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Approximate solutions, thermodynamic properties and expectation values with the Hua Plus modified Eckart (HPME) potential.

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ABSTRACT

The approximate solutions of Schrodinger equation for the Hua plus modified Eckart (HPME) potential is obtained via the Formula method. The vibrational partition function and other thermodynamic properties were investigated. Using the Hellmann-Feynman theorem, the expectation values of r^{-2} , T and p^2 and their numerical values are also presented. Some cases of this potential are also studied. The results of our study are consistent with those in literature.

Keywords: Schrodinger equation; Formula method; Hua plus modified Eckart potential; Expectation values; Thermodynamic properties

1. Introduction

For many decades, the Schrodinger equation under various interactions, has been a subject of study owing to its applications in physical systems. A major task in such studies is to obtain exact solutions. As there are many systems which do not have exact solutions, approximate solutions, despite their drawbacks, are very essential. The approximate solutions of Schrodinger equation with different potentials have been reported [1-6]. One of such potentials is the Hua plus modified Eckart (HPME) potential [2, 3]. This potential is given as

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

where $V_0, V_1, V_2, V_3, \alpha, q$ are parameters. The HPME potential reduces to Eckart potential when $V_0 = V_1 = 0$ and $q = 1$, Hua potential for $V_0 = V_2 = V_3 = 0$, and Poschl-Teller potential if $V_0 = V_1 = V_3 = 0$ and $q = -1$. It is seen that the HPME potential incorporates Eckart potential, Hua potential and Poschl-Teller potential as special cases. Interesting reports on the special cases are also known [7-10], and clearly highlights their applications in various areas of physics [11-13]. Consequently, one can describe the HPME potential as an important realistic model in physics. Some authors have investigated this potential using different methods under Dirac, Schrodinger and Klein-Gordon equations [2,3, 14-15].

Recently, many researchers have studied thermodynamic properties [16-26] and expectation values [27-30] for different systems.

The objectives of this study are as follows: First, to solve the radial Schrodinger equation for the HPME potential via the formula approach [31]. Secondly, we study the thermodynamic properties of the HPME potential. Then, finally we obtain the expectation values of the HPME potential using the Hellmann-Feynman theorem [32, 33]. This has not been reported in previous studies.

We prepare the work as follows: Section 2 contains a brief review of Formular method. The energy levels and eigenfunction are calculated in sec. 3. Sec. 4 gives the partition function and thermodynamic properties. In sect. 5, we evaluate the expectation values. Discussion of results appears in sec. 6. Finally, conclusion is presented in sec. 7.

2. Formula Method

Given the following second order hypergeometric ordinary differential equation of the form [34]

$$\frac{d^2\psi(s)}{ds^2} + \frac{c_1 - c_2s}{s(1 - c_3s)} \frac{d\psi(s)}{ds} + \frac{\xi_1s^2 + \xi_2s + \xi_3}{s^2(1 - c_2s)^2} \psi(s) = 0, \quad (2)$$

where ξ_1, ξ_2, ξ_3 are constants. A method of solving such equation was proposed by Falaye et al. [31]. To derive the energy expression, the following condition is given

$$\left[\frac{c_4^2 - c_5^2 - \left[\frac{1-2n}{2} - \frac{1}{2c_3^2} \left(c_2 - \sqrt{(c_3 - c_2)^2 - 4\xi_1} \right) \right]^2}{2 \left[\frac{1-2n}{2} - \frac{1}{2c_3^2} \left(c_2 - \sqrt{(c_3 - c_2)^2 - 4\xi_1} \right) \right]} \right]^2 - c_5^2 = 0, c_3 \neq 0, \quad (3)$$

where,

$$\left. \begin{aligned} c_4 &= \frac{(1-c_1) + \sqrt{(1-c_1)^2 - 4\xi_3}}{2} \\ c_5 &= \frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3} + \sqrt{\left(\frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3} \right)^2 - \left(\frac{\xi_1}{c_3^2} + \frac{\xi_2}{c_3} + \xi_3 \right)} \end{aligned} \right\}. \quad (4)$$

To obtain the wave function in terms of the generalized hypergeometric functions, we use

$$\psi(s) = N_n s^{c_4} (1-c_3 s)^{c_5} {}_2F_1 \left(-n, n + 2(c_4 + c_5) + \frac{c_2}{c_3} - 1; 2c_4 + c_1; c_3 s \right), \quad (5)$$

where N_n is a normalization constant.

For the case where $c_1 = c_2 = c_3 = 1$, Onate et al. [35], put forward a simplified energy equation from eq. (3)

$$\sqrt{-\xi_3} \left(1 + \sqrt{1 - 4(\xi_1 + \xi_2 + \xi_3) + 2n} \right) = \xi_3 - \xi_1 - n(n+1) - n \sqrt{1 - 4(\xi_1 + \xi_2 + \xi_3)} - \left(\frac{1}{2} + \frac{1}{2} \sqrt{1 - 4(\xi_1 + \xi_2 + \xi_3)} \right)^2. \quad (6)$$

3. Schrodinger equation for HPME potential

The Schrodinger equation in spherical coordinates is given in eq. (7) as [36]

$$-\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Psi(r, \theta, \phi) = E_{nl} \Psi(r, \theta, \phi), \quad (7)$$

E, \hbar, μ and Ψ are the energy, reduced Planck constant, reduced mass and wave function, respectively. If we set $\Psi(r, \theta, \phi) = \frac{R(r)}{r} \psi_{nl}(\theta, \phi)$ into eq. (7), the equation reduces to a radial form given as

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} (E_{nl} - V(r)) - \frac{l(l+1)}{r^2} \right] R_{nl}(r) = 0, \quad (8)$$

where n and l are the radial and orbital angular momentum quantum numbers, respectively.

