Solutions of Schrödinger equation and thermal properties of generalized trigonometric Pöschl-Teller potential

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Analytical solutions of the Schrödinger equation for the generalized trigonometric Pöschl-Teller potential by using an appropriate approximation to the centrifugal term within the framework of the Functional Analysis Approach have been considered. Using the energy equation obtained, the partition function was calculated, and other relevant thermodynamic properties. More so, we use the concept of superstatistics to evaluate the thermodynamics properties of the system. It is noted that the well-known normal statistics results are recovered in the absence of the deformation parameter \((q = 0)\), and this is displayed graphically for the clarity of our results. We also obtain the normalized wave function in terms of the hypergeometric function. The numerical energy spectra for different values of the principal and orbital quantum numbers are obtained. To show the accuracy of our results, we discuss some special cases by adjusting some potential parameters and also compute the numerical eigenvalue of the trigonometric Pöschl-Teller potential for comparison sake. However, it was found out that our results agree excellently with the results obtained via other methods.

Keywords: Trigonometric Pöschl-Teller potential; factorization method; superstatistics; Schrödinger equation.

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1. Introduction

The solutions of the radial Schrödinger equation is of immense importance in nonrelativistic quantum mechanics because it is well established that the wave function contains all the necessary information required to describe a quantum system [1-3]. From the early days of quantum mechanics, the study of exactly solvable problems has attracted considerable attention in many branches of physics. In particular, the applications of quantum mechanics to nuclear physics, information theory, molecular physics, and particle physics need not be overemphasized [4,5].

It is well known that exact solutions of this equation are only possible for a few potential models, such as the Kramers [6-7], Eckart potential [8-10], shifted Deng-Fan [11-14], Molecular Tietz potential [15-18], etc. The exact analytical solutions of the Schrödinger equation with some of these potentials are only possible for \(\ell = 0\). For \(\ell \neq 0\) states, one has to employ some approximations, such as the Pekeris approximation [17,18], to deal with the orbit centrifugal term or solve numerically [19,20]. Several mathematical approaches have been developed to solve differential equations arising from these considerations. They include the supersymmetric approach [21-24], Nikiforov-Uvarov method [25-27], asymptotic iteration method (AIM) [28-30], Feynman integral formalism [31-34], factorization formalism [35,36], Formula Method [37] exact quantization rule method [38-43], proper quantization rule [44-48], Wave Function Ansatz Method [49] etc...

The trigonometric Pöschl-Teller potential was proposed by Pöschl and Teller [50] in 1933, and it has been used in describing diatomic molecular vibration. This potential can be written as

\[ V(r) = V_1 \cos \alpha r^2 + V_2 \sec^2 \alpha r, \]  

(1)

where parameters \(V_1\) and \(V_2\) describe the property of the potential well, whereas the parameter \(\alpha\) is related to the range of this potential [51].

This potential has been applied to study diatomic molecular vibration. Ever since it was proposed in 1933, researchers have given much attention to the molecular potential. For example, Liu \textit{et al.} [51] carried out a fermionic analysis with this potential. The bound state solutions have also been carried out in the relativistic regime by Falaye and Ikhdair [52], Chen [53], Candemir [54], and Hamzavi [55].

Very recently, Hamzavi and Rajabi [56] also studied the s-wave solutions of the Schrödinger equation for this potential using the Nikiforov-Uvarov method. Hamzavi and Ikhdair [57] obtained the approximate solutions of the radial Schrödinger equation for the rotating trigonometric PT potential using the Nikiforov-Uvarov method. The energy eigenvalues and their corresponding eigenfunctions were calculated for arbitrary \(\ell\)-states in closed form.

Motivated by Ref. [50-57], we propose a modification to the trigonometric Pöschl-Teller potential, called the Generalized trigonometric Pöschl-Teller potential. This potential is given as:
\[ V(r) = V_1 \cos cc^2(\alpha r) + V_2 \sec^2(\alpha r) + V_3 \tan^2(\alpha r) + V_4 \cot^2(\alpha r), \] (2)

where parameters \( V_1, V_2, V_3, \) and \( V_4 \) describe the property of the potential well, whereas the parameter \( \alpha \) is related to the range of this potential. For what obtains in previous studies of the molecular potential, we modified the potential to allow for more physical application and comparative analysis to existing studies of the molecular potential. Besides, in molecular physics, it has also been established that potential energy functions with more parameters tend to fit experimental data than those with fewer parameters, and researchers have recently paid great attention to obtaining modified version of potential functions by employing dissociation energy and equilibrium bond length for molecular systems as explicit parameters. This model will be an important tool for spectroscopists to represent experimental data, verify measurements, and make predictions.

The first step in obtaining the thermodynamics properties of a given system is to calculate its vibrational partition function. The partition function, which explicitly depends on temperature, aids us to obtain other thermodynamics properties. The vibrational partition function for certain potential models can easily be obtained by calculating the rotation-vibrational energy levels of the system whose applications are widely used in statistical mechanics and molecular physics [58,59]. Different mathematical approaches have been employed by many researchers in evaluating partition functions, such as Poisson the summation formula [60], commulant expansion method [61], standard method [62], and Wigner-Kirkwood formulation [63]. Superstatistics is the topic of interest in statistical mechanics.

Superstatistics is a superposition of different statistics: One given by ordinary Boltzmann factor and another given by the fluctuation of the intensive parameter such as the inverse temperature. Superstatistics describe non-equilibrium systems with a stationary state and intensive parameter fluctuations and contains Tsallis statistics as a special case [64-72].

Therefore, it is the primary objective of the present work to study the Schrödinger equation for non-zero angular momentum with the generalized trigonometric Pöschl-Teller potential using the Functional Analysis Approach. We will also use the resulting energy equation to find the partition function, which will enable us to calculate other thermodynamics properties via statistical mechanics and superstatistics mechanics approach.

