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Approximate solutions and the thermodynamic properties of a potential model

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The solution of the radial Schrödinger equation for a Pöschl-Teller type of potential with two main parameters is obtained via the supersymmetric approach. The energy equation and its corresponding wave function are obtained explicitly. The energy equation obtained was used to calculate the partition function via the Poisson summation formula. The calculated partition was used to studied the enthalpy, Gibbs free energy and entropy of the system. The result obtained showed that the two parameters have the same effect on the energy of the system but different effects on the thermodynamic properties. It was also shown that the rise in temperature of the system only increases enthalpy but decreases partition function, Gibbs free energy an entropy.

Keywords: Bound state; thermal property; enthalpy; Gibbs free energy; entropy.

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1. Introduction

The introduction of thermodynamic properties can be traced back as early as 18th century when the concept of heat was conceived. This also led to the development of heat engines via the caloric theory that analyzes the efficiency of the steam engines. This proposition gave birth to the formulation of the second law of thermodynamics. In the middle of the 18th century, the concept of energy conservation arose leading to the development of the first law of thermodynamics. An increase in knowledge brought about the concept of entropy as a measure of the disorderliness in a system by Clausius. This formalized the second law of thermodynamic governing the entropy of an isolated system. For diverse applications and usefulness, the macroscopic properties of the thermodynamic systems were linked to the microscopic behaviour of particles via statistical mechanics. The development of the concept of free energy and chemical potential leads to the understanding of chemical reactions and phase transitions in thermodynamic systems [1-7]. Thermodynamic properties are fundamental characteristics of different physical systems that analyze the transformation of energy as well as the states of matter under various conditions. These properties play a crucial role in the responsiveness of systems to changes in the foundation of thermodynamics. There is a connection between energy levels and thermodynamic properties which is a foundational concept in statistical mechanics, where the behaviour of systems at the quantum level is linked to the macroscopic thermodynamic properties. This connection allows the derivation of properties such as temperature, entropy, specific heat, Gibbs free energy, and enthalpy from the distribution of energy levels of particles via the partition function. These energy levels are obtained from the solutions of the Schrödinger equation with different potential models. One such potential model is the Pöschl-Teller potential. The Pöschl-Teller potential is an important model in quantum mechanics that is widely used in both quantum mechanics and mathematical physics as a result of its exact solvability and numerous applications in atomic and molecular physics making it a valuable tool for theoretical studies. It provides insight into phenomena like tunneling, bound states, and scattering, maintaining its relevance in both theoretical research and practical applications. There are different forms of Pöschl-Teller potential models reported by different authors. The different form of the Pöschl-Teller potential reported include the generalized Pöschl-Teller potential [8-10], the second Pöschl-Teller potential [11-16], improved Pöschl-Teller potential [17-19], modified Pöschl-Teller potential [20-22], new Pöschl-Teller potential [23], trigonometric Pöschl-Teller potential model [24, 25] and other forms of Pöschl-Teller potential such as that reported by Agboola [26-28]. Motivated by the interest in thermodynamic properties and the usefulness of the Pöschl-Teller potential, this research wants to study the thermodynamic properties under another form of Pöschl-Teller potential. The form of Pöschl-Teller potential to be studied in the work is given as

$$V(r) = -\frac{4V_0 e^{-2\alpha r}}{(1+e^{-2\alpha r})^2}, \tag{1}$$

where V_0 is the potential depth. To the best of our understanding, the form of Pöschl-Teller potential model above has not been widely reported in the literature except in Ref. [29]. The solutions of the potential with the Schrödinger equation is possible with different traditional methods. For the purpose of this study, the authors decided to adopt the supersymmetric approach for the energy levels. The reason for the choice of the method is due to the familiarity of the method by the authors.