If we incorporate eq. (1) into (8), we obtain

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} \left(E_{nl} - V_0 - V_1 \left(\frac{1 - e^{-2\alpha r}}{1 - qe^{-2\alpha r}} \right) - V_2 \left(\frac{4e^{-2\alpha r}}{(1 - qe^{-2\alpha r})^2} \right) - V_3 \left(\frac{1 + e^{-2\alpha r}}{1 - qe^{-2\alpha r}} \right) \right) - \frac{l(l+1)}{r^2} \right] R_{nl}(r) = 0. \quad (9)$$

An exact solution to eq. (9) is not feasible due to $\frac{1}{r^2}$. Therefore, to solve (9), an approximation must be adopted for the centrifugal term [37]

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{(1 - qe^{-2\alpha r})^2}. \quad (10)$$

Using eq. (10) in (9) and making the transformation $s = qe^{-2\alpha r}$, (9) becomes

$$\frac{d^2 R_{nl}(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR_{nl}(s)}{ds} + \frac{As^2 + Bs + C}{s^2(1-s)^2} R_{nl}(s) = 0, \quad (11)$$

where

$$A = \frac{\mu \left(E_{nl} - V_0 - \frac{V_1}{q} \right)}{2\alpha^2 \hbar^2}, \quad (12)$$

$$B = \frac{\mu \left(2V_0 - 2E_{nl} + \frac{2V_1}{q} - \frac{4V_2}{q} - \frac{V_3}{q} \right)}{2\alpha^2 \hbar^2} - \frac{l(l+1)}{q}, \quad (13)$$

$$C = \frac{\mu(E_{nl} - V_0 - V_1 - V_3)}{2\alpha^2 \hbar^2}. \quad (14)$$

Using the procedure outlined in section 2 above, the constants, $c_1 = c_2 = c_3 = 1$. Thus, we derive the constants in (4) as

$$\left. \begin{aligned} c_4 &= \sqrt{-C} \\ c_5 &= \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{l(l+1)}{q} + \frac{V_1(q-1)^2}{q} + \frac{4V_2}{q} + \frac{V_3(q+1)}{q}} \end{aligned} \right\}. \quad (15)$$

Using the simplified energy expression in eq. (6), the energy expression of the HPME potential is given as

$$E_{nl} = V_0 + V_1 + V_3 - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{\frac{\mu(2V_1(q-1) + 4V_2 + V_3(1+2q))}{2\alpha^2 \hbar^2} + qn(n+1) + \frac{q}{2} + l(l+1) + \left(n + \frac{1}{2}\right) \sqrt{q^2 + 4ql(l+1) + \frac{2\mu(V_1(q-1)^2 + 4qV_2 + qV_3(1+q))}{\alpha^2 \hbar^2}}}{q + 2qn + \sqrt{q^2 + 4ql(l+1) + \frac{2\mu(V_1(q-1)^2 + 4qV_2 + qV_3(1+q))}{\alpha^2 \hbar^2}}} \right)^2. \quad (16)$$

The corresponding wave function is

$$R_{nl}(s) = N_n s^{\sqrt{-C}} (1-s)^{c_5} {}_2F_1\left(-n, n + 2(\sqrt{-C} + c_5); 2\sqrt{-C} + 1; s\right) \quad (17)$$

4. Thermodynamic properties of the HPME potential

Setting $l = 0$, the pure vibrational energy of the HPME potential is given as

$$E_n = V - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{Q}{2(n+\sigma)} + \frac{(n+\sigma)}{2} \right)^2, \quad (18)$$

where,

$$\left. \begin{aligned} P &= \frac{\mu}{2\alpha^2 \hbar^2} (2V_1(q-1) + 4V_2 + V_3(1+2q)), \\ \sigma &= \frac{1}{2} + \frac{1}{2q} \sqrt{\frac{2\mu}{\alpha^2 \hbar^2} (V_1(q-1)^2 + 4qV_2 + qV_3(1+q)) + q^2}, \\ Q &= \frac{P + q\sigma(1-\sigma)}{q}, V = V_0 + V_1 + V_3 \end{aligned} \right\} \quad (19)$$

The partition function for the pure vibrational energy is gotten from the following expression

$$Z(\beta) = \sum_{n=0}^{\lambda} e^{-\beta E_n}, \beta = \frac{1}{k_B T}, \quad (20)$$

where k_B and β are the Boltzmann constant and temperature parameter, respectively. T is the

temperature and λ is the upper bound quantum number, realised from $\left. \frac{dE_n}{dn} \right|_{n=\lambda} = 0$.

$$\lambda = \left[-\sigma \pm \sqrt{Q} \right]. \quad (21)$$

Using eq. (18), eq. (20) becomes

$$Z(\beta) = \sum_{n=0}^{\lambda} \exp \left(-\beta \left(V - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{(n+\sigma)}{2} + \frac{Q}{2(n+\sigma)} \right)^2 \right) \right). \quad (22)$$

For classical thermodynamics, we set $\rho = n + \sigma$, the partition function becomes

$$Z(\beta) = \int_{\sigma}^{\lambda+\sigma} e^{-Y\rho^2\beta - \frac{W}{\rho^2}\beta + X\rho} d\rho \quad . \quad (23)$$

