

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 in-

terval (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

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

(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:

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

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

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

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:

$$\hat{N} = e^{i\mu} \begin{bmatrix} m_0 - im_3 & -im_1 \\ -im_1 & m_0 + im_3 \end{bmatrix}, \quad (23)$$

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:

$$\begin{bmatrix} \phi_1(b, t) \\ \phi_2(b, t) \end{bmatrix} = \hat{V} \begin{bmatrix} \phi_1(a, t) \\ \phi_2(a, t) \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} \phi'_1(b, t) \\ \phi'_2(b, t) \end{bmatrix} = \hat{V} \begin{bmatrix} \phi'_1(a, t) \\ \phi'_2(a, t) \end{bmatrix}, \quad (25)$$

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 equating 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

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

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:

$$\begin{aligned} (\hat{\Pi} \Phi)(b, t) &= \hat{V} (\hat{\Pi} \Phi)(a, t) \quad \text{and} \\ (\hat{\Pi} \Phi)'(b, t) &= \hat{V} (\hat{\Pi} \Phi)'(a, t), \end{aligned} \quad (36)$$

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:

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

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. (B10) and (B13) 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. (B17) and (B18) 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, $j^0 = c\varrho$ 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, $\hat{E}\varrho - \hat{p}j = 0$ (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 $K^0_0 = \varrho_{\text{en}}$ 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, $\hat{E}\varrho_{\text{en}} - \hat{p}j_{\text{en}} = 0$, 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

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

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

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

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:

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

($m_0 = +1$). 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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