VIBRATIONAL SPECIFIC HEAT CAPACITY FOR SPINLESS PARTICLES

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Abstract

In this paper we have applied the concepts of proper quantization rule and ansatz solution technique to obtain polynomial solutions of the Schrödinger equation for spinless particles in a Rosen-Morse potential. Closed form expressions for energy eigenvalues and radial eigenfunctions were obtained, in tackling the spin-orbit term of the Schrödinger equation, a Pekeris-like approximation recipe was used. For a suitable choice of potential parameters, bound state ro-vibrational energies of the improved Rosen-Morse potential were deduced from the expression of the energy eigenvalues of the Rosen-Morse potential. The results we obtained for the ro-vibrational energy eigenvalues were in perfect agreement with the expression for ro-vibrational energy eigenvalues of the improved Rosen-Morse potential in the literature. We have employed the expression for energy eigenvalues obtained in this work to derive formula for classical ro-vibrational partition function, Z and ro-vibrational specific capacity, C. Results of studies carried out on this functions show that Z decreases monotonically with increase in temperature while C decreases sharply from a large positive value to zero and remains fairly constant at zero as temperature is further increased.

Keywords: Rosen-Morse potential, Schrödinger equation, Pekeris approximation, spinless particles, partition function

1.   Introduction

Much attention has been paid to the exact solutions of wave equations in quantum mechanics because they are embedded with information about the system being studied, this information allows many physical properties about the system to be explored [1-2]. Quantum mechanical systems are usually represented by potential energy functions, up to the present time, as a result of different system behaviors, a universal potential energy model that will explain all atomic and molecular interactions has not been realized, this has necessitated researchers to device different potential energy functions for the purpose of explaining interactions [3-5]. The Schrödinger equation is used for the description of nonrelativistic spinless particles, a major challenge often encountered with the exact solution of Schrödinger equation is that it is characterized by the quantum state of the system, defined by the principal (n) and angular momentum quantum (ℓ) numbers as well as the potential energy function, only a few potential energy models are known to have exact solution with the Schrödinger equation for all quantum states, few other potential models have exact solution only for state $\ell = 0$, such solutions are described as s-wave solutions [6-8]. For the state $\ell \neq 0$, a vast number of potential energy functions have no exact solution with the Schrödinger equation because of the presence of the spin-orbit term of the effective potential in the Schrödinger equation. Approximate analytical or numerical solutions are calculated for these class of potentials [9-10]. So many analytical solution methods have been proposed in the literature, these include exact quantization rule (EQR) [11], proper quantization rule (PQR) [12-13], ansatz solution approach [14], Nikiforov-Uvarov method [15] and supersymmetric quantum mechanics approach [16] amongst others. Ro-vibrational or eigenenergies derived from Schrödinger equation

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have been used to study the physical properties of a system [17-18]. The Rosen-Morse potential has been reported to be a good potential for modeling the interaction of polyatomic molecules and has various applications in nuclear physics, molecular physics, chemical physics and solid-state physics, it is given by [19-20]:

$$V(r) = -V_1 \operatorname{sech}^2(\alpha r) + V_2 \tanh(\alpha r) \tag{1}$$

where V_1 and V_2 are potential parameters, α is the screening parameter and $r \in (0, \infty)$ is the internuclear separation. The Rosen-Morse potential and its modified forms have received considerable attention in the literature. The Schrödinger equation has been solved with the Rosen-Morse potential for different approximation schemes applied to the spin-orbit term of the effective potential [21-25]. Ro-vibrational energies obtained from solutions of Schrödinger equation with asymmetric trigonometric Rosen-Morse potential has been employed in the studies of spherical quantum dots [22]. In the present work, we propose to obtain the vibrational specific heat capacity for spinless particles in a Rosen-Morse potential, our specific objectives include: (a) solve the Schrödinger equation with the Rosen-Morse potential using the PQR and ansatz solution method to obtain energy eigenvalues and radial wave eigenfunctions respectively (b) derive expressions for partition function and ro-vibrational specific heat capacity, (c) compare results with those in the literature where they exists.

2. Theoretical Formalism
2.1 Basic Ideas of the Proper Quantization Rule

Here we will provide the basic ideas of PQR relevant to the present work, a comprehensive description of this concept is given elsewhere in the literature [2]. The PQR was proposed to overcome the difficulties arising from the application of EQR to obtaining eigenenergies from the effective potential of the Schrödinger equation. Initially, the EQR was proposed to solve the one-dimensional Schrödinger equation [11] given by:

$$u''(x) + k^2(x)u(x) = 0 \tag{2}$$

where prime designates derivative with respect to argument x, $u(x)$ is the radial wave function and $k(x)$ is the momentum, defined as:

$$k(x) = \sqrt{\frac{2\mu}{\hbar^2}\{E - V_{eff}(x)\}} \tag{3}$$

E is the energy eigenvalue and $V_{eff}(x)$ is the effective potential energy of the system. In the usual notation, Eq. (2) is expressed as a Riccati differential equation given as:

$$\phi'(x) + \phi^2(x) + k^2(x) = 0 \tag{4}$$

the logarithmic derivative $\phi(x) = u'(x)/u(x)$ of the wave function $u(x)$ is known as the phase angle. Yang explained that for the Sturm-Liouville problem [2], the phase angle must be monotonic with respect to the energy. From Eq. (2), $u(x)$ decreases monotonically with respect to x between two turning points where $E \geq V_{eff}(x)$ specifically, as x increases across a node of the wave function $u(x)$, $\phi(x)$ decreases to $-\infty$, jumps to $+\infty$, and then decreases again. After a careful study of the Schrödinger equation, the EQR was proposed by Ma and Xu [11] as:

$$\int_{x_A}^{x_B} k(x)dx = N\pi + \int_{x_A}^{x_B} k'(x)\frac{\phi(x)}{\phi'(x)}dx \tag{5}$$

where x_A and x_B are two turning points determined by the equation $V_{eff}(x) = E$, $N = n+1$ is the number of nodes of $\phi(x)$ in the region $E \geq V_{eff}(x)$ and is larger by 1 than the number v of the nodes of the wave function $u(x)$ [2, 11]. The term $N\pi$ in Eq. (5) is the contribution from the nodes of the phase angle while the second term is the quantum correction, it is independent of v for all exactly solvable quantum systems, accordingly, it can be evaluated at the ground state ($n = 0$). For a spherically symmetric potential, Eqs. (2) - (4) are expressed as:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)\right\}u_{vJ}(r) = E_{vJ}u_{vJ}(r) \tag{6}$$

$$k_{n\ell}(r) = \sqrt{\frac{2\mu}{\hbar^2}\{E_{n\ell} - V_{eff}(r)\}} \tag{7}$$

$$\phi'_{n\ell}(r) + \phi^2_{n\ell}(r) + k^2_{n\ell}(r) = 0 \tag{8}$$

where

$$V_{eff}(r) = V(r) + \frac{L\hbar^2}{2\mu r^2} \tag{9}$$

with $L = \ell(\ell+1)$. In spherical coordinates, Eq. (5) is written in compact form as:

$$I_{n\ell} = N\pi + Q_c \tag{10}$$

where

$$I_{n\ell} = \int_{r_{nA}}^{r_{nB}} k_{n\ell}(r)\,dr \tag{11}$$

$$Q_c = \int_{x_{nA}}^{x_{nB}} \frac{\phi_{0J}(r)}{\phi'_{0J}(r)} k'_{0J}(r)\,dr \tag{12}$$

Letting $v = 0$ in Eq. (11) and eliminating Q_c, the expression PQR [2] is given in compact form as:

$$I_{n\ell} = I_{0\ell} + n\pi \tag{13}$$

2.2 Energy Eigenvalues of the Rosen-Morse Potential
Upon substituting Eq. (1) in Eq. (9), the effective potential becomes:

$$V_{eff}(r) = -V_1 \operatorname{sech}^2(\alpha r) + V_2 \tanh(\alpha r) + \frac{L\hbar^2}{2\mu r^2} \tag{14}$$

Solving Eq. (6) in the presence of Eq. (14) for an all ℓ-state analytical solution requires employing a suitable approximation scheme on the spin-orbit term, in the present work the Pekeris-like approximation model will be used, it is given by [4]:

$$\frac{1}{r^2} \approx \frac{1}{r_e^2}\left\{a_0 + a_1 \operatorname{sech}^2(\alpha r) + a_2 \tanh(\alpha r)\right\} \tag{15}$$

where r_e is the equilibrium bond length and the parameters a_{j-1} $(j=1,2,3)$ are given in terms of constant coefficients a_{j-1} $(j=1,2,3)$ by [26]:

$$a_0 = c_0 + \tfrac{1}{2}(c_1 + c_2) \tag{16}$$

$$a_2 = -\tfrac{1}{4}c_2 \tag{17}$$

$$a_1 = -\tfrac{1}{2}(c_1 + c_2) \tag{18}$$

where

$$c_0 = 1 - \frac{1}{2\alpha r_e}\left(3 - e^{-2\alpha r_e}\right)\left(1 + e^{-2\alpha r_e}\right) + \frac{3}{4\alpha^2 r_e^2}\left(1 + e^{-2\alpha r_e}\right)^2 \tag{19}$$

$$c_1 = \frac{e^{2\alpha r_e}}{\alpha r_e}\left(2 - e^{-2\alpha r_e}\right)\left(1 + e^{-2\alpha r_e}\right)^2 - \frac{3e^{2\alpha r_e}}{2\alpha^2 r_e^2}\left(1 + e^{-2\alpha r_e}\right)^3 \tag{20}$$

$$c_2 = -\frac{e^{4\alpha r_e}}{2\alpha r_e}\left(1 - e^{-2\alpha r_e}\right)\left(1 + e^{-2\alpha r_e}\right)^3 + \frac{3e^{4\alpha r_e}}{4\alpha^2 r_e^2}\left(1 + e^{-2\alpha r_e}\right)^4 \tag{21}$$

