metrics in almost every species, with nonlinear correlation. In the case of adaptive nonlinear correlation, only two species do not achieve a value of one for the four metrics. Looking at the averages, adaptive nonlinear correlation has slightly better performance in accuracy, sensitivity, and precision than nonlinear correlation, with the same performance in specificity for both types of correlation.

Tables IV and V show the FrMT results with nonlinear and adaptive nonlinear correlation, respectively. For this transformation, working with nonlinear correlation, the results also show a value of one for the four metrics in almost every species. With adaptive nonlinear correlation, only two species do not achieve a value of one for the four metrics. Again, looking at the averages, only in specificity did both types of correlation have the same performance, with a slightly better performance for adaptive nonlinear correlation in the other three metrics.

Comparing both transformations, in the case of nonlinear correlation, both transforms have the same mean accuracy and mean specificity, and for the mean sensitivity and mean

Confusion Matrix																														
Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	1	0	19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
7	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	9	0
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	18	0
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0

FIGURE 8. Confusion matrix obtained with the FrMT using nonlinear correlation. Rows represent true classes, while columns represent the predicted classes.

Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
True Label	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0	0
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0	0
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	1	0
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0
28	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0
29	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0
30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21
Predicted Label	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30

FIGURE 9. Confusion matrix obtained with the FrMT using adaptive nonlinear correlation. Rows represent true classes, while columns represent the predicted classes.

precision, the FrMT had slightly better performance than the FrST. With adaptive nonlinear correlation, both transformations performed similarly with all four metrics. The performance of both transforms with adaptive nonlinear correlation was better than that obtained with nonlinear correlation for mean accuracy, mean sensitivity, and mean precision. In contrast, mean specificity had the same performance in both types of correlations for both transformations.

Figures 6-9 present the confusion matrices for both transformations and both correlation types.

5. Conclusion

The results show similar performance across the two fractional transformations when using nonlinear correlation, achieving high performance across all metrics, with the FrMT performing slightly better than the FrST. In the case of adaptive nonlinear correlation, the results are the same for both transforms and are better than those obtained with nonlinear correlation. Therefore, the adaptive nonlinear correlation was the better option for both transformations. The results show that using fractional orders yields better discrimination performance for both transforms. Therefore, the fractional scale transform introduced in this work is a good new pattern recognition tool capable of scale-invariant identification with high performance.

The species analyzed determines the scale range used in this work. However, integral transformations of this type can be applied to a broader range, as demonstrated by Pech-Pacheco *et al.* (2003) [25], who used the classical scale transform to classify Arial font letters across scale ranges from 50 % to 150 %. Therefore, the fractional scale transform, being a generalization of the classical scale transform, can operate effectively over a broader range.

This methodology does not require a training stage; there is no need to know the scale, rotation, and position parameters in advance to achieve the performance reported in this work.

Conflicts of interest

The authors declare no conflict of interest related to this study.

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Data statement

The data supporting is not publicly available, but they can be shared if you send an Email to the corresponding author.

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Experimental observation of frequency of oscillation, amplitude and temporal symmetry of a clapp oscillator incorporating a physical memristor

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The Clapp oscillator consists of one voltage amplifier, one inductor, three capacitors, and three resistors. The proposed work analyses the Clapp oscillator when two resistors are replaced by a commercially available physical memristor, *e.g.* the Knowm memristor, and a third case when the polarity of the memristor is inverted. In this manner, three cases are analyzed and compared with the responses of the Clapp oscillator without a memristive element. The responses of the experiments show how the position and polarity of the Knowm memristor influence the steady-state behavior of the LC resonant oscillator. The results show that the three cases, using the Knowm memristor, produce measurable changes in frequency of oscillation, amplitude, and temporal symmetry of the output waveform, whereas reversing the memristor polarity, reverses both frequency and temporal asymmetry trends. As a conclusion, the observed behaviors indicate that the memristor acts as a dynamic and history-dependent element, *i.e.* it modifies the oscillation conditions of the Clapp oscillator beyond the effects of a static resistive component. These findings establish that the Clapp oscillator topology is a suitable experimental platform for studying memristive effects in LC resonant systems. The results provide insights into the role of memristive devices position and polarity in shaping oscillatory dynamics.

Keywords: Knowm memristor; clapp oscillator; frequency; amplitude; symmetry.

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1. Introduction

Oscillators based on LC resonant networks, as the Colpitts, Hartley and Clapp, remain fundamental building blocks in analog and radio-frequency systems, where frequency stability, spectral purity, and robustness against parameter variations are essential. In such oscillatory systems, the balance between reactive elements and system losses determines whether sustained oscillations exist, how they are sustained, and their quality [1].

The Colpitts oscillator was modified by James Kilton Clapp in 1948 through the introduction of an additional capacitor in series with the inductor. This modification improved frequency stability by making the frequency of oscillation primarily dependent on the series capacitor and the inductor, thereby reducing the influence of parasitic capacitances and active device variations. The modified circuit was named Clapp oscillator. For instance, the resonant tank of the Clapp oscillator consists of three capacitors and one inductor, forming a capacitive divider that provides the necessary feedback to satisfy the Barkhausen criteria. By selecting the series capacitor to dominate the equivalent capacitance, the circuit achieves greater frequency precision while maintaining stable sinusoidal oscillations, which makes it suitable for high-frequency and variable frequency applications [2].

The proposed work reaffirms that the inclusion of nonli-

near or time-varying elements in an oscillator topology can significantly affect not only the oscillation frequency but also the signal's stability and waveform integrity. In this context, memristors have attracted increasing attention as circuit elements that introduce nonlinearity and history-dependent impedance into electrical systems.

Since the theoretical formulation as the fourth fundamental circuit element [3], the memristor has been characterized by a constitutive relationship between voltage and current that depends on the past excitation history. This memory effect enables behaviors that conventional passive components cannot replicate and has motivated its application in analog and nonlinear systems, and emerging electronic architectures. For instance, early works on memristor-based oscillators have been focused predominantly on non-resonant, or RC-based topologies. Among them, the Wien bridge oscillator is the most extensively studied topology.

The authors in Refs. [4,5] introduced a theoretical framework based on time-domain oscillatory poles to analyze the stability of memristor-based Wien oscillators, primarily relying on mathematical models and numerical simulations. In parallel, memristive nonlinearity has been exploited to generate complex dynamics, including chaotic oscillations, often through fractional-order memristor emulators [6]. More recently, memristor-based relaxation oscillators and reconfigurable signal generators have been explored in configurations

lacking resonant networks, revealing a strong dependence of the oscillatory dynamics on control signals and memristor state evolution [7,8]. Recent experimental studies have shown the influence of real physical memristors on RC-based oscillators, including both relaxation and Wien-bridge configurations, demonstrating that non-ideal memristive dynamics can induce significant frequency shifts and waveform modifications compared to conventional implementations [9].

Despite the widespread practical relevance of LC resonant oscillators, experimental studies integrating memristors into highly stable LC topologies remain scarce. Recent review articles on memristor-based sinusoidal oscillators explicitly highlight this gap and emphasize the lack of experimental validation using real physical memristors in such configurations [10]. Although related oscillatory structures have been reported, they have been investigated predominantly through simulation-based approaches [11].

The availability of commercial physical memristors has recently enabled experimental studies beyond idealized models and active emulators. In particular, Self-Directed Channel (SDC) devices manufactured by Knowm Technologies provide a platform for evaluating memristive behavior under realistic laboratory conditions. Unlike idealized models, physical memristors exhibit non-ideal dynamics that depend on excitation frequency, polarity, and prior stimulus history, which may critically influence the operation of resonant oscillators [12]. In this manner, the proposed work uses the Clapp oscillator—a topology that provides enhanced frequency stability and reduced sensitivity to parasitic capacitances—to be employed as a test platform to experimentally assess the impact of a nonlinear, history-dependent resistive element on an LC resonant system.

Section 2 shows the experimental waveform responses of the Clapp oscillator considering three characteristics, namely: frequency of oscillation, amplitude, and temporal symmetry. The measurement setup is implemented using the Analog Discovery Studio kit from Digilent, and three cases are established by replacing two passive resistors by the physical Knowm memristor, and a third case by changing the polarity of the memristor. Section 3 shows the experimental observation of the changes in the output waveform for each of the three cases, and shows the procedures to observe the frequency of oscillation, amplitude, and temporal symmetry when using the Knowm memristor and changing its polarity. Section 4 discusses the experimental observations of the output waveforms for the three cases. Finally, Sec. 5 summarizes the main conclusions.

2. Experimental methodology

A Clapp oscillator can be understood as a slight modification of the famous Colpitts topology [13]. The design of the

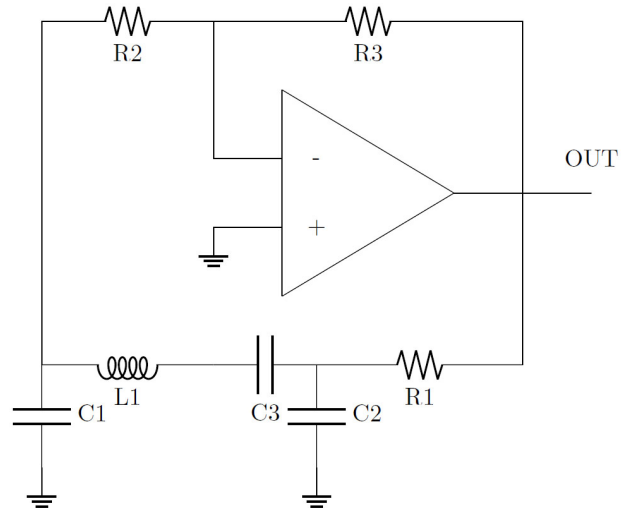


FIGURE 1. Clapp oscillator circuit topology consisting of one voltage amplifier, one inductor, three capacitors and three resistors.

experiment begins by the implementation of the topology of the Clapp oscillator shown in Fig. 1, whose experimental results are taken as the baseline for all subsequent comparisons. This topology is used herein as a stable, well-characterized resonant system, with its nominal behavior assumed known.

The oscillator topology shown in Fig. 1 is implemented to operate in a steady-state sinusoidal regime, where the oscillation frequency is primarily determined by the LC resonant tank, which has low sensitivity to parasitic capacitances. Throughout the analysis, all reactive and active components of the circuit are kept constant to ensure that any observed variation in oscillatory behavior can be attributed exclusively to modifications in the resistive elements, which are changed by the Knowm memristor one at a time, rather than to changes in the resonant network or the amplification stage.

In the proposed work, no adaptive tuning mechanisms, automatic gain control, or compensation strategies are implemented during the oscillator circuit operation. This omission is deliberate, as the main goal is not to restore or enforce ideal oscillation conditions, but rather to observe how the intrinsic dynamics of a nonlinear, history-dependent element, as the Knowm memristor, perturb an oscillator topology that is inherently designed for spectral stability. Under these assumptions, the topology shown in Fig. 1 is taken as a reference configuration that defines the experimental framework to perform a comparison between the stable and previously characterized LC oscillator against the impact of incorporating a physical memristive device by interchanging the memristor with one of the resistors given in the classical Clapp oscillator topology. This experimental approach allows isolating the effects induced by the memristor without conflating them with a circuit reconfiguration or parameter readjustment.

The experimental evaluation of the Clapp oscillator shown in Fig. 1, is based on a set of directly observable criteria selected to reflect relevant changes resulting from incor-

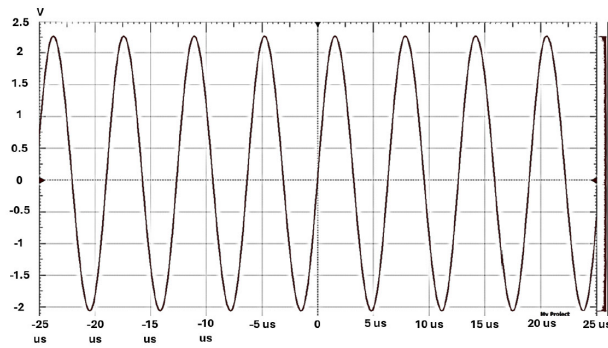


FIGURE 2. Experimental output waveform of the Clapp oscillator shown in Fig. 1.

porating a nonlinear, history-dependent resistive element. These criteria are defined before the memristor is included to avoid post hoc interpretations and ensure consistent comparisons across the three cases when each resistor is replaced by the Knownm memristor.

The first evaluation parameter is the frequency of oscillation of the Clapp topology, defined as the dominant component in the output voltage spectrum under steady-state conditions. The second parameter that is considered in the experimental observations is the amplitude of the output signal, which is analyzed and quantified by the maximum, minimum, and peak-to-peak values of the oscillatory voltage waveform. The amplitude parameter enables assessment of the memristive element's impact on the system gain balance and identification of potential saturation or attenuation effects associated with nonlinear resistive dynamics. The third parameter being measured concerns the temporal symmetry of the output waveform, which is examined through the time distribution of the positive and negative half-cycles. Alterations in this symmetry may indicate that the circuit behavior depends on the instantaneous signal polarity, which is particularly relevant for physical memristive devices, as the Knownm memristor, which exhibits asymmetric dynamics.

