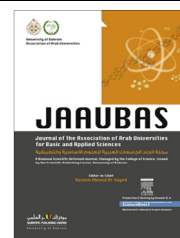




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ORIGINAL ARTICLE

Thermodynamic properties and approximate solutions of the ℓ -state Pöschl–Teller-type potential

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Abstract In this study, the solutions of the ℓ -state Pöschl–Teller-type potential for the Schrödinger and Klein–Gordon equations are obtained using the parametric Nikiforov–Uvarov method. Solving the Schrödinger and Klein–Gordon wave equations, the energy eigenvalues and wave functions are obtained. For the case $\ell = 0$, we made comparison with previous results where the solutions of Schrödinger equation for the Pöschl–Teller-type potential were obtained for s-wave ($\ell = 0$) state. We also obtain the thermodynamic properties such as vibrational mean energy, vibrational specific heat, vibrational mean free energy and vibrational entropy for the Pöschl–Teller-type potential in the classical limit.

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1. Introduction

The exact solutions of the wave equations in non-relativistic and relativistic quantum mechanics are very important. The Schrödinger wave equation is used to describe non-relativistic spinless particles. The Klein–Gordon, Dirac, and Duffin–Kemmer–Petiau equations are used to describe spin zero, spin half and spin one particles, respectively. The Duffin–Kemmer–Petiau equation can also be used to describe spin zero particles. To obtain the exact and approximate solutions of the wave equations, various methods have been used ranging from Nikiforov–Uvarov method (Ikhdair, 2012; Yahya et al., 2010), supersymmetry quantum

mechanics (Hassanabadi et al., 2012; Oyewumi and Akoshile, 2010), asymptotic iteration method (Champion et al., 2008; Fernandez, 2004), improved AIM (Boztosun and Karakoc, 2007; Yahya et al., 2014a), Laplace integral transform (Ortakaya, 2012), factorization method (Dong et al., 2007), proper quantization rule and exact quantization rule (Dong and Gonzalez-Cisneros, 2008; Qiang and Dong, 2010). The results obtained by solving wave equations for certain potential models are increasingly being applied. Recently, the solution of the two-dimensional spinless Klein–Gordon equation for scalar–vector harmonic oscillator potentials with and without the constant perpendicular magnetic and Aharonov–Bohm (AB) flux fields was studied by Ikhdair and Falaye (2013b). The energies and wave functions of certain potential models have also been used to obtain information-theoretic measures such as Fisher information, Shannon entropy, Renyi entropy, Tsallis entropy among other information-theoretic measures (see e.g. Yahya et al., 2014b).

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In this work, the solutions of Schrödinger and Klein–Gordon equations for the Pöschl–Teller-type potential are obtained for all ℓ (orbital angular momentum). The Pöschl–Teller potential is used to account for the Physics of many systems which includes the excitons, quantum wires and quantum dots (Ikhdair and Falaye, 2013a). The dynamical group of the modified Pöschl–Teller potential was studied by Dong and Lemus in 2002, and it was realized as $SU(1,1)$ group by factorization method (Dong and Lemus, 2002). Also the solutions of the Dirac equation with the generalized Pöschl–Teller potential including the pseudo-spin-centrifugal term have been obtained by Jia et al. (2009). The Pöschl–Teller-type potential to be considered is given as (Chen et al., 2013)

$$V(r) = \frac{\hbar^2 \alpha^2 \lambda (\lambda + 1)}{2M} \tanh^2(\alpha r), \quad (-\infty < r < \infty), \quad (1)$$

where M is the mass of the particle, λ denotes the potential depth and α is related with the range of the potential.

We also study the thermodynamic properties such as vibrational mean energy, vibrational specific heat, vibrational mean free energy and vibrational entropy for the Pöschl–Teller-type potential. Thermodynamic properties of some model potentials were investigated recently. In Ref. (Baria and Jani, 2012), a new model potential was used with the exchange and correlation effects to calculate internal energy (enthalpy), entropy and Helmholtz free energy of liquid Na, K, Rb and Cs at various temperatures with the variational approach. The thermodynamic properties have also been studied for the modified Rosen–Morse potential (Dong and Cruz-Irisson, 2012), harmonic oscillator plus an inverse square term (Dong et al., 2007), shifted Deng–Fan potential (Oyewumi et al., 2013) and Pöschl–Teller potential (Ikhdair and Falaye, 2013a) which is of course different from the Pöschl–Teller-type potential to be considered in this study.