2. Energy level and the Pöschl-Teller potential

The energy levels of the Pöschl-Teller potential is obtained by first considered the radial Schrödinger equation of the form

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} - E_n + V(r)\right] R_n(r) = 0, \tag{2}$$

where E_n is the nonrelativistic energy, $V(r)$ is the radial potential, $\hbar$ is the reduced Planck's constant, μ is the reduced mass of the particle, n is the quantum number and $R_n(r)$ is the wave function. Substituting Eq. (1) into Eq. (2) gives

$$\frac{d^2R_n(r)}{dr^2} = -\frac{2\mu E_n}{\hbar^2} - \frac{\frac{8\mu V_0 e^{-2\alpha r}}{\hbar}}{(1+e^{-2\alpha r})^2}. \tag{3}$$

Following the supersymmetric approach, the ground state wave function $R_0(r)$ is written in the form [30-34]

$$R_0(r) = \exp\left(-\int W(r)dr\right), \tag{4}$$

where is the superpotential in supersymmetry quantum mechanics. Substituting Eq. (4) into Eq. (3) leads to Riccati equation of the form

$$W^2(r) - W'(r) = -\frac{\frac{8\mu V_0 e^{-2\alpha r}}{\hbar}}{(1+e^{-2\alpha r})^2} - E_0. \tag{5}$$

To begin the deduction of the energy levels of the system, the solution of the Riccati equation given in Eq. (5) must be known. The solution is only given by the superpotential function. Following the interacting potential in Eq. (1) and the Riccati equation in Eq. (5), we propose a superpotential of the form

$$W(r) = \lambda_0 - \frac{\lambda_1 e^{-2\alpha r}}{1+e^{-2\alpha r}}. \tag{6}$$

The parameters λ_0 and λ_1 are superpotential constants whose values are determined by considering Eq. (5) when the property of the left-hand side equals the property of the right-hand side. Substituting Eq. (6) into Eq. (5) and with some mathematical simplifications, the two constants in Eq. (6) can be obtain as

$$\lambda_0^2 = -\frac{2\mu E_n}{\hbar^2}, \tag{7}$$

$$\lambda_1 = \alpha\left(-1 \pm \sqrt{1+\frac{8\mu V_0}{\alpha^2\hbar^2}}\right), \tag{8}$$

$$\lambda_0 = \lambda_1. \tag{9}$$

To determine the correct value of Eq. (8), we construct the family potentials using Eq. (6).

$$V_+(r) = W^2(r) + W'(r) = \lambda_0^2 + \frac{\lambda_1(\lambda_1 - 2\lambda_0)e^{-2\alpha r}}{1+e^{-2\alpha r}} + \frac{\lambda_1(\lambda_1 + 2\alpha)e^{-2\alpha r}}{(1+e^{-2\alpha r})^2}, \tag{10}$$

$$V_-(r) = W^2(r) - W'(r) = \lambda_0^2 + \frac{\lambda_1(\lambda_1 - 2\lambda_0)e^{-2\alpha r}}{1+e^{-2\alpha r}} + \frac{\lambda_1(\lambda_1 - 2\alpha)e^{-2\alpha r}}{(1+e^{-2\alpha r})^2}. \tag{11}$$

The family potentials in Eq. (10) and Eq. (11) are shape invariants and thus, satisfied the shape invariance condition. These shape invariant potentials are related by a simple formula

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1). \tag{12}$$

Via mapping of the form $a_1 = f(a_0) = a_0 - 2\alpha$ where a_0 is an old set of parameters and a_1 is a new set of parameters uniquely determined from the old set of parameters a_0 as $a_0 \rightarrow \lambda_1$. The term is a residual term and is independent of the variable r. This established a recurrence relation of the form $a_1 = \lambda_0 - 2\alpha$, $a_2 = \lambda_0 - 2(2\alpha)$, $a_3 = \lambda_0 - 3(2\alpha)$, and subsequently $a_n = \lambda_0 - 2n\alpha$ Considering the residual term, Eq. (12) can be written in a generalized form following

$$R(a_1) = a_0 - a_1, \tag{13}$$

$$R(a_2) = a_1 - a_2, \tag{14}$$

$$R(a_3) = a_2 - a_3, \tag{15}$$

$$R(a_4) = a_3 - a_4, \tag{16}$$

$$R(a_n) = a_{n-1} - a_n. \tag{17}$$

Following the formalism of the shape invariance and supersymmetric techniques, the deduction of the energy levels begins as follows [35-41]

$$E_n = \sum_{K=1}^{n} R(a_K) = R(a_1) + R(a_2) + R(a_3) + R(a_4) + ... + R(a_n). \tag{18}$$