This paper is organized as follows. In Sec. 2, we derive the bound states of the Schrödinger equation with the generalized trigonometric PT potential using the FAA. In Sec. 3, we obtain the thermodynamic properties, which will be calculated using the expression for the partition function. In Sec. 4, we calculate the effective Boltzmann factor considering modified Dirac delta distribution in the deformed formalism. We obtain the statistical properties of the systems by using the superstatistics. In Sec. 5, we obtain the rotation-vibrational energy spectrum for some diatomic molecules with numerical results and discussion. In Sec. 6, we present special cases of the potential under consideration. Finally, in Sec. 7, we give a concluding remark.

2. Energy levels and wavefunctions

The radial part of the Schrödinger equation is given by [60]:

\[ \frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E_{n\ell} - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \right] R_{n\ell}(r) = 0. \] (3)

Considering the generalized trigonometric Pöschl-Teller potential (Eq. (2)), we obtain the radial Schrödinger equation, Eq. (3) is rewritten as follows:

\[ \frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E_{n\ell} - \left( V_1 \cos cc^2(\alpha r) + V_2 \sec^2(\alpha r) + V_3 \tan^2(\alpha r) + V_4 \cot^2(\alpha r) \right) - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \right] R_{n\ell}(r) = 0. \] (4)

This equation cannot be solved analytically for \( \ell \neq 0 \) due to the centrifugal term. Therefore, we must use an approximation to the centrifugal term. We use the following approximation [57]

\[ \frac{1}{r^2} \approx \alpha^2 \left[ d_0 + \frac{1}{\sin^2(\alpha r)} \right], \] (5)

where \( d_0 = 1/12 \) is a dimensionless shifting parameter, and \( \alpha \) is the screening parameter. It is noted that for a short-range potential, the relation Eq. (5) is a good approximation to \( 1/r^2 \), as proposed by Greene and Aldrich [19,53] approximation. This implies that Eq. (5) is not a good approximation to the centrifugal barrier when the screening parameter becomes large. Thus, the approximation is valid when \( \alpha r = 1 \).

Inserting Eqs. (5) into Eq. (4), we have:

\[ \frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E_{n\ell} - \left( V_1 \cos cc^2(\alpha r) + V_2 \sec^2(\alpha r) + V_3 \tan^2(\alpha r) + V_4 \cot^2(\alpha r) \right) - \frac{\hbar^2 \ell(\ell+1)\alpha^2}{2\mu} \right] \times \left( d_0 + \frac{1}{\sin^2(\alpha r)} \right) R_{n\ell}(r) = 0. \] (6)

Using the coordinate transformation \( \rho = \sin^2(\alpha r) \), Eq. (6) translates into,

\[ 4\rho(1 - \rho) \frac{d^2 R_{n\ell}(\rho)}{d\rho^2} + (2 - 4\rho) \frac{dR_{n\ell}(\rho)}{d\rho} + \frac{1}{\rho(1 - \rho)} \times \left[ -((\varepsilon + \eta_3 + \eta_4 - \gamma d_0)^2 + (\varepsilon + \eta_1 - \eta_2 + 2\eta_4 - \gamma d_0 + \gamma)\rho - (\eta_1 + \eta_3 + \gamma) \right] R_{n\ell}(\rho) = 0. \] (7)
For Mathematical simplicity, let us introduce the following dimensionless notations:

\[ \varepsilon = \frac{2\mu E_{nt}}{\hbar \alpha^2}, \quad \eta_i = \frac{2\mu V_i}{\hbar^2 \alpha^2}, \]

\[ i = 1, 2, 3, 4, \quad \gamma = \ell(n + 1). \quad (8) \]

To solve Eq. (6), we propose the physical wave function as:

\[ R_{nt}(\rho) = \rho^\beta(1 - \rho)^\delta f(\rho), \quad (9) \]

where

\[ \beta = \frac{1}{4} + \sqrt{\frac{1}{16} + \frac{(\eta_1 + \eta_4 + \gamma)}{4}} \]

(10)

and

\[ \delta = \frac{1}{4} + \sqrt{\frac{1}{16} + \frac{(\eta_3 + \eta_2)}{4}}. \quad (11) \]

On substitution of Eq. (9) into Eq. (7) leads to the following hypergeometric equation:

\[ \rho(1 - \rho)f''(\rho) + \left[ \left( 2\beta + \frac{1}{2} \right) - (2\beta + 2\delta + 1) \right] f'(\rho) \]

\[ - \left[ (\beta + \delta)^2 - \frac{(\varepsilon + \eta_3 + \eta_4 - \gamma d_0)}{4} \right] f(\rho) = 0 \quad (12) \]

whose solutions are the hypergeometric functions

\[ f(\rho) = 2F_1(a, b; c; \rho), \quad (13) \]

where

\[ a = (\beta + \delta) - \frac{\sqrt{\varepsilon + \eta_3 + \eta_4 - \gamma d_0}}{2}, \]

\[ b = (\beta + \delta) + \frac{\sqrt{\varepsilon + \eta_3 + \eta_4 - \gamma d_0}}{2}, \]

\[ c = 2\beta + \frac{1}{2}. \quad (14) \]

By considering the finiteness of the solutions, the quantum condition is given by

\[ (\beta + \delta) - \frac{\sqrt{\varepsilon + \eta_3 + \eta_4 - \gamma d_0}}{2} = -n \quad n = 0, 1, 2... \quad (15) \]

from which we obtain, the energy expression as

\[ \varepsilon = \gamma d_0 - \eta_3 - \eta_4 + \frac{1}{4} \left[ 4n + 2 + \sqrt{1 + 4(\eta_3 + \eta_2)} \right. \]

\[ + \sqrt{1 + 4(\eta_1 + \eta_4 + \gamma)} \left. \right] ^2. \quad (16) \]