It follows that by substituting Eq. (15) in (14), one obtains:

$$V_{eff}(r) = \left(\frac{L\hbar^2 a_1}{2\mu r_e^2} - V_1\right)\operatorname{sech}^2(\alpha r) - \left(\frac{L\hbar^2 a_2}{2\mu r_e^2} + V_2\right)\tanh(\alpha r) + \frac{L\hbar^2 a_0}{2\mu r_e^2} \tag{22}$$

Incorporating the coordinate transformation defined by:

$$\zeta = \tanh(\alpha r) \tag{23}$$

Eq. (22) assumes the form:

$$V_{eff}(\zeta) = \frac{\hbar^2}{2\mu}\sum_{j=1}^{3}\chi_{-1+j}^2\,\zeta^{3-j} \tag{24}$$

where

$$\chi_0^2 = -\frac{2\mu V_1}{\hbar^2} - \frac{La_1}{r_e^2} \tag{25}$$

$$\chi_1^2 = \frac{2\mu V_2}{\hbar^2} + \frac{L a_2}{r_e^2} \tag{26}$$

$$\chi_2^2 = -\frac{2\mu V_1}{\hbar^2} + \frac{L}{r_e^2}(a_0 + a_1) \tag{27}$$

The turning points $\zeta_{nA} = \tanh(\alpha r_{nA})$ and $\zeta_{nB} = \tanh(\alpha r_{nB})$ can be obtained by solving the equation $V_{eff}(\zeta) = E_{n\ell}$ [2], inserting Eq. (24) in this relation, this results in:

$$\sum_{j=1}^{3} \chi_{-1+j}^2 \zeta^{3-j} = \frac{2\mu E_{n\ell}}{\hbar^2} \equiv \chi_{n\ell}^2 \tag{28}$$

Solving for ζ in Eq. (28), we obtain the sum and products of the roots as:

$$\zeta_{nA} + \zeta_{nB} = -\frac{\chi_1^2}{\chi_0^2} \tag{29}$$

$$\zeta_{nA}\zeta_{nB} = \frac{\chi_2^2 - \chi_{n\ell}^2}{\chi_0^2} \tag{30}$$

Transforming the relation (7) to one in terms of the turning points, the momentum of the system translates to:

$$k_{n\ell}(\zeta) = \sqrt{\chi_{n\ell} - \chi_0^2 \zeta^2 - \chi_1^2 \zeta - \chi_2^2} \equiv \chi_0\sqrt{(\zeta - \zeta_{nA})(\zeta_{nB} - \zeta)} \tag{31}$$

Substituting Eq. (23) in (8), we have the Riccati equation in terms of our new variable ζ as:

$$\alpha(1 - \zeta^2)\phi_{n\ell}'(\zeta) + \phi_{n\ell}^2(\zeta) + \chi_{n\ell}^2 - \chi_0^2\zeta^2 - \chi_1^2\zeta - \chi_2^2 = 0 \tag{32}$$

Due to Sturm-Liouville condition, we select a trial wave function of the form:

$$\phi_{0\ell}(\zeta) = -\gamma\zeta + \sigma \tag{33}$$

where $\gamma < 0$ and σ are constants, with $n = 0$ and replacing Eq. (33) in (32), we have the following relation:

$$(\alpha\gamma + \gamma^2 - \chi_0^2)\zeta^2 + (-2\gamma\sigma - \chi_1^2)\zeta - \alpha\gamma + \sigma^2 + \chi_{0\ell}^2 - \chi_2^2 = 0 \tag{34}$$

Eq. (34) only if each of the coefficients of ζ^2, ζ and ζ^0 are each equal to zero, leading to:

$$\alpha\gamma + \gamma^2 = \chi_0^2 \tag{35}$$

$$-2\gamma\sigma = \chi_1^2 \tag{36}$$

$$-\alpha\gamma + \sigma^2 = \chi_2^2 - \chi_{0\ell}^2 \tag{37}$$

Solving for γ in Eq. (35) we have that:

$$\gamma = \alpha\omega \tag{38}$$

where, for mathematical brevity we have used:

$$\omega = -\frac{1}{2} - \sqrt{\frac{1}{4} - \frac{L c_1}{\alpha^2 r_e^2} + \frac{2\mu V_1}{\alpha^2 \hbar^2}} \tag{39}$$