Figure 2, shows the output waveform of the classical Clapp oscillator using the circuit element values given in Table I. To ensure the reliability of the baseline circuit, a theoretical estimation of the expected oscillation frequency was carried out based on the resonant tank of the Clapp topology.

TABLE I. Circuit element values to implement the Clapp topology shown in Fig. 1.

Element	Identifier	Value
Resistor	R1	100 Ω
Resistor	R2	1 k Ω
Resistor	R3	47 k Ω
Capacitor	C1, C2, C3	100 nF
Inductor	L1	30.5 μ H
Supply	V ⁺	12 V
Supply	V ⁻	-12 V

In this configuration, the effective capacitance C_{eq} is deter-

mined by the series combination of C_1 , C_2 , and C_3 , as given in Eq. (1),

$$C_{eq} = \frac{C_1 C_2 C_3}{C_1 C_2 + C_1 C_3 + C_2 C_3} = \frac{(100 \text{ nF})^3}{3(100 \text{ nF})^2} = 33,3 \text{ nF}. \quad (1)$$

The frequency of oscillation depends on the LC values, so that it is evaluated by Eq. (2),

$$f = \frac{1}{2\pi\sqrt{(L_1)(C_{eq})}} = \frac{1}{2\pi\sqrt{(30,5 \times 10^{-6})(33,3 \times 10^{-9})}} \approx 1,5814 \times 10^5 \text{ Hz}. \quad (2)$$

This theoretical value is used as a reference for the subsequent analysis of both the classical and memristor-based configurations, enabling a consistent comparison among theoretical predictions, simulation results, and experimental measurements.

The experimental measurement setup is implemented using the Analog Discovery Studio kit from Digilent. Table II summarizes the experimental characteristics of the Clapp oscillator. All measurements are performed with the supply conditions, load, and connection topology held constant, so that any differences observed between the Clapp oscillator configurations without and with memristor, can be attributed to the memristive element rather than to external variations in the experimental environment.

Prior to perform the measurements, each oscillator configuration was allowed to operate continuously until transient effects associated with the memristive dynamics had settled. All circuits maintained stable operation for over one hour, with no appreciable variations in the frequency of oscillation, waveform shape, or amplitude beyond normal measurement uncertainty. This confirms that, under the considered conditions, the system reaches a steady-state regime without long-term drift or transitions to alternative dynamical behaviors, and the reported results therefore correspond to steady-state operation.

It is worth noting that the experimentally measured frequency of oscillation (158.14 kHz) shows strong agreement with the theoretical estimation (158 kHz). The minimal deviation observed falls within expected tolerances and can be attributed to non-ideal effects such as component tolerances, parasitic elements, and the finite bandwidth of the active

TABLE II. Standard Clapp oscillator: voltage, frequency, and duty cycle measurements.

V Max	2.2133 V
V Min	-2.0592 V
Vpp	4.2725 V
Frequency	158.14 kHz
Duty cycle (+ / -)	48.33 % / 51.66 %

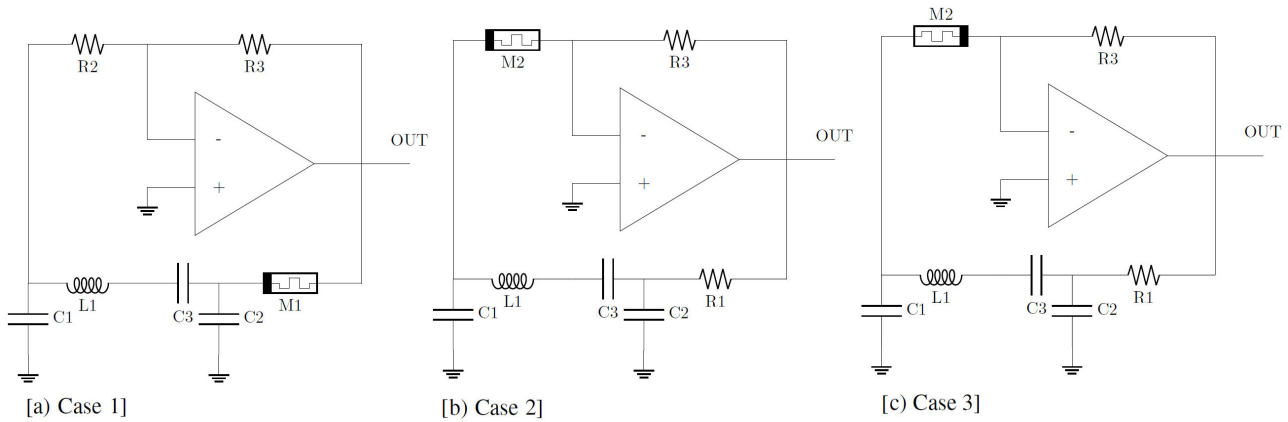


FIGURE 3. Three representative cases by replacing the resistors shown in Fig. 1 by the Known memristor: a) memristor M1 replaces resistor R1, b) memristor M2 replaces resistor R2, and c) memristor M2 replaces resistor R2 but in an opposite polarity compared to b).

device. This close correspondence validates the theoretical model used as a reference for subsequent analysis.

Taken as reference the topology of the classical Clapp oscillator shown in Fig. 1, three experimental scenarios are defined herein in which the physical Known memristive device is integrated into specific resistive positions within the electrical circuit. In the proposed work, the experimental analysis is deliberately restricted to three representative cases denoted as: Case 1, where the memristor M1 replaces resistor R1 as shown in Fig. 3a); Case 2, where the memristor M2 replaces resistor R2 as shown in Fig. 3b); and Case 3, where the memristor M2 replaces resistor R2 as shown in Fig. 3c), but in an opposite polarity compared to Fig. 3b). As one can infer, specifically these three cases show that the memristor is used as a replacement for R1 and R2, in which Case 3 considers the effect of inverted polarity of the memristor. These three cases exhibit clearly distinguishable behaviors in terms of oscillation frequency, signal amplitude, and temporal symmetry, as shown in the following section.

3. Experimental results

The comparison between the reference Clapp oscillator and Cases 1, 2 and 3 shown in Fig. 3, is performed in this section by using the circuit element values given in Table I. Figure 4 shows the experimental steady-state output waveforms corresponding to Cases 1, 2, and 3 of the Clapp oscillators incorporating the physical memristive device. It can be appreciated that in the three configurations using the Known memristor, sustained oscillatory operation appears, confirming that the inclusion of the memristor does not suppress the fundamental oscillation condition. However, noticeable differences in waveform shape, amplitude, and temporal characteristics are evident among the three cases, indicating a strong dependence on both the position and orientation of the memristive element within the circuit.

Observing the experimental output waveform shown in Fig. 4a), which is associated to the topology for Case 1 shown

in Fig. 3a), the signal has the largest amplitude among the three configurations and deviates from the sinusoidal behavior of the classical Clapp oscillator shown in Fig. 2. Figure 4a) shows the experimental output waveform with slightly sharper transitions and mild asymmetry between the positive and negative half-cycles, suggesting that the memristor directly influences the steady-state oscillatory regime when placed in a configuration that strongly interacts with the resonant loop.

Figure 4b) shows an experimental output waveform associated to Case 2, which behavior is closer to a sinusoidal signal, with less distortion than in Case 1, but also a little bit different to the experimental sinusoidal response shown in Fig. 2. In this Case 2, which is associated to the topology shown in Fig. 3b), although the memristor is located outside the LC tank network, its presence still affects the oscillatory behavior, resulting in observable but less pronounced deviations from the reference configuration of the Clapp oscillator shown in Fig. 1. This indicates that the memristive dynamics influence the oscillator indirectly by modifying the loop conditions rather than directly participating in the resonance mechanism.

A different behavior is observed in Case 3 in Fig. 4c). Here, the memristor M2 replaces R2 as done in Fig. 3c) but now with an inverted polarity. The experimental output waveform of Case 3 causes a distinct reduction in waveform amplitude and increases the number of oscillation cycles in a similar time window, indicating a higher frequency of oscillation. Notably, the distortion of the waveform is particularly pronounced during the negative half-cycle. This demonstrates that the memristor effect on the oscillating circuit is polarity-dependent, driven by the asymmetric internal dynamics of its structure.

The general experimental results show that incorporating the memristor in Cases 1 and 2 leads to a significant increase in the output signal amplitude relative to the reference configuration of the classical Clapp oscillator, whose characteristics are given in Table II. This effect is accompanied by a notable reduction in the frequency of oscillation. In contrast, Case 3 exhibits a distinctly different behavior: although the

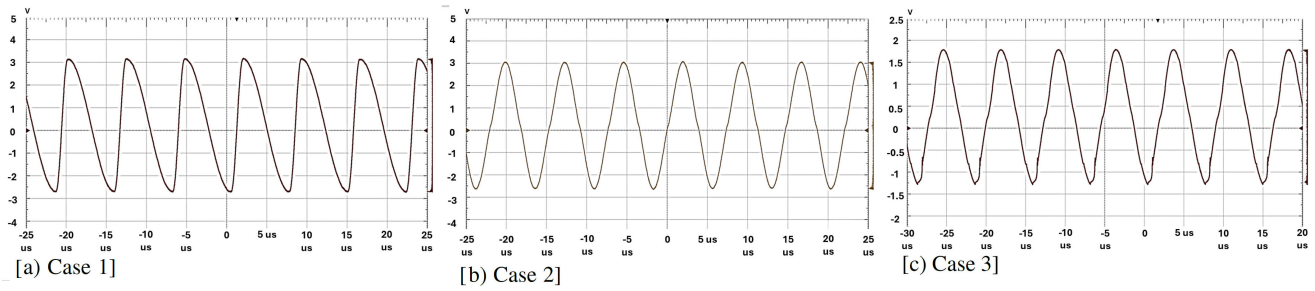


FIGURE 4. Experimental output waveforms of the three representative cases shown in Fig. 3.

oscillation frequency approaches the value of the reference oscillator, the signal amplitude is considerably reduced.

Across the experimental results of the output waveform for all three cases, slight temporal asymmetries are evident in the relative durations of the positive and negative half-cycles. These features suggest that the observed behavior is influenced not only by instantaneous signal conditions but also by specific memristive effects, such as the device's sensitivity to signal polarity and the evolution of its internal state over time.

3.1. Variation of the frequency of oscillation

The frequency of oscillation constitutes a primary indicator of how the inclusion of a memristive element alters the dynamics of the Clapp oscillator. Table III summarizes the experimentally measured frequencies for the reference configuration of the classical Clapp oscillator and for Cases 1, 2 and 3.

As one can appreciate, the experimental oscillation shown in Fig. 2 for the reference Clapp oscillator, indicates that it operates at 158.14 kHz. This measured frequency is consistent with the expected behavior of a stable LC resonant circuit. However, when the physical Knowm memristor is introduced to replace resistors, as shown in Fig. 3, the experimental measured frequencies diminishes. For instance, the experimental waveform shown in Fig. 4a) associated to Case 1, shows that the frequency of oscillation decreases significantly, dropping to 137.41 kHz. This change represents about 13 % deviation from the reference configuration of the classical Clapp circuit.

A similar reduction is observed in the experimental output waveform shown in Fig. 4b), associated to Case 2, where the frequency of oscillation decreases to 135.89 kHz, but in general the frequency shift remains comparable to that of Case 1. This confirms that the memristive device's influence on the frequency of oscillation is not limited to direct interaction with the resonant tank but can also arise from indirect modifications to the loop dynamics.

TABLE III. Frequencies of oscillation for the classical Clapp oscillator shown in Fig. 1 and the three cases shown in Fig. 3.

Clapp	Case 1	Case 2	Case 3
158.14 kHz	137.41 kHz	135.89 kHz	155.37 kHz

In contrast, the experimental output waveform shown in Fig. 4c), associated to Case 3 shows a markedly different behavior. When the memristor is placed in the same circuit position as in Case 2 but with reversed polarity, the frequency of oscillation is also lower than that of the reference one shown in Fig. 2, but compared to the experimental output waveform shown in Fig. 4b), reversing the polarity of the memristor makes an increase to 155.37 kHz, approaching the value of the classical Clapp oscillator. This change in frequency trend underscores the strong dependence of oscillatory behavior on the orientation of the physical memristor's polarity.

Overall, the results demonstrate that integrating a physical memristive device can either reduce or increase the oscillation frequency of a Clapp oscillator, depending on its position and polarity within the circuit. These findings support the idea that the memristor acts as a dynamic element that alters the effective oscillation conditions of an LC resonant system, rather than merely introducing a static resistive perturbation.

3.2. Amplitude behavior

The effect of the physical Knowm memristor on the amplitude of the oscillation waveform is evaluated herein by the maximum, minimum, and peak-to-peak voltages of the output signal. These parameters provide direct insight into how the memristive dynamics influence the balance between loop gain and effective losses in the Clapp oscillator. For clarity, the measured amplitude values for the Classical Clapp configuration and for Cases 1, 2 and 3, are summarized in Table IV.

The reference Clapp oscillator exhibits a peak-to-peak voltage of 4.2725 V, corresponding to a stable oscillatory regime with moderate amplitude. When the memristor is in-

TABLE IV. Maximum, minimum, and peak-to-peak voltages comparison for the classical Clapp oscillator and Cases 1, 2 and 3.