Considering Eq. (7) to Eq. (9) and Eq. (13) to Eq. (17) into Eq. (19), the complete energy levels for the Pöschl-Teller potential in Eq. (1) become

$$E_n = \frac{2\alpha^2\hbar^2}{\mu}\left[n + \frac{1}{2} + \frac{1}{2}\sqrt{1+\frac{8\mu V_0}{\alpha^2\hbar^2}}\right]^2. \tag{19}$$

3. Partition function and the energy levels

The partition function (Z) and energy levels of any system is given by [42-47]

$$Z = \sum_{n=0}^{\eta_{\max}} e^{-\beta E_n}, \tag{20}$$

where β is the inverse of the product of the Boltzmann constant (k_β) and the absolute temperature (T) given as $\beta = (Tk_\beta)^{-1}$. The upper bound of the summation $\eta_{\max}$ is the maximum quantum state obtained from the first derivative of

Eq. (19) equated to zero $(dE_n/dn = 0)$. Thus, the maximum quantum state becomes

$$\eta_{\max} = \frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{8\mu V_0}{\alpha^2\hbar^2}}. \tag{21}$$

Using Poisson summation formula [48] and consider the lowest order approximation, Eq. (20) becomes

$$Z = \sum_{n=0}^{\eta_{max}} f(\eta) = \frac{1}{2}\left(f(0) - f(\eta_{max}+1)\right) + \int_0^{\eta_{max}+1} f(x)dx. \tag{22}$$

Substituting Eq. (19) and Eq. (21) into Eq. (22), we have

$$Z = \frac{1}{2}\left(e^{-\beta\lambda_2^2\eta_{max}^2} - e^{-\beta\lambda_2^2(2\eta_{max}+1)^2}\right) + \int_0^{\eta_{max}+1} e^{-\beta\lambda_2^2(x+\eta_{max})^2}dx, \tag{23}$$

where

$$\lambda_2^2 = \frac{2\alpha^2\hbar^2}{\mu}. \tag{24}$$

Defining $\theta = -\lambda_2\sqrt{2\beta}(x+\eta_{max})$ Eq. (23) turns out to be

$$Z = \frac{1}{2}\left(e^{-\beta\lambda_2^2\eta_{max}^2} - e^{-\beta\lambda_2^2(2\eta_{max}+1)^2}\right) - \frac{1}{\lambda_2\sqrt{\beta}}\int_{-\lambda_3}^{-\lambda_4} e^{\theta^2}d\theta, \tag{25}$$

where

$$\lambda_3 = \lambda_2\eta_{max}\sqrt{\beta}, \lambda_4 = \lambda_2(2\eta_{max}+1)\sqrt{\beta}. \tag{26}$$

Using maple program software, the partition function in Eq. (25) finally becomes

$$Z = \frac{1}{2}\left(e^{-\beta\lambda_2^2\eta_{max}^2} - e^{-\beta\lambda_2^2(2\eta_{max}+1)^2}\right) + \frac{\sqrt{\pi}[erfi(\lambda_3) - erfi(\lambda_4)]}{2\lambda_2\sqrt{\beta}}.$$

4. Thermodynamic properties and the partition function

In this section, the thermodynamic properties such as the enthalpy, the Gibbs free energy and the entropy are calculated from the partition function.