Evaluating eq. (23), the partition function becomes

$$Z(\beta) = \frac{e^{\beta X} \sqrt{\pi}}{4\Omega\sqrt{\beta Y}} \left(\Omega^2 (\operatorname{erf}(\chi_2) - \operatorname{erf}(\chi_1)) + \operatorname{erf}(\chi_2) - \operatorname{erf}(\chi_1) \right), \quad (24)$$

where

$$\left. \begin{aligned} \Omega &= e^{2\sqrt{-\beta W} \sqrt{-\beta Y}} \\ \chi_1 &= \sigma \sqrt{-\beta Y} + \frac{\sqrt{-\beta W}}{\sigma} \\ \chi_2 &= (\sigma + \lambda) \sqrt{-\beta Y} + \frac{\sqrt{-\beta W}}{(\sigma + \lambda)} \\ X &= \frac{\alpha^2 \hbar^2}{\mu} Q - V \\ Y &= \frac{\alpha^2 \hbar^2}{2\mu} \\ W &= \frac{\alpha^2 \hbar^2}{2\mu} Q^2 \\ \operatorname{erfi}(x) &= \frac{\operatorname{erf}(ix)}{i} = \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2} dt \end{aligned} \right\} \quad . \quad (25)$$

Other thermodynamic properties of the HPME are obtained as:

Vibrational Internal Energy

$$U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta} \quad (26)$$

Vibrational Free Energy

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta) \quad . \quad (27)$$

Vibrational Entropy

$$S(\beta) = k \ln Z(\beta) - k\beta \frac{\partial \ln Z(\beta)}{\partial \beta} \quad . \quad (28)$$

Vibrational Specific Heat Capacity

$$C(\beta) = k\beta^2 \frac{\partial^2 \ln Z(\beta)}{\partial \beta^2} \quad (29)$$

5. Expectation values of the HPME potential

The expectation values of the HPME potential are obtained using the Hellmann-Feynman theorem [32, 33]. The theorem states that the derivative of the energy of a system with respect to a parameter, v , is equal to the expectation value for the Hamiltonian with respect to the same parameter. The basic equation governing the Hellmann-Feynman theorem is given by

$$\frac{\partial E_{nl}(v)}{\partial v} = \left\langle \psi_{nl} \left| \frac{\partial H(v)}{\partial v} \right| \psi_{nl} \right\rangle \quad (30)$$

The effective Hamiltonian for the HPME potential is

$$H = \frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V_0 + V_1 \left(\frac{1-e^{-2\alpha r}}{1-qe^{-2\alpha r}} \right)^2 + V_2 \left(\frac{4e^{-2\alpha r}}{(1-qe^{-2\alpha r})^2} \right) + V_3 \left(\frac{1+e^{-2\alpha r}}{1-qe^{-2\alpha r}} \right) \quad (31)$$

By setting q to be l and μ , the expectation values for r^{-2} and T , respectively are obtained. The expectation value p^2 is obtained using the formula $\langle T \rangle = \frac{\langle p^2 \rangle}{2\mu}$.

$$\langle r^{-2} \rangle = \frac{8(qn)^2}{\hbar^2 \delta \Delta (q + 2qn + \Delta)^3} \left[\left\{ \delta \left(1 + \frac{\Delta}{qn} \left(1 + \frac{1}{2n} \right) + \frac{l}{qn^2} (1+l) + \frac{1}{2n^2} \right) + 2\mu + \frac{3\phi}{4} \right\} \right. \quad (32)$$

$$\left. \times \left\{ \delta \left(\frac{\Delta}{q^2 n} \left(1 + \frac{1}{2n} \right) + \frac{l}{(qn)^2} (1+l) + \frac{1}{q} \left(1 + \frac{1}{n} + \frac{1}{2n^2} \right) \right) + \phi + 3\mu \right\} \right]$$

$$\langle T \rangle = \frac{-(qn)^2}{\mu \delta \Delta (q + 2qn + \Delta)^3} \left[\left\{ \delta \left(\frac{1}{q} + \frac{2}{qn} + \frac{1}{2qn^2} + \frac{\Delta}{q^2 n} \left(1 + \frac{1}{2n} \right) + \frac{l}{(qn)^2} (1+l) \right) + \phi + 3\mu \right\} \right. \quad (33)$$

$$\left. \times \left\{ \delta \left[\frac{1}{n^2} \left(\frac{4l^2 \left(l^2 + 2l + 1 + \frac{1}{l} \right)}{q} + q + 5l(l+1) + 3q \right) + 12l \left(l + \frac{l}{n} + \frac{1}{n} + 1 \right) + 3q \right] \right. \right.$$

$$\left. \left. + \Delta \left(\frac{1}{qn} \left(\frac{\Delta^2}{2qn} + \frac{\Delta^2}{q} + \frac{l^2}{n} + \frac{2}{q} \right) + \frac{1}{n} \left(\frac{1}{2n} - l^2 + l \right) + 2n + 3 \right) \right\} \right.$$

$$\left. \left. + q\phi \left(4qn(n+1) + 6n(n+1) - \Delta(1+2n) + \frac{9}{4} \right) + \phi \left(l \left(3l + \frac{2l}{\mu} + \frac{2}{q} \right) - \frac{3\Delta}{2} \left(\frac{1}{2} + n \right) + 2n^2 + 1 \right) \right\} \right]$$

$$\langle p^2 \rangle = \frac{-2(qn)^2}{\delta \Delta (q + 2qn + \Delta)^3} \times \left\{ \delta \left[\frac{1}{q} + \frac{2}{qn} + \frac{1}{2qn^2} + \frac{\Delta}{q^2 n} \left(1 + \frac{1}{2n} \right) + \frac{l}{(qn)^2} (1+l) \right] + \phi + 3\mu \right\} \quad (34)$$

$$\times \left\{ \frac{1}{n^2} \left[\frac{4l^2 \left(l^2 + 2l + 1 + \frac{1}{l} \right)}{q} + q + 5l(l+1) + 3q \right] + 12l \left(l + \frac{l}{n} + \frac{1}{n} + 1 \right) + 3q \right. \\ \left. + \Delta \left[\frac{1}{qn} \left(\frac{\Delta^2}{2qn} + \frac{\Delta^2}{q} + \frac{l^2}{n} + \frac{2}{q} \right) + \frac{1}{n} \left(\frac{1}{2n} - l^2 + l \right) + 2n + 3 \right] \right. \\ \left. + q\phi \left(4qn(n+1) + 6n(n+1) - \Delta(1+2n) + \frac{9}{4} \right) + \phi \left[l \left(3l + \frac{2l}{\mu} + \frac{2}{q} \right) - \frac{3\Delta}{2} \left(\frac{1}{2} + n \right) + 2n^2 + 1 \right] \right\}$$

where,

$$\left. \begin{aligned} \delta &= 2(\alpha \hbar n q)^2 \\ \Delta &= \sqrt{q^2 + 4ql(l+1) + \frac{2\mu((q-1)^2 + 4q + q(1+q))}{\alpha^2 \hbar^2}} \\ \phi &= 4\mu q \end{aligned} \right\} \quad (35)$$