Case	V_{Max}	V_{Min}	V_{pp}	Amplitude
Clapp	2.2133 V	-2.0592 V	4.2725 V	2.1363 V
Case 1	3.2022 V	-2.5892 V	5.7921 V	2.8961 V
Case 2	3.1627 V	-2.6002 V	5.7630 V	2.8815 V
Case 3	1.8350 V	-1.2386 V	3.0692 V	1.5346 V

troduced in Case 1, a substantial increase in signal amplitude is observed, with the peak-to-peak voltage rising to

5.7921 V. This increase is consistent with the waveform shown in Fig. 4a), where the signal exhibits larger excursions together with mild distortion.

A similar amplitude enhancement is observed in Case 2, where the peak-to-peak voltage reaches 5.763 V. This behavior indicates that the memristive element can significantly affect the oscillation amplitude by indirectly modifying the loop conditions.

In contrast, Case 3 displays a markedly different amplitude response. When the memristor is placed with inverted polarity, the peak-to-peak voltage decreases to 3.0692 V, representing a substantial reduction relative to both the reference configuration and the other memristor-based cases. This reduction is clearly reflected in the waveform shown in Fig. 4c), where the signal exhibits smaller voltage excursions and increased distortion.

Overall, the amplitude results demonstrate that the physical memristor can either enhance or suppress the oscillation amplitude depending on its placement and polarity within the circuit.

4. Discussion

The experimental observations of the frequency of oscillation, amplitude and symmetry of the temporal responses performed in the proposed work, indicate that the behavior of an LC resonant oscillator can be significantly reshaped by adding a memristive element, even when the overall circuit topology remains unchanged. The dependence of the oscillatory regime on the device's position and polarity highlights that the memristor introduces additional dynamic degrees of freedom into the system.

From a physical perspective, the observed frequency shifts suggest that the memristor alters the dynamic balance between energy storage and dissipation within the oscillation loop. Rather than contributing a constant resistive term, the memristor serves as a state-dependent resistive and memory element. Its instantaneous influence on the oscillation cycle arises from its internal state changing in response to the voltage and current history, directly affecting circuit dynamics. This state dependence provides a clear explanation for the different frequency trends observed across the tested configurations.

The polarity-dependent changes in amplitude and temporal symmetry further support this interpretation. The inversion of waveform asymmetry observed when the memristor orientation is reversed indicates that the device's internal dynamics are not symmetric with respect to voltage polarity. Such asymmetry implies that the memristor interacts differently with the oscillatory loop during positive and negative signal excursions, leading to unequal energy exchange between the two halves of each cycle.

Importantly, these effects persist even when the memristor is not embedded in the LC tank. This indicates that the memristor's role is not limited to simply modifying the reso-

nant network. Rather, the memristor modulates the oscillator by altering the global loop conditions, thus influencing gain, losses, and phase throughout the system. This demonstrates that memristive effects in resonant oscillators arise from the memristor's system-wide interactions, rather than being confined to a single circuit element or described by purely static models.

Overall, this highlights that the memristor acts as an active element in oscillation dynamics: its state evolution and polarity sensitivity directly shape the system's steady-state behavior. Recognizing these roles is essential for understanding and predicting how resonant circuits incorporating memristive devices will behave.

5. Conclusions

The proposed work experimentally demonstrates that a physical memristive device can be integrated into a Clapp oscillator without suppressing sustained oscillation. The presence of the memristor leads to reproducible changes in oscillation frequency, output amplitude, and temporal symmetry, which depend on both the device's position and polarity within the circuit.

The experimental analysis shows that the frequency of oscillation is strongly influenced by both the placement and orientation of the memristor. Circuit configurations corresponding to Cases 1 and 2 exhibit a clear reduction in frequency relative to the reference oscillator, whereas reversing the polarity of the device in Case 3 produces an increase in frequency approaching the reference value. These observations confirm that the memristor introduces a dynamic contribution to the oscillation conditions that cannot be described as a fixed resistive effect.

Amplitude measurements further reveal that the memristor can either enhance or suppress the output signal depending on the configuration. While Cases 1 and 2 lead to a significant increase in peak-to-peak voltage, Case 3 results in a pronounced reduction in amplitude. This contrasting behavior, observed under otherwise identical circuit conditions, highlights the oscillation loop's sensitivity to the device's internal state and polarity-dependent dynamics.

In addition to frequency and amplitude variations, all memristor-based configurations exhibit measurable temporal asymmetries between positive and negative half-cycles. These temporal features reinforce the interpretation of the memristor as a history-dependent element that modifies the steady-state oscillatory regime beyond conventional linear expectations.

The results confirm that the memristor cannot be treated as a static resistive element in an LC resonant oscillator, as its dynamic and polarity-dependent behavior directly influences the steady-state oscillatory regime. The Clapp topology has been shown to provide a stable, well-defined platform for observing these effects under controlled experimental conditions.

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Elastic, optical and thermodynamic properties of the double perovskites $\text{Ba}_2\text{DySbO}_6$: Applications in spintronic devices

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In this research, we employed an ab initio calculation approach based on the full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT), integrated into the WIEN2k code. By examining in detail the structural, elastic, electronic, magnetic, optical, and thermodynamic characteristics of the double perovskite compound $\text{Ba}_2\text{DySbO}_6$. Firstly, our study focused primarily on magnetic stability. The results presented in this work are in good agreement with the available experimental and theoretical data. Subsequently, we studied the electronic properties in which we calculated the band structure and the density of states. Regarding the magnetic properties of the compound $\text{Ba}_2\text{DySbO}_6$, it was found that the total magnetic moment is mainly due to the magnetic moment of the lanthanide atom. The optical properties, such as the real and imaginary parts of the dielectric function, the refractive index, the extinction coefficient, the reflectivity, the optical conductivity, and the absorption coefficient of the $\text{Ba}_2\text{DySbO}_6$ compound, were calculated for all photon energies. The thermodynamic study of our compound has shown that it is stable at high temperatures. The predictive calculations of the thermal properties of our compound show that it follows the same behavior with temperature variation.

Keywords: Elastic; optical; thermodynamic; DFT, $\text{Ba}_2\text{DySbO}_6$.

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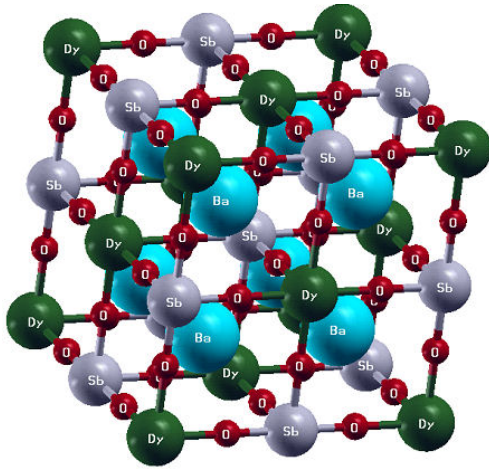
1. Introduction

In recent years, double perovskites have gained enormous interest and have become one of the most motivating subjects in the field of scientific research due to the extraordinary physical and electrical properties that characterize this family of compounds. Some of the double perovskites with the general formula $\text{A}_2\text{B}'\text{B}''\text{O}_6$ (where A is generally an alkaline earth or rare earth metal, B' and B'' are transition metals or lanthanides) have been proposed as ferroelectric, such as $\text{Ba}_2\text{GdMoO}_6$ [1]. Furthermore, it has been well known that these compounds possess particular characteristics of interest among them; their structural and physical properties are very sensitive to small changes in chemical composition. Therefore, depending on the choice of cations A, B', and B'', they can exhibit a wide variety of crystalline structures, including structures with monoclinic ($\text{P}2_1/\text{n}$), tetragonal ($\text{I}4/\text{m}$), and cubic ($\text{Fm}\bar{3}\text{m}$) symmetries [2, 3], as well as electrical and magnetic properties that include metallicity and magnetoelectric response [4]. Perovskite compounds with the basic structure $\text{Ba}_2\text{RESbO}_6$, (where RE = Nd, Eu, and Dy), were prepared as single-phase materials using standard solid-state methods. These compounds are isostructural and exhibit a complex perovskite structure, as shown by powder X-ray diffraction measurements [5–7]. Ab initio simulation studies, within the framework of DFT, have been dedicated to this promising class of double perovskite oxides containing magnetic ions in B' sites. But, despite these recent advances in understanding the physical properties of these compounds, several other questions regarding electronic, magnetic, elastic, optical, and thermodynamic structures are still debatable. For the-

se reasons, in this work, we performed first-principles calculations based on the full-potential linearized augmented plane wave (FP-LAPW) method, implemented in the Wien2k code, with the generalized gradient approximation (GGA-PBE) of the double perovskite compound $\text{Ba}_2\text{DySbO}_6$.

2. Computational details

By examining in detail the structural, elastic, electronic, magnetic, optical, and thermodynamic properties of the double perovskite compound $\text{Ba}_2\text{DySbO}_6$, we were able to obtain useful information for this compound using methods based on DFT [8, 9] with the generalized gradient approximation (GGA-PBE) [10–12]. Within the framework of these studies, the application of DFT generally begins with total energy calculations and structural optimization steps. Therefore, in this work, we studied the cubic double perovskite $\text{Ba}_2\text{DySbO}_6$. This compound crystallizes in the space group (No. 225) described by $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$. The positions of the Ba, Dy, Sb, and O atoms, respectively, are Ba (0.25, 0.25, 0.25), Ba (0.75, 0.75, 0.75), Dy (0.0, 0.0, 0.0), Sb (0.5, 0.5, 0.5), and O ($u=0.2851$, 0, 0) [7]. The cubic structure of $\text{Ba}_2\text{DySbO}_6$ is illustrated in Fig. 1. The Wien2k program, which is directly based on the application of the FP-LAPW method [13] allows for the calculation of various properties, such as the total energy. This code uses DFT-based techniques and considers both the space group symmetry and the Bravais lattice. The exchange-correlation functional was described using the GGA-PBE approximation [10]. The value

FIGURE 1. Crystal structure of double perovskites Ba₂DySbO₆.

of $\ell_{\text{max}} = 10$ defines the cutoff used to determine the angular momentum of the functions inside the sphere. The parameter $G_{\text{max}} = 14$ indicates the largest wave vector norm (K) used to carry out the Fourier (plane-wave) expansion of the charge density. The cutoff parameter $R_{\text{MT}} \times K_{\text{max}} = 8$ determines the basis functions to be used in the calculation, where RMT is the smallest radius of the Muffin-tin (MT) spheres in the unit cell, and K_{max} is the norm of the largest wave vector (K) associated with the plane-wave expansion of the eigenfunctions. These parameters proved suitable for achieving convergence with an energy tolerance of 10^{-4} Ry and the cut-off energy between the valence states and the core states was set at -6 eV. The integration in reciprocal space is performed with a mesh of $14 \times 14 \times 14$, resulting in 3000 k-points in the irreducible Brillouin zone (IBZ) [14]. The radii of the MT spheres (RMT) of the Ba, Dy, Sb, and O atoms chosen in our calculations are respectively, 2.5, 2.25, 1.98, and 1.7 a.u. (atomic unit). To verify the crystal structures of double perovskites, the tolerance factor was calculated using the expression $t = (r_A + r_O) / (\sqrt{2}(r_B + r_O))$. The Shannon ionic radii of Ba²⁺, Dy³⁺, Sb⁵⁺, and O²⁻ were used to deter-

mine the tolerance factor t of the four cations: 1.61 Å (Ba²⁺), 0.912 Å (Dy³⁺), 0.6 Å (Sb⁵⁺), and 1.4 Å (O²⁻). The average radius of Dy and Sb was used for the B site to give an average B -cation radius of 0.756 Å and a tolerance factor of about $t \approx 0.99$, indicating that the B -site cations have a stable configuration in a cubic structure. Depending on the value of the tolerance factor, the structure of double perovskites is cubic since t is between 0.9-1 [15].

3. Results and discussion

3.1. Structural and elastic properties

The calculation of the physical properties of double perovskites requires the determination of their ground state. To achieve this, we evaluated the total energy of the system for different volume values. In order to determine the magnetic stability (ferromagnetic and non-magnetic configurations) and structural properties (lattice parameter a , compressibility modulus B , and its derivative B') in the vicinity of equilibrium, we analyzed the energy differences and structural responses for each configuration. The obtained results were then fitted by the third-order Birch-Murnaghan equation of state [16]. Figure 2 represents the variation of total energy as a function of volume for both the magnetic and non-magnetic phases, using the GGA-PBE approximation with and without spin polarization. The results obtained regarding the ground state energy and structural parameters such as, the lattice parameter, the bulk modulus B , and its derivative B' , are compiled in Table I, along with the experimental values and those obtained by other theoretical calculations for comparison. The most stable ferromagnetic state is identified because it corresponds to the phase with the minimum energy. The results presented in Table I above are in good agreement with the available experimental and theoretical data [6, 17–22]. Comparing these data in percentage, we find a slight overestimation of the lattice parameters cal-

TABLE I. Lattice constant a_0 (in Å), bulk modulus B (in GPa), its pressure derivative B' , and minimum energy at equilibrium E_0 (in Ryd) using GGA (PBE).