I: Enthalpy. Enthalpy is given by

$$H = RT^2\frac{\partial \ln Z}{\partial T}, \tag{27}$$

substituting Eq. (27) into Eq. (28) gives

$$H = \frac{R}{2}\left(\frac{\lambda_2^2\eta_{\max}^2 e^{-\frac{\lambda_2^2\eta_{\max}^2}{k_\beta T}} - \lambda_2^2(2\eta_{\max}+1)^2 e^{-\frac{\lambda_2^2(\eta_{\max}+1)^2}{k_\beta T}}}{k_\beta} + \frac{\sqrt{\pi}[erfi(\lambda_3) - erfi(\lambda_4)]}{2\lambda_2 k_\beta^{-1/2}T^{-3/2}}\right) \Big/ \frac{1}{2}\left(e^{-\beta\lambda_2^2\eta_{\max}^2} - e^{-\beta\lambda_2^2(2\eta_{\max}+1)^2}\right) + \frac{\sqrt{\pi}[erfi(\lambda_3) - erfi(\lambda_4)]}{2\lambda_2(k_\beta T)^{-1/2}}. \tag{28}$$

II: Gibbs free energy. The Gibbs free energy is calculated using the formula

$$G = -RT\ln Z. \tag{29}$$

Substituting Eq. (27) into Eq. (30) gives the Gibbs free energy as

$$G = -RT\ln\left[\frac{1}{2}\left(e^{-\beta\lambda_2^2\eta_{max}^2} - e^{-\beta\lambda_2^2(2\eta_{max}+1)^2}\right) + \frac{\sqrt{\pi}[erfi(\lambda_3) - erfi(\lambda_4)]}{2\lambda_2(k_\beta T)^{-1/2}}\right]. \tag{30}$$

III: Entropt. The entropy of a system is given by

$$S = -R\ln Z + RT\frac{\partial \ln Z}{\partial T}. \tag{31}$$

Substituting Eq. (27) into Eq. (32) gives

$$S = \frac{H-G}{T}. \tag{32}$$

TABLE I. The partition function and the thermodynamic properties as a function of temperature with $V_0 = 2.5$ and $\alpha = 0.5$.

$T(K)$	$-Z$ (ev/J)	H (J/mol/K)	$-G$ (J/mol/K)	S (J/mol/K)
0	6.032335961	446.3331850	1494.137479	19.40470664
100	8.301923479	435.1419486	1759.647485	21.94789433
200	7.011150201	862.8299386	3238.305940	20.50567938
300	6.645183744	1283.842093	4723.746282	20.02529458
400	6.473305585	1702.494464	6211.179515	19.78418495
500	6.373627867	2120.067646	7699.465830	19.63906695
600	6.308590625	2537.060490	9188.195297	19.54209298
700	6.262821448	2953.706058	10677.18429	19.47270051
800	6.228867189	3370.127529	12166.33836	19.42058236
900	6.202678027	3786.396053	13655.60387	19.37999992
1000	6.181864590	4202.555563	15144.94818	19.34750375
1100	6.164926305	4618.634650	16634.35024	19.32089535
1200	6.150873414	5034.652715	18123.79592	19.29870718
1300	6.139026675	5450.623394	19613.27531	19.27992207
1400	6.128904506	5866.556532	21102.78131	19.26381274
1500	6.120155947	6282.459437	22592.30869	19.24984541

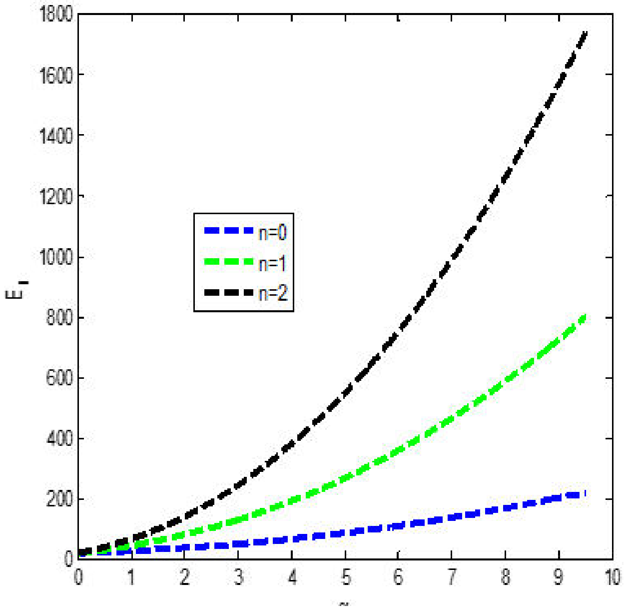

FIGURE 1. Variation of energy against the screening parameter for three quantum states with $\mu = \hbar = 1$ and $V_0 = 5$.