The paper is organized as follows: In Section 2, the parametric NU method will be reviewed. The bound state solutions for the Pöschl–Teller-type potential are obtained for Schrödinger and Klein–Gordon equations using the parametric Nikiforov–Uvarov method in Section 3. In Section 4, the thermodynamic properties such as vibrational mean energy, vibrational specific heat, vibrational mean free energy and vibrational entropy are studied for the Pöschl–Teller-type potential. The conclusion is given in Section 5.

2. The parametric Nikiforov–Uvarov (NU) method

By using the parametric NU method, the solutions of a second order differential equation of the form (Tezcan and Sever, 2009)

$$\frac{d^2 \Psi}{ds^2} + \left[\frac{c_1 - c_2 s}{s(1 - c_3 s)} \right] \frac{d\Psi}{ds} + \left[\frac{-As^2 + Bs - C}{s^2(1 - c_3 s)^2} \right] \Psi = 0 \quad (2)$$

are

$$\begin{aligned} c_2 n - (2n + 1)c_5 + (2n + 1)(\sqrt{c_9} + c_3 \sqrt{c_8}) + n(n - 1)c_3 \\ + c_7 + 2c_3 c_8 + 2\sqrt{c_3 c_9} \\ = 0 \end{aligned} \quad (3)$$

and

$$\Psi_n = s^{c_{12}} (1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{(c_{10}-1, \frac{c_{11}}{c_3} - c_{10}-1)} (1 - 2c_3 s), \quad (4)$$

where $P_n^{(a,b)}(x)$ is the Jacobi polynomials and

$$\begin{aligned} c_4 &= \frac{1}{2}(1 - c_1), \quad c_5 = \frac{1}{2}(c_2 - 2c_3), \quad c_6 = c_5^2 + A, \quad c_7 = 2c_4 c_5 - B \\ c_8 &= c_4^2 + C, \quad c_9 = c_3(c_7 + c_3 c_8) + c_6, \quad c_{10} = c_1 + 2c_4 + 2\sqrt{c_8} \\ c_{11} &= c_2 - 2c_5 + 2(\sqrt{c_9} + c_3 \sqrt{c_8}), \quad c_{12} = c_4 + \sqrt{c_8}, \\ c_{13} &= c_5 - (\sqrt{c_9} + c_3 \sqrt{c_8}) \end{aligned} \quad (5)$$

In the special case $c_3 = 0$, we have

$$\lim_{c_3 \rightarrow 0} P_n^{(c_{10}-1, \frac{c_{11}}{c_3} - c_{10}-1)} (1 - 2c_3 s) = L_n^{c_{10}-1}(c_{11} s), \quad (6)$$

$$\lim_{c_3 \rightarrow 0} (1 - 2c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} = e^{c_{13} s}, \quad (7)$$

and the wave function in Eq. (4) turns to

$$\Psi = s^{c_{12}} e^{c_{13} s} L_n^{c_{10}-1}(c_{11} s), \quad (8)$$

where $L_n^a(x)$ is the Laguerre polynomials.

3. Solution of the Pöschl–Teller-type potential

3.1. Solution of the Schrödinger equation

The radial part of Schrödinger equation in spherical polar coordinate can be written as

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left(E_{n\ell} - V(r) - \frac{\hbar^2 \ell(\ell + 1)}{2\mu r^2} \right) R_{n\ell}(r) = 0, \quad (9)$$

where μ is the mass of the particle and $E_{n\ell}$ is the energy spectrum. The exact solution of Eq. (9) cannot be obtained except by using an approximation. It is found that the following approximation (Ikhdair and Falaye, 2013a,b; Ikhdair and Hamzavi, 2012)

$$\frac{1}{r^2} \approx \alpha^2 \left(4d_0 + \frac{1}{\sinh^2(\alpha r)} \right) \quad (10)$$

is a good one to the centrifugal term in short range potential, with $d_0 = 1/12$. The approximation used in Eq. (10) above is a slightly better approximation than $1/r^2 \approx \alpha^2 (d_0 + 1/\sinh^2(\alpha r))$ at certain small values of αr like when $\alpha = 0.1$. Substituting Eqs. (1) and (10) into Eq. (9), we obtain