Method / Work	a_0 (Å)	B (GPa)	B'	E_0 (Ry)
NM-GGA-PBE	8.7097	105.1572	5.3211	-70738.804736
FM-GGA-PBE	8.5372	129.2429	4.8769	-70765.738955
Experimental	8.431 [6]	-	-	-
	8.4247 [17]	-	-	-
	8.4289 [18]	-	-	-
	8.4374 [18]	-	-	-
	8.4247 [20]	-	-	-
	8.4297 [21]	-	-	-
	8.4376 [22]	-	-	-
Theoretical	8.4243 [19]	-	-	-

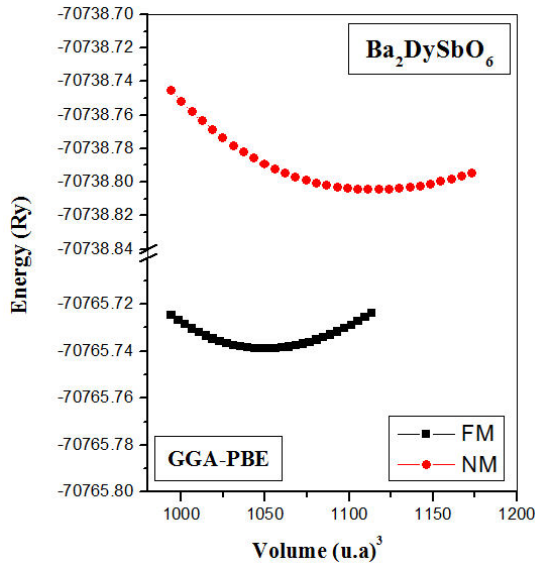


FIGURE 2. The total energy for both non-magnetic (NM) and ferromagnetic (FM) configurations with the GGA (PBE) approximation as a function of volume.

TABLE II. Calculated elastic constants C_{11} , C_{12} , C_{44} (in GPa), bulk modulus B (in GPa), Young's modulus E and shear modulus G (in GPa), Poisson's ratio ν , the anisotropic parameter A and the B/G ratio, longitudinal, transverse and average sound velocities (v_l , v_t , v_m) (in m s^{-1}), and Debye temperature θ_D (in K) calculated using GGA (PBE) at $T = 0$ K and $P = 0$ GPa.

Elastic constants (GPa)				
C_{11}	C_{12}	C_{44}	$B = \frac{C_{11}+2C_{12}}{3}$	
211.8	98.7	80.7	136.36	
Mechanical properties				
E (GPa)	G (GPa)	ν	A	B/G
181.5861	71.04	0.28	1.42	1.92
Sound velocities (m s ⁻¹) and Debye temperature				
v_l	v_t	v_m	θ_D (K)	
3182.955	5740.639	3545.581	195.2865	

culated by the GGA (PBE) approximation on the order of: 3.32 % and 1.26 % for the non-magnetic and ferromagnetic states, respectively, due to the use of GGA(PBE).

To determine the elastic properties of the $\text{Ba}_2\text{DySbO}_6$ compound, we first applied orthorhombic and monoclinic constraints, respectively. The requirement of mechanical stability of the cubic structure leads to the following restrictions on the elastic constants, $C_{11} > 0$, $C_{12} > 0$, $C_{44} > 0$, and $(C_{11} + 2C_{12}) > 0$ [23, 24]. Our obtained elastic constants listed in Table II, obey these stability conditions for cubic structures, including the fact that $C_{12} > 0$ must be less than $C_{11} > 0$. Furthermore, our calculated elastic constants also meet the stability conditions for cubic structures, which implies that $C_{12} < B < C_{11}$. The value of the bulk modulus B , calculated from the elastic constants, is nearly the sa-

me as the value obtained from the smoothing points $E_{\text{tot}}(V)$ using the Murnaghan equation of state (EOS). This gives us a good estimate of the precision and accuracy of the elastic constants of $\text{Ba}_2\text{DySbO}_6$. The calculated value of A , which is listed in Table II, indicates that $\text{Ba}_2\text{DySbO}_6$ is a material exhibiting anisotropic behavior (if $A \neq 1$, indicates anisotropic behavior, while $A = 1$ corresponds to isotropic behavior). The typical value of the Poisson coefficient for covalent materials is around 0.1, while for ionic materials it is around 0.25 [23, 24]. In our case, the value of the Poisson's ratio is 0.28, which suggests a stronger intra-atomic ionic bonding contribution for this compound. According to Pugh's empirical formula [23, 24], which states that the critical value of the B/G ratio separating the ductile and brittle behavior of materials is approximately 1.75, i.e., if $B/G > 1.75$, the material behaves in a ductile manner; otherwise, it behaves in a brittle manner, the $\text{Ba}_2\text{DySbO}_6$ compound is classified as ductile.

3.2. Electronic and magnetic properties

The band structure calculation of the double perovskite $\text{Ba}_2\text{DySbO}_6$ was performed along the high-symmetry directions of the first Brillouin zone [25] based on the GGA-PBE approximation. The results obtained are illustrated in Fig. 3 for both spin-up and spin-down. According to these figures, it is evident that the band structure of minority spins (spin-down) has a spin polarization around the Fermi level, which indicates that this electronic structure has a purely metallic character, while the majority spins (spin-up) exhibit a semi-conducting behavior, with the maximum and minimum of the valence band and conduction band located at the Γ point, indicating the presence of a direct band gap in the $(\Gamma - \Gamma)$ direction for the $\text{Ba}_2\text{DySbO}_6$ material, which confirms that this compound is typically ferromagnetic semi-metallic by GGA-PBE. The energy gap value, from the spin-up band structure diagram, is equal to 3.19 eV for the $\text{Ba}_2\text{DySbO}_6$ compound. In our study, we calculated the density of states (DOS) of this material $\text{Ba}_2\text{DySbO}_6$. Figure 4 shows the partial density of

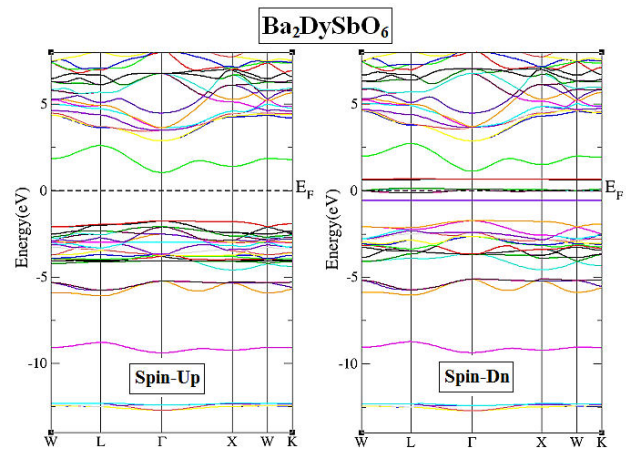
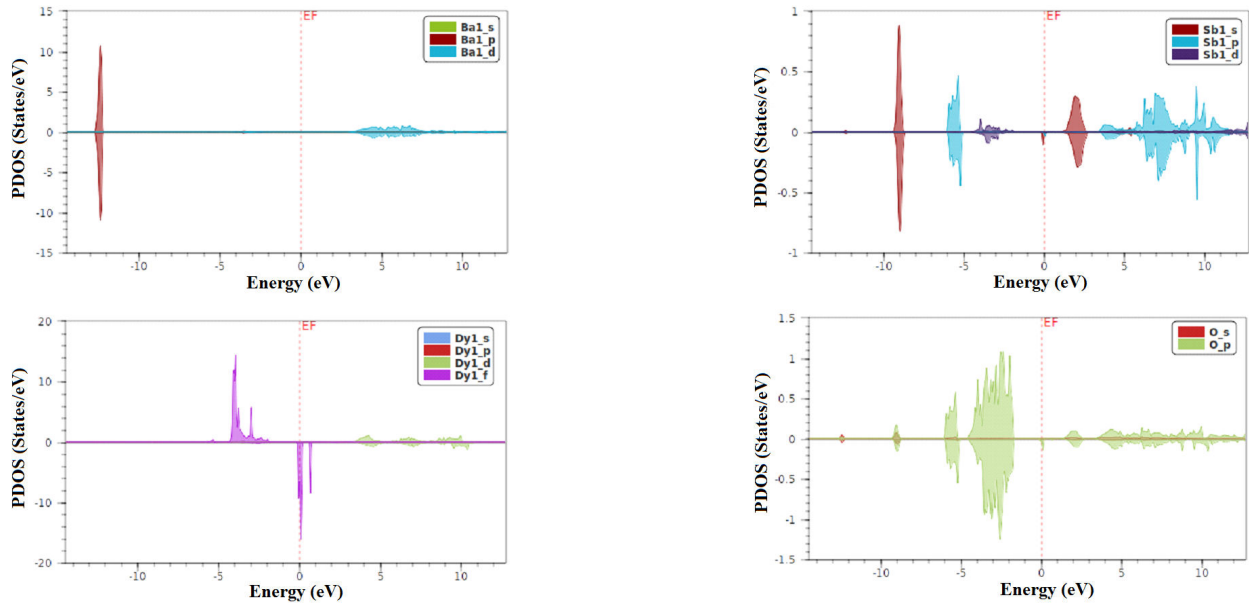


FIGURE 3. The band structure of $\text{Ba}_2\text{DySbO}_6$ at the equilibrium structure using PBE-GGA approximation with spin polarization.

FIGURE 4. The partial density of states of Ba₂DySbO₆ at the equilibrium structure using PBE-GGA approximation with spin polarization.TABLE III. Total and local magnetic moments of Ba₂DySbO₆ obtained by the GGA-PBE approximation, with spin polarization.

Method	Ba	Dy	Sb	O	Interstitial	Total
GGA-PBE (at $T = 0$ K)	-0.00047	4.86657	-0.00731	0.01815	0.03000	5.0
Theoretical (at $T \neq 0$ K)	—	—	—	—	—	7.7 [7]
Experimental (at $T \neq 0$ K)	—	—	—	—	—	8.9 [7]
	—	—	—	—	—	10.55 [21]
	—	—	—	—	—	10.63 [21]

states (PDOS) calculated using the generalized gradient approach (GGA-PBE) with spin polarization between -13 and 15 eV relative to the Fermi level. We observe for this compound Ba₂DySbO₆ below the Fermi level, the valence band is strongly dominated by Ba-p (up and down) and Dy-f (up) states with, however, a minor contribution from Sb-s,p and O-p (up and down) states around the Fermi level, the states are dominated by Dy-f (down) orbitals. Above the Fermi level (states located about 1 eV and higher), in the conduction band, the PDOS is weakly dominated by Sb-p (up and down) and O-p (up and down) states. We also note that the partial density of states (PDOS) calculated using (GGA-PBE) with spin polarization of this Ba₂DySbO₆ compound for both spin-up and spin-down cases are not similar, which confirms that the material is magnetic. The results presented in Figs. 3 and 4 are in good agreement with the available theoretical data [7, 19]. We calculated the total, partial, and interstitial magnetic moments of the double perovskite compound Ba₂DySbO₆ using the GGA-PBE approximation and with spin polarization. According to Table III, the compound Ba₂DySbO₆ has a significant total magnetic moment, indicating the presence of ferromagnetic behavior in this material in its ground state. We also notice that the total contributions are

much more localized on the lanthanide atom Dy. The experimental and theoretical data are represented in Table III. The difference in total magnetic moments is due to the change in temperature ($T \neq 0$ K).

3.3. Optical properties

The GGA-PBE approximation was adopted to study the optical properties of the Ba₂DySbO₆ compound. In this section, optical properties such as the real and imaginary parts of the dielectric function, reflectivity, refractive index, extinction coefficient, optical conductivity, and absorption coefficient of the Ba₂DySbO₆ compound were calculated for all photon energy, and they are presented in Figs. 5-10 respectively. In Fig. 5, the fixed value of the real part $\epsilon_1(0)$, which relates to the material's interaction with low-frequency, is quite high, suggesting a strong polarization capacity. $\epsilon_1(\omega)$ peaks at about 0.67 eV, indicating a strong coupling of the material to the incoming photons in this energy range. After this point, $\epsilon_1(\omega)$ decreases and becomes negative at about 1.01 eV, showing that the material enters a metallic reflection phase. The disappearance of $\epsilon_1(\omega)$ signifies the presence of a bulk plasmon, which is a collective excitation of conduction electrons. The real part $\epsilon_1(\omega)$ starts very high (ranging

from approximately 25 to 30), then decreases with increasing

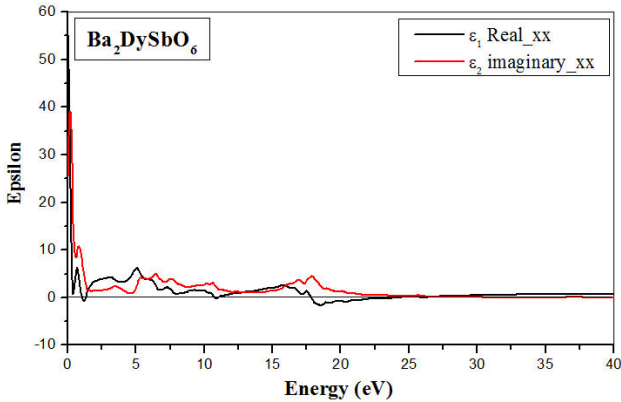


FIGURE 5. The real part $\varepsilon_1(\omega)$ and imaginary part $\varepsilon_2(\omega)$ of dielectric function of $\text{Ba}_2\text{DySbO}_6$ compound.