5. Discussion

Figure 1 presents the variation of energy against the screening parameter for various quantum state at constant V_0. At various quantum states studied, the energy of the Pöschl-Teller rises as the screening parameter increases. The higher the quantum state, the higher the energy. The variation of energy as a function of the potential parameter V_0 is shown in Fig. 2.

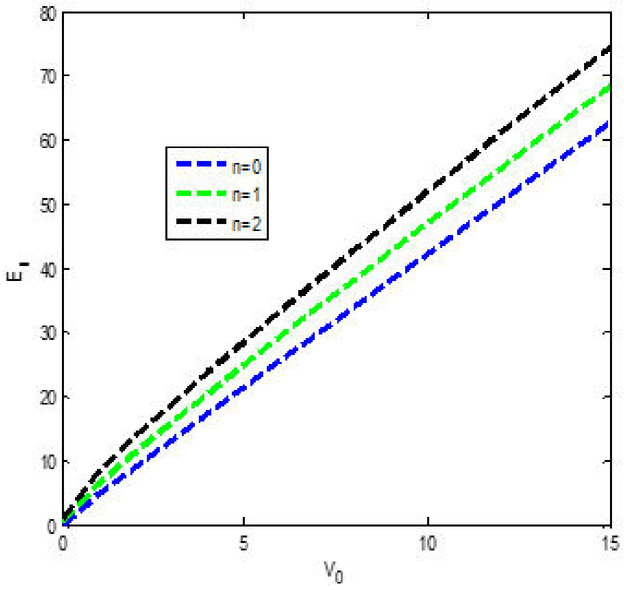

FIGURE 2. Variation of energy against the potential parameter V_0 with $\alpha = 0.25$ for three quantum states.

The rise in energy also correspond to the quantum state. This shows that the higher the quantum state the more the energy. An increase in the potential parameter leads to a significant rise in the energy of the system for the three quantum states. This system as a function of the potential parameter has unbounded energy. In Fig. 3, the variation of energy as a function of the quantum state is presented. The energy of the Pöschl-Teller potential increases monotonically as the quantum state increases gradually. The figure shows that even at the ground state, the energy of the system is not zero. The

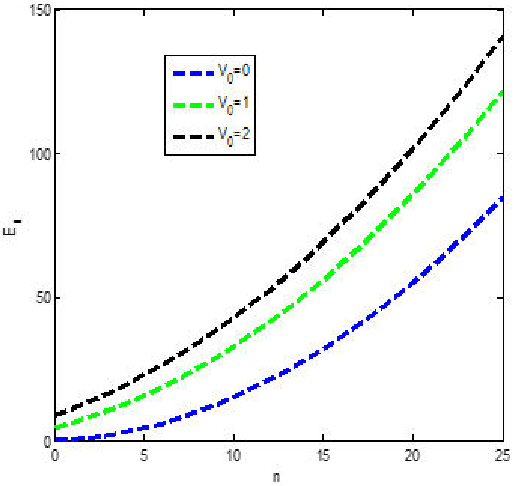

FIGURE 3. Variation of energy as a function of the quantum state with $\alpha = 0.25$ for three values of the potential parameter V_0 .