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \left[\epsilon - \frac{\alpha^2 \ell(\ell + 1)}{\sinh^2(\alpha r)} - \alpha^2 \lambda(\lambda + 1) \tanh^2(\alpha r) \right] R_{n\ell}(r) = 0, \quad (11)$$

where

$$\epsilon = \frac{2\mu E}{\hbar^2} - 4d_0 \alpha^2 \ell(\ell + 1). \quad (12)$$

Also, if we make the substitution $s = \sinh^2(\alpha r)$, we obtain

$$\begin{aligned} \frac{d^2 R_{n\ell}(s)}{ds^2} + \frac{1/2 + s}{s(1 + s)} \frac{dR_{n\ell}(s)}{ds} + \frac{1}{s^2(1 + s)^2} \\ \left[s^2 \left(\frac{\epsilon - \tau}{4} \right) + s \left(\frac{\epsilon - \Lambda}{4} \right) - \frac{\Lambda}{4} \right] R_{n\ell}(s) = 0, \end{aligned} \quad (13)$$

where

$$\Lambda = \alpha^2 \ell(\ell + 1), \quad \tau = \alpha^2 \lambda(\lambda + 1). \quad (14)$$

Comparing Eq. (13) with Eq. (2), we have that

$$A = \frac{\tau - \epsilon}{4}, \quad B = \frac{\epsilon - \Lambda}{4}, \quad C = \frac{\Lambda}{4}$$

$$c_1 = \frac{1}{2}, \quad c_2 = -1, \quad c_3 = -1. \quad (15)$$

If we make use of Eq. (5), we obtain

$$c_4 = \frac{1}{4}, \quad c_5 = \frac{1}{2}, \quad c_6 = \frac{1}{4} + \frac{\tau - \epsilon}{4}, \quad c_7 = \frac{1}{4} - \frac{\epsilon - \Lambda}{4},$$

$$c_8 = \frac{1}{16} + \frac{\Lambda}{4}, \quad c_9 = \frac{1}{16} + \frac{\tau}{4}, \quad c_{10} = 1 + 2\zeta,$$

$$c_{11} = -2 + 2(\gamma - \zeta), \quad c_{12} = \frac{1}{4} + \zeta, \quad c_{13} = \frac{1}{2} - (\gamma - \zeta), \quad (16)$$

where

$$\gamma = \sqrt{\frac{1}{16} + \frac{\tau}{4}}, \quad \zeta = \sqrt{\frac{1}{16} + \frac{\Lambda}{4}}. \quad (17)$$

Substituting Eq. (16) into Eq. (3), we obtain after simplification

$$\epsilon = -4n^2 - 4n + 8n\gamma + 4\gamma - 8n\zeta - 4\zeta - \frac{3}{2} - \Lambda + 8\gamma\zeta, \quad (18)$$

from which we obtain the energy eigenvalues as

$$E_{n\ell} = \frac{\hbar^2}{2\mu} \left[4d_0\alpha^2\ell(\ell+1) - 4n^2 - 4n + 8n\gamma + 4\gamma - 8n\zeta - 4\zeta - \frac{3}{2} - \Lambda + 8\gamma\zeta \right], \quad (19)$$

where $n = 0, 1, 2, \dots, [\lambda]$ and $[\lambda]$ denotes the largest integer inferior to λ . Also, substituting Eq. (16) into Eq. (4), we obtain the wave function as

$$R_{n\ell} = s^{\frac{1}{4} + \zeta} (1+s)^{\frac{1}{4} - \gamma} P_n^{(2\zeta, -2\gamma)} (1+2s). \quad (20)$$

The numerical results of the energy eigenvalues for the non-relativistic Pöschl–Teller-type potential are obtained in Table 1 for $\ell = 0$ (s-wave), and compared with the result obtained in Ref. (Chen et al., 2013) where the s-wave state of the Pöschl–Teller-type potential was studied. It can be observed that our results are in good agreement. It can also be noticed from Fig. 1 that the energy eigenvalue increases with increasing n and ℓ .

3.2. Solutions of the Klein–Gordon equation

The radial part of time-independent Klein–Gordon equation with equal scalar $S(r)$ and vector $V(r)$ potentials, describing spin-zero particle can be written as

Table 1 Energy eigenvalues for the non-relativistic Pöschl–Teller-type potential with $\lambda = 50$, $\hbar = 2\mu = 1$, $\alpha = 1$, $\ell = 0$.

n	E_n (our result)	E_{n+1} (Ref. Chen et al., 2013)
0	149.00	149.00
1	341.00	341.00
2	525.00	525.00
3	701.00	701.00
4	869.00	869.00
5	1029.0	1029.0
6	1181.0	1181.0
7	1325.0	1325.0
8	1461.0	1461.0
9	1589.0	1589.0
10	1709.0	1709.0