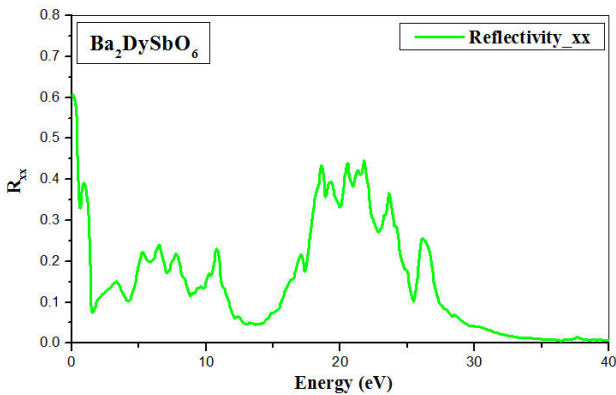


FIGURE 6. The reflectivity $R(\omega)$ of $\text{Ba}_2\text{DySbO}_6$ compound.

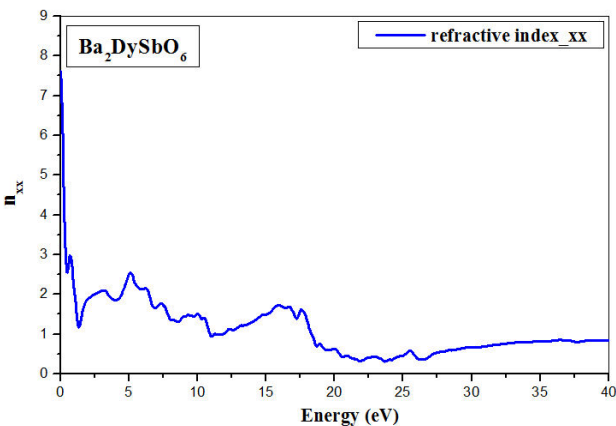


FIGURE 7. The refractive index $n(\omega)$ of $\text{Ba}_2\text{DySbO}_6$ compound.

energy, eventually crossing zero at approximately 16 to 17 eV, indicating the presence of a plasmon resonance. The imaginary part $\varepsilon_2(\omega)$ can be directly linked to the material's optical absorption, indicating electronic transitions between the bands. A distinct peak is observed at 0.16 eV, which is ascribed to electronic transitions into the upper conduction bands. For energy values larger than 0.18 eV, $\varepsilon_2(\omega)$ gradually

decreases indicating that the absorption decreases as interband transitions become less available. The intermediate energy region has multiple smaller peaks (around 4 to 5) at approximately 5 eV, (around 2 to 3) at approximately 10 eV, and (around 3 to 4) between 16 and 18 eV, which correspond to multiple electronic transitions related to the band gap energy. Above 22 eV, both $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ tend to zero, and the material approaches transparency. Overall, there is strong interaction between the material and light in the low and intermediate energy ranges. Figure 6 illustrates the evolution of reflectivity R according to photon energy for the material $\text{Ba}_2\text{DySbO}_6$. Reflectivity is a crucial factor for evaluating the proportion of light reflected by the material's surface during electromagnetic excitation and is directly related to the refractive index and extinction coefficient. We observe a low reflectivity value at energies $E < 3$ eV, indicating a high degree of absorption or transmission by the material of most of the incident illumination, followed by a significant increase from 3 eV onward, still with oscillations that most often coincide with the peaks we observe earlier in the extinction coefficient. The region beyond 30 eV shows a stabilized reflectivity value; the slight oscillations observed could be due to plasmonic effects and secondary electronic transitions. The $\text{Ba}_2\text{DySbO}_6$ material refractive index (n) evolution is illustrated in Fig. 7, as a function of photon energy, progressively increasing from 0.51 eV before reaching maximal n around 3 at a photon energy of 0.70 eV. The enhancement of refractive index (n) is due to the contribution of interband electron transitions that increase the optical response of the material, and refractive index (n) begins to decrease slightly after 17.67 eV due to related absorption increasing as more electrons are excited into higher energy levels. Starting from 25 eV, the refractive index (n) becomes really low, which means the materials are not effectively transmitting light in this spectral region. Analyzing the refractive index is very useful to understand the optical properties of the material and its different utilizations, especially in optoelectronics and photonics, where a high refractive index is desirable to serve as a waveguide for some wavelength ranges, for nonlinear optical devices, or even for antireflective applications. Therefore, the analysis of this curve provides a better understanding of the light-electron interaction mechanism in $\text{Ba}_2\text{DySbO}_6$ and thus progresses its potential applications. It appears from Fig. 8 that a significant peak around 0.24 eV is observed in the extinction coefficient of about 0.45, indicating strong optical absorption resulting from allowed electronic transitions. These transitions are determined by the band structure of the solid, which can also cause several secondary peaks that reflect other modes of electronic transitions. In Fig. 9, we represent the variation of optical conductivity (σ_x) as a function of energy for the material $\text{Ba}_2\text{DySbO}_6$, whose appearance is characterized by a very significant peak located in the vicinity of 17.92 eV, which could correspond to a strong absorption of incident photons due to dominant interband electronic transitions. We indeed observe that after this peak, the conductivity decreases with some oscillation, with

secondary electronic transitions and

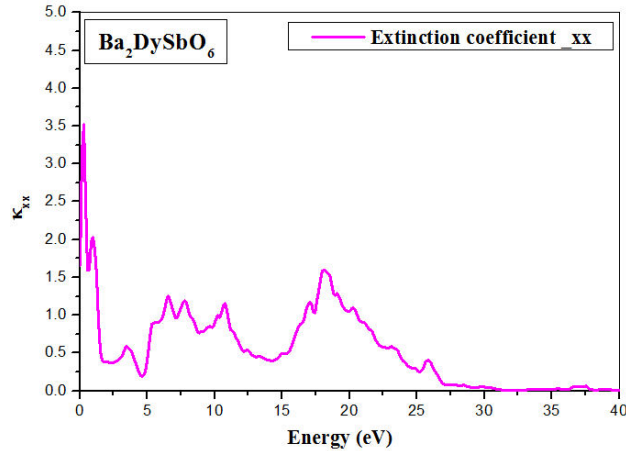


FIGURE 8. The extinction coefficient $k(\omega)$ of $\text{Ba}_2\text{DySbO}_6$ compound.

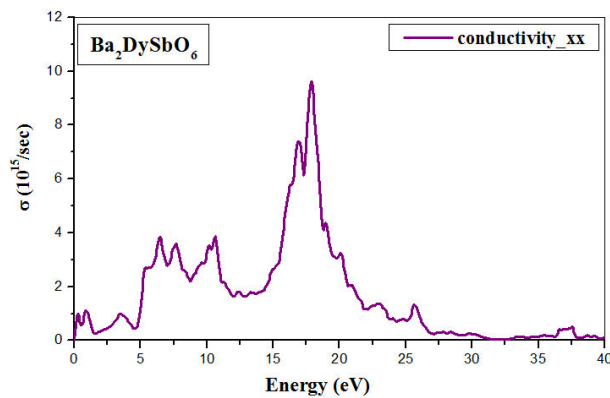


FIGURE 9. The conductivity $\sigma(\omega)$ of $\text{Ba}_2\text{DySbO}_6$ compound.

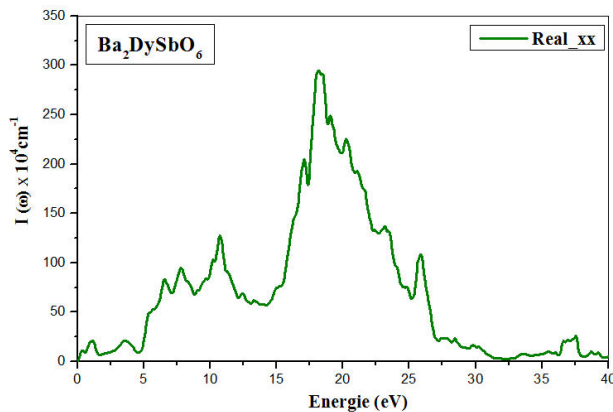


FIGURE 10. The absorption $I(\omega)$ of $\text{Ba}_2\text{DySbO}_6$ compound.

density of states effects opposing the main transition. Figure 10 shows the evolution of the absorption coefficient of the $\text{Ba}_2\text{DySbO}_6$ material as a function of the energy of the incident photons. Optical absorption is indeed an important parameter for understanding the electronic and optical properties of a material, both for optoelectronic and photovoltaic

applications, and here, the absorption coefficient gradually increases until it reaches a maximum around 18,17 eV, then decreases. This trend is generally observed for materials undergoing inter-band transitions between the valence and the conduction band, where the absorption peak is related to direct electronic transitions.

3.4. Thermodynamic properties

To address the thermodynamic properties of the double perovskite compound $\text{Ba}_2\text{DySbO}_6$, we apply the quasi-harmonic Debye model to the GIBBS program [11, 14, 26]. This model allows the extraction of all thermodynamic properties from the energy and volume properties, provided at equilibrium. To study the thermal properties of the double perovskite compound $\text{Ba}_2\text{DySbO}_6$ at high temperature and high pressure, we applied the quasi-harmonic Debye approximation. To begin, a calculation of the total energy as a function of the unit volume $E(V)$, was performed and associated with the numerical equation of state (EOS) to determine the structural parameters at room temperature and zero pressure, and to deduce the macroscopic properties as a function of pressure and temperature from classical thermodynamic relations. The thermal properties are calculated over the temperature range of 0 – 700 K using the GGA-PBE method, where the quasi-harmonic model is fully valid. In Fig. 11, the curve of the lattice parameter is shown as a function of temperature and for different pressures for the double perovskite compound $\text{Ba}_2\text{DySbO}_6$. The lattice parameter increases with increasing temperature, but the percentage increase is more significant for the temperature range above 150 K. On the other hand, when the pressure (P) increases (from 0 to 40 GPa), the lattice parameter decreases at a given temperature (from 0 to 700 K). The graph plotted in Fig. 12 illustrates the variation of the compressibility modulus (B) with temperature at the considered pressure. It appears that, (from 0 to 150 K), the compressibility modulus is almost constant, while at high temperatures ($T > 150$ K), a linear decrease is observed with increasing temperature. At a given pressure, the compressibility increases with temperature, and at a given temperature, it increases as the pressure decreases. At the temperature

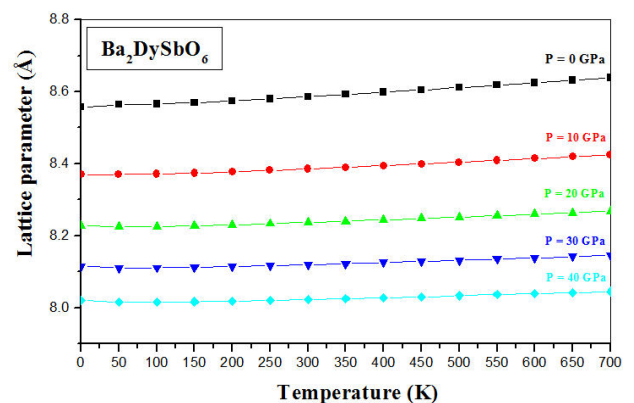


FIGURE 11. The variation of lattice parameter as a function of temperature of $\text{Ba}_2\text{DySbO}_6$: at different pressures.

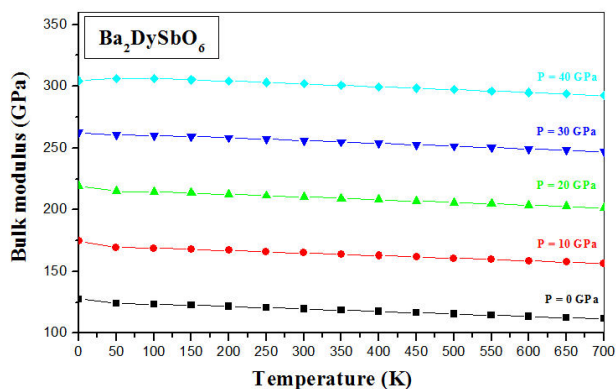


FIGURE 12. The variation of bulk modulus B as a function of temperature for $\text{Ba}_2\text{DySbO}_6$: at different pressures.