energy of the system for the various potential parameter diverges as the quantum state increases. The variation of the partition function as a function of the potential parameter V_0 is shown in Fig. 4a) while Fig. 4b) shows the variation of the partition function as a function of the screening parameter α. The partition function decreases monotonically as the potential parameter V_0 increases from zero making the partition function negative. When is V_0 zero, the partition function is also zero, hence, an increase in V_0 leads to a strong negativity of the partition function. However, in Fig. 4b), an increase in the screening parameter α causes a tremendous rise in the partition function. Though the partition function is negative for all values of the screening parameter but, as the screening parameter increases, the less negativity is the parathion function. While the decrease in partition function is gradual at the lower values of V_0, the increase in partition function is gradual at the higher values of the screening parameter. The two Figures showed that the potential parameter V_0 and the

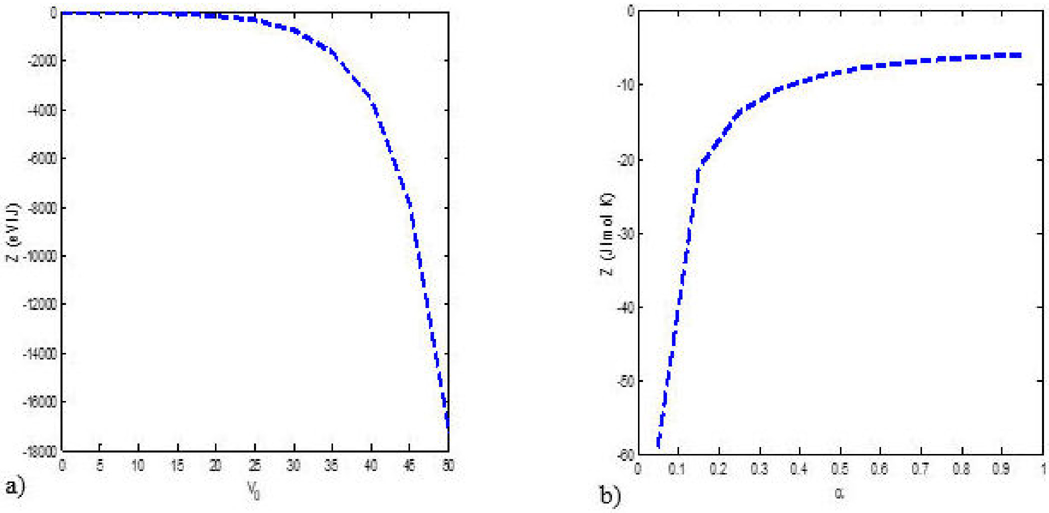

FIGURE 4. a) Variation of partition function against V_0 and b) against α with $\alpha = 0.2$ and $V_0 = 5$.

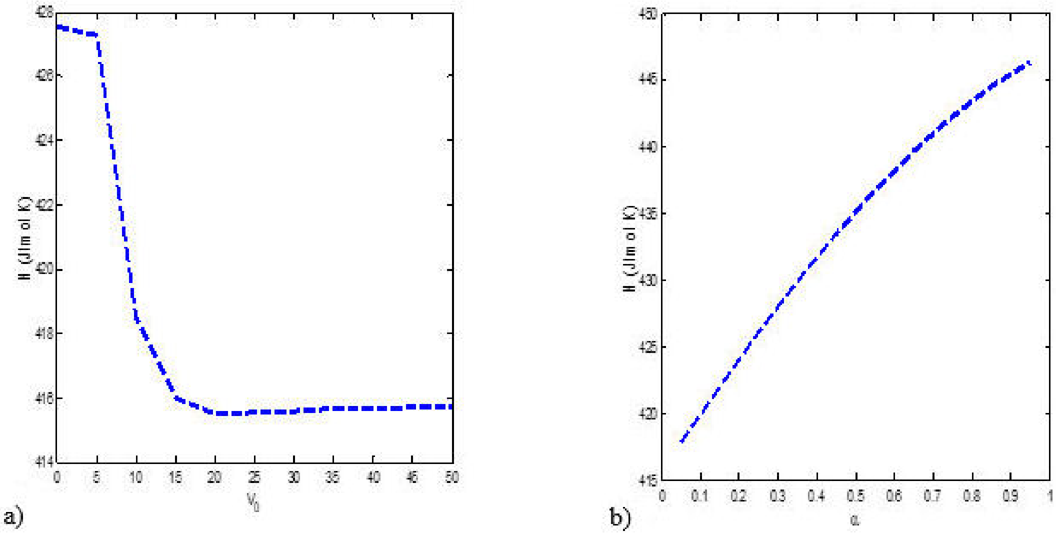

FIGURE 5. a) Variation of the enthalpy as a function of the potential parameter V_0 and b) as a function of the screening parameter.

