ANALYSIS

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DISCOVERY

Thermodynamic Properties of Quantum Mechanical Gravitational plus Harmonic Oscillator Potential using the Proper Quantization Rule

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We obtained by using the proper quantization rule, the analytical solutions of the Schrödinger equation for the Deformed Harmonic Oscillator potential. The energy levels of all bound states as well as the normalized wave-functions are obtained. The vibrational entropy, heat capacity, partition function, mean free energy and, chemical potential were analyzed to further investigate the behavior of the mixed potential under investigation.

INTRODUCTION

The exact solution of both relativistic and non-relativistic equation for most of the physical potential possesses difficulties in area where the application of the approximation becomes necessary. i.e, in the case of the Schrödinger equation when the arbitrary angular momentum quantum number l is present, one can only solve the non-relativistic equation approximately using a suitable approximation scheme [1]. Some of such approximations which has successfully produced results include conventional approximation scheme proposed by Greene and Aldrich [2], improved approximation scheme by Jia *et al.* [3], elegant approximation scheme [4], the pekeris approximation which is based on a Taylor expansion series of the centrifugal potential [5] and recently a good approximation by Yazarloo *et al.* [6]. Some of these potentials include the Manning-Rosen potential [7], Rosen-Morse potential [8], Mobius square potential [9], Shifted Deng-Fan potential [10], Shioberg potential [11], Morse and generalised Morse potential [12].The Manning–Rosen potential have been widely investigated both in its pure state and when mixed for relativistic and non-relativistic equations using various methods where different approximation scheme were employed in the literature [13-23].

In this present work, a mixed potential known as the Quantum Mechanical Gravitational plus Harmonic Oscillator Potential, is investigated through the proper quantization rule (PQR). Recently, the thermodynamic properties of different potentials have been studied. Oyewumi *et al*. [24] studied the thermodynamic properties of the Schrodinger equation with a shifted Deng-Fanpotential via AIM method. Larkin and Filinov [25] investigated the thermodynamics of relativistic Newton–Wigner particle in external potential field. Suparmi *et al*. [26] studied the thermodynamics properties of diatomic molecules with q-deformed modified Poschl-Teller plus Manning Rosen non-central potential in D dimensions using SUSYQM approach. Sincethen, different authors have investigated the thermodynamic properties for some physical systems [27, 28]

We organize our work as follows; firstly, we give a brief introduction in section one. Secondly, in section two we discussed briefly the proper quantization rule. In section three, we obtained the approximate solution of the Schrodinger equation for any l-state. Section four will be dedicated to the thermodynamic properties of the MRHP model. Section four will present results and discuss the work. Finally the conclusion will be given in the last section.

PROPER QUANTIZATION RULE

The proper quantization rule has been used to investigate different quantum potential to obtain both exact and approximate solutions of non-relativistic particle equation by Qiang–Dong [29]. For the non-relativistic equation, the one dimensional Schrodinger equation expressed as

$$\frac{d^2}{dr^2}\psi(r) = -\frac{2m}{\hbar^2}[E - U(r)]\psi(r) \qquad (1)$$

Can be written as

$$\frac{d}{dr}\phi(r) = -\frac{2\mathrm{m}}{\hbar^2}[E - U(r)] - \phi(r)^2, \qquad (2)$$

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where $\phi(r) = \psi(r)^{-1}\, d\psi(r)/dr$ is the logarithmic derivative of the wavefunction $\psi(r)$ and the potential $U(r)$ is a piecewise continuous real function of the variable r. By investigating the one-dimensional Schrodinger equation via the exact quantization rule, Qiang and Dong obtained a proper quantization rule expressed as

$$\int_{r_1}^{r_2} k_n(r)\, dr - \int_{r_{01}}^{r_{02}} k_0(r)\, dr = n\pi, \tag{3}$$