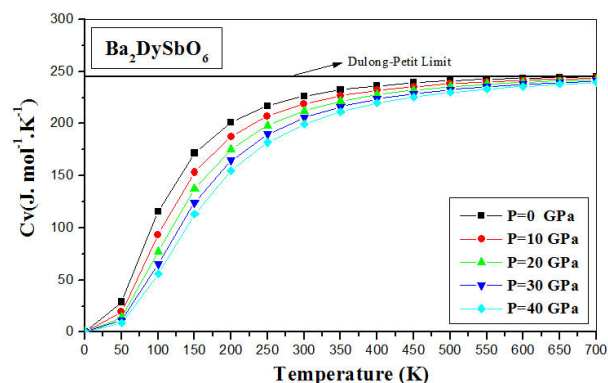


FIGURE 13. The variation of heat capacity C_v as a function of temperature for $\text{Ba}_2\text{DySbO}_6$: at different pressures.

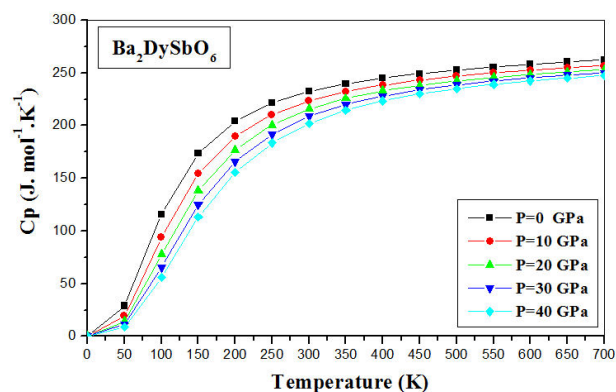


FIGURE 14. The variation of heat capacity C_p as a function of temperature for $\text{Ba}_2\text{DySbO}_6$: at different pressures.

$T = 0$ K and $P = 0$ GPa, the modulus $B = 127,6789$ GPa. At elevated temperatures, the specific heat (or heat capacity at constant volume C_v) changes only slightly with temperature and approaches the Dulong-Petit limit [11, 14, 26], which all solids attain at high temperature in the limit. The variation of the heat capacity C_v as a function of temperature at pressures ranging from 0–40 GPa is shown in Fig. 13. We then obser-

ve that for $T < 300$ K, the heat capacity C_v increases rapidly with temperature. At higher temperatures ($T > 300$ K), C_v

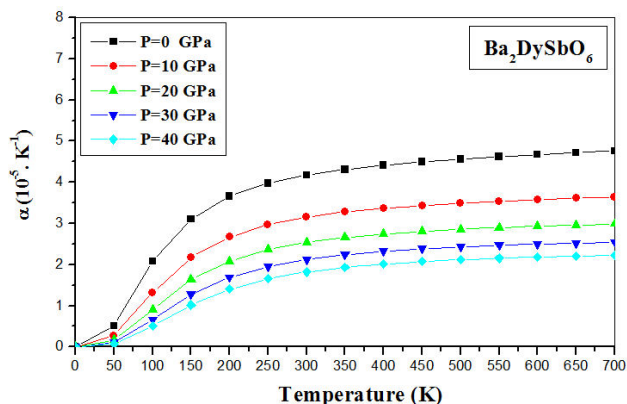


FIGURE 15. The variation of thermal expansion coefficient α as a function of temperature for $\text{Ba}_2\text{DySbO}_6$: at different pressures.

approaches the Dulong-Petit limit, as is common for most solid materials at high temperatures. At high temperature, it reaches a value of $245,2951 \text{ J mol}^{-1} \text{ K}^{-1}$. Figure 14 shows how C_p varies with temperature under different pressures for the double perovskite based on $\text{Ba}_2\text{DySbO}_6$. The variation of C_p with temperature is comparable to that of C_v at low temperatures; at high temperatures, C_p is different from C_v which becomes constant. The effect of pressure on the heat capacity at constant pressure C_p is substantially identical to that of C_v . Figure 15 illustrates the effect of temperature on the thermal expansion coefficient (α), which increases with temperature. At a given pressure, the thermal coefficient (α) increases quite significantly with temperature up to 300 K, beyond which α becomes progressively more linear with temperature. At $P = 0$ GPa and $T = 300$ K, the thermal expansion coefficient α is found to be $4,17409 \times 10^{-5} \text{ K}^{-1}$. Entropy (S) could be defined as a measure of the disorder of a system at the microscopic level. When the entropy of the system decreases, its constituents become more ordered, bound, and capable of producing mechanical effects. The increase in temperature can easily be translated into an increase in disorder as measured by entropy, as evidenced by the increase in possible positions of the molecules. Figure 16 shows the variation of entropy (S) as a function of temperature and pressure for the double perovskite $\text{Ba}_2\text{DySbO}_6$.

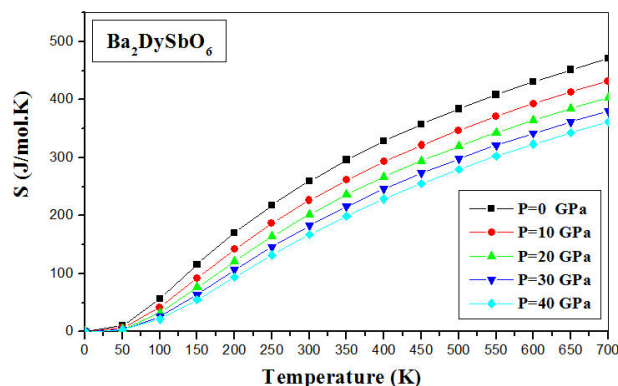


FIGURE 16. The variation of entropy as a function of temperature for Ba₂DySbO₆: at different pressures.

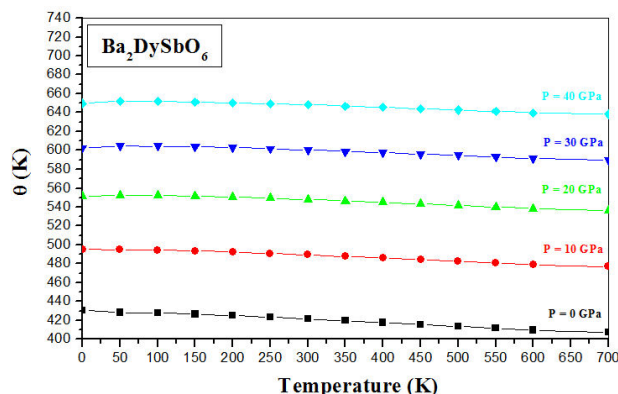


FIGURE 17. The variation of Debye temperature as a function of temperature for Ba₂DySbO₆: at different pressures.

For a given pressure, it is observed that the entropy (S) has a strong temperature dependence (which increases very rapidly with increasing temperature), but conversely, the entropy (S) decreases at a given temperature with increasing pressure. Heating favors the vibrational contribution to entropy, therefore, the entropy (S) increases with temperature. In Fig. 17, the Debye temperatures θ^D are represented as a function of temperature for several pressure values. It appears that θ^D remains constant from 0–40 K, then decreases linearly with increasing temperature. At a fixed temperature, the Debye temperature increases with the rise in pressure. By superimposing this curve with Fig. 12, related to the compressibility modulus, we note that θ^D and (B) follow the same evolution. Due to the type of approximation chosen, there is a non-negligible difference between the Debye temperatures θ^D obtained by the elastic method ($\theta^D = 195,2865$ K) and the thermodynamic method ($\theta^D = 430,6$ K), at $T = 0$ K and $P = 0$ GPa. Indeed, only low-frequency acoustic modes are taken into account by the elastic approach, thus leading to an underestimation of the Debye temperature; whereas the thermodynamic approach pays attention to the entire photon spectrum by including optical modes, thus providing a higher and therefore more representative estimate of the Debye temperature for the material's behavior. The Debye temperature cannot be considered a unique quantity but only as a function

of the evaluation method adopted.

4. Conclusion

In the present study, we used an ab initio method based on the full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT). The method focused on the structural, elastic, electronic, magnetic, and thermodynamic properties of the Ba₂DySbO₆ compound in its GGA-PBE version. After studying the magnetic stability, we found that the ferromagnetic state is the most stable configuration, because it is associated with the phase that has the lowest total energy. The results of the present study are in good agreement with the experimental and theoretical data found in the literature. The elastic constants obtained meet the stability conditions; the calculated value of the factor (A) indicates that Ba₂DySbO₆ is an anisotropic material. In our case, the Poisson's ratio value of 0.28 means that the intra-atomic ionic bonding contribution would be higher for this compound. From our results, the material displays semi-metallic characteristics with a direct ($\Gamma - \Gamma$) gap in the spin-up channel while the spin-down channel remains metallic. Thus, spin polarization is quite evident at the Fermi level in both channels, making it a unique property for spintronic applications. Consequently, Ba₂DySbO₆ may be a suitable candidate for spintronic devices such as spin filters, spin injectors, and magnetic tunnel junctions in which the performance is determined by a spin-dependent transport property. The compound Ba₂DySbO₆ demonstrates in the partial density of states (PDOS) calculated with (GGA-PBE) that the valence band, below the Fermi level, is strongly dominated by Ba-p (up and down) and Dy-f (up) states, while around the Fermi level, the states are dominated by Dy-f (down). Above the Fermi level, the PDOS in the conduction band is weakly dominated by Sb-s and Sb-p (up-down) states. Regarding the magnetic properties of the compound Ba₂DySbO₆, we have shown that the total magnetic moment is primarily due to the magnetic moment of the lanthanide atom Dy. The results of the density of states and band structure show that the compound has a semi-metallic character and is a good candidate for spintronic applications. According to the calculations of optical properties, this material exhibits high sensitivity in the energy region between visible light and extreme ultraviolet (UV). Materials with broad peaks in the UV range are used in various fields such as disinfection, spectroscopy, and printing. Finally, the thermodynamic parameters such as the heat capacity at constant volume (C_V), the heat capacity (C_p) at constant pressure, the thermal expansion coefficient (α), the Debye temperature (θ^D), and the entropy (S) of our product Ba₂DySbO₆ were determined and discussed. Next, the effect of pressure on the lattice parameter and the compressibility modulus (B) was also studied. All things considered, the thermodynamic properties of our Ba₂DySbO₆ material are good and efficient.

Declarations conflict of interest

The authors declare no competing financial interest.

Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Long-term reliability analysis of bipolar stress in SiC power MOSFETs

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This paper examines the reliability of SiC DMOS power transistors in a DC-DC boost converter circuit. This reliability analysis focuses on the impact of bias temperature instabilities (BTI) on the electrical performance of the transistor, taking into account the variation of one of the most critical parameters of a SiC power MOSFET: the on-resistance (R_{on}). The study presented in this work also provides an insight into the importance of using an accurate physical reliability model to estimate the transistor's real threshold voltage drift for a long operating time. We demonstrate that SiC DMOS technology exhibits a higher threshold voltage (V_{th}) and R_{on} stability when operated in a bipolar mode. As a result, data derived from measure-stress-measure (MSM) sequences are used to calibrate the defect parameters of a two-state non-radiative multi-phonon model (NMP) that captures the charge trapping kinetics of oxide and interface defects in a reliability simulation framework, Comphy. The analysis shows that an extrapolation of device deterioration at operating conditions settings reduces bias temperature instabilities (BTI), leading to a minimal on-state loss degradation.

Keywords: Reliability; charge trapping; bias temperature instabilities; on-resistance.

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1. Introduction

Power converter circuits are widely used in many applications where their continuous operation is required. However, these converters are continuously under stressful conditions like overvoltage, overcurrent, high temperature, and harsh environments, which leads to an unavoidable degradation of the components of the circuit, causing, in some cases, irreversible damage. In real operating conditions, power devices are frequently subjected to coupled thermo-mechanical and electrical stresses, such as those induced by power cycling, which can simultaneously affect both chip-level and package-level reliability. These conditions have been shown to induce progressive degradation in key parameters such as threshold voltage, on-state resistance, and switching performance, ultimately impacting device lifetime and system reliability [1].

Under high switching speeds and voltage slew rates, additional dynamic stress mechanisms may arise, further challenging device reliability [2]. In addition to long-term aging mechanisms, recent studies have shown that extreme operating conditions such as short-circuit events and high electrical stress can significantly accelerate degradation processes and trigger failure mechanisms such as gate oxide breakdown and thermal runaway, severely impacting device reliability [3].

In this sense, power semiconductor switches are well known to be the most affected and, hence, the main cause for the system failure [4, 5]. Some reports and studies indicate that almost a third of the total failure is due to the aging phenomena of semiconductor switches, which are generally MOSFET transistors [6]. With the integration of wide-bandgap materials, such as SiC, it has been possible to design more efficient power electronics systems. This mate-

rial exhibits notable advantages in terms of electrical breakdown field, thermal conductivity, and high electron mobility [7], which result in lower on-resistance (R_{on}) values than conventional silicon technology.

However, it is well known that the bias temperature instabilities (BTI) degradation phenomena for SiC MOSFETs may lead to thermal stress of the device, a decrease in efficiency, electrical stress at the gate area, an increase of the transistor leakage current due to breakdown, as well as an increase of the R_{on} and other undesirable effects [8–13]. Recent works have highlighted that extreme electric field stress can activate additional degradation pathways, such as hole injection and trap generation in the gate oxide, which significantly accelerate threshold voltage instability [14].