Thus, if one substitutes the value of the dimensionless parameters in Eq. (8) into Eq. (16), we obtain the energy eigenvalues as:

\[ E_{nt} = \frac{\hbar^2 \alpha^2 \ell(\ell + 1)d_0}{2\mu} - V_3 - V_4 \frac{\hbar^2 \alpha^2}{8\mu} \]

\[ \times \left[ 4n + 2 + \sqrt{1 + \frac{8\mu V_3}{\hbar^2 \alpha^2} + \frac{8\mu V_2}{\hbar^2 \alpha^2}} \right. \]

\[ + \sqrt{\frac{8\mu V_3}{\hbar^2 \alpha^2} + \frac{8\mu V_2}{\hbar^2 \alpha^2} + (2\ell + 1)^2} \right]^2. \quad (17) \]

The corresponding unnormalized wave function is obtained as

\[ R_{nt}(\rho) = N_{nt}\rho^\beta(1 - \rho)^\delta 2F_1 \]

\[ \times \left( -n, n + 2(\beta + \delta), 2\beta + \frac{1}{2}, \rho \right), \quad (18) \]

where \( N_{nt} \) is the normalization constant. \( N_{nt} \) can be calculated by the normalization conditions of the wave function:

\[ \int_0^\infty |R_{nt}(r)|^2 dr = 1, \quad (19) \]

Putting Eq. (18) into the Eq. (19) yields

\[ \frac{|N_{nt}(r)|^2}{\alpha} I_n = 1, \quad (20) \]

where

\[ I_n = \int_0^1 \rho^{2\beta-(1/2)}(1 - \rho)^{2\delta-(1/2)} \]

\[ \times \left[ 2F_1(-n, n + 2\beta + 2\delta, \frac{1}{2} + 2\beta, \rho) \right]^2 d\rho. \quad (21) \]

The integral \( I_n \) is calculated for different \( n \) values using the Mathematica software program for \( \text{Re}[\beta] > -(1/4) \) and \( \text{Re}[\delta] > -(1/4) \) as follows:

\[ n = 0 \Rightarrow I_0 = \frac{\Gamma \left( \frac{1}{2} + 2\beta \right) \Gamma \left( \frac{3}{2} + 2\delta \right)}{2(\beta + \delta)\Gamma(2\beta + 2\delta)}, \]

\[ n = 1 \Rightarrow I_1 = \frac{2\Gamma \left( \frac{3}{2} + 2\beta \right) \Gamma \left( \frac{5}{2} + 2\delta \right)}{(1 + 4\beta)^2(\beta + \delta + 1)\Gamma(2\beta + 2\delta + 1)}, \]
n = 2 ⇒ I_2 = \frac{16\Gamma \left( \frac{5}{2} + 2\beta \right) \Gamma \left( \frac{5}{2} + 2\delta \right)}{(1 + 4\beta)^2(3 + 4\beta)^2(\beta + \delta + 2)\Gamma(2\beta + 2\delta + 2)}, \\
n = 3 ⇒ I_3 = \frac{192\Gamma \left( \frac{7}{2} + 2\beta \right) \Gamma \left( \frac{7}{2} + 2\delta \right)}{(1 + 4\beta)^2(3 + 4\beta)^2(5 + 4\beta)^2(\beta + \delta + 3)\Gamma(2\beta + 2\delta + 3)}, \\
\vdots \\
n = m ⇒ I_m = m!2^{4m-1} \frac{\Gamma \left( \frac{m + \frac{1}{2} + 2\beta \right) \Gamma \left( m + \frac{7}{2} + 2\delta \right) [\Gamma(m + 2\beta)\Gamma(4\beta)]^2}{(\beta + \delta + m)\Gamma(2\beta + 2\delta + m)\Gamma(2\beta)\Gamma(2m + 4\beta)^2}, (22)

Hence, we find

\[ N_{nl} = \left( \frac{\alpha(\beta + \delta + n)\Gamma(2\beta + 2\delta + n)\Gamma(2\beta)\Gamma(2n + 4\beta)}{n!2^{4n-1}\Gamma(n + \frac{1}{2} + 2\beta)\Gamma(n + \frac{7}{2} + 2\delta)\Gamma(n + 2\beta)\Gamma(4\beta)} \right)^{1/2}. (23) \]

By using Eqs. (23) and (18) one can plot the radial wave functions for arbitrary quantum states through the Mathematica software program.

3. Thermal Properties of generalized trigonometric Pöschl-Teller potential

We consider the contribution of the bound state to the vibrational partition function at a given temperature T [58,60]

\[ Z(\beta) = \sum_{n=0}^{n_{max}} e^{-\beta E_{nl}}, \quad \beta = \frac{1}{k_B T}, \quad (24) \]

Here, \( k_B \) is the Boltzmann constant, and \( E_{nl} \) is the rotational-Vibrational energy of the nth bound state.