$$k(r) = \sqrt{\frac{2m\left(E-U(r)\right)}{\hbar^2}} \tag{4}$$

where r_1 and r_2 are two turning points determined by $E = U(x)$. n is the number of nodes of $\phi(r)$ in the region $E \geq U(r)$ and it is larger by one than the number of nodes of wave function ψ(x). In a similar way, they generalized the quantization rule (3) to three-dimensional Schrodinger equation with a spherically symmetric potential. This is realized by taking $\psi(r) = r^{-1}R(r)Y_m^l\,(\theta,\phi)$. Substituting this into the Schrodinger equation allows us to obtain the following radial Schrodinger equation

$$\frac{d^2}{dr^2}R(r) = -\frac{2m}{\hbar^2}\left[E - V_{eff}(r)\right]R(r), \quad V_{eff}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2} \tag{5}$$

from eq.3, the two integrals have the same mathematical form. Accordingly, when applying it to calculate the energy levels, we can calculate its first integral with respect to $k(r)$ and then replace energy levels E_n in the result by the ground state energy E_0 to obtain the second integral.

QUANTUM MECHANICAL GRAVITATIONAL PLUS HARMONIC OSCILLATOR POTENTIAL

In this work, we study the one dimensional Schrodinger equation for the QMGHOP model [30],

$$V(r) = \gamma r + V_0 e^{-\alpha r} + \frac{1}{2}m\omega^2 r^2, \tag{6}$$

Eq. (6) can also be written as

$$V(r) = V + (\gamma - \alpha V_0)r + \left(\left(\alpha^2 V_0 + \frac{1}{2}m\omega^2\right)\right)r^2,$$

Where the turning points r_a and r_b are determined by $E = U(r)$,

$$E = V_0 + (\gamma - \alpha V_0)r + \left(\left(\alpha^2 V_0 + \frac{1}{2}m\omega^2\right)\right)r^2 \tag{7}$$

For simplicity, we can assume the following

$$\left(\left(\alpha^2 V_0 + \frac{1}{2}m\omega^2\right)\right) = A, (\gamma - \alpha V_0) = B, E - V_0 = C \tag{8}$$

$$r_1 = \frac{-b-\sqrt{b^2-4c}}{2}, \quad r_2 = \frac{-b+\sqrt{b^2-4c}}{2} \tag{9}$$

where we have obtained the two turning points

$$b = -\frac{B}{A} = r_1 + r_2 = -\frac{\gamma-\alpha V_0}{\left(\alpha^2 V_0 + \frac{1}{2}m\omega^2\right)}, \; c = -\frac{C}{A} = r_1 r_2 = -\frac{E-V_0}{\left(\alpha^2 V_0 + \frac{1}{2}m\omega^2\right)} \tag{10}$$

The momentum $k(r)$ between the two turning points is given by

$$k(r) = \sqrt{\frac{2m}{\hbar^2}(C - Ar^2 - Br)} \tag{11}$$

The corresponding non-linear Riccati equation (2) becomes

$$\frac{d}{dr}\phi(r) = -\frac{2\mathrm{m}}{\hbar^2}(C_0 - Ar^2 - Br) - \phi(r)^2 \tag{12}$$

Based on the Sturm–Liouville theorem, after taking $\phi_0(r) = -C_1 r + C_2 (C_1 > 0)$, substituting this into the above Riccati equation (11) we obtain

$$C_0 = \frac{\hbar\sqrt{A}}{\sqrt{2m}} - \frac{B^2}{4A} \tag{13}$$

on considering the first integral in eq.3, we obtained

$$\int_{r_1}^{r_2} k_n(r)\,dr = \sqrt{\frac{2mA}{\hbar^2}} \int_{r_1}^{r_2} \sqrt{(r-r_a)(r_b-r)}\,dr \tag{14}$$

$$= \frac{\pi\sqrt{2mA}}{8\hbar A^2}(B^2 + 4AC_n) \tag{15}$$

Where we used the following integral formula [31]

$$\int_{r_1}^{r_2} \sqrt{(r-r_1)(r_2-r)}dr = \frac{\pi}{8}(r_2-r_1)^2 \qquad 0<r