6. Discussion of Results

Table 1 gives numerical results of the energy of the HPME potential. The energy is observed to increase as quantum numbers n and l increase for $\alpha = 0.02$. For $\alpha = 0.04$ and $\alpha = 0.06$, a similar trend is observed up to $n = 4$, for $\alpha = 0.04$ and $n = 3$ for $\alpha = 0.06$, when the energy is observed to decrease as n and l increase. In Tables 2 and 3, the energies of the Hua and modified Eckart potentials are observed to respectively increase as n and l increase. Table 4 gives the numerical results of the energy of the HPME potential for the exact case ($l = 0$). The results are seen to be in agreement with results presented in the literature [3]. The slight variation can be attributed to the approximation used in this study for the centrifugal term. This is a validation of the accuracy of our result. In table 5, the expectation values of r^{-2} , T and p^2 . $\langle r^{-2} \rangle$ is observed to increase with increasing values of n and l . On the other hand $\langle T \rangle$ and $\langle p^2 \rangle$ are observed to decrease as n and l increase.

Table 1

Energy eigenvalues of the HPME potential with $V_0 = 0.2$; $V_1 = 0.3$; $V_2 = 0.4$; $V_3 = 0.5$; $q = 0.6$; $\mu = \hbar = 1$.

n	l	$\alpha=0.02$	$\alpha=0.04$	$\alpha=0.06$
0	0	-3.619049188	-3.612007524	-3.605479238
1	0	-3.605661530	-3.589503802	-3.577840660
2	0	-3.594410214	-3.574976406	-3.567002288
	1	-3.594158232	-3.574452926	-3.566810462
3	0	-3.585197952	-3.567749014	-3.570970628
	1	-3.584995216	-3.567570370	-3.571806502
	2	-3.584593530	-3.567262546	-3.573682348
4	0	-3.577934194	-3.567232644	-3.588114770
	1	-3.577778544	-3.567371746	-3.589869772
	2	-3.577470824	-3.567694314	-3.593553398
	3	-3.577018158	-3.568287244	-3.599497586
5	0	-3.572534554	-3.572912462	-3.617090056
	1	-3.572423976	-3.573345600	-3.619674292
	2	-3.572206208	-3.574251670	-3.624990422
	3	-3.571887984	-3.575708680	-3.633320882
	4	-3.571479334	-3.577829734	-3.645059054

Table 2

Energy eigenvalues of the Hua Potential with $V_l = 0.3$, $q = 0.6$, $\mu = \hbar = 1$.

n	l	$\alpha=0.02$	$\alpha = 0.04$	$\alpha=0.06$
0	0	-0.7809716160	-0.6713865654	-0.5706923194
1	0	-0.5841478244	-0.3544360644	-0.1837755158
2	0	-0.4258086732	-0.1427734612	0.0346777498
	1	-0.4077766632	-0.1008333914	0.0900595578
3	0	-0.2969653902	0.0030111898	0.1631793406
	1	-0.2822075860	0.0322931780	0.1959006104
	2	-0.2541791478	0.0811508340	0.2402541104
4	0	-0.1911327284	0.1052391708	0.2385139512
	1	-0.1789535734	0.1258871810	0.2570112626
	2	-0.1557905398	0.1603519429	0.2806519423
	3	-0.1237610570	0.1994277045	0.2966774614
5	0	-0.1035365656	0.1773211871	0.2797772796
	1	-0.0934184652	0.1918341819	0.2886963321
	2	-0.0741544756	0.2159346321	0.2979437493
	3	-0.0474726272	0.2428997367	0.2991872456
	4	-0.0155109256	0.2672122693	0.2885176998

Table 3

Energy eigenvalues of the modified Eckart with $V_2 = 0.4$, $V_3 = 0.5$, $q = 0.6$.

n	l	$\alpha=0.02$	$\alpha=0.04$	$\alpha=0.06$
-----	-----	---------------	---------------	---------------

0	0	-5.266622496	-5.248221248	-5.230507222
1	0	-5.231021126	-5.183233712	-5.141885066
2	0	-5.198529476	-5.129781682	-5.077401056
	1	-5.197749730	-5.127375336	-5.073422772
3	0	-5.168993044	-5.086793584	-5.033904078
	1	-5.168285848	-5.084888414	-5.031398536
	2	-5.166877596	-5.081158460	-5.026720226
4	0	-5.142268178	-5.053338510	-5.008824958
	1	-5.141630044	-5.051890962	-5.007618236
	2	-5.140359588	-5.049068068	-5.005489420
	3	-5.138468368	-5.045011236	-5.002982046
5	0	-5.118221184	-5.028604624	-5.000052112
	1	-5.117648868	-5.027576624	-5.000000648
	2	-5.116509728	-5.025585608	-5.000141662
	3	-5.114814720	-5.022758826	-5.000941248
	4	-5.112580096	-5.019280634	-5.003047726