One crucial aspect to be considered for the SiC power MOSFETs, precisely, is the threshold voltage drift (ΔV_{th}) under long-term operation. The BTI impact caused by continuous bias at the gate has been well studied [15–20]. However, recent studies have shown that the degradation behavior of SiC MOSFETs strongly depends on the device structure, particularly in trench gate configurations, where electric field crowding and oxide/interface quality can lead to significantly different reliability characteristics compared to planar devices. In particular, distinct threshold voltage instability mechanisms, including electron and hole trapping, have been reported to vary with gate architecture, bias polarity, and temperature [21]. At the physical level, this degradation is mainly attributed to charge trapping and detrapping processes associated with defects at the SiC/SiO₂ interface and within the gate oxide, which govern the threshold voltage shift under both DC and AC stress conditions [22].

The different properties of the semiconductor-dielectric interface and the nature of the wide-bandgap material silicon carbide (SiC) compared to its silicon counterpart cause some peculiar characteristics in the V_{th} variation and BTI. On the other hand, while these SiC properties are suitable for circuit applications, the degradation of SiC MOSFETs under several operating conditions, including switching frequency, needs to be fully understood, especially under dynamic operating conditions where recent studies have reported complex interactions between gate bias, temperature, and switching cycles affecting threshold voltage stability [23]. In particular, recent studies have highlighted that conventional static stress tests are not sufficient to capture the complex degradation mechanisms occurring under dynamic high dV/dt conditions, where electric field enhancement and gate oxide stress can significantly impact device reliability [2]. It could be beneficial to determine the useful lifetime of commercially introduced and available devices [24].

Another significant advantage of the commercially SiC power transistors is the switching-speed performance (speed between on and off states), where a R_{on} as low as possible is required [25]. However, R_{on} is significantly influenced by the driving voltage, *i.e.*, the gate voltage. Therefore, to know how the R_{on} behaves under the instabilities introduced by the gate voltage stress, the reliability study of power MOSFETs based on SiC gains more critical importance.

The threshold voltage of SiC power MOSFETs, besides the drift caused by static stress, may undergo an additional shift triggered by switching events (turn-On and turn-Off of the transistor). Under more extreme operating conditions, such as high-amplitude gate voltage transients or electrostatic discharge-like events, the degradation can be further accelerated due to strong electric field effects in the gate oxide. Recent studies have shown that hole trapping and field-assisted charge injection dominate the threshold voltage instability under such ultra-high gate stress conditions, leading

to significant V_{th} shifts and oxide degradation [14]. It is only possible to identify this other component in long-term switching tests. Recent studies have shown that under dynamic gate stress conditions, this threshold voltage drift can be significantly enhanced and is strongly dependent on operating conditions such as temperature and gate bias, directly impacting on-resistance and long-term device reliability [22]. The effect is related to gate-oxide trap dynamics [12, 26]. The increase of V_{th} causes a slight rise in R_{on} , which translates into increased on-state losses over time. For this reason, to account for a very accurate physical trapping model to predict the V_{th} drift behavior over time, it is essential to consider defect-dependent charge trapping mechanisms at the atomic scale, which directly influence the long-term instability of SiC MOSFETs [22], as well as degradation under cyclic electrothermal stress conditions, where the interaction between static and dynamic degradation mechanisms significantly influences long-term device reliability and lifetime prediction [1].

Finally, in this work, we highlight the importance of using a very accurate physical defect model to estimate the threshold voltage drift (ΔV_{th}) over time. We also present the remarkable difference when the transistors work under bipolar V_G operation and unipolar V_G operation in terms of R_{on} variation due to the impact of the BTI degradation mechanism, which is critical for the lifetime projection operation of the devices.

2. Stress pattern definition and physical charge trapping model calibration

SiC DMOSFETs commonly use a bipolar gate drive, where a slightly negative voltage is applied during the off-state. This technique helps suppress long-term changes in both V_{th} and R_{on} , which are typically affected by BTI.

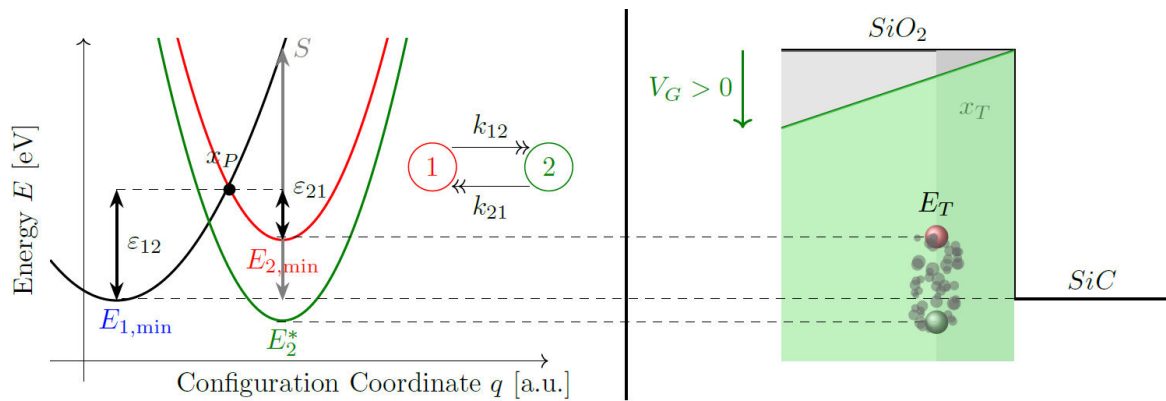


FIGURE 1. Configuration coordinate diagram illustrating the two-state non-radiative multi-phonon (NMP) model for oxide defects. The potential energy surfaces $E_1(q)$ and $E_2(q)$ represent the defect in two different charge states as a function of the configuration coordinate q . Transitions between states, governed by phonon-assisted capture and emission rates k_{ij} , depend on the energy barriers E_{12} and E_{21} . The diagram includes alignment of defect levels relative to the conduction band edge E_C , valence band edge E_V , and trap level E_T . This model is used within the Comphy simulation framework to evaluate the occupancy dynamics of defects over time, which directly influence the effective threshold voltage shift (ΔV_{th}) observed in BTI-stressed MOSFETs.

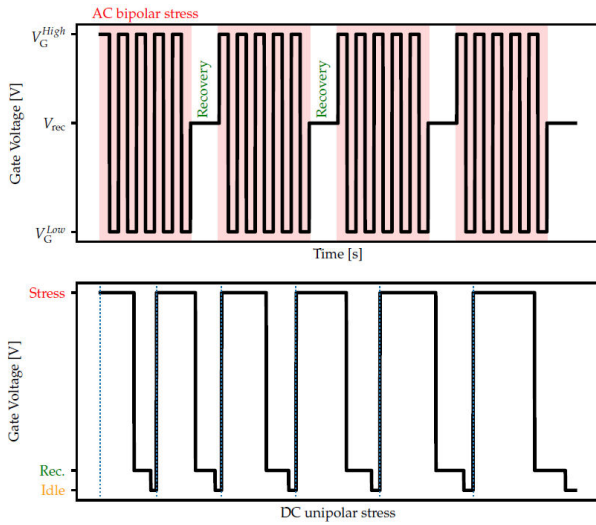


FIGURE 2. AC (top) and extended DC (bottom) MSM stress schemes are used to extract threshold voltage shift (ΔV_{th}) over time. The AC scheme applies pulsed gate stress with recovery, while the DC scheme uses prolonged stress phases to capture long-term degradation behavior in SiC MOSFETs.

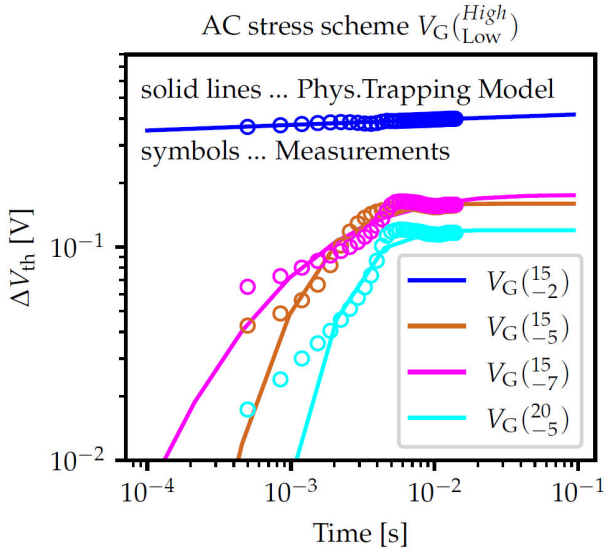


FIGURE 3. Experimental threshold voltage drift values can be reproduced accurately by using the Comphy reliability simulator based on the Physical Charge Trapping Model (NMP) for an AC MSM scheme.

BTI is mainly caused by charge trapping at defects near the interface between the channel and gate oxide. To analyze and predict this behavior, researchers use a non-radiative multi-phonon (NMP), as depicted in Fig. 1, which is based on detailed physical parameters of the materials and defects involved.

To accurately model the charge trapping behavior of oxide and interface defects, we calibrate a two-state non-radiative multi-phonon model within our simulation framework, Comphy [26]. This calibration is based on experimental data derived from measure-stress-measure (MSM)

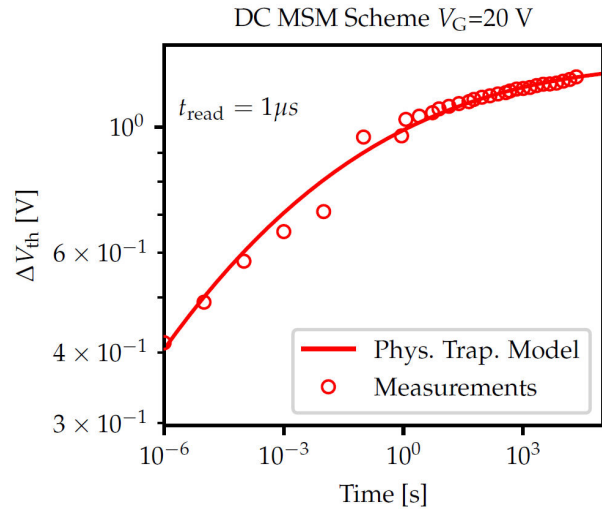


FIGURE 4. Experimental threshold voltage drift values can be reproduced accurately by using the Comphy reliability simulator based on the Physical Charge Trapping Model (NMP) for a DC MSM scheme.

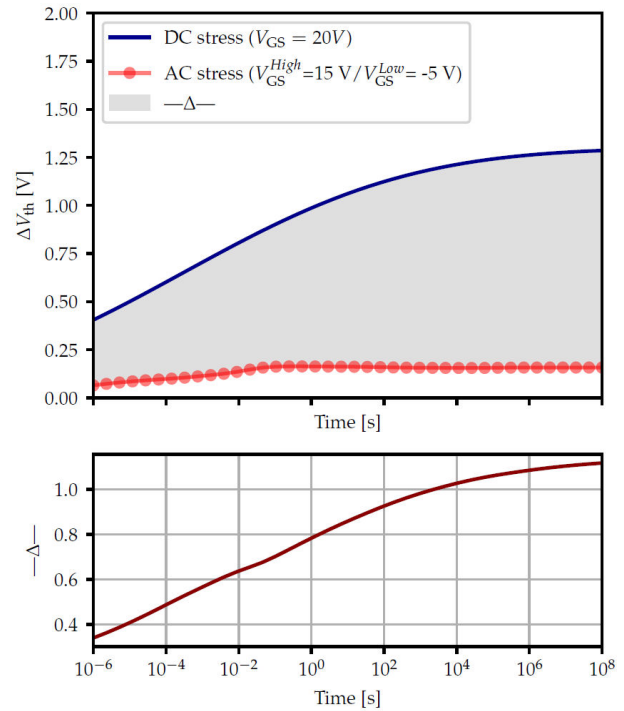


FIGURE 5. Threshold voltage shift (ΔV_{th}) over time under AC and DC stress, extrapolated up to 10 years after calibrating the reliability simulation framework, highlighting stronger degradation from constant high-voltage DC stress compared to pulsed AC stress conditions.

sequences, which provide insights into the underlying defect dynamics. A comprehensive dataset collected from a commercially available SiC DMOSFET, which includes both long-term DC stress and short-term AC MSM (measure-stress-measure) sequences, as shown in Fig. 2, is utilized to extract the characteristics of the underlying defects.

TABLE I. Boost converter circuit parameters.

Parameter	Value
V_{in}	400 V
V_{out}	800 V
f_{sw}	100 kHz
I_{in}	6.18 A
V_{GS}	(PWM) +15/ - 4
C	20.15 μ F
P_{out}	2600 W

The results of both short-term AC V_{th} data for bipolar gate drive and long-term DC V_{th} data for accelerated V_G at $T = 300$ K stress situations and standard operating circumstances are displayed in Figs. 3 and 4, respectively. As can be seen, the physical charge trapping model (NMP) accurately reproduces the observed behavior of ΔV_{th} for both stress conditions. This allows the calibration of our simulation framework to reproduce the ΔV_{th} behavior for extended operating times, for instance, up to 10 years. Simulation results show that bipolar gate operation significantly improves reliability and reduces degradation, making it possible to maintain stable performance with minimal efficiency loss even over extended lifetimes, such as 10 years, as shown in Fig. 5.