We can rewrite Eq. (17) to be of the form

\[ E_{nl} = \sigma_1 + \frac{\hbar^2 \alpha^2}{8\mu}(4n + \sigma_2)^2, \quad (25) \]

where

\[ \sigma_1 = \frac{\hbar^2 \alpha^2(\ell + 1)d_0}{2\mu} - V_3 - V_4; \]

\[ \sigma_2 = 2 + \sqrt{1 + \frac{8\mu V_3}{\hbar^2 \alpha^2} + \frac{8\mu V_2}{\hbar^2 \alpha^2}} + \sqrt{\frac{8\mu V_1}{\hbar^2 \alpha^2} + \frac{8\mu V_4}{\hbar^2 \alpha^2} + (2\ell + 1)^2}. \quad (26) \]

We substitute Eq. (25) into Eq. (24) to have

\[ Z(\beta) = \sum_{n=0}^{n_{max}} e^{-\beta[n(\sigma_1 + (\hbar^2 \alpha^2/8\mu)(4n + \sigma_2)^2)]} \]

where

\[ n_{max} = \left\lfloor \frac{\sigma_2}{4} \right\rfloor. \quad (28) \]

Replacing the sum in Eq.(27) by an integral in the classical limit, we obtain

\[ Z(\beta) = \int_0^{n_{max}} e^{-\beta(An^2 + Bn + C)} dn, \quad (29) \]

where

\[ A = \frac{2\hbar^2 \alpha^2}{\mu}; \quad B = \frac{\hbar^2 \alpha^2 \sigma_2}{\mu}; \quad C = \frac{\hbar^2 \alpha^2 \sigma_2^2}{8\mu}. \quad (30) \]

Therefore, we use the mathematica software to evaluate the integral in Eq. (29), thus obtaining the partition function for generalized trigonometric Pöschl-Teller potential model.

\[ Z(\beta) = \frac{\sqrt{\pi} e^{\beta B^2/4A}}{2\sqrt{\beta A}} \left( Erf \left( \frac{\beta(2An_{max} + B)}{2\sqrt{\beta A}} \right) - Erf \left( \frac{\beta B}{2\sqrt{\beta A}} \right) \right) e^{-\beta C}. \quad (31) \]

The imaginary error function can be defined as [62]

\[ Erf (z) = i Erf (z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{u^2} du. \quad (32) \]

Thermodynamic functions such as: free energy, entropy, internal energy, and specific heat capacity functions can be obtained from the partition function (31) as follows [20].
3.1. Helmholtz free energy

\[ F(\beta) = -\frac{1}{\beta} \ln z(\beta), \]  
\[ \ln \left( \frac{e^{(\beta B^2/4A) - \beta C} \sqrt{\pi} \left( \text{Erf} \left( \frac{\beta(2A\text{max}+B)}{2\sqrt{3A}} \right) - \text{Erf} \left( \frac{\beta B}{2\sqrt{3A}} \right) \right)}{2\sqrt{3A}} \right) \]  
\[ F(\beta) = \frac{e^{(\beta B^2/4A) - \beta C} \sqrt{\pi} \left( \text{Erf} \left( \frac{\beta(2A\text{max}+B)}{2\sqrt{3A}} \right) - \text{Erf} \left( \frac{\beta B}{2\sqrt{3A}} \right) \right)}{2\sqrt{3A}} \]  
\[ (33a) \]
\[ (33b) \]

3.2. Entropy

\[ S(\beta) = -k_B \frac{\partial F(\beta)}{\partial \beta}, \]  
\[ S(\beta) = \Delta_0 - \frac{1}{2} \text{Erf} \left( \frac{B\sqrt{\beta}}{2\sqrt{A}} \right) + \text{Erf} \left( \frac{\sqrt{\beta}(B + 2A\text{max})}{2\sqrt{A}} \right) \]  
\[ \text{where} \]  
\[ \Delta_0 = \ln \left( \frac{e^{(\beta B^2/4A) - \beta C} \sqrt{\pi} \left( \text{Erf} \left( \frac{\beta(2A\text{max}+B)}{2\sqrt{3A}} \right) - \text{Erf} \left( \frac{\beta B}{2\sqrt{3A}} \right) \right)}{2\sqrt{3A}} \right) \]  
\[ \Delta_1 = \text{Erf} \left( \frac{B\sqrt{\beta}}{2\sqrt{A}} \right) - \text{Erf} \left( \frac{\sqrt{\beta}(B + 2A\text{max})}{2\sqrt{A}} \right), \]  
\[ \Delta_2 = 2 \left( \frac{B^2}{4A} - C \right) \beta \left( -\text{Erf} \left( \frac{B\sqrt{\beta}}{2\sqrt{A}} \right) + \text{Erf} \left( \frac{\sqrt{\beta}(B + 2A\text{max})}{2\sqrt{A}} \right) \right), \]  
\[ \Delta_3 = \frac{e^{-(\beta[B+2A\text{max}]^2)/2A\sqrt{\beta}(B-B\text{e}^{B\text{max}(B+An_{\text{max}})}+2A\text{max})}}{2A\sqrt{\pi}} \]  
\[ (34a) \]
\[ (34b) \]

3.3. Internal energy

\[ U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta}, \]  
\[ U(\beta) = \frac{1}{8A^3/2\beta^3/2} e^{-\beta[C+n_{\text{max}}(B+A\text{max})]} \left( e^{\beta[B+2A\text{max}]^2}/4A \sqrt{\pi}(-B^2+2A+2+4C\beta) \right) \]  
\[ \times \left( -\text{Erf} \left( \frac{B\sqrt{\beta}}{2\sqrt{A}} \right) + \text{Erf} \left( \frac{\sqrt{\beta}(B + 2A\text{max})}{2\sqrt{A}} \right) \right) - 2\sqrt{A}\sqrt{\beta} \left( B - B\text{e}^{B\text{max}(B+An_{\text{max}})} + 2A\text{max} \right) \]  
\[ (35a) \]
\[ (35b) \]