Table 4

Energy eigenvalues of the HPME potential with $V_0 = 2.5$; $V_I = 0.3$; $V_2 = -0.05$; $V_3 = 0.4$; $q = 0.09$; $\mu = 0.5$; $\hbar = 1$; $l = 0$

n	Present study	Hassanabadi et al. [3]
0	2.932998240	3.1024
1	2.954999940	3.1152
2	2.975979327	3.1270
3	2.995947646	3.13792
4	3.014915950	3.1478
5	3.032895106	3.15695
6	3.049895796	3.1651
7	3.065928522	3.1724
8	3.081003609	3.1788
9	3.095131210	3.1843

Table 5

Numerical results of the expectation values of the HPME potential with $V_0 = 0.2$, $V_1 = 0.3$, $V_2 = 0.4$; $V_3 = 0.5$, $q = 0.6$, $\alpha = 0.01$, $\mu = \hbar = 1$

n	l	$\langle r^{-2} \rangle \left(\frac{\text{\AA}^{-2}}{A} \right)$	$\langle T \rangle (\text{eV})$	$\langle p^2 \rangle (\text{eV}/c)^2$
0	0	0.0001659961078	-0.005517931840	-0.01103586368
1	0	0.0001667639368	-0.01660535193	-0.03321070386
2	0	0.0001675315157	-0.02779459478	-0.05558918957
	1	0.0001675315893	-0.02796308568	-0.05592617137
3	0	0.0001682988499	-0.03908561192	-0.07817122384
	1	0.0001682988954	-0.03925525346	-0.07851050692
	2	0.0001682989866	-0.03959453656	-0.07918907312
4	0	0.0001690659447	-0.05047835625	-0.1009567125
	1	0.0001690659622	-0.05064914790	-0.1012982957
	2	0.0001690659977	-0.05099073100	-0.1019814620
	3	0.0001690660505	-0.05150310565	-0.1030062113
5	0	0.0001698328054	-0.06197278205	-0.1239455640
	1	0.0001698327951	-0.06214472325	-0.1242894466
	2	0.0001698327748	-0.06248860560	-0.1249772111
	3	0.0001698327440	-0.06300442850	-0.1260088569
	4	0.0001698327030	-0.06369219075	-0.1273843815

In figs. 1(a-f), the energy of the HPME potential is plotted against various potential parameters for various values of n and $l = 1$. In figs. 1a & b, the energy is observed to decrease as the screening parameter, α and deformation parameter, q , increase, respectively. In figs. 1c & d, the energy is seen to increase in a monotonic manner as V_0 and V_1 increase, respectively. In fig. 1e, the energy decreases as V_2 increases, while, in fig. 1f, energy increases as V_3 increases.

In fig. 2a, the vibrational partition function, Z , is observed to increase as the parameter, β , increases, i.e., as temperature decreases. The implication of this is that as the temperature drops, the probability that the system occupies a given microstate also decreases. In fig. 2b, Z is seen to first increase slowly, then sharply as the upper bound vibrational quantum number, λ , increases. In figs. 3a & b, respectively, the vibrational internal energy, U , increases sharply as β and λ increase, but cuts off at a point for all values of λ and β . In fig. 4a, the vibrational free energy, F , of the system is observed to increase as β increases up to about $\beta = 0.01$, then begins to approach to a constant value. In fig. 4b, F is observed to decrease as λ increases. In figs. 5a & b, the vibrational entropy, S , of the system first increases slowly, then sharply rises as both β and λ respectively increase. For the vibrational specific heat capacity, C , as can be seen in figs. 6a & b, there is an increase in C with respective increase in β and λ .