Having obtained γ and σ as given by Eqs. (38) and (36) respectively, our next task is to obtain the momentum integral, using the transformation Eq. (23) in (11) and substituting the relation (31) in the resulting expression, we have:

$$I_{n\ell} = \frac{\chi_0}{\alpha} \int_{\zeta_{nA}}^{\zeta_{nA}} \frac{\sqrt{(\zeta - \zeta_{nA})(\zeta_{nB} - \zeta)}}{1 - \zeta^2} d\zeta \tag{40}$$

to evaluate the integral of Eq. (40), we consider the standard integral due to Serrano *et al.* [2] given as:

$$\int_a^b \frac{\sqrt{(x-a)(b-x)}}{1 - x^2} dx = \frac{\pi}{2}\left\{2 + \sqrt{(1-a)(1-b)} - \sqrt{(1+a)(1+b)}\right\} \tag{41}$$

Using Eq. (41) to evaluate the definite integral in (40) and simplifying, we have:

$$I_{n\ell} = \frac{\pi}{2\alpha}\left\{2\chi_0 + \sqrt{\chi_0^2 + \chi_1^2 + \chi_2^2 - \chi_{n\ell}^2} - \sqrt{\chi_0^2 - \chi_1^2 + \chi_2^2 - \chi_{n\ell}^2}\right\} \tag{42}$$

For the ground state ($n = 0$), Eq. (42) gives:

$$I_{0\ell} = \frac{\pi}{2\alpha}\left\{2\chi_0 + \sqrt{\chi_0^2 + \chi_1^2 + \chi_2^2 - \chi_{0\ell}^2} - \sqrt{\chi_0^2 - \chi_1^2 + \chi_2^2 - \chi_{0\ell}^2}\right\} \tag{43}$$

Substituting the Eqs. (35) – (37) and replacing Eq. (35) in the resulting relation leads to:

$$I_{0\ell} = \frac{\pi}{2\alpha}(2\chi_0 + 2\alpha\omega) \tag{44}$$

With the help of Eqs. (42), (44) and the proper quantization rule given by (13), we have:

$$\chi_{n\ell}^2 = \chi_0^2 + \chi_1^2 + \chi_2^2 - \alpha^2 \left\{ n - \omega + \frac{\chi_1^2}{2\alpha^2(n-\omega)} \right\}^2 \tag{45}$$

Using Eqs. (25) – (27) to eliminate $\chi_j^2 (j = 1,2,3)$ from Eq. (45), we have the energy eigenvalues of the Rosen-Morse potential as:

$$E_{n\ell} = V_2 + \frac{L\hbar^2}{2\mu r_e^2}(a_0 + a_2) - \frac{2\alpha^2\hbar^2}{\mu} \left\{ \frac{n^2 - (2n+1)\omega + \frac{\mu}{\alpha^2\hbar^2}(2V_1 + V_2) - \frac{L}{2\alpha^2 r_e^2}(2a_1 - a_2)}{2(n-\omega)} \right\}^2 \tag{46}$$

2.3 Eigenfunctions of the Rosen-Morse Potential

The eigenfunctions of the Rosen-Morse potential can be obtained with the help of the substitution $\varphi = \frac{1}{2}(1 + \zeta)$ and employing the phase angle – wave function relationship, Riccati equation (32) gives:

$$\varphi(1-\varphi)R_{n\ell}''(\varphi) + (1-2\varphi)R_{n\ell}'(\varphi) + \left\{ -\frac{\chi_0^2}{4\alpha^2}\frac{(2\varphi-1)^2}{\varphi(1-\varphi)} - \frac{\chi_1^2}{4\alpha^2}\frac{2\varphi-1}{\varphi(1-\varphi)} - \frac{\chi_2^2 - \chi_{n\ell}^2}{4\alpha^2}\frac{1}{\varphi(1-\varphi)} \right\}R_{n\ell}(\varphi) = 0 \tag{47}$$

$R_{n\ell}(\varphi)$ being the radial wave function. Following procedures similar to Tang *et al.* [24], Eq. (47) has a polynomial solution by:

$$R_{n\ell}(\varphi) = N_{n\ell}\varphi^\nu(1-\varphi)^\varepsilon \, _2F_1(-n, n + 2\nu + 2\varepsilon + 1; 2\nu + 1; \varphi) \tag{48}$$

where $N_{n\ell}$ and $_2F_1(-n, n + 2\nu + 2\varepsilon + 1; 2\nu + 1; \varphi)$ are respectively the normalization constant and the Gauss hypergeometric function. The parameters ν and ε are given by:

$$\nu = \sqrt{\frac{L}{4\alpha^2 r_e^2}(a_0 - a_2) - \frac{\mu}{2\alpha^2\hbar^2}(V_2 + E_{n\ell})} \tag{49}$$

$$\varepsilon = \sqrt{\frac{L}{4\alpha^2 r_e^2}(a_0 + a_2) + \frac{\mu}{2\alpha^2\hbar^2}(V_2 - E_{n\ell})} \tag{50}$$

