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Klein–Gordon equation and thermodynamic properties with the Hua plus modified Eckart potential (HPMEP)

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Abstract We apply the Nikiforov–Uvarov method to solve the Klein–Gordon equation with the Hua plus modified Eckart potential (HPMEP). The energy eigenvalues and corresponding wave functions are obtained analytically. We show that in the non-relativistic limit, the solution of Klein–Gordon equation reduces to that of Schrodinger equation. Special cases of HPMEP such as modified Eckart, Hua, Morse and Poschl–Teller Potentials are also reported. Furthermore, the partition function and other thermodynamic properties are studied for H_2, CO, NO and N_2 molecules.

1 Introduction

Since the inception of quantum mechanics, the study of exactly solvable potentials has attracted research interest in many areas of physics. Studies on exponential-type potentials are known [1–4]. The exponential potential of interest in this study is the Hua plus modified Eckart potential (HPMEP). This potential has been reported with respect to some wave equations [5–7]. The HPMEP is a superposition of the Hua potential [8, 9] and Eckart potential [10] in modified version. In molecular physics and quantum chemistry, the Hua potential is widely applied as an intermolecular potential. The Hua potential has been investigated within the framework of relativistic and non-relativistic wave equations [11–13] and reduces to the Morse potential [14] when the deformation parameter, q, equals zero. The Eckart potential is very useful in chemical physics [15, 16] and has been investigated in the fields of quantum mechanics (relativistic and non-relativistic aspects) [17, 18]. Dong et al. [19] derived the bound states of Schrodinger equation with Eckart potential via approximate technique. In a related work, the authors in Ref. [20] obtained scattering states of l-wave Schrodinger equation for Eckart potential. The bound and scattering state of l-wave Klein–Gordon equation for mixed Eckart potentials are reported [21]. Other reports on Eckart potential can also be found in Refs. [22, 23].

Recently, the study of thermodynamic properties in various potential models has become the subject of research [24–27]. This has become possible through statistical mechanics which allows the interpretation of thermodynamic properties of a system [28, 29]. In Sta-

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tistical physics, the partition function [30] contains the whole thermodynamic information such as the entropy, the free energy, the specific heat and internal energy. Within the last decade, the thermodynamic properties have been studied in various potential models such as deformed Hylleraas plus deformed Woods–Saxon potential [31], screened Kratzer potential [32], Mobius square potential [33], improved Tietz potential [34], Morse potential [35], improved deformed exponential-type potential [29], improved Rosen–Morse potential [36], improved Manning–Rosen potential [37], improved Tietz potential [38], general molecular potential [39] and others. Further literature on the thermodynamic properties of various systems can be found in Refs. [40–44]. However, thermodynamic properties with HPMEP have not been studied, which is a motivation for the present work.

In relativistic limits, the motion of a particle is described using either Klein–Gordon or Dirac equations [45, 46] depending on the particle's spin. The spin-zero particles are reported by the Klein–Gordon equation. Klein–Gordon equation with equal scalar-vector potential is very interesting. The Klein–Gordon equation with various potentials is vital because one can discuss the physics and properties of a system described by such solutions. Many techniques are applied to solve Klein–Gordon equation for various potentials. These techniques include Nikiforov–Uvarov (NU) method [47–51], factorization method [52], path integral method [53], Ansatz method [54, 55] etc. The exact solutions of the Klein–Gordon equation with equal scalar and vector ring-shaped potentials have been reported [56]. The Klein–Gordon equation with equal scalar and vector Mobius square potential has been reported [57]. A number of studies on Klein–Gordon equation in different potentials abound in literature [58–62]. The study is therefore aimed at investigating thermodynamic properties of Klein–Gordon equation with HPMEP. To achieve this, we solved the Klein–Gordon equation to derive the energy levels and corresponding wave functions. Then, we can obtain the thermodynamic properties. The HPMEP is expressed as [5–7]

$$V(r) = V_0 + V_1 \left(\frac{1 - e^{-2\alpha r}}{1 - q e^{-2\alpha r}} \right)^2 + V_2 \left(\frac{4 e^{-2\alpha r}}{1 - q e^{-2\alpha r}} \right) + V_3 \left(\frac{1 + e^{-2\alpha r}}{1 - q e^{-2\alpha r}} \right), \quad (1)$$

where V_0, V_1, V_2, V_3, α and q are constants.