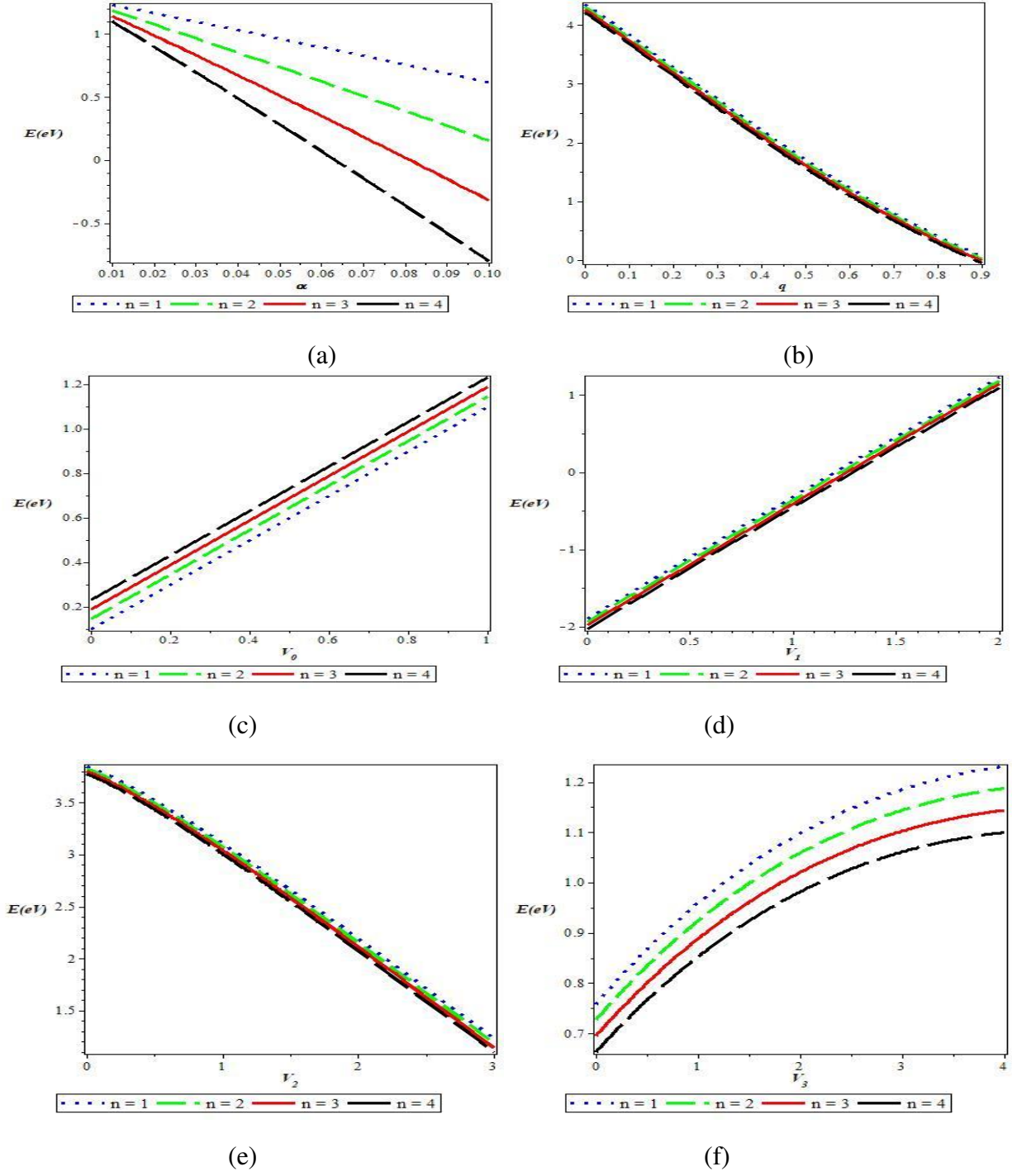


Fig. 1. Variation of Energy of the HPME potential with various potential parameters with $V_0=1$, $V_1=2$, $V_2=3$, $V_3=4$, $l=1$, $q=0.6$ and $\alpha=0.01$

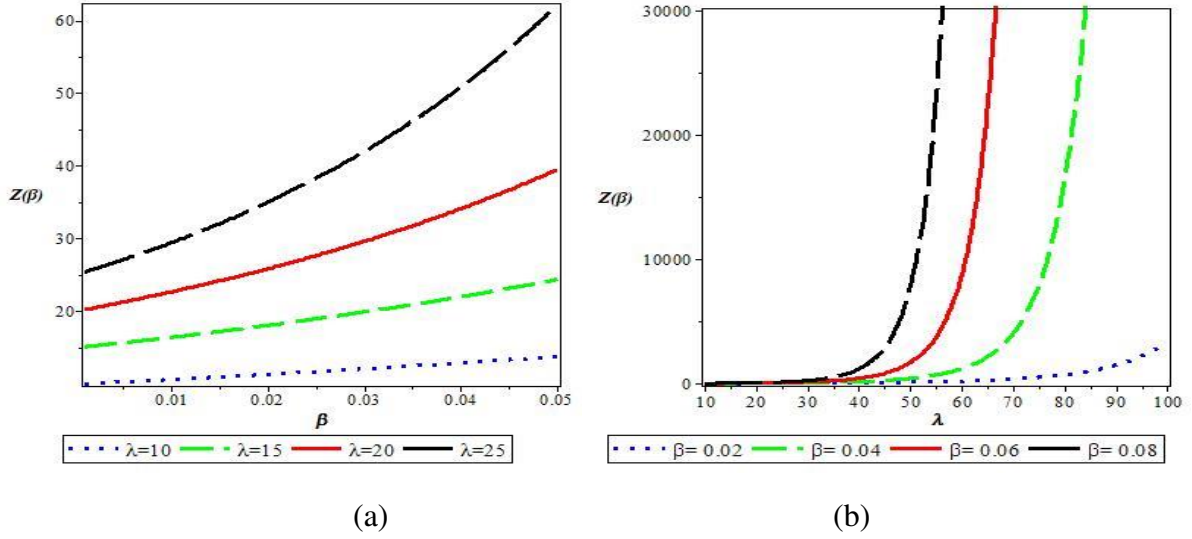


Fig. 2. Variation of vibrational partition function of the HPME potential with β and λ with $V_0=1$, $V_1=2$, $V_2=3$, $V_3=4$, $l=1$, $q=0.6$ and $\alpha=0.2$

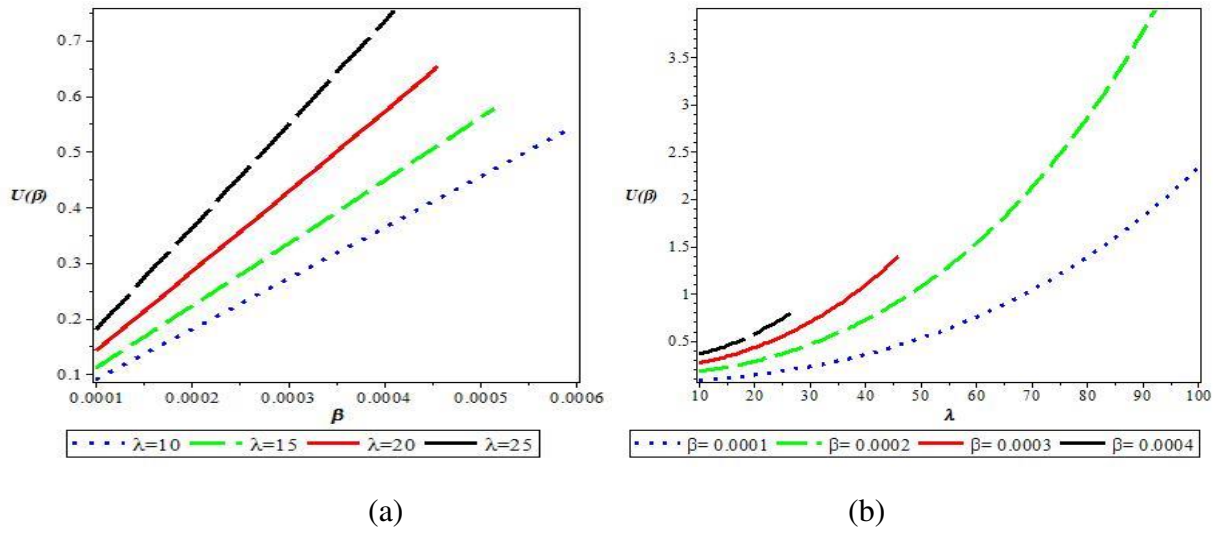


Fig. 3. Variation of vibrational internal energy of the HPME potential with β and λ with $V_0=1$, $V_1=2$, $V_2=3$, $V_3=4$, $l=1$, $q=0.6$ and $\alpha=0.2$