2.4 Ro-Vibrational specific Heat Capacity of the Rosen-Morse Potential

In statistical mechanics and other branches of physics, knowledge of the ro-vibrational partition function is necessary because it shows how particles of the system are distributed in a given ensemble and is essential in the derivation of other useful thermodynamic functions of the system, it is given as [14-15]:

$$Z(\beta) = \sum_{\nu=0}^{\lambda} e^{-\beta E_{\nu J}} \tag{51}$$

where $\beta = (k_B T)^{-1}$, T is the temperature, k_B is the Boltzmann constant and parameter λ is the maximum vibrational quantum number. Substituting Eq. (46) into (51), we have that:

$$Z(\beta) = \sum_{\nu=0}^{\lambda} e^{\beta\theta\left\{(n-\omega)^2 + \frac{\kappa^2}{(n-\omega)^2} + \frac{\tau}{\theta}\right\}} \tag{52}$$

where

$$\theta = \frac{\alpha^2\hbar^2}{2\mu} \tag{53}$$

$$\tau = -V_2 - \frac{L\hbar^2}{2\mu r_e^2}(a_0 + a_2) + \kappa\theta \tag{54}$$

$$\kappa = \frac{V_2}{\theta} + \frac{La_2}{\alpha^2 r_e^2} \tag{55}$$

In the classical limit, at high temperatures and for large λ and small β, the summation in Eq. (52) can be replaced with a definite integral [15], this gives:

$$Z(\beta) = \int_0^{\lambda} e^{\left(\beta\theta\rho^2 + \frac{\beta\theta\kappa^2}{\rho^2} + \beta\tau\right)} d\rho \tag{55}$$

where

$$\rho = n - \omega \tag{56}$$

Following Ikot *et al.* [15], the integral in Eq. (55) is obtained as:

$$Z(\beta) = \lambda\, e^{\beta\theta\rho^2 + \beta\tau} \left\{ e^{x^2} - \sqrt{\pi}\, x\, erfi(x) - \sqrt{\pi}\, x \right\} \tag{57}$$

where

$$x = \left(\frac{\beta\theta\kappa^2}{\lambda^2} \right)^{\frac{1}{2}} \tag{58}$$

and *erfi (x)* is the imaginary error function of the argument *x*, it is given as:

$$erfi(x) = -i\, erf(ix) = \frac{2}{\sqrt{\pi}} \int_0^x e^{y^2}\, dy \tag{59}$$

The ro-vibrational specific heat capacity $C(\beta)$ is expressed in terms of ro-vibrational partition function by the following relation [15]:

$$C(\beta) = k_B\, \beta^2\, \frac{\partial^2}{\partial\beta^2} \ln Z(\beta) \tag{60}$$

which, upon substituting Eq. (57) in (60) gives:

$$C(\beta) = \frac{\sqrt{\pi}\,\theta\kappa k_B\, \beta^2}{2\lambda^2 x} \frac{1 + erfi(x)}{\Omega\, e^{\Omega}} \left\{ \frac{\theta\kappa^2}{2\lambda^2 x} - \frac{2}{\sqrt{\pi}} \frac{e^{x^2}}{1 + erfi(x)} - \frac{\sqrt{\pi}\,\theta\kappa^2}{\lambda^2 x} \frac{1 + erfi(x)}{\Omega\, e^{\Omega}} \right\} \tag{61}$$

where

$$\Omega = \ln\left\{ e^{x^2} - \sqrt{\pi}\, x\, erfi(x) - \sqrt{\pi}\, x \right\} \tag{62}$$

3.   Results and Discussion

To verify the accuracy of our results, it is pertinent to note that by appropriately choosing $V_1 = \frac{1}{4} D_e \left(e^{2\alpha r_e} + 1 \right)^2$ and $V_2 = -\frac{1}{2} D_e \left(e^{4\alpha r_e} - 1 \right)$ in accordance with Jia *et al.* [27], from Eq. (1) we have that:

$$\tilde{V}(r) = V(r) + s \tag{63}$$

where $\tilde{V}(r)$ is the improved Rosen-Morse potential [27], $s = \frac{1}{2} D_e \left(e^{4\alpha r_e} + 1 \right)$ is a constant and D_e is the dissociation energy.

Eq. (63) reveals that with the above choice of parameters for V_1 and V_2, the Rosen-Morse potential is transformed to the improved Rosen-Morse potential and a constant *s* is added as a result of the transformation. However, it must be remarked that *s* merely shifts the equilibrium minimum of the Rosen-Morse potential but the molecular properties of the system which it represents are retained. Eq. (63) also suggest that the ro-vibrational energy spectra for the improved Rosen-Morse potential can be predicted by adding *s* to Eq. (46). Substituting the above expressions for V_1 and V_2 into Eq. (46), and adding the constant *s* to the resulting expression leads to:

$$E_{n\ell} = D_e + \frac{L\hbar^2}{2\mu r_e^2}(a_0 + a_1) - \frac{\alpha^2\hbar^2}{2\mu} \left\{ \frac{2n+1 - \sqrt{1 + \frac{2\mu D_e}{\alpha^2\hbar^2}\left(e^{2\alpha r_e}+1\right)^2 - \frac{4La_2}{\alpha^2 r_e^2}}}{2} - \frac{\frac{\mu D_e}{\alpha^2\hbar^2}\left(e^{4\alpha r_e}-1\right) - \frac{La_1}{\alpha^2 r_e^2}}{2n+1 - \sqrt{1 + \frac{2\mu D_e}{\alpha^2\hbar^2}\left(e^{2\alpha r_e}+1\right)^2 - \frac{4La_2}{\alpha^2 r_e^2}}} \right\}^2 \tag{64}$$

where Eq. (39) has been employed to eliminate ω and the mapping $\alpha \to \frac{1}{2}\alpha$ has been considered. Eq. (64) is identical to the expression for rotation-vibrational energy levels of diatomic molecules in the presence of improved Rosen-Morse potential energy model [26]. Also, if we express Eq. (46) in natural units, that is ($\hbar = \mu = 1$) and make the identification $\omega = -1 - \delta$, Eq. (46) is reduced to the expression for the energy eigenvalues of the Schrödinger equation with Rosen-Morse potential in ref. [24]. Evidently, we conclude that Eq. (46) is the correct expression for the energy eigenvalues for the Rosen-Morse potential for spinless particles. In Figure 1, we have plotted the variation of $E_{n\ell}$ as a function of principal quantum number *n*, the plot shows that as *n* is increased from zero, the energy of the system decreases approximately in a linear trend. The plot in Figure 2 shows the variation of $E_{n\ell}$ as a function of ℓ, from the plot it can be seen that $E_{n\ell}$ slightly increases to a maximum in the range $0 \le \ell < 2$, it decreases to a minimum for $3 < \ell < 10$ and eventually begins to increase as ℓ is further increased. To show that the eigenfunctions obtained in this work are physically realistic wave functions, we have used Eq. (48) to plot radial wave function for arbitrary quantum state $n = 5$, $\ell = 3$, the wave function is shown in Figure 3. We have also applied Eq. (57) to study the variation of vibrational partition function *Z* with temperature β, this is

shown by the plot in Figure 4, from the plot Z is observed to decrease monotonically as β is increased from zero. Eq. (61) shows the relation between vibrational specific heat capacity C with temperature, this relation is represented by the plot in Figure 5, as revealed by the plot, C decreases sharply from a large positive value to zero as β is slightly increased, C remains fairly constant at zero with a further increase in β
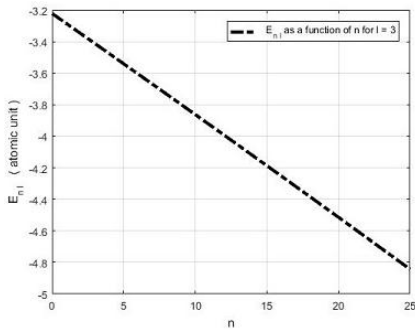

Figure1: Variation of $E_{n\ell}$ (in atomic units $\mu = \hbar = 1$) as a function of *n* for $V_1 = 3$, $V_2 = -2$, $r_e = 10$ and $\alpha = 0.01$
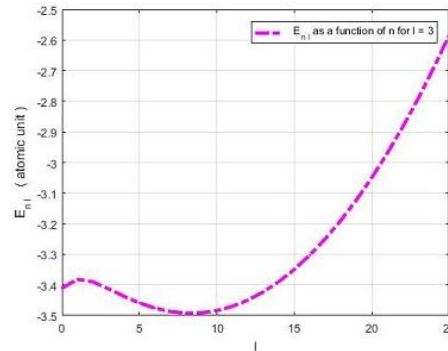
Figure 2: Variation of $E_{n\ell}$ (in atomic units $\mu = \hbar = 1$) as a function of ℓ for $V_1 = 3$, $V_2 = -2$, $r_e = 10$ and $\alpha = 0.01$
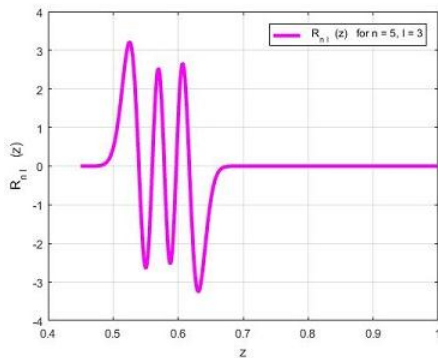

Figure 3: Plot of unnormalized radial wave function (in atomic unit, $\mu = \hbar = 1$) vs. z for $V_1 = 3$, $V_2 = -2$, $r_e = 10$ and $\alpha = 0.01$
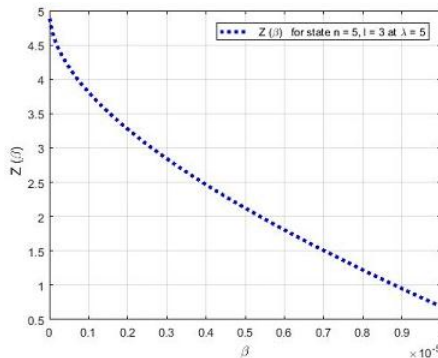