3.4. Specific heat capacity

\[ C_v = k_B \frac{\partial U(\beta)}{\partial \beta}, \]  
\[ C_v = \frac{1}{32A^5/2} e^{(B^2\beta/4A) - C\beta} \left( H_0 + 2\sqrt{A} e^{-\beta(B+2A\text{max})^2}/4A (H_1 + H_2) \right), \]  
\[ H_0 = \frac{\sqrt{\pi}(12A^2 + 4A(-B^2 + 4AC)\beta + (B^2 - 4AC)^2\beta^2)}{\beta} \left( \text{Erf} \left( \frac{B\sqrt{\beta}}{2\sqrt{A}} \right) - \text{Erf} \left( \frac{\sqrt{\beta}(B + 2A\text{max})}{2\sqrt{A}} \right) \right), \]  
\[ H_1 = B\text{e}^{B\text{max}(B+An_{\text{max}})}(B^2\beta - 2A(3+4C\beta)), \]  
\[ H_2 = (B + 2A\text{max})(-B^2 + A(6 + 8C\beta) + 4A\beta n_{\text{max}}(B + An_{\text{max}})). \]
4. Superstatistics mechanics

In this section, we introduce the necessary conditions of superstatistics. The effective Boltzmann factor of the system can be written as [73,74]

\[ B(E) = \int_0^\infty e^{-\beta' E} f(\beta', \beta) d\beta', \] (37)

where

\[ f(\beta', \beta) = \delta(\beta' - \beta), \] (38a)

is the probability density. Besides we state here the modified form of Dirac delta function used in this study as [75]:

\[ f(\beta', \beta) = a' \delta(\beta' - \beta) + b' \beta' \frac{\partial}{\partial \beta'(\delta(\beta' - \beta))} + c' \beta'^2 \frac{\partial^2}{\partial \beta'^2} (\delta(\beta' - \beta)), \] (38b)

Finally, we find the generalized Boltzmann factor as in Ref. [75]

\[ B(E) = e^{-\beta E} \left(1 + \frac{q}{2} \beta^2 E^2\right). \] (39)

where \( q \) is the deformation parameter. Details of Eq. (39) can be found in Appendix A of Ref. [75] and references therein.

The partition function for the modified Dirac delta distribution has the following form [75]:

\[ Z_S = \int_0^\infty B(E) d\beta'. \] (40)

We substitute Eq. (25) into Eq. (40) to have

\[ Z_S = \int_0^\infty e^{-\beta(\sigma_1 + \lambda \sigma_2)} \left(1 + \frac{q}{2} \beta^2 \left(\sigma_1 + \frac{\hbar^2 \alpha^2}{8\mu} (4n + \sigma_2)^2\right)^2\right) d\beta. \] (41)

Therefore, we use Mathematica software to evaluate the integral in Eq. (41), thus obtaining the partition function with generalized trigonometric Pöschl-Tellerpotential model in superstatistics as follows:

\[ Z_q(\beta) = \frac{e^{-\beta(\sigma_1 + \lambda \sigma_2)} \left(e^{\beta \lambda \sigma_2} \sqrt{\pi} (8 + 3q + 4q \beta_1 (1 + \beta \sigma_1)) - \sqrt{\beta \lambda}(\xi) \sigma_2 + 4q(\beta \lambda)^{3/2} \sigma_3^2\right)}{64\sqrt{\beta \lambda}} \] (42a)

where

\[ \xi = -6q - 8q \beta_1 \sigma_1 + \frac{e^{\beta \lambda \sigma_2} \sqrt{\pi} Erf[\sqrt{\beta \lambda} \sigma_2]}{\sqrt{\beta \lambda} \sigma_2}. \] (42b)

Other thermodynamic functions such as Helmholtz free energy, \( F_q(\beta) \), entropy, \( S_q(\beta) \), internal energy, \( U_q(\beta) \), and specific heat, \( C_q(\beta) \), functions can be obtained from the partition function (42a) as follows:

4.1. Helmholtz free energy

The Helmholtz free energy is obtained in superstatistics formalism with the aid of Eq. (33a) as follows:

\[ F_q(\beta) = \frac{1}{\beta} \ln \left(\frac{1}{64\sqrt{\beta \lambda}} e^{-\beta(\sigma_1 + \lambda \sigma_2)} \left(N_0 - \sqrt{\beta \lambda}(-6q - 8q \beta_1 + N_1) \sigma_2 + 4q(\beta \lambda)^{3/2} \sigma_3^2\right)\right) \] (43a)

where

\[ N_0 = e^{-\beta \lambda \sigma_2} \sqrt{\pi} (8 + 3q + 4q \beta_1 (1 + \beta \sigma_1)), \]
\[ N_1 = \frac{e^{-\beta \lambda \sigma_2} \sqrt{\pi} Erf[\sqrt{\beta \lambda} \sigma_2] (8 + 3q + 4q \beta_1 (1 + \beta \sigma_1))}{\sqrt{\beta \lambda} \sigma_2}. \] (43b)

4.2. Entropy

The entropy is obtained in superstatistics formalism with the aid of Eq. (34a) as follows:

\[ S_q(\beta) = \Omega_0 + \frac{\Omega_1 + \Omega_2 - \Omega_3 + \Omega_4}{(2(\Omega_5 + \Omega_6)^4)}. \] (44a)
where

\[ \Omega_0 = \ln \left[ \frac{1}{64\sqrt{\lambda}} e^{-\beta(\sigma_1 + \lambda \sigma_2^2)} \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + 3q + 4q\beta \sigma_1(1 + \beta \sigma_1)) - \sqrt{3\lambda}(-6q - 8q\beta \sigma_1 + N_1)\sigma_2 + 4q(\beta \lambda)^{3/2} \sigma_2^3} \right) \right], \]

\[ \Omega_1 = e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + 3q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) + 8e^{\beta \lambda \sigma_2^2} \sqrt{\pi} q \beta^3 \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \sigma_1^4, \]