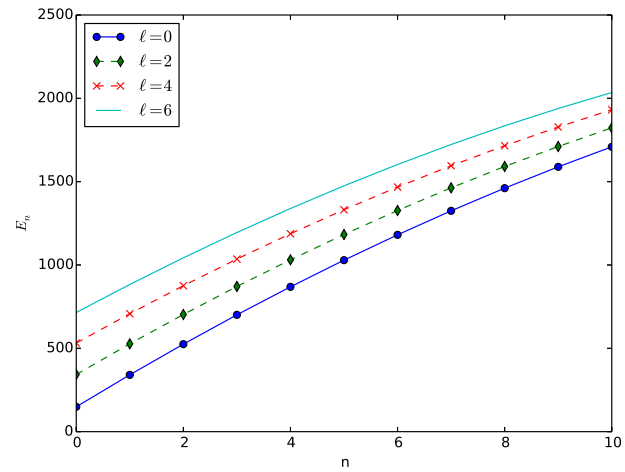


Figure 1 Energy eigenvalues of the non-relativistic Pöschl–Teller potential against n for various values of ℓ with $\alpha = 1$.

$$\left\{ \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{1}{\hbar^2 c^2} [E^2 - M^2 c^4] - \frac{2}{\hbar^2 c^2} [E + M c^2] V(r) \right\} u(r) = 0, \quad (21)$$

where E refers to the energy spectrum and M is the rest mass of the confined particle. If we make use of Eqs. (1) and (10), we obtain

$$\frac{d^2 u(r)}{dr^2} + \left[\epsilon - \frac{\Lambda}{\sinh^2 \alpha r} - \kappa \tanh^2 \alpha r \right] u(r) = 0, \quad (22)$$

where

$$\epsilon = \frac{E^2 - M^2 c^4}{\hbar^2 c^2} - 4\alpha^2 d_0 \ell(\ell+1), \quad \kappa = \frac{(E + M c^2)}{M c^2} \alpha^2 \lambda(\lambda+1). \quad (23)$$

Substituting $s = \sinh^2(\alpha r)$ in Eq. (22), we obtain

$$\frac{d^2 u(s)}{ds^2} + \frac{1/2 + s}{s(1+s)} \frac{du(s)}{ds} + \frac{1}{s^2(1+s)^2} \left[s^2 \frac{(\epsilon - \kappa)}{4} + s \frac{(\epsilon - \Lambda)}{4} - \frac{\Lambda}{4} \right] u(s) = 0. \quad (24)$$

Comparing Eq. (24) with Eq. (2), we have that

$$A = \frac{\kappa - \epsilon}{4}, \quad B = \frac{\epsilon - \Lambda}{4}, \quad C = \frac{\Lambda}{4}$$

$$c_1 = \frac{1}{2}, \quad c_2 = -1, \quad c_3 = -1. \quad (25)$$

Using Eqs. (5) and (25), we obtain

$$c_4 = \frac{1}{4}, \quad c_5 = \frac{1}{2}, \quad c_6 = \frac{1}{4} + \frac{\kappa - \epsilon}{4}, \quad c_7 = \frac{1}{4} - \frac{\epsilon - \Lambda}{4},$$

$$c_8 = \frac{1}{16} + \frac{\Lambda}{4}, \quad c_9 = \frac{1}{16} + \frac{\kappa}{4}, \quad c_{10} = 1 + 2\zeta,$$

$$c_{11} = -2 + 2(\delta - \zeta), \quad c_{12} = \frac{1}{4} + \zeta, \quad c_{13} = \frac{1}{2} - (\delta - \zeta), \quad (26)$$

where

$$\delta = \sqrt{\frac{\kappa}{4} + \frac{1}{16}}, \quad \zeta = \sqrt{\frac{\Lambda}{4} + \frac{1}{16}}. \quad (27)$$

Substituting Eq. (26) into Eq. (3), we obtain after simplification

$$\varepsilon = -4n^2 - 4n + 8n\delta + 4\delta - 8n\zeta - 4\zeta - \frac{3}{2} - \Lambda + 8\delta\zeta, \quad (28)$$

from which we obtain the relativistic energy eigenvalues as

$$E_{n\ell} = \left[h^2 c^2 \left(-4n^2 - 4n + 8n\delta + 4\delta - 8n\zeta - 4\zeta - \frac{3}{2} - \Lambda + 8\delta\zeta + 4x^2 d_0 \ell(\ell+1) \right) + M^2 c^4 \right]^{\frac{1}{2}}. \quad (29)$$

The wave function is also obtained as

$$u_{n\ell} = s^{\frac{1}{2}+\zeta} (1+s)^{\frac{1}{2}-\delta} P_n^{(2\zeta, -2\delta)}(1+2s). \quad (30)$$

The numerical results of the eigenvalues for the relativistic Pöschl–Teller-type potential are displayed in Table 2 for some values of n and ℓ . It is observed that when $\ell(n)$ is kept constant, the energy eigenvalue increases with increasing $n(\ell)$.