Figure 4: Plot of vibrational partition function as a function of temperature (in atomic unit, $\mu = \hbar = 1$) for $V_1 = 3$, $V_2 = -2$, $r_e = 10$ and $\alpha = 0.01$
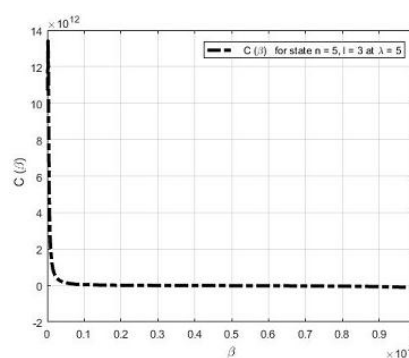

Figure 5: Plot of vibrational specific heat capacity (in atomic unit, $\mu = \hbar = 1$) as a function of temperature for $V_1 = 3$, $V_2 = -2$, $r_e = 10$ and $\alpha = 0.01$

4. Conclusion

In this work, we have obtained the vibrational specific heat capacity for spinless particles by solving the radial Schrödinger equation with the Rosen-Morse potential via the proper quantization rule to obtain equations for bound state energy eigenvalues and unnormalized eigenfunctions, a Pekeris-like approximation model was introduced to deal with the spin-orbit term of the effective potential. For some chosen values of potential depths of the Rosen-Morse potential, expressions for bound state ro-vibrational energy eigenvalues and eigenfunctions of the improved Rosen-Morse potential were deduced from those of the energy eigenvalues and radial wave functions for the Rosen-Morse potential, the results obtained were in total agreement with available results in the literature. With the help of our formula for the energy eigenvalues, we have

obtained expressions for classical ro-vibrational partition function and ro-vibrational specific heat capacity for the Rosen-Morse potential. Studies of these thermal functions show that as temperature is increased, the partition function decreases monotonically while the specific heat capacity drops from a large positive value to zero and remains approximately constant as temperature is further increased

References
[1]   Berkdemir, C., Berkdemir, A. and Sever, R. (2005a). Polynomial Solution of the Schrödinger Equation for the Generalized Woods-Saxon Potential. *Phys. Rev. C* **72** 027001 https://doi.org/10.1103/PhysRevC.72.027001

[2]   Serrano, F.A., Gu, X-Y. and Dong, S-H. (2010). Qiang-Dong Proper Quantization Rule and its Applications to Exactly Solvable Quantum Systems. *J. Math Phys.* **51**, 082103 https://doi.org/10.1063/1.3466802

[3]   Erkol, H. and Demiralp, E. (2007). The Woods-Saxon Potential with Point Interactions. *Phys. Lett. A* **365** 55-63 https://doi.org/10.1016/j.physleta.2006.12.050

[4]   Ikhdair, S.M. and Sever, R. (2010a). Any ℓ-state Solutions of the Woods-Saxon Potential in Arbitrary Dimensions within the New improved Quantization Rule. *Int. J. Mod. Phys. A.* **25**, 3941-3952 https://doi.org/10.1142/ S0217751X10050160

[5]   Sun, Y., He, S. and Jia C-S. (2013). Equivalence of the Deformed Modified Rosen-Morse Potential Energy Model and The Tietz Potential Energy Model. *Phys. Scr.* **87**, 025301 https://doi.org/10.1088/0031-8949/87/02/025301

[6]   Berkdemir, C., Han, J. (2005b). Any ℓ-state Solutions of the Morse Potential through the Pekeris Approximation and Nikiforov-Uvarov Method. *Chem. Phys. Lett.* **409** 203-207 https://doi.org/10.1016/j.cplett.2005.05.021

[7]   Qiang, W-C., Chen, W-L., Li, K. and Wei, G-F. (2009). The Scattering States of the ℓ-wave Schrödinger Equation with the Second Pöschl-Teller-like Potential. *Phys. Scr.* **79** 025005 https://doi.org/10.1088/0031-8949/79/02/025005

[8]   Taskin, F. and Kocal, K. (2010). Approximate Solutions of Schrödinger Equation for Eckart Potential with Centrifugal Term. *Chin. Phys. B*. **19** 090314 https://doi.org/10.1088/1674-1056/19/9/090314

[9]   Secrest, D., Cashion, K. and Hirchfelder, J.O. (1962). Power-Series Solutions for Energy Eigenvalues. *J. Chem. Phys.* **17**, 830-835

[10]   Qiang, W-C. and Dong, S-H. (2007). Arbitrary ℓ-state Solutions of the Rotating Morse Potential through Exact Quantization Rule Method. *Phys. Lett. A* **363**, 169-176 https://doi.org/10.1016/j.physleta.2006.10.091