\[ \Omega_2 = 2(8 + 3q) \sqrt{\beta \lambda} \lambda \sigma_2 + 4q\beta^{3/2} \lambda^{3/2} \sqrt{3\lambda} \sigma_2^3 + 8q\beta^{5/2} \lambda^{5/2} \sqrt{3\lambda} \sigma_2^5, \]

\[ \Omega_3 = 4q\beta^2 \sigma_1^2 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) - 6\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 \right), \]

\[ \Omega_4 = 2\beta \sigma_1 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) - 2q\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 + 12q\beta^{3/2} \lambda^{3/2} \sqrt{3\lambda} \sigma_2^3 \right) \]

\[ \Omega_5 = e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + 3q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) + 4e^{\beta \lambda \sigma_2^2} \sqrt{\pi} \beta^2 \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \sigma_1^4, \]

\[ \Omega_6 = 6q\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 + 4q\beta^{3/2} \lambda^{3/2} \sqrt{3\lambda} \sigma_2^3 + 8q\beta \sigma_1 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \right. \]

\[ + 2\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 \right) \]

(44b)

4.3. Internal energy

The internal energy is obtained in superstatistics formalism with the aid of Eq. (35a) as follows:

\[ U_q(\beta) = \frac{1}{128(\beta \lambda)^{3/2}} e^{-\beta(\sigma_1 + \lambda \sigma_2^2)} \sqrt{\beta \lambda}^{3/2} \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + 3q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \right. \]

\[ + 8e^{\beta \lambda \sigma_2^2} \sqrt{\pi} q \beta^3 \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \sigma_1^4 - 4q\beta^2 \sigma_1^2 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \right. \]

\[ - 6\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 \right) \left( 2 + \sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2(8 + 3q + 2q\beta \lambda \sigma_2(1 + 2\beta \lambda \sigma_2)) \right) \]

\[ + 2\beta \sigma_1 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) + 2q\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2(1 + 6\beta \lambda \sigma_2^3) \right) \right) \] \tag{45}

4.4. Specific heat capacity

The specific heat is obtained in superstatistics formalism with the aid of Eq. (36a) as follows:

\[ C_q = \frac{1}{256(\beta \lambda)^{3/2}} e^{-\beta(\sigma_1 + \lambda \sigma_2^2)} \sqrt{\beta \lambda} \left( \Xi_0 - \Xi_1 - 6(8 + 3q) \sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 - 4(8 + 3q) \beta^{3/2} \lambda^{3/2} \sqrt{\beta \lambda} \sigma_2^3 \right. \]

\[ + 8q\beta^{5/2} \lambda^{5/2} \sqrt{\beta \lambda} \sigma_2^5 - \Xi_2 - \Xi_3 - \Xi_4 \right), \] \tag{46a}

where

\[ \Xi_0 = -3e^{\beta \lambda \sigma_2^2} \sqrt{\pi(8 + 3q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right), \]

\[ \Xi_1 = 16e^{\beta \lambda \sigma_2^2} \sqrt{\pi} q \beta^4 \left( \sqrt{\beta \lambda} \lambda \sigma_2 \right) \sigma_1^4, \]

\[ \Xi_2 = 16q^{3/2} \lambda^{7/2} \sqrt{\beta \lambda} \sigma_2 + 32q\beta^3 \sigma_1^4 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi} \left( \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) \right. \right) \]

\[ - 2\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 \right), \]

\[ \Xi_3 = 8q^2 \sigma_1^2 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi(4 + q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) - 6q\sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 + 12q\beta^{3/2} \lambda^{3/2} \sqrt{\beta \lambda} \sigma_2^3 \right) \]

\[ \Xi_4 = 8q \beta \sigma_1 \left( e^{\beta \lambda \sigma_2^2} \sqrt{\pi(4 + q)} \left( \sqrt{\beta \lambda} - \sqrt{3\lambda} \text{Erf} \left[ \sqrt{3\lambda} \sigma_2 \right] \right) + 2(4 + q) \sqrt{\beta \lambda} \sqrt{\beta \lambda} \sigma_2 \right. \]

\[ - 4q\beta^{3/2} \lambda^{3/2} \sqrt{\beta \lambda} \sigma_2^3 + 8q\beta^{5/2} \lambda^{5/2} \sqrt{\beta \lambda} \sigma_2^5 \right). \] \tag{46b}
To show the accuracy of our work, we calculate the energy eigenvalues using Eq. (18) for different quantum numbers \( n \) and \( \ell \) with parameters \( V_1 = 5 \text{ fm}^{-1} \), \( V_2 = 3 \text{ fm}^{-1} \), \( V_3 = 2 \text{ fm}^{-1} \), and \( V_4 = 0.5 \text{ fm}^{-1} \). In Table I, it is observed that the energy decreases for a fixed value of the principal quantum number for varying orbital angular momentum. Furthermore, we have computed the energy eigenvalues of the trigonometric Pöschl-Teller potential using the reduced energy equation given in Eq. (33) and Eq.(34) as a special case. Our results, shown in Tables II- V., are in good agreement with the results given in Ref. [56-57,76].

In Fig. 1a) and b), we plot the shape of the potential for clarity and understanding of the system we are studying. Figure 1a) we plot the shape of the generalized trigonometric Pöschl-Teller potential against the interatomic distance. Figure 1b) shows a comparative plot of the shapes of the trigonometric Pöschl-Teller potential model and generalized trigonometric Pöschl-Teller potential. However, we note that our generalized model fits appropriately with the trigonometric Pöschl-Teller potential.