2 Klein–Gordon equation in D-dimensions

The D-dimensional Klein–Gordon equation ($c = 1$) is [63]

$$\left(\hbar^2 \nabla_D^2 - (\mu + S(r))^2 + (E - V(r))^2 \right) \Psi(r, \Omega_D) = 0, \quad (2)$$

D is the spatial dimensionality, $D \geq 2$, ∇_D^2 is the D-dimensional Laplace operator, $S(r)$ and $V(r)$ are, respectively, the attractive scalar and repulsive vector potentials, c and E are the speed of light and relativistic energy, respectively.

$$\Psi(r, \Omega_D) = r^{-\frac{D-1}{2}} R_{nl}(r) \Upsilon_{lm}(\Omega_D), \quad (3)$$

where $\Upsilon_{lm}(\Omega_D)$ is the spherical harmonic function. The eigenvalues equation for the generalized angular momentum operator is $L_D^2 \Upsilon_{lm}(\Omega_D) = l(l + D - 2)\Upsilon_{lm}(\Omega_D)$. With this we write the radial D-dimensional Klein–Gordon equation as.

$$\left[\hbar^2 \frac{d^2}{dr^2} + \left(E^2 - \mu^2 \right) - 2(\mu S(r) + E V(r)) + V^2(r) - S^2(r) - \frac{K(K + 1)\hbar^2}{r^2} \right] R_{nl}(r) = 0, \quad (4)$$

where $K = l + \frac{1}{2}(D-3)$, n and l are the radial and orbital angular momentum quantum numbers. For equal scalar and vector potentials, i.e., $S(r) = V(r)$, Eq. (4) becomes

$$\left[\hbar^2 \frac{d^2}{dr^2} + (E^2 - \mu^2) - 2(\mu + E)\, V(r) - \frac{K(K+1)\hbar^2}{r^2}\right] R_{nl}(r) = 0 \qquad (5)$$

Adopting Alhaidari et al.'s scheme [64], we rescale the potential under the non-relativistic limit as $V(r) = S(r) \rightarrow \frac{V(r)}{2}$ and setting, $V(r) = V_0 + V_1\left(\frac{1-e^{-2\alpha r}}{1-qe^{-2\alpha r}}\right)^2 + V_2\left(\frac{4e^{-2\alpha r}}{1-qe^{-2\alpha r}}\right) + V_3\left(\frac{1+e^{-2\alpha r}}{1-qe^{-2\alpha r}}\right)$, thus, Eq. (5) becomes

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\left(\frac{E^2 - \mu^2}{\hbar^2}\right) + \left(\frac{\mu + E}{\hbar^2}\right)\left\{V_0 + V_1\left(\frac{1-e^{-2\alpha r}}{1-qe^{-2\alpha r}}\right)^2 \right.\right.$$
$$\left.\left. + V_2\left(\frac{4e^{-2\alpha r}}{1-qe^{-2\alpha r}}\right) + V_3\left(\frac{1+e^{-2\alpha r}}{1-qe^{-2\alpha r}}\right)\right\} - \frac{K(K+1)}{r^2}\right] R_{nl}(r) = 0 \qquad (6)$$

To solve Eq. (6), we include the approximation [65]

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{\left(1 - qe^{-2\alpha r}\right)^2}. \qquad (7)$$

Inserting Eq. (7) in Eq. (6) and using $s = e^{-2\alpha r}$ gives

$$\frac{d^2 R(s)}{ds^2} + \frac{(1-qs)}{s(1-qs)}\frac{dR(s)}{ds} + \frac{-\Omega s^2 + \varphi s - \chi}{s^2(1-qs)^2} R(s) = 0, \qquad (8)$$

where

$$\Omega = -\left(\varepsilon_1 q^2 - \varepsilon_2 V_0 q^2 - \varepsilon_2 V_1 + \varepsilon_2 V_3 q^2\right), \qquad (9)$$

$$\phi = 2\varepsilon_2 V_0 q + 2\varepsilon_2 V_1 - 4\varepsilon_2 V_2 + \varepsilon_2 V_3(q-1) - 2\varepsilon_1 q - k(k+1), \qquad (10)$$

$$\chi = -(\varepsilon_1 - \varepsilon_2 V_0 - \varepsilon_2 V_1 - \varepsilon_2 V_3), \qquad (11)$$

with

$$\left.\begin{array}{c}\varepsilon_1 = \dfrac{E^2 - \mu^2}{4\alpha^2} \\[2mm] \varepsilon_2 = \dfrac{E^2 + \mu^2}{4\alpha^2}\end{array}\right\} \qquad (12)$$

To get the eigenvalues and eigenfunctions, we solve Eq. (8) using NU method [47–51]. First, we consider the equation:

$$\frac{d^2\psi(s)}{ds^2} + \frac{c_1 - c_2 s}{s(1-c_3 s)}\frac{d\psi(s)}{ds} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{s^2(1-c_3 s)^2}\psi(s) = 0. \qquad (13)$$