[11]   Ma, Z-Q. and Xu, B-W. (2005). Quantum Correction in Exact Quantization Rules. *EPL* **69**, 685 https://doi.org/10.1209/epl/i2004-10418-8

[12]   Ma, Z-Q., Gonzalez-Cisneros, A., Xu, B-W. and Dong, S-H. (2007). Energy Spectrum of the Trigonometric Rosen-Morse Potential Using an Improved Quantization Rule. *Phys. Lett. A* **371**, 180-184 https://doi.org/10.1016/j.physleta.2007.06.021

[13]   Ikhdair, S.M. and Sever, R. (2010b). Approximate Analytical Solutions of the Generalized Woods-Saxon Potentials Including the Spin-Orbit Coupling Term and Spin Symmetry. *Cent. Eur. Phys.* **8**, 652-666 10.2478/s11534-009-0118-5

[14]   Okorie, U.S., Ikot, A.N., Chukwuocha, E.O. and Rampho, G.J. (2020). Thermodynamic Properties of Improved Deformed Exponential-Type Potential (IDEP) for Some Diatomic Molecules. *Results Phys.* **17** 103078 https://doi.org/10.1016/j.rinp.2020.103078

[15]   Ikot, A.N., Okorie, U.S., Sever, R. and Rampho, G.J. (2019). Eigensolution, Expectation Values and Thermodynamic Properties of the Screened Kratzer Potential. *Eur. Phys. J. Plus* **134**, 386 10.1140/epjp/i2019-12783-x

[16]   Onate, C.A. Ojonuba, J.O. (2015). Eigensolutions of the Schrödinger Equation with a Class of Yukawa Potentials via Supersymmetric Approach. *J. Theor. Phys.* **10**, 21-26 https://doi.org/10.1007/s40094-015-0196-2

[17]   Gordillo-Vázquez, F.J. and Kunc, J. (1998). Statistical-Mechanical Calculations of Thermal Properties of Diatomic Molecules. *J. Appl. Phys.* **84** 4693-4703 https://doi.org/10.1063/1.368712

[18]   Oyewumi, K.J., Falaye, B.J., Onate, C.A., Oluwadare, O.J. and Yahya, W.A. (2014). Thermodynamic Properties and the Approximate Solutions of the Schrödinger Equation with the Shifted Deng-Fan Potential Model. *Mol. Phys.* **112**, 127-141 https://doi.org/10.1080/00268976.2013.804960

[19]   Rosen, N. and Morse, P.M. (1932). On the Vibrations of Polyatomic Molecules. *Phys. Rev.* **42** 210-217 https://doi.org/10.1103/PhysRev.42.210

[20]   Zhang, G-D., Liu, J-Y., Zhang, L-H., Zhou, W. and Jia, C-S. (2012). Modified Rosen-Morse Potential-Energy Model for Diatomic Molecules. *Phys. Rev. A.* **86** 062510 https://doi.org/10.1103/PhysRevA.86.062510

[21]   Englefield, M.T. (1987). Algebra Representation of Eigenfunctions of the Rosen-Morse Potential. *J. Math Phys.* **28**, 827 https://doi.org/10.1063/1.527570

[22]   Khordad, R. and Mirhosseini, B. (2015). Linear and Nonlinear Optical Properties in Spherical Quantum Dots: Rosen-Morse Potential. *Condens. Matter Phys.* **117**, 434-440 10.1134/S0030400X14090100

[23]   Sun, G.H., Dong, S-H. and Saad, N. (2013). Quantum Information Entropies for Asymmetric Trigonometric Rosen-Morse Potential. *Ann. Phys.* (*Berlin*), **1**, 10 https://doi.org/10.1002/andp.201300089

[24]   Taskin. (2009). Approximate Solutions of Schrödinger Equation with the Rosen-Morse Potential Including the Centrifugal Term. *Int. J. Theor. Phys.* **48**, 2692-2697 https://doi.org/10.1007/s10773-009-0059-1

[25]   Ikot, A.N. and Akpabio, L.E. (2010). Approximate Solution of the Schrödinger Equation with Rosen-Morse Potential Including the Centrifugal Term. *Applied Physics Research* **2**, 202-208 doi.10.5539/apr.v2n2p202

[26]   Liu, J-Y., Hu, X-T. and Jia, C-S. (2014). Molecular Energies of Improved Rosen-Morse Potential Energy Model. *Can. J. Chem.* **92**, 40-44 dx.doi.org/10.1139/cjc-2013-0396

[27]   Jia, C-S., Diao, Y-F., Liu, X-J., Wang, P-Q., Liu, X-Y. *et. al.* (2012). Equivalence of Wei Potential Model and Tietz Potential Model for Diatomic Molecules. *J. Chem. Phys.* **137** 014101 http://dx.doi.org/10.1063/1.4731340.