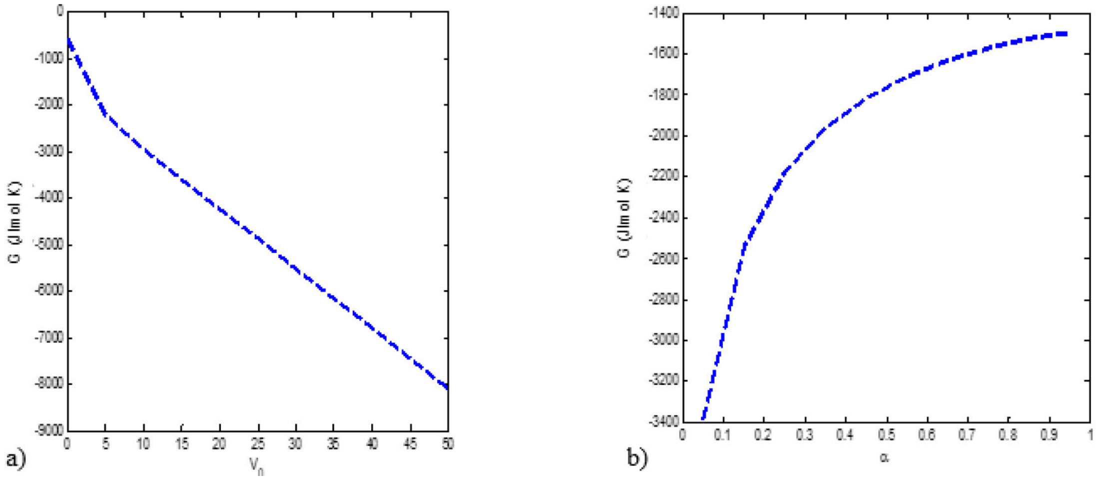

FIGURE 6. Variation of the Gibbs free energy as a function of the potential parameter V_0 and screening parameter α respectively.

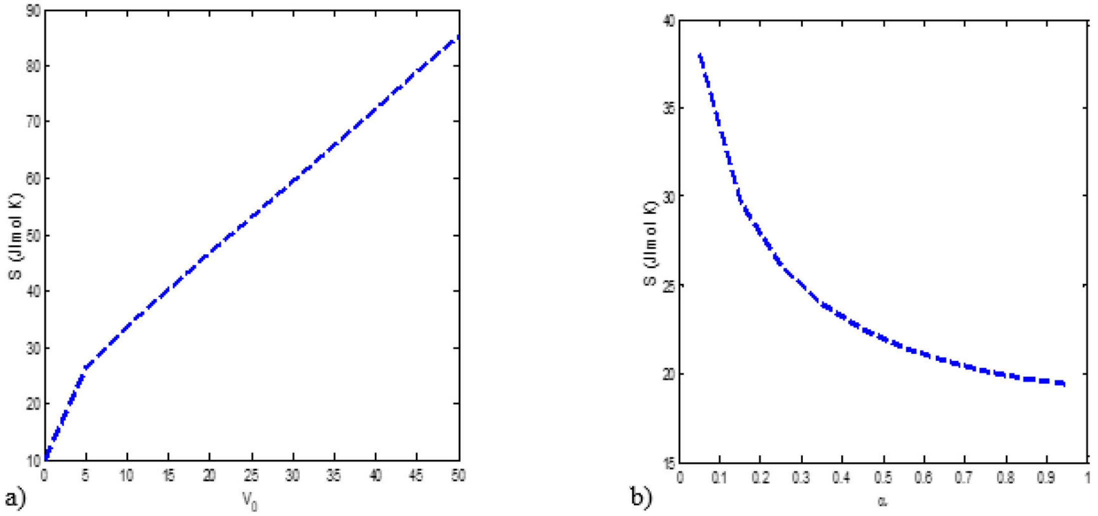

FIGURE 7. Variation of entropy against the potential parameter V_0 and the screening parameter α respectively.