Applying parametric NU method [48], we have solution of Eq. (13) as

$$\psi(s) = N_{nl}\, s^{c_{12}}(1 - c_3 s)^{-c_{12} - \left(\frac{c_{13}}{c_3}\right)} P_n^{\left(c_{10} - 1,\, \frac{c_{11}}{c_3} - c_{10} - 1\right)}(1 - 2c_3 s), \qquad (14)$$

where $P_n^{(\alpha, \beta)}$ are Jacobi polynomials. The equation of the energy is expressed as:

$$(c_2 - c_3)n + \alpha_3 n^2 - (2n+1)c_5 + (2n+1)(\sqrt{c_9} + c_3\sqrt{c_8}) + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0, \qquad (15)$$

with

$$
\left.
\begin{aligned}
& c_4 = \frac{1}{2}(1 - c_1), \ c_5 = \frac{1}{2}(c_2 - 2c_3), \ c_6 = c_5^2 + \xi_1, \ c_7 = 2c_4c_5 - \xi_2, \\
& c_8 = c_4^2 + \xi_3, \ c_9 = c_3c_7 + c_3^2 c_8 + c_6, \ c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}, \\
& c_{11} = c_2 - 2c_5 + 2\left(\sqrt{c_9} + c_3\sqrt{c_8}\right), \ c_{12} = c_4 + \sqrt{c_8}, \ c_{13} = c_5 - \left(\sqrt{c_9} + c_3\sqrt{c_8}\right).
\end{aligned}
\right\}
\tag{16}
$$

Comparing Eqs. (13) with (8), we obtain

$$
\left.
\begin{aligned}
& c_1 = 1, c_2 = c_3 = q, c_4 = 0, c_5 = -\frac{q}{2}, c_6 = \frac{q^2}{4} + \Omega, c_7 = -\varphi, c_8 = \chi, c_9 = -q\varphi + q^2\chi + \Omega + \frac{q^2}{4} \\
& c_{10} = 1 + 2\sqrt{\chi}, c_{11} = 2\left(1 + \sqrt{\chi}\right) + \frac{1}{2}\sqrt{4\varepsilon_2\left(V_1(q-1)^2 + 4qV_2\right) + 4qK(K+1) + q^2}, c_{12} = \sqrt{\chi}, \\
& c_{13} = -\frac{1}{2}\sqrt{4\varepsilon_2\left(V_1(q-1)^2 + 4qV_2\right) + 4qK(K+1) + q^2} - q\left(\frac{1}{2} + \sqrt{\chi}\right)
\end{aligned}
\right\}
\tag{17}
$$

Substitution of Eqs. (17) into (15) and Eq. (14) gives the energy eigenvalue as

$$
\begin{aligned}
(E^2 - \mu^2) = & (\mu + E^2)(V_0 + V_1 + V_3) \\
& - 4\alpha^2 \\
& \left(\frac{\frac{(\mu+E^2)}{4\alpha^2}(V_1(q-1) + 4V_2 + V_3(q+1)) + \frac{q}{2} + qn(n+1) + K(K+1) + \left(n+\frac{1}{2}\right)\sqrt{\frac{\mu+E}{\alpha^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4qK(K+1) + q^2}}{q + 2qn + \sqrt{\frac{\mu+E}{\alpha^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4qK(K+1) + q^2}} \right)^2
\end{aligned}
\tag{18}
$$

According to Eq. (14), the corresponding wave function is obtained as

$$
R(s) = N_{nls} s^{\sqrt{\chi}} (1 - s)^{\delta} P_n^{(2\sqrt{\chi}, 2\delta - 1)}(1 - 2qs)
\tag{19}
$$

where

$$
\delta = \frac{1}{2} + \frac{1}{2}\sqrt{\frac{2\mu}{\alpha^2\hbar^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4ql(l+1) + q^2}
\tag{20}
$$

and P_n is the Jacobi polynomial expressed as

$$
P_n^{(2\sqrt{\chi}, 2\delta - 1)}(1 - 2qs) = \frac{\Gamma\left(n + 2\sqrt{\chi} + 1\right)}{n!\,\Gamma\left(n + 2\sqrt{\chi} + 1\right)^2} F_1\left(-n, 2\sqrt{\chi} + 2\delta + n, 2\sqrt{\chi} + 1; qs\right)
\tag{21}
$$

2.1 Non-relativistic limit

In the non-relativistic limit, the transformations $E + \mu \to \frac{2\mu}{\hbar^2}$ and $E - \mu \to E$ can be used to get the corresponding non-relativistic energy of Eq. (18) as

$$
\begin{aligned}
E = & V_0 + V_1 + V_3 \\
& - \frac{2\alpha^2\hbar^2}{\mu} \\
& \left(\frac{\frac{\mu}{2\alpha^2\hbar^2}(V_1(q-1) + 4V_2 + V_3(q+1)) + \frac{q}{2} + qn(n+1) + K(K+1) + \left(n+\frac{1}{2}\right)\sqrt{\frac{2\mu}{\alpha^2\hbar^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4qK(K+1) + q^2}}{q + 2qn + \sqrt{\frac{2\mu}{\alpha^2\hbar^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4qK(K+1) + q^2}} \right)^2
\end{aligned}
\tag{22}
$$