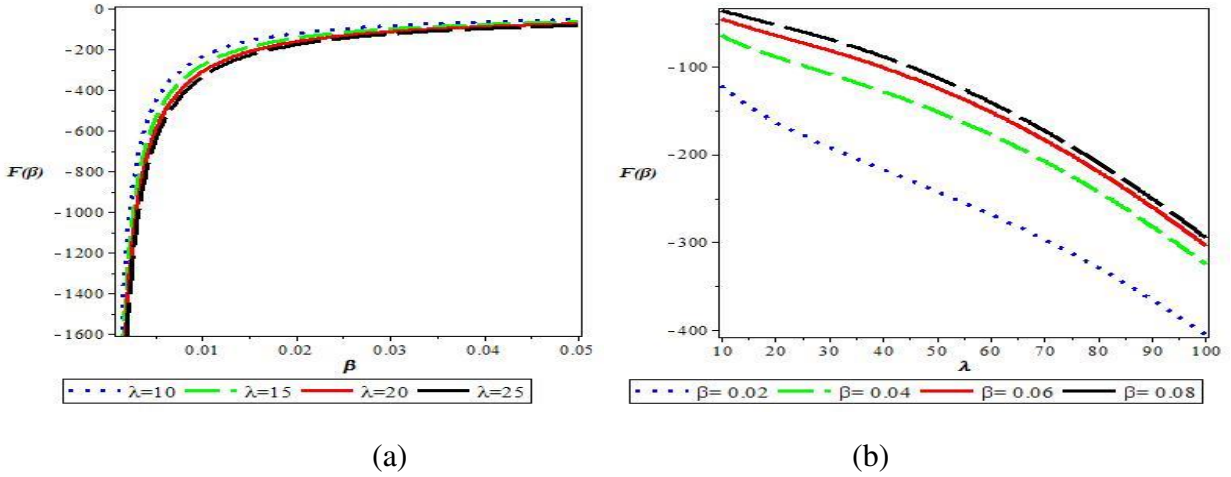


Fig. 4. Variation of vibrational free energy of the HPME potential with β and λ with $V_0=1, V_1=2, V_2=3, V_3=4, l=1, q=0.6$ and $\alpha=0.2$

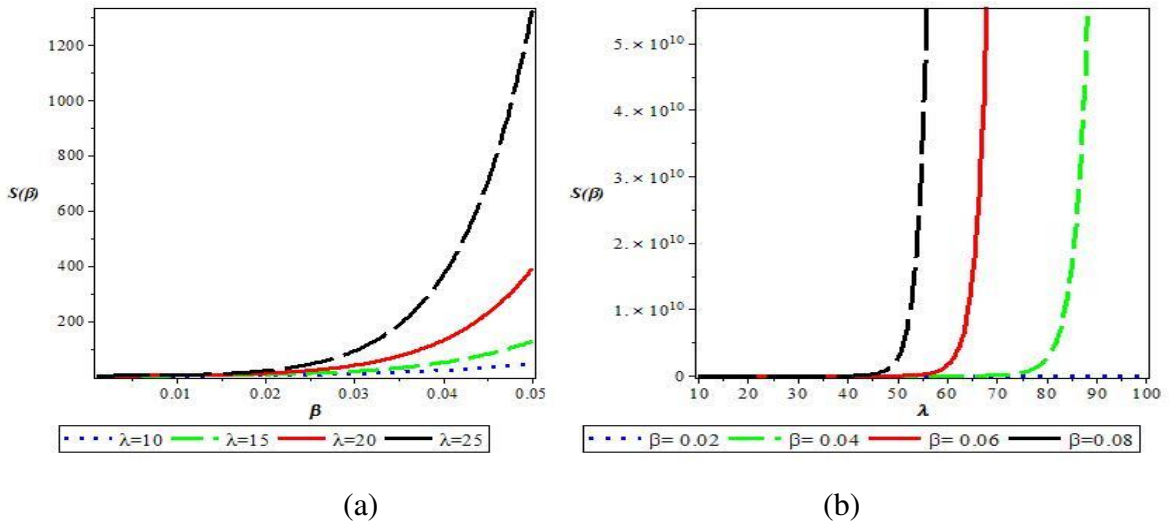


Fig. 5. Variation of vibrational entropy of the HPME potential with β and λ with $V_0=1, V_1=2, V_2=3, V_3=4, l=1, q=0.6$ and $\alpha=0.2$