Figures 2 a)-f) clearly shows the energy eigenvalues variation with parameters \( V_1 \), \( V_2 \), \( V_3 \), \( V_4 \), \( \mu \) and \( \alpha \) for various quantum states. It can be easily observed from these Figs. 2a)-d) that the parameters increase directly as the energy increases. Figure 2e) shows the energy eigenvalues variation with the particle’s reduced mass \( \mu \) for different quantum states. It is seen that in the region \( \mu \approx 0.1-0.1 \text{ a.m.u} \), the energy eigenvalue is at its maximum, beyond this region, there is a drop and this continues in a linear trend. The energy is only high in the region where the mass is low but decreases as the particle’s mass increases monotonically. The energy is very similar for \( 0.2 < \mu < 1.0 \). Figure 2f) shows the energy eigenvalues variation with screening parameter \( \alpha \) for different quantum states. It can be seen explicitly that in all the quantum states, the representation curves spreads out uniformly from the origin. It is shown that the energy eigenvalue increases as the screening parameter increases.

### Table I. Bound state energy levels \( E_{nl} \) for the Generalised trigonometric Pöschl-Teller potential obtained with parameters \( V_1 = 5 \text{ fm}^{-1} \), \( V_2 = 3 \text{ fm}^{-1} \), \( V_3 = 0.5 \), \( V_4 = 0.5 \), and \( \mu = 10 \text{ fm}^{-1} \).

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Figure 2. Energy eigenvalues variation with (a) parameter for various quantum states (b) parameter for various quantum states. (c) with parameter for various quantum states. (d) with parameter for various quantum states (e) with particle’s mass for various quantum states. (f) with screening parameter for quantum states.

Table II. Comparison of s-wave energy eigenvalues (in eV) obtained by using the Functional Analysis Approach with other methods for the trigonometric Pöschl-Teller potential with other methods obtained with parameters $V_1 = 5 \text{ fm}^{-1}$, $V_2 = 3 \text{ fm}^{-1}$, and $\mu = 10 \text{ fm}^{-1}$.

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Table III. Comparison of s-wave energy eigenvalues (in eV) obtained by using the Functional Analysis Approach with other methods for the trigonometric Pöschl-Teller potential with other methods obtained with parameters $V_1 = 5 \text{ fm}^{-1}$, $V_2 = 3 \text{ fm}^{-1}$, and $\mu = 10 \text{ fm}^{-1}$.

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SOLUTIONS OF SCHRÖDINGER EQUATION AND THERMAL PROPERTIES OF GENERALIZED TRIGONOMETRIC...

Figure 3. a) Partition Function variation with $\beta$ for various values of $n_{\text{max}}$. b) Free energy variation with $\beta$ for different values of $n_{\text{max}}$. c) Entropy variation with $\beta$ for different values of $n_{\text{max}}$. d) Mean energy variation with $\beta$ for different values of $n_{\text{max}}$. e) Specific heat capacity variation with $\beta$ for different values of $n_{\text{max}}$.

Figure 4. a) Partition Function variation with $n_{\text{max}}$ for various values of $\beta$. b) Free energy variation with $n_{\text{max}}$ for different values of $\beta$. c) Entropy variation with $n_{\text{max}}$ for different values of $\beta$. d) Mean energy variation with $n_{\text{max}}$ for different values of $\beta$. e) Specific heat capacity variation with $n_{\text{max}}$ for different values of $\beta$. 

Rev. Mex. Fís. 66 (6) 824–839
In Figs. 3a)-(e), we show a graphical representation of the thermal properties obtained via the standard Boltzmann-Gibbs statistical mechanical approach. We analyze how these properties vary with $\beta$ for different discrete values of $n_{\text{max}}$. Figure 3(a) shows the partition function variation with $\beta$ for various values of $n_{\text{max}}$. It can be seen that the partition function decreases as the temperature increases. It is also shown that in the high temperature limits, there’s a uniform convergence of all the curves and the partition function reaches its minimum. Figure 3(b) shows the mean free energy variation with $\beta$ for different values of $n_{\text{max}}$. Again, it is seen that the free energy reduces monotonically with $\beta$. Figure 3(c) shows the entropy variation with $\beta$ for different values of $n_{\text{max}}$. It is seen that the entropy declines as temperature increases. Figure 3(d) shows the mean energy variation with $\beta$ for various values of $n_{\text{max}}$. The mean energy decreases as $\beta$ increases. It is also observed that the mean energy has its minimum in the high $\beta$ region. Figure 3(e) clearly shows the specific heat capacity variation with $\beta$ for different values of $n_{\text{max}}$. An asymmetric shaped formed for increasing value of $n_{\text{max}}$. At $n_{\text{max}} = 300$, its trough is reached and heat capacity monotonically growth with $\beta$. We see that at some point in $\beta$, the values of $n_{\text{max}}$ might become invariant.

In Fig 4(a)-(e), we graphically display the thermal properties obtained via the standard Boltzmann-Gibbs statistical mechanical approach. We analyze how these properties vary with $n_{\text{max}}$ for different values of $\beta$. Figure 4a) clearly shows the Partition Function variation with $n_{\text{max}}$ for various values of $\beta$. From this plot, we observe that there is spread from the zero point; the partition function increases as $n_{\text{max}}$ increases. It is also observed that the partition function has its maximum in the high region of $n_{\text{max}}$. Figure 4b) clearly shows the free energy variation with $n_{\text{max}}$ for different values of $\beta$. It is clearly shown that the mean free energy rises logarithmically as $n_{\text{max}}$ rises. Figure 4c) shows a plot of entropy variation with different values of $\beta$. It is seen that the entropy up-

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FIGURE 5. Superstatistics plots of: a) Partition Function variation with $\beta$ for various values of $q$. b) Free energy variation with $\beta$ for different values of $q$. c) Entropy variation with $\beta$ for different values of $q$. d) Mean energy variation with $\beta$ for different values of $q$. e) Specific heat capacity variation with $\beta$ for different values of $q$.