4. Thermodynamic properties

To study the thermodynamic properties of the Pöschl–Teller-type potential, we first obtain the vibrational partition function defined as

$$Z(\beta) = \sum_{n=0}^{[\lambda]} e^{-\beta E_n}, \quad (31)$$

where $\beta = 1/kT$, k is the Boltzmann constant and $[\lambda]$ is the largest integer inferior to λ , the potential depth. The principal quantum number n ranges from 0, 1, 2, ... $[\lambda]$. In the classical limit, at high temperature T for large $[\lambda]$, the sum can be replaced by an integral and $[\lambda]$ can be replaced by λ (since $[\lambda] = \lambda - 1$). By substituting Eq. (19) into Eq. (31) and replacing the sum by an integral, the partition function for the Pöschl–Teller-type potential gives, for large λ :

$$Z(\beta) = \int_0^\lambda e^{-\beta E_n} dn = \sqrt{\frac{m\pi}{8\beta\hbar^2}} e^{-J} \left[\operatorname{erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} Q \right) - \operatorname{erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} L \right) \right], \quad (32)$$

where

$$J = \frac{\hbar^2 \beta}{12\mu} [2\ell(\ell+1)\alpha^2 + 3(-1+8\gamma^2+8\zeta^2-2\Lambda)],$$

$$L = 1 - 2\gamma + 2\zeta, \quad Q = 1 - 2\gamma + 2\zeta + 2\lambda,$$

$$\operatorname{erfi}(z) = \frac{\operatorname{erf}(iz)}{i}, \quad \operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt. \quad (33)$$

The thermodynamic properties can now be obtained from the partition function as follows:

Table 2 Energy eigenvalues for the relativistic Pöschl–Teller-type potential with $\lambda = 50$, $\hbar = 2M = c = 1$, $\alpha = 1$.

ℓ	n	$E_{n\ell}$
0	0	-0.488561, 7.66370
0	1	-0.440421, 13.1143
0	2	-0.352923, 17.3663
0	3	-0.226206, 20.9756
1	1	-0.439820, 13.1606
1	2	-0.351936, 17.4046
1	3	-0.224834, 21.0089
1	4	-0.058249, 24.1800
2	2	-0.350064, 17.4771
2	3	-0.222230, 21.0717
2	4	-0.054909, 24.2360
2	5	0.152284, 27.0754

(1) The vibrational mean energy U :

$$U(\beta) = -\frac{\partial}{\partial \beta} \ln Z(\beta) \quad (34)$$

$$U(\beta) = \frac{-1}{\sqrt{\mu\Omega}} \left\{ e^J \sqrt{\frac{8\hbar^2 \beta}{\pi}} \left[\sqrt{\frac{\mu\pi}{8\hbar^2 \beta}} e^{-J} \left(\frac{\hbar Q}{\sqrt{2\mu\pi\beta}} e^{\frac{\hbar^2 \beta L^2}{2\mu}} - \frac{\hbar L}{\sqrt{2\mu\pi\beta}} e^{\frac{\hbar^2 \beta Q^2}{2\mu}} \right) \right. \right. \\ \left. \left. - \frac{1}{4\hbar\beta^{3/2}} \sqrt{\frac{\mu\pi}{2}} e^{-J} \Omega - \frac{1}{24\sqrt{\mu\beta}} e^{-J} \sqrt{\frac{\hbar^2 \pi}{2}} \Upsilon \Omega \right] \right\}, \quad (35)$$

where

$$\Upsilon = 2\ell(\ell+1)\alpha^2 + 3(-1+8\gamma^2+8\zeta^2-2\Lambda),$$

$$\Omega = \operatorname{erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} Q \right) - \operatorname{erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} L \right). \quad (36)$$