For $D = 3$, Eq. (22) becomes

$$
\begin{aligned}
E = & V_0 + V_1 + V_3 \\
& - \frac{2\alpha^2\hbar^2}{\mu} \\
& \left(\frac{\frac{\mu}{2\alpha^2\hbar^2}(V_1(q-1) + 4V_2 + V_3(q+1)) + \frac{q}{2} + qn(n+1) + l(l+1) + \left(n+\frac{1}{2}\right)\sqrt{\frac{2\mu}{\alpha^2\hbar^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4ql(l+1) + q^2}}{q + 2qn + \sqrt{\frac{2\mu}{\alpha^2\hbar^2}\left(V_1(q-1)^2 + 4qV_2\right) + 4ql(l+1) + q^2}} \right)^2
\end{aligned}
\tag{23}
$$

3 Thermodynamic properties with HPMEP

The first step to evaluate the thermodynamic properties of any system is to establish the partition function. One can obtain all microstate energies, and thus partition function Z, which enables us to have the thermodynamic properties. The partition function for the vibrational energy is given as

$$Z(\beta, \lambda) = \sum_{n=0}^{\lambda} e^{-\beta E_{nl}}, \beta = \frac{1}{kT} \tag{24}$$

where λ is the upper bound quantum number. T and k are the absolute temperature and Boltzmann constant, respectively. Setting $l = 0$, Eq. (23) can be simplified as:

$$E = V - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{(n+\sigma)}{2} + \frac{Q}{2(n+\sigma)} \right)^2, \tag{25}$$

where

$$\left. \begin{array}{l} P = \dfrac{\mu}{2\alpha^2 \hbar^2} (V_1(q-1) + 4V_2 + V_3(q+1)), \\[2mm] \sigma = \dfrac{1}{2} + \dfrac{1}{2q} \sqrt{\dfrac{2\mu}{\alpha^2 \hbar^2} \left(V_1(q-1)^2 + 4qV_2 \right) + q^2} \\[2mm] Q = \dfrac{P + q\sigma(1-\sigma)}{q}, \\[2mm] V = V_0 + V_1 + V_2. \end{array} \right\} \tag{26}$$

Substituting Eqs. (25) into (24) gives

$$Z(\beta, \lambda) = \sum_{n=0}^{\lambda} \exp \left(-\beta \left(V - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{(n+\sigma)}{2} + \frac{Q}{2(n+\sigma)} \right)^2 \right) \right) \tag{27}$$

In the classical limit, if we set $\rho = n + \sigma$, the partition function becomes

$$Z(\beta, \lambda) = \int_0^{\lambda} e^{Y\rho^2 \beta - \frac{W}{\rho^2}\beta + X\beta} d\rho \tag{28}$$

Evaluating the integral using Maple software, the partition function becomes

$$Z(\beta, \lambda) = \frac{1}{2} e^{(\beta Y \rho^2 + X\beta)} \sqrt{\beta W} \left(\frac{2\lambda e^{\frac{\beta W}{\lambda^2}}}{\sqrt{\beta W}} - \frac{2\sqrt{\beta W}\sqrt{\pi} erfi\left(\frac{\sqrt{\beta W}}{\lambda}\right)}{\sqrt{\beta W}} - 2\sqrt{\pi} \right), \tag{29}$$

where

$$X = \frac{\alpha^2 \hbar^2 Q}{\mu} - V, Y = \frac{\alpha^2 \hbar^2}{2\mu}, W = \frac{\alpha^2 \hbar^2 Q^2}{2\mu} \tag{30}$$

The imaginary error function erf$i(x)$ is defined by

$$\text{erf}i(x) = \frac{erf(ix)}{i} = \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2} dt \tag{31}$$

Using Eq. (29), we obtain other thermodynamic properties of the HPMEP as follows:

- *Vibrational Internal Energy*

$$U(\beta,\lambda) = -\frac{\partial \ln Z(\beta,\lambda)}{\partial \beta} \qquad (32)$$

- *Vibrational Free Energy*

$$F(\beta,\lambda) = -\frac{1}{\beta}\ln Z(\beta,\lambda) \qquad (33)$$

- *Vibrational Entropy*

$$S(\beta,\lambda) = k\ln Z(\beta,\lambda) - k\beta\frac{\partial \ln Z(\beta,\lambda)}{\partial \beta} \qquad (34)$$

- *Vibrational Specific Heat Capacity*

$$C(\beta,\lambda) = k\beta^2\frac{\partial^2 \ln Z(\beta,\lambda)}{\partial \beta^2} \qquad (35)$$