screening parameter α have different opposite effect on the parathion function. The variation of the enthalpy as a function of the potential parameter V_0 is shown in Fig. 5a) while the variation of the enthalpy as a function of the screening parameter is shown in Fig. 5b). The enthalpy as a function of the potential parameter V_0 decreases radically as V_0 increases from 0 to 15. From 15 to 20, there is a gradual decrease in the enthalpy. After 20, the enthalpy seems to be stable as the potential parameter V_0 increases. The decreasing effect on enthalpy is more as V_0 increase from 5 to 20. There is an irregular behavior as the enthalpy decreases which captured the underlying physical phenomena like phase transitions, molecular reconfigurations, or nonlinear interaction responses. However, in Fig. 5b), the enthalpy increases linearly with increase in the screening parameter. In the absence of the screening parameter, there is no enthalpy on like the potential parameter when enthalpy has a significant value for $V_0 = 0$. In both cases, the enthalpy is endothermic. The variation of the Gibbs free energy as a function of the potential parameter V_0 is shown in Fig. 6a) while the variation of the Gibbs free energy as a function of the screening parameter is shown in Fig. 6b). The Gibbs free energy decreases radically as the potential parameter V_0 increases as shown in Fig. 6a). However, in Fig. 6b), the Gibbs free energy rises gargantuanly as the screening parameter increases towards one. It is observed that going above unity, the Gibbs free energy tends to be constant. The variation of the entropy as a function of the potential parameter V_0 is shown in Fig. 7a). The entropy and the potential parameter V_0 vary directly with one another for a constant screening parameter. This means that as the potential parameter increases, the entropy also increases. The entropy for constant screening parameter with increase in the potential parameter V_0 is positive even in the absence of the potential parameter V_0. In Fig. 7b), we presented the variation of the entropy of the Pöschl-Teller potential for various screening parameter at constant potential parameter V_0. The entropy decreases monotonically as the screening parameter increases from zero to one. It is observed that an increase in the potential parameter V_0 decreases the three thermodynamic properties studied while and increase in the screening parameter increases the three thermodynamic properties studied. Table 1 shows the partition function, enthalpy, Gibbs free energy and entropy as a function of temperature. As the temperature of the Pöschl-Teller type of potential in Eq. (1) increase, the partition function reduces, the enthalpy of the system increases, the Gibbs free energy and the entropy respectively, decreases. At every 100K change in temperature, there is a very small change in the partition function and the entropy respectively but a significant change in observed in the enthalpy and Gibbs free energy.

6. Conclusion

The solutions of one-dimensional Schrödinger equation is obtained for a certain type of Pöschl-Teller potential model with two main parameters. The two parameters exhibited the same variation with the energy of the system but exhibited opposite characteristics with the thermodynamic properties such as enthalpy, Gibbs free energy and entropy. The parameter V_0 varies inversely with the thermodynamic properties while the screening parameter α varies directly with the thermodynamic properties. The thermodynamic properties such as Gibbs free energy and entropy are negatively sensitive to temperature while the enthalpy is positively sensitive to temperature. To the best of our understanding, this is the first time this Pöschl-Teller potential model is examined for thermodynamic properties. This potential type has a unique behaviour based on the effects of its parameters on the quantities studied. This study has applications in both theoretical research and practical fields such as material science, chemistry, and also condensed matter physics particularly for modeling molecular or atomic interactions, predicting and optimizing the thermodynamic properties of materials.

Data availability

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Declaration:

There is no conflict of interest.

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