(2) Vibrational specific heat C :

$$C(\beta) = \frac{\partial U}{\partial T} = -k\beta^2 \frac{\partial U}{\partial \beta}. \quad (37)$$

$$C(\beta) = -\frac{k\beta^2}{\sqrt{\mu\Omega}} \left\{ 2e^J \sqrt{\frac{2\hbar^2}{\pi}} \Phi \left[\sqrt{\frac{\mu\pi}{8\hbar^2 \beta}} e^{-J} \Phi - \sqrt{\frac{\mu\pi}{32\hbar^2 \beta^3}} e^{-J} \Omega - \frac{1}{24} \sqrt{\frac{\hbar^2 \pi}{2\mu\beta}} e^{-J} \Upsilon \Omega \right] \right. \\ + \frac{k\beta^{3/2}}{\sqrt{\mu\Omega}} \left\{ e^J \sqrt{\frac{2\hbar^2}{\pi}} \left[\sqrt{\frac{\mu\pi}{8\hbar^2 \beta}} e^{-J} \Phi - \sqrt{\frac{\mu\pi}{32\hbar^2 \beta^3}} e^{-J} \Omega - \frac{1}{24} \sqrt{\frac{\hbar^2 \pi}{2\mu\beta}} e^{-J} \Upsilon \Omega \right] \right\} \\ + \frac{k\beta^2}{\sqrt{18\mu^3 \pi \Omega}} \left\{ e^J \hbar^3 \sqrt{\beta \Upsilon} \left[\sqrt{\frac{\mu\pi}{8\hbar^2 \beta}} e^{-J} \Phi - \sqrt{\frac{\mu\pi}{32\hbar^2 \beta^3}} e^{-J} \Omega - \frac{1}{24} \sqrt{\frac{\hbar^2 \pi}{2\mu\beta}} e^{-J} \Upsilon \Omega \right] \right\} \\ + \frac{k\beta^2}{\sqrt{\mu\Omega}} \left\{ e^J \sqrt{\frac{8\hbar^2}{\pi}} \left[\frac{-1}{2\hbar\beta^{3/2}} e^{-J} \sqrt{\frac{\mu\pi}{2}} \Phi + \sqrt{\frac{\mu\pi}{8\hbar^2 \beta}} e^{-J} \left(\frac{e^{\hbar^2 \beta L^2/2\mu} \hbar L}{\sqrt{8\mu\pi\beta^3}} \right. \right. \right. \\ \left. \left. - \frac{e^{\hbar^2 \beta Q^2/2\mu} \hbar^3 L^3}{\sqrt{8\mu^3 \pi \beta}} - \frac{e^{\hbar^2 \beta Q^2/2\mu} \hbar Q}{\sqrt{8\mu\pi\beta^3}} + \frac{e^{\hbar^2 \beta Q^2/2\mu} \hbar^3 Q^3}{\sqrt{8\mu^3 \pi \beta}} \right) - \frac{1}{12} \sqrt{\frac{\hbar^2 \pi}{2\mu\beta}} e^{-J} \Phi \Upsilon \right. \right. \\ \left. \left. + \frac{9}{8} \sqrt{\frac{\mu\pi}{2\hbar^2 \beta^5}} e^{-J} \Omega + \frac{1}{24} \sqrt{\frac{\hbar^2 \pi}{2\mu\beta^3}} e^{-J} \Upsilon \Omega + \frac{\hbar^3}{288\mu^{3/2}} \sqrt{\frac{\pi}{2\beta}} e^{-J} \Upsilon^2 \Omega \right] \right\}, \quad (38)$$

where

$$\Phi = \frac{\hbar Q}{\sqrt{2\mu\pi\beta}} e^{\frac{\hbar^2 \beta L^2}{2\mu}} - \frac{\hbar L}{\sqrt{2\mu\pi\beta}} e^{\frac{\hbar^2 \beta Q^2}{2\mu}}. \quad (39)$$

(3) Vibrational mean free energy F :

$$F(\beta) = -kT \ln Z(\beta) \quad (40)$$

$$F(\beta) = -\frac{1}{\beta} \ln \left\{ \sqrt{\frac{m\pi}{8\beta\hbar^2}} e^{-J} \left[\operatorname{Erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} Q \right) - \operatorname{Erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} L \right) \right] \right\}. \quad (41)$$