FIGURE 6. Comparison of superstatistics at $q = 0$ and normal statistics: a) Partition Function variation with $\beta$. b) Free energy variation with $\beta$. c) Entropy variation with $\beta$. d) Mean energy variation with $\beta$. e) Specific heat capacity variation with $\beta$. 
surges monotonically with \( n_{\text{max}} \). Figure 4d) displays the plot of mean energy variation with \( n_{\text{max}} \) for different values of \( \beta \). The mean energy surges in an linear-monotonic pattern. Figure 4e) presents the plot of specific heat capacity variation with \( n_{\text{max}} \) for different values of \( \beta \). As predicted in Fig. 3e), it clearly shows for the different values of \( \beta \), at some point in \( n_{\text{max}} \), heat capacity becomes invariant. We can deduce that for the values of \( n_{\text{max}} \), specific heat and \( \beta \) is invariant.

In Fig S(a-e), we show graphically the thermal properties obtained via this superstatistical mechanical approach. We analyze how these properties vary with \( \beta \) for different values of the deformation parameter \( q \). Figure 5a) shows a plot of the partition function variation with \( \beta \) for various values of \( q \). It is seen that the partition function decreases as \( \beta \) increases. More so, the partition function increases as \( q \) increases. Figure 5b) shows the variation of mean free energy with \( \beta \) for various values of \( q \). The mean free energy decreases monotonically as \( \beta \) increases. A plot of entropy variation with \( \beta \) for different values of \( q \) is shown in Fig. 5c). The entropy of the system reduces as \( \beta \) rises. For different values of the deformation parameter \( q \), the entropy of the system increases with increasing \( q \). Figure 5d) shows the variation of the mean energy with \( \beta \) for various values of \( q \). The mean energy decreases with increasing \( \beta \) and increases with increasing \( q \). Figure 5e) depicts a plot of specific heat capacity variation with \( \beta \) for different values of \( q \). It is seen explicitly that the specific heat capacity of the system increases monotonically with increasing \( \beta \) but decreases with increasing \( q \).

It is interesting to note also that when \( q = 0 \), normal statistics or the conventional Boltzmann-Gibbs statistics is recovered from the superstatistics. However, to further strengthen this claim, we show a graphical comparative plot in Figs. 6a)-e) of all thermal properties obtained via the superstatistics at \( q = 0 \) and B-G statistics at maximum quantum number. It is interesting to see that there’s no discernable difference in the curves as they’re both adequately fitted.

The shape of the radial wave functions is shown in Fig. 7 for 2p, 3d, and 4f quantum states. If we examine the shapes of Fig. 7 carefully, we see that the wave functions have different number of radial nodes and different amplitudes.

6. Special Cases

In this section, we shall study one special case of the Generalized Trigonometric Pöschl-Teller potential and its energy eigenvalues, respectively

6.1. Trigonometric Pöschl-Teller potential

Choosing \( V_3 = V_4 = 0 \), the Generalized Trigonometric Pöschl-Teller potential takes [76,56]

\[
V(r) = \frac{V_1}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)},
\]

and the energy eigenvalue becomes

\[
E_{n\ell} = \frac{\hbar^2 \alpha^2 (\ell + 1) d_0}{2\mu} + \frac{\hbar^2 \alpha^2}{8\mu} \left[ 4n + 2 \right. \\
+ \sqrt{1 + \frac{8\mu V_2}{\hbar^2 \alpha^2}} + \sqrt{\frac{8\mu V_1}{\hbar^2 \alpha^2} + (2\ell + 1)^2} \bigg].
\]

This is in excellent agreement with Eq. (3) of Ref. [76] and Eq. (19) of Ref. [57].

By setting \( \ell \), we obtain the s-wave energy equation for the potential understudy as:

\[
E_{n0} = \frac{\hbar^2 \alpha^2}{8\mu} \left[ 4n + 2 + \sqrt{1 + \frac{8\mu V_2}{\hbar^2 \alpha^2}} + \sqrt{\frac{8\mu V_1}{\hbar^2 \alpha^2} + 1} \right].
\]

This is in excellent agreement with Eq. (15) of Ref. [56].

7. Conclusion

In this article, we have solved the Schrödinger equation using the Functional Analysis Approach and suitable approximation to overcome the centrifugal barrier. We have also presented the rotational-vibrational energy spectra with the Generalized Trigonometric Pöschl-Teller potential. We have expressed the solutions by the generalized hypergeometric functions \( \text{}_2F_1(a, b, c; \rho) \). Results have been discussed extensively using plots. We discussed some special cases by adjusting the potential parameters and compute the numerical energy spectra for the trignometric Pöschl-Teller potential for both the \( \ell = 0 \) and \( \ell \neq 0 \) cases, respectively. It was found that our results agree with the existing literature. In detail, we evaluated the vibrational partition functions \( Z(\beta) \), which we used to study the thermodynamics properties of vibrational mean energy \( U(\beta) \), vibrational entropy \( S(\beta) \), vibrational mean free energy \( F(\beta) \), and vibrational specific heat capacity \( C(\beta) \). Besides, the effective Boltzmann factor is calculated by using superstatistics, and the results is compared with the case where the deformation parameter vanished. It is noted that the results, in the special case of the vanished
deformation parameter, are in agreement with the ordinary statistics. Finally, this study has many applications in different areas of physics, and chemistry such as atomic physics, molecular physics and chemistry amongst others.


61. G. Herzberg, Molecular spectra and molecular structure II. Infrared and Raman spectra of polyatomic molecules (Van Nosstrand, New York, 1945).