4 Discussions

Our results are based on Eq. (23). Table 1 shows the spectroscopic values of the molecules [66, 67]. In Fig. 1, it is seen that for all the diatomic molecules studied, the partition function, Z, increases monotonically as β, increases. In Fig. 2, a monotonic increase in Z as the upper bound vibrational quantum number, λ, increases for all the diatomic molecules. As seen in Fig. 3, the internal energy for all the diatomic molecules decreases progressively as β increases for all the diatomic molecules. This implies that at higher temperatures, the diatomic molecules have higher values of internal energy, U. In Fig. 4, all the diatomic molecules show an increase in U as λ increases up to a value around $\lambda = 15$. Beyond this point, U tends to a constant value for the molecules. In Fig. 5, the vibrational specific heat, C, for all the molecules decreases as β increases. This implies that at lower temperatures, the diatomic molecules have lower values of vibrational specific heat and vice versa. The variation of C with upper bound vibrational quantum number, λ (Fig. 6), shows a similar trend to the variation of internal energy, U, with λ. In Fig. 7, entropy, S, is seen to decrease with increasing β for all the diatomic molecules studied, implying an increase in entropy at higher temperatures, consistent with the predictions of statistical physics. Figure 8 shows entropy increasing progressively as λ increases for all the diatomic molecules. This can be explained by the fact that the molecules gain more energy as temperature increases and are able to attain higher energy states. The variation of vibrational free energy, F, with β (Fig. 9), shows that F first increases rapidly up to a point, then the increase becomes less rapid beyond $\beta = 0.001$ for all the diatomic molecules. The variation of F with λ (Fig. 10) shows that F decreases for all the diatomic molecules as λ increases.

4.1 Cases and deductions from HPMEP

Modified Eckart Potential: Substituting $V_0 = V_1 = 0$, $q = 1$ in Eq. (1), the potential yields modified Eckart potential

$$V(r) = V_2\left(\frac{4e^{-2\alpha r}}{1 - qe^{-2\alpha r}}\right) + V_3\left(\frac{1 + e^{-2\alpha r}}{1 - qe^{-2\alpha r}}\right), \qquad (36)$$

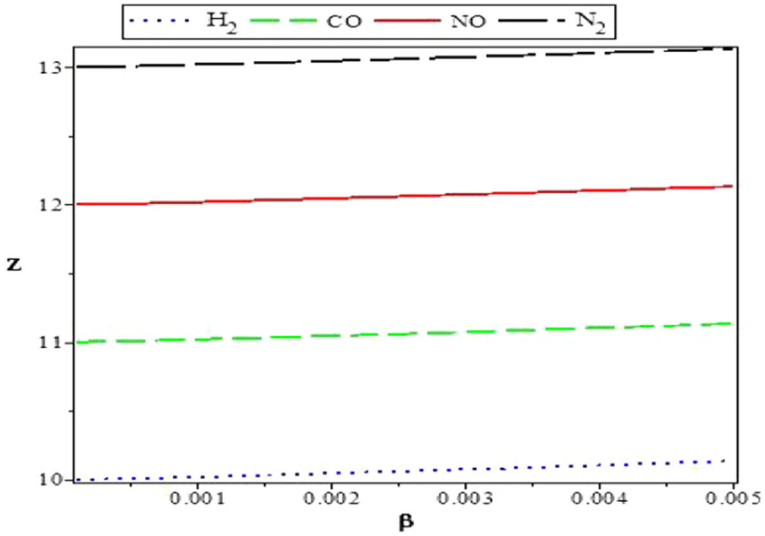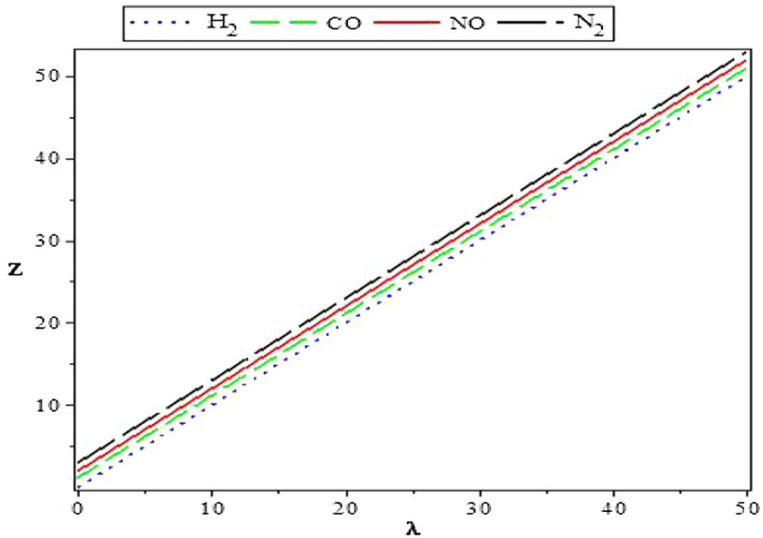| **Table 1** Spectroscopic parameters of the selected diatomic molecules [66, 67]	Molecule	μ(amu)	α (Å^{-1})
	H$_2$	0.50391	0.7416
	CO	6.8606719	1.1283
	NO	7.468441	1.1508
	N$_2$	7.00335	2.6986

Fig. 1 Variation of vibrational partition function Z with β for the selected diatomic molecules