3. Analyzed circuit and reliability analysis strategy through SPICE simulation

Figure 6 shows the schematic representation of the DC-DC boost converter circuit analyzed in this work. The value of a

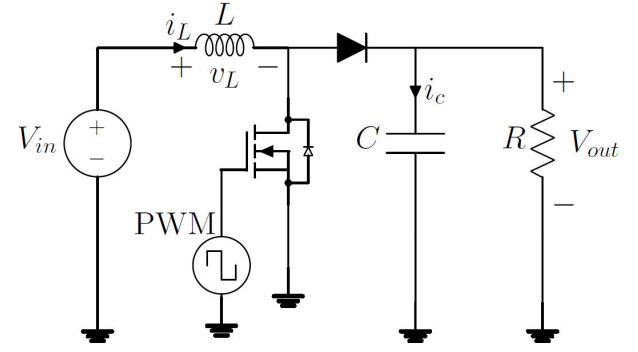
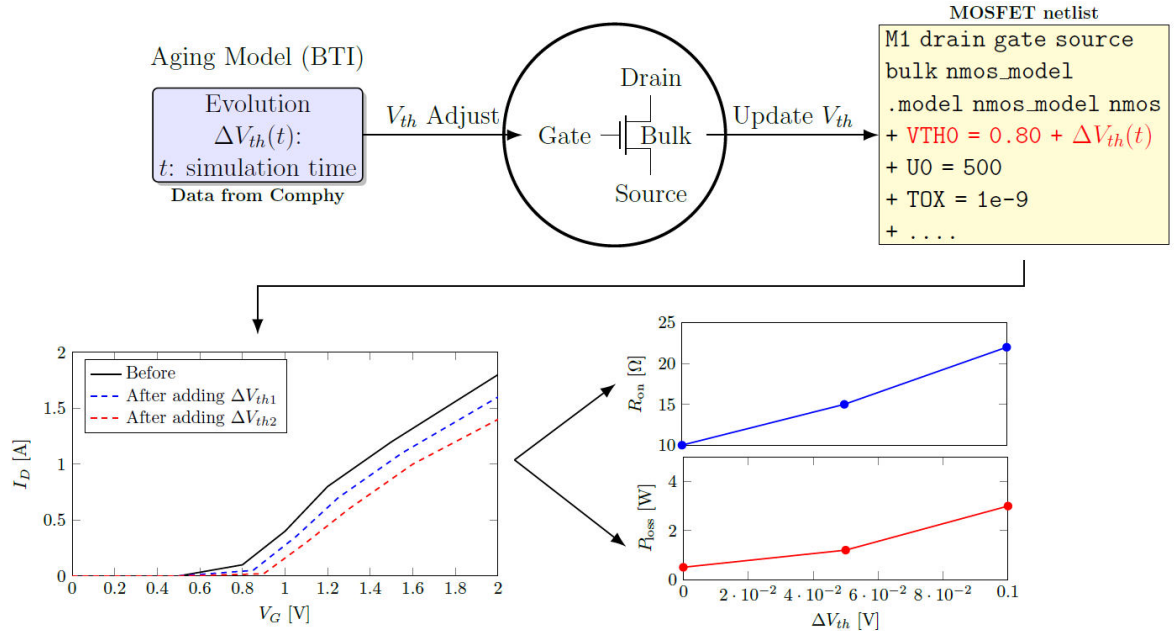


FIGURE 6. Schematic of the boost converter circuit analyzed in this work.

typical operating frequency for SiC devices is 100 kHz, a duty cycle of 0.5, and V_{High} and V_{Low} of 15 V and -4 V, respectively, for the PWM pulse applied to the gate of transistors.

In this study, we used a commercially available SiC power MOSFET produced by Wolfspeed. To improve the accuracy of our analysis, we utilized the manufacturer-provided SPICE model. For engineers developing silicon carbide (SiC) power systems, Wolfspeed's SPICE models offer significant advantages, particularly in achieving accurate simulations and optimizing overall system performance. These models account for critical parasitic components—such as capacitances and inductances—that are vital for the behavior of high-speed SiC devices. Including these effects in simulations leads to results that more closely reflect real-world performance. The results from the simulation analysis were obtained considering the circuit performance parameters shown in Table I.

FIGURE 7. SPICE simulation of MOSFET aging using a BTI-induced threshold voltage shift model ($\Delta V_{th}(t)$), integrated into the device netlist. The figure illustrates transfer characteristics, on-resistance (R_{on}), and power loss evolution as ΔV_{th} is updated over time.

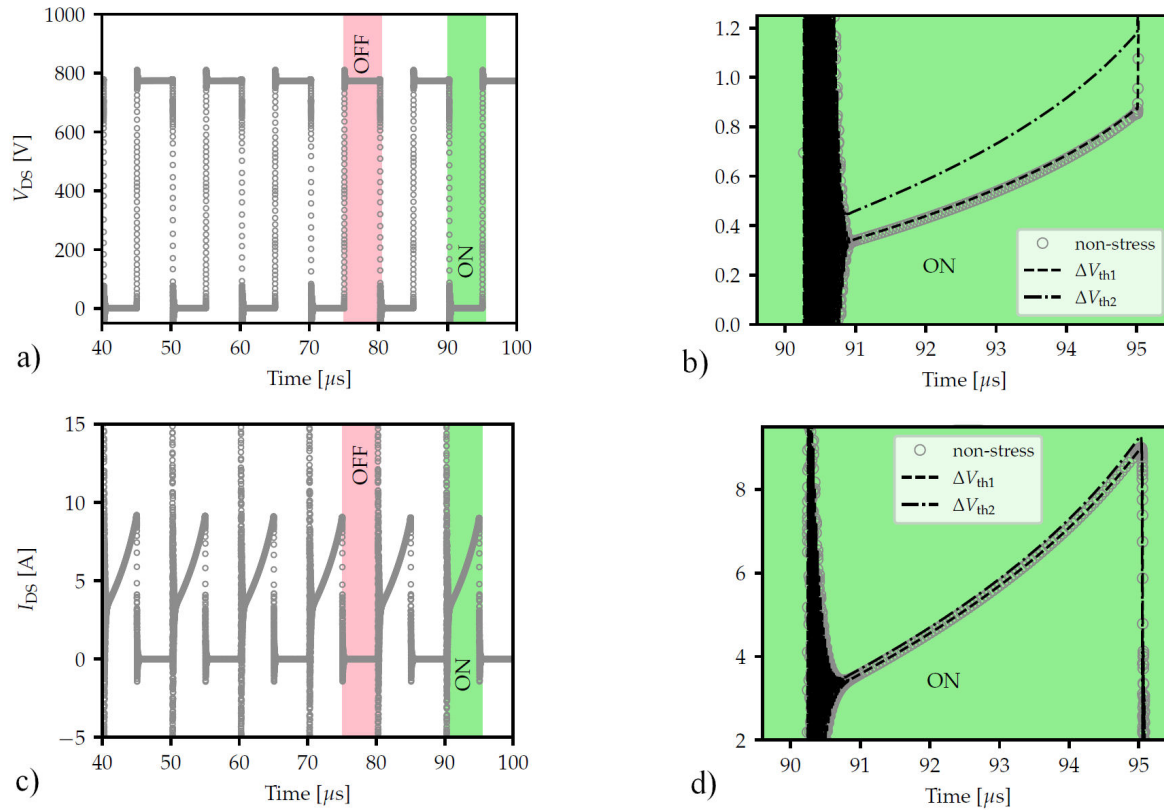


FIGURE 8. a) Drain-to-source voltage (V_{DS}) and c) drain current (I_{DS}) waveforms during switching events of boost converter circuit performance, illustrating ON and OFF states. b) Zoomed-in view highlighting the increase of R_{on} due to the rise of the V_{DS} minimum value when it drops during the ON state affected by the threshold voltage shift ΔV_{th} . d) ΔV_{th} has negligible impact on I_{DS} .

To represent the BTI impact on the transistor behavior, an equivalent modification is done to the netlist of the transistor model. It was considered adding an independent constant voltage source connected in series to the internal gate of the MOSFET to take into account the degradation of the device due to the known aging mechanisms, which means the drift of the threshold voltage (ΔV_{th}) [27,28], as shown in the diagram from Fig. 7.

Figure 8 shows the drain-to-source voltage (V_{DS}) and drain-to-source current (I_{DS}) during boost converter circuit performance. The extracted signals correspond to non-degraded operation conditions, *i.e.*, $\Delta V_{th} = 0$, and consider degradation due to BTI impact for two different ΔV_{th} values. As can be seen, BTI has a negligible impact on I_{DS} . During on-state operating time, V_{DS} drops to a value close to zero due to an increase in the on-resistance caused by the threshold voltage drift (ΔV_{th}).

The increase in V_{DS} during the on-state suggests a progressive rise in R_{on} , which can be linked to degradation of the channel region due to charge trapping at the SiC/SiO₂ interface. This trapping modifies the inversion layer formation and reduces effective carrier mobility, thereby increasing the conduction resistance. Furthermore, additional contributions from contact resistance and package parasitics cannot be neglected under prolonged stress conditions.

On the other hand, the oscillations observed in the switching waveforms are primarily caused by the interaction between parasitic inductances in the circuit loop and the intrinsic capacitances of the device, forming an underdamped LC network. During fast switching transitions, this results in ringing phenomena in both voltage and current waveforms. The effect is further amplified by the high dv/dt and di/dt characteristics of SiC MOSFETs, as well as the presence of packaging parasitics such as bond wire inductance. Therefore, these oscillations are mainly attributed to circuit-level parasitic effects rather than intrinsic device degradation mechanisms.

Using the well-known Ohm's law, the value R_{on} can be extracted as follows:

$$R_{on} = \frac{V_{DS-on}}{I_{DS-on}}. \quad (1)$$

3.1. Impact of BTI on device and circuit parameters

In Fig. 9a), the computed parameter R_{on} extrapolation is presented for each ΔV_{th} value over 10 years of operating time when both bipolar gate-drive and unipolar gate-drive operations are considered. Each ΔV_{th} value contains singular degradation information at a specific time value during circuit performance.

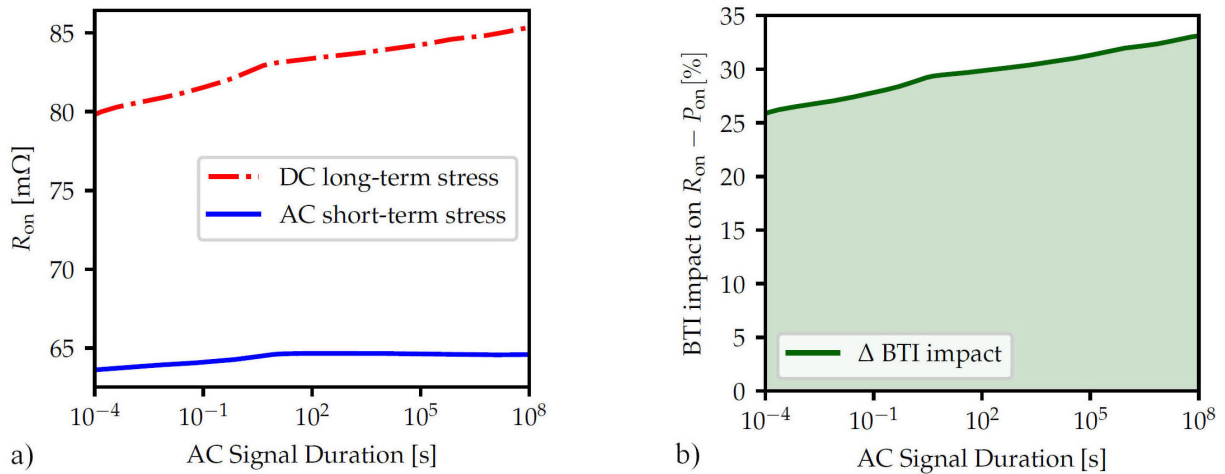


FIGURE 9. According to the extracted values of ΔR_{on} a) for each ΔV_{th} from our calibrated framework, static on-state losses after 10 years can be reduced around 30 % when bipolar AC gate-drive operation is considered b).

It is noteworthy that, after a decade, the ΔR_{on} shows an increase of around 30 % in on-state loss for unipolar gate-drive operation (long-term stress scheme) in comparison to bipolar AC mode (short-term stress scheme) at a duty cycle of $d = 0.5$, Fig. 9b). The higher gate stress in unipolar drive accelerates BTI degradation, leading to more pronounced shifts in device behavior. This degradation is particularly critical in high-frequency or high-load scenarios, where elevated R_{on} has a larger impact on converter performance. These findings highlight the importance of considering BTI effects during the design phase and suggest that gate-drive strategies should be carefully chosen to balance performance and long-term reliability.

4. Conclusions

In conclusion, our calibrated simulations estimate a 30 % reduction in on-state loss at bipolar (AC) V_G operation over unipolar (DC) V_G gate-drive signals. According to these findings, BTI-induced degradation has only a minor impact to power conversion efficiency under the suggested operating circumstances. However, special attention has to be paid during the design phase for gate-driving strategies to mitigate BTI impact, especially in long-lifetime applications like automotive or industrial power converters.

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