(4) Vibrational entropy S :

$$S(\beta) = k \ln Z(\beta) + kT \frac{\partial}{\partial T} \ln Z(\beta) = k \ln Z(\beta) - k\beta \frac{\partial}{\partial \beta} \ln Z(\beta). \quad (42)$$

$$S(\beta) = k \ln \left\{ \sqrt{\frac{m\pi}{8\beta\hbar^2}} e^{-J} \left[\operatorname{Erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} Q \right) - \operatorname{Erfi} \left(\hbar \sqrt{\frac{\beta}{2\mu}} L \right) \right] \right\} \\ - \frac{1}{\sqrt{\mu T \Omega}} \left\{ e^J \sqrt{\frac{8\hbar^2 \beta}{\pi}} \left[\sqrt{\frac{\mu\pi}{8\hbar^2 \beta}} e^{-J} \left(\frac{\hbar Q}{\sqrt{2\mu\pi\beta}} e^{\frac{\hbar^2 \beta L^2}{2\mu}} - \frac{\hbar L}{\sqrt{2\mu\pi\beta}} e^{\frac{\hbar^2 \beta Q^2}{2\mu}} \right) \right. \right. \\ \left. \left. - \frac{1}{4\hbar\beta^{3/2}} \sqrt{\frac{\mu\pi}{2}} e^{-J} \Omega - \frac{1}{24\sqrt{\mu\beta}} e^{-J} \sqrt{\frac{\hbar^2 \pi}{2}} \Upsilon \Omega \right] \right\} \quad (43)$$

The plots of the thermodynamics properties against λ for the diatomic molecules HCl and H₂ with $\beta = 0.001$ are shown in Figs. 2–6. The spectroscopic constants of the diatomic molecules studied in this work are displayed in Table 3 and taken from (Yahya et al., 2014a). We have also used the conversions $\hbar c = 1973.29 \text{ eV } \text{\AA}^{-1}$ and $1 \text{ amu} = 931.494028 \times 10^6 \text{ eV } c^{-2}$. It is observed from Fig. 2 that the partition function Z decreases monotonically with increasing λ for the two diatomic molecules considered, and reaches a constant value for some typical values of λ . From the variations of the mean energy U with λ in Fig. 3, it can be observed that the vibrational mean energy initially decreased to a minimum after which it increases with increasing λ for the two diatomic molecules studied. Fig. 4 shows that the vibrational specific heat decreases exponentially with increasing λ unlike the vibrational mean free energy F that increases monotonically with increasing λ for the two diatomic molecules, as depicted in Fig. 5. In Fig. 6, the variations of the vibrational entropy S with λ are shown. It is observed that the vibrational entropy decreases monotonically with increasing λ .

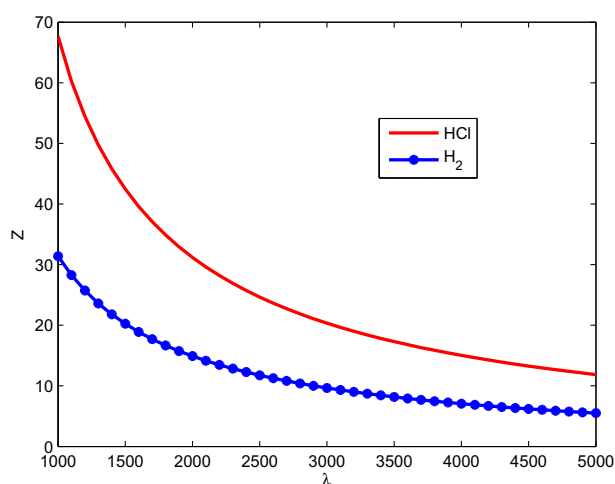


Figure 2 Vibrational partition function Z against λ for the diatomic molecules HCl and H₂ with $\beta = 0.001$.

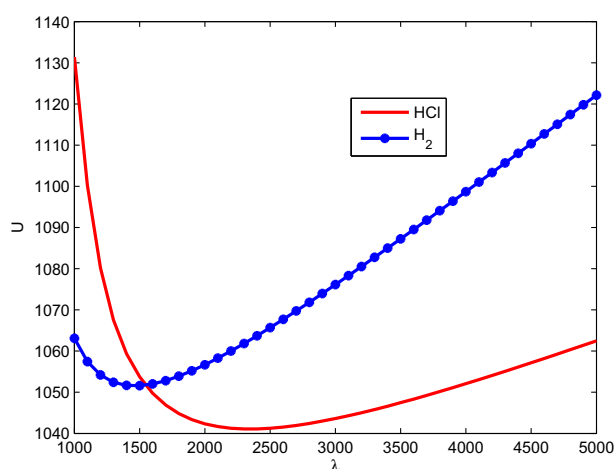


Figure 3 Vibrational mean energy U against λ for the diatomic molecules HCl and H₂ with $\beta = 0.001$.