Fig. 2 Variation of vibrational partition function Z with λ for the selected diatomic molecules
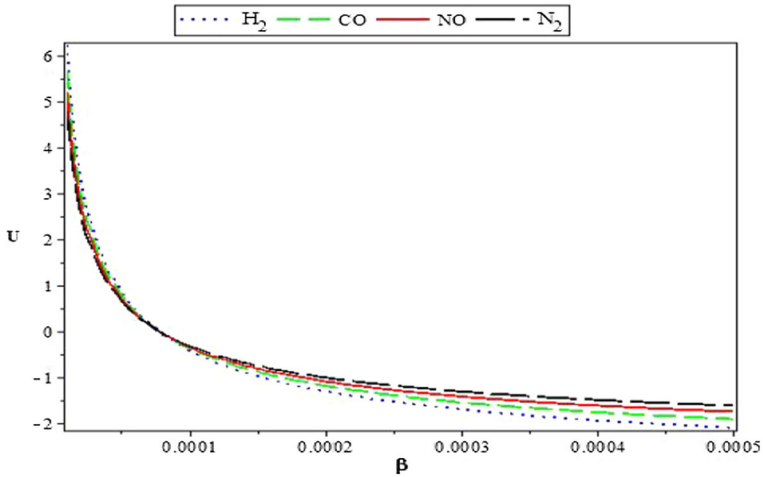
Fig. 3 Variation of vibrational internal energy U with β for the selected diatomic molecules
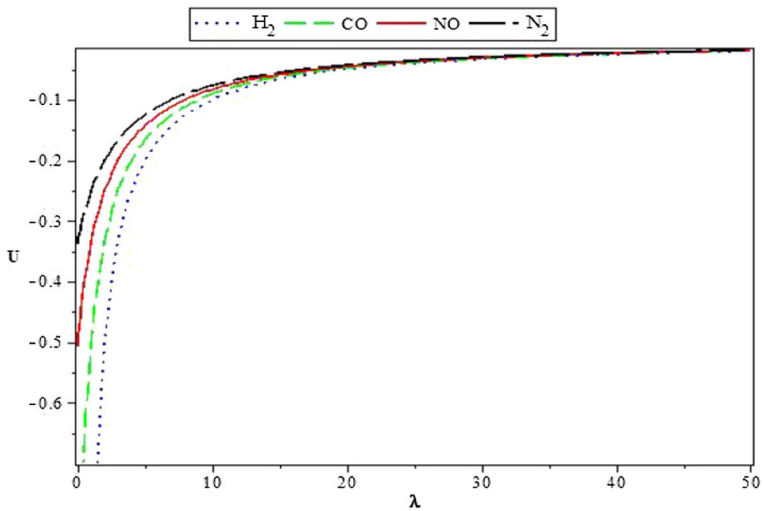
Fig. 4 Variation of vibrational internal energy U with λ for the selected diatomic molecules

with the energy equation as

$$E = V_3 - \frac{2\alpha^2\hbar^2}{\mu}\left(\frac{\frac{\mu}{2\alpha^2\hbar^2}(2V_2 + V_3) + \frac{1}{2} + n(n+1) + l(l+1) + \left(n + \frac{1}{2}\right)\sqrt{\frac{8\mu V_2}{\alpha^2\hbar^2} + (2l+1)^2}}{1 + 2n + \sqrt{\frac{8\mu V_2}{\alpha^2\hbar^2} + (2l+1)^2}}\right)^2$$

(37)

If we assign $V_3 = \alpha$, $\frac{1}{2\alpha} = a$, $V_2 = \beta$, $2V_2 + V_3 = 4\alpha$ and $\hbar = \mu = 1$, the result of Eq. (37) is seen to be consistent with Eq. (22) of Ref. [30], when expanded.
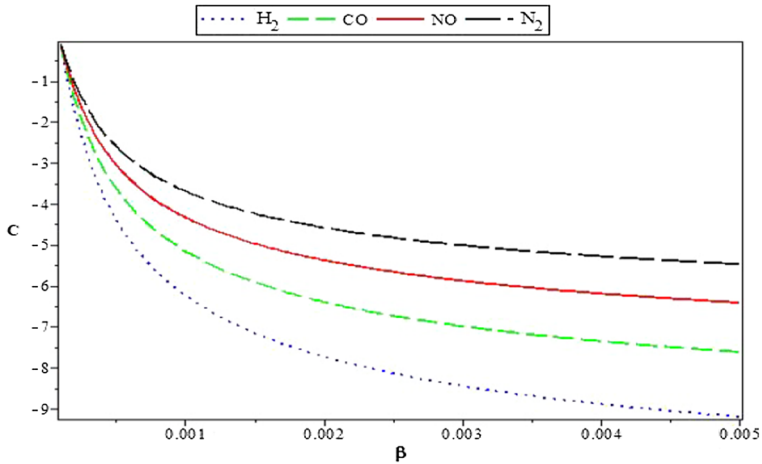
Fig. 5 Variation of vibrational specific heat capacity C with β for the selected diatomic molecules
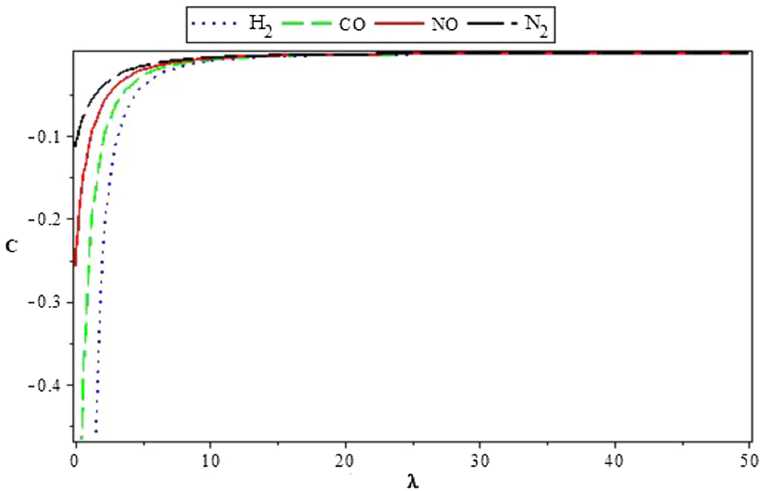

Fig. 6 Variation of vibrational specific heat capacity C with λ for the selected diatomic molecules

Hua Potential: Substituting $V_0 = V_2 = V_3 = 0$ in Eq. (1) gives the Hua potential

$$V(r) = V_1 \left(\frac{1 - e^{-2\alpha r}}{1 - q e^{-2\alpha r}} \right)^2 \tag{38}$$

with corresponding energy as

$$E = V_1 - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{\frac{\mu V_1(q-1)}{2\alpha^2 \hbar^2} + \frac{q}{2} + q\,n(n+1) + l(l+1) + \left(n + \frac{1}{2}\right)\sqrt{\frac{2\mu V_1(q-1)^2}{\alpha^2 \hbar^2} + 4ql(l+1) + q^2}}{q + 2qn + \sqrt{\frac{2\mu V_1(q-1)^2}{\alpha^2 \hbar^2} + 4ql(l+1) + q^2}} \right)^2 \tag{39}$$
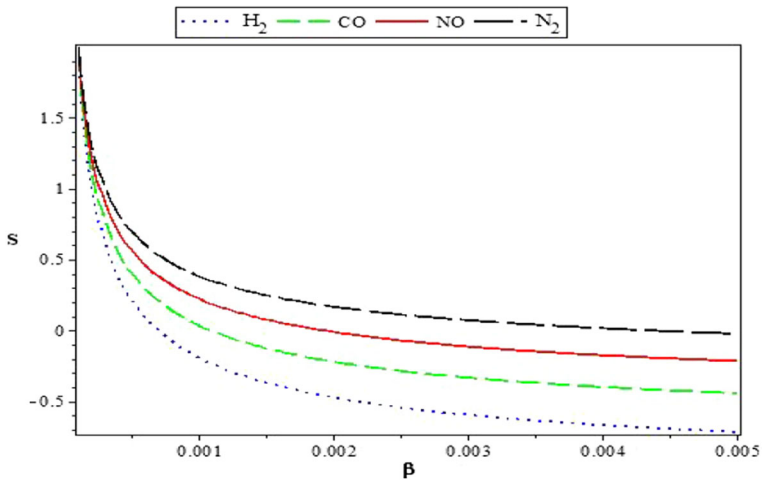
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Fig. 7 Variation of vibrational entropy for S with β for the selected diatomic molecules
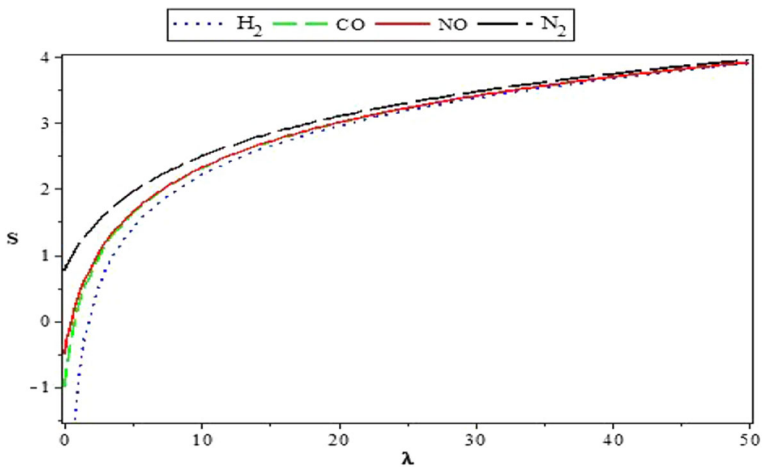

Fig. 8 Variation of vibrational entropy S with λ for the selected diatomic molecules

Morse Potential: Substituting $V_0 = V_2 = V_3 = 0, q = 0$ into Eq. (1), we have

$$V(r) = V_1\left(\frac{1 - e^{-2\alpha r}}{1 - e^{-2\alpha r}}\right)^2,\tag{40}$$

and the energy equation

$$E = V_1 - \frac{2\alpha^2\hbar^2}{\mu}\left(\frac{\frac{-\mu V_1}{2\alpha^2\hbar^2} + l(l+1) + \left(n + \frac{1}{2}\right)\sqrt{\frac{-2\mu V_1}{\alpha^2\hbar^2}}}{\sqrt{\frac{-2\mu V_1}{\alpha^2\hbar^2}}}\right)^2\tag{41}$$
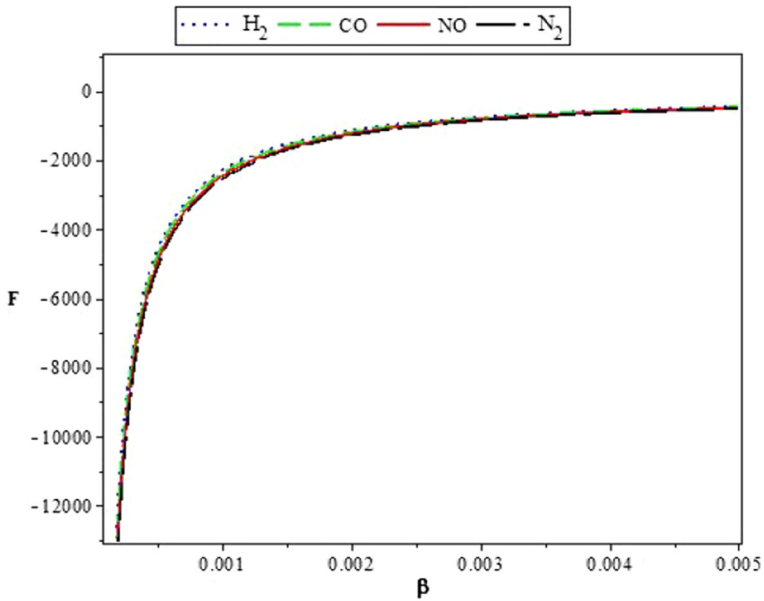
Fig. 9 Variation of vibrational free energy F with β for the selected diatomic molecules
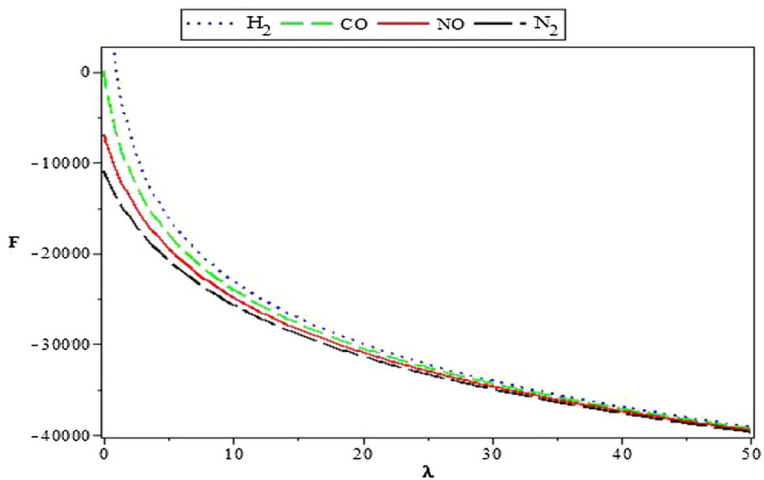

Fig. 10 Variation of vibrational free energy F with λ for the selected diatomic molecules

Poschl–Teller Potential: If we set $V_0 = V_1 = V_3 = 0$, and $q = -1$ in Eq. (1), we obtain the Poschl–Teller potential

$$V(r) = V_2\left(\frac{4e^{-2\alpha r}}{1 + e^{-2\alpha r}}\right) \tag{42}$$

with energy equation

$$E = -\frac{2\alpha^2\hbar^2}{\mu}\left(\frac{\frac{-\mu V_2}{\alpha^2\hbar^2} + \frac{1}{2} + n(n+1) + l(l+1) - \left(n+\frac{1}{2}\right)\sqrt{1 - 4l(l+1) + \frac{8\mu V_2}{\alpha^2\hbar^2}}}{1 + 2n - \sqrt{1 - 4l(l+1) + \frac{8\mu V_2}{\alpha^2\hbar^2}}}\right)^2 \quad (43)$$

The result of Eq. (43) is consistent with Eq. (20) in Ref. [68], when $V_2 = -V_1$.

5 Conclusion

This study presents the approximate solutions of Klein–Gordon equation and thermodynamic properties of HPMEP using the NU method. In the non-relativistic limit, the energy spectrum is used to calculate the partition function and other thermodynamic properties such as the internal energy U, mean free energy F, entropy S and specific heat capacity C. Various plots showing the variation of these thermodynamic properties with β and λ for H_2, CO, NO and N_2 molecules are presented. Special cases of the HPMEP are also reported and are found to be consistent with literature. Our work will find applications in molecular physics.

Author contributions CPO designed the work. IJN and CJO drafted the manuscript. AO and UMU prepared all the figures and table. EEO supervised the work. All the authors reviewed the manuscript.

Declarations

Conflict of interest The authors declare that they have no known conflict of interest.

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