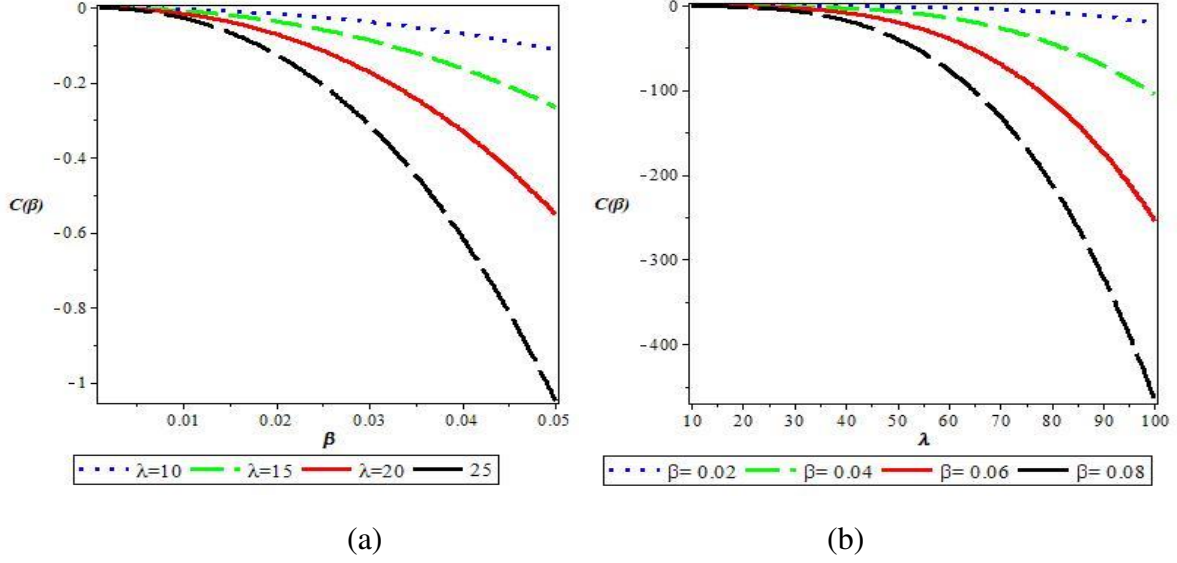


Fig. 6. Variation of vibrational specific heat capacity of the HPME potential with β and λ with $V_0=1$, $V_1=2$, $V_2=3$, $V_3=4$, $l=1$, $q=0.6$ and $\alpha=0.2$

6.1 Special cases

Case 1: Modified Eckart Potential

If we make $V_0=V_1=0$, $q=1$, the HPME potential reduces to the modified Eckart potential

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

Thus, (16) reduces to

$$E = V_3 - \frac{2\alpha^2 \hbar^2}{\mu} \left(\frac{\frac{\mu}{2\alpha^2 \hbar^2} (4V_2 + 3V_3) + \frac{1}{2} + n(n+1) + l(l+1) + \left(n + \frac{1}{2}\right) \sqrt{\frac{8\mu(V_2 + V_3)}{\alpha^2 \hbar^2} + (2l+1)^2}}{1 + 2n + \sqrt{\frac{8\mu(V_2 + V_3)}{\alpha^2 \hbar^2} + (2l+1)^2}} \right)^2. \quad (37)$$

Case 2: Hua Potential

If we set $V_0=V_2=V_3=0$, the HPME potential reduces to the Hua potential

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

Consequently, (16) becomes

$$E = V_1 - \frac{2\alpha^2\hbar^2}{\mu} \left(\frac{\left(\frac{\mu V_1(q-1)}{2\alpha^2\hbar^2} + \frac{q}{2} + qn(n+1) + l(l+1) + \left(n + \frac{1}{2}\right) \sqrt{\frac{2\mu V_1(q-1)^2}{\alpha^2\hbar^2} + 4ql(l+1) + q^2} \right)^2}{q + 2qn + \sqrt{\frac{2\mu V_1(q-1)^2}{\alpha^2\hbar^2} + 4ql(l+1) + q^2}} \right). \quad (39)$$

If we set $\alpha r = b_h(r - r_e)$ and using the approximation $\frac{1}{r^2} \approx \frac{1}{r_e} \left(D_0 + \frac{D_1 e^{-b_h(r-r_e)}}{1 - qe^{-b_h(r-r_e)}} + \frac{D_2 e^{-2b_h(r-r_e)}}{(1 - qe^{-b_h(r-r_e)})^2} \right)$, the energy in eq. (39) will become exactly the same as eq. (14) in ref. [17].

Case 4: Poschl-Teller Potential

Adjusting $V_0=V_l=V_3=0$, $q=-1$, the HPME potential reduces to the Poschl-Teller potential

$$V(r) = V_2 \left(\frac{4e^{-2\alpha r}}{1 + e^{-2\alpha r}} \right). \quad (40)$$

Hence, (16) reduces to

$$E = -\frac{2\alpha^2\hbar^2}{\mu} \left(\frac{\left(\frac{-\mu V_2}{\alpha^2\hbar^2} + \frac{1}{2} + n(n+1) - l(l+1) - \left(n + \frac{1}{2}\right) \sqrt{1 - 4l(l+1) + \frac{8\mu V_2}{\alpha^2\hbar^2}} \right)^2}{1 + 2n - \sqrt{1 - 4l(l+1) + \frac{8\mu V_2}{\alpha^2\hbar^2}}} \right). \quad (41)$$

If we set $V_2 = -V_l$, eq. (41) will be similar to eq. (20) in Ref. [38]. Also, if we set $q = 1$ and $l = 0$, the energy (16) becomes very identical to eq. (32) in ref. [3].

7. Conclusions

In this paper, we solved the Schrodinger equation for the HPME potential via the Formula method. In addition, we obtain the partition function and other thermodynamic properties of the HPME potential. Furthermore, the expectation values of the HPME potential were determined using the powerful Hellmann-Feynman theorem. Numerical values of the energies and the expectation values are presented. The results of the study are in good agreement with literature.

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Author contribution statement

IJN: conceptualization of the manuscript and wrote the manuscript. CJO and CPO: performed the calculations and wrote the manuscript. EO and PN: prepared all the figures and took part in the investigation. FUN: prepared all the tables and edited the manuscript. All the authors reviewed the manuscript.

Additional Information

Competing Interest

The authors declare no conflict of interest.