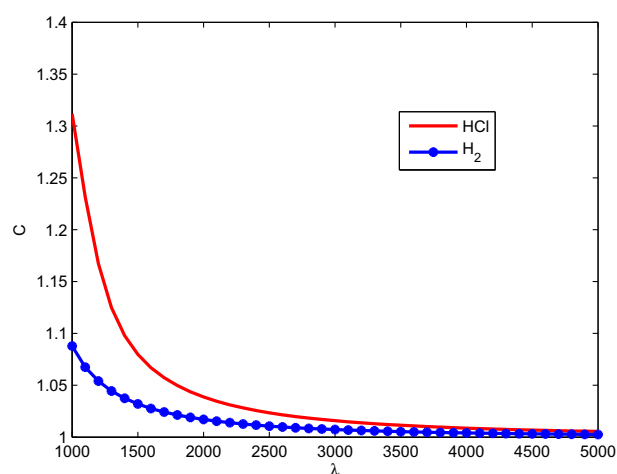


Figure 4 Vibrational specific heat C against λ for the diatomic molecules HCl and H₂ with $\beta = 0.001$.

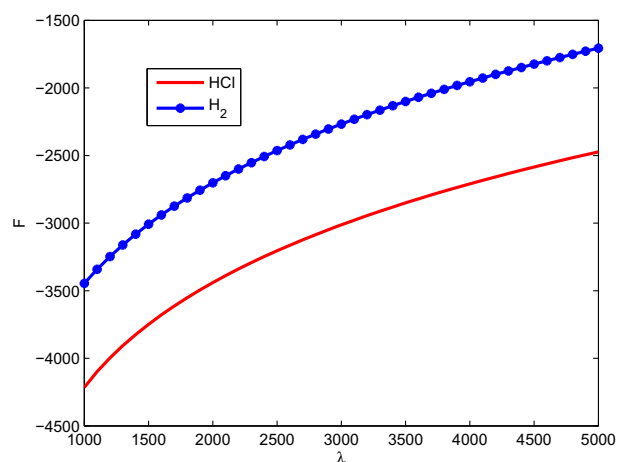


Figure 5 Vibrational mean energy F against λ for the diatomic molecules HCl and H₂ with $\beta = 0.001$.

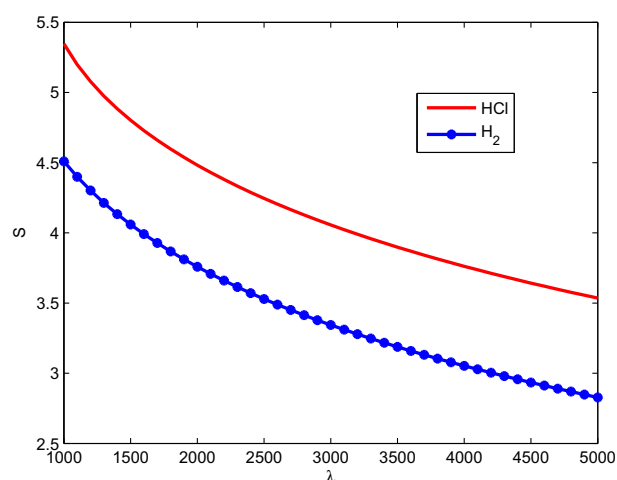


Figure 6 Vibrational entropy S against λ for the diatomic molecules HCl and H₂ with $\beta = 0.001$.

Table 3 Spectroscopic constants of the diatomic molecules studied in this work.

Molecule	μ (amu)	α ($\text{\AA}^{-1}$)
HCl	0.9801045	1.8677
H_2	0.5039100	1.9425

5. Conclusion

The solutions of the Pöschl–Teller-type potential for the Schrödinger and Klein–Gordon equations have been obtained via the parametric Nikiforov–Uvarov method. We made comparison between the energy eigenvalues obtained for the Schrödinger equation (when $\ell = 0$) and that of the result obtained in the literature where s-wave ($\ell = 0$) state of the Pöschl–Teller-type potential was considered in the non-relativistic case. The results are in perfect agreement. We have also obtained, from the high temperature partition function, the thermodynamic properties such as vibrational mean energy, vibrational specific heat, vibrational mean free energy and vibrational entropy for the model potential. From the plots of the various thermodynamic properties with λ , we have observed that the vibrational entropy and vibrational specific heat decrease with increasing λ while the vibrational free energy F increases monotonically with increasing λ . The mean energy U on the other hand initially decreases to a minimum after which it continues to rise with increase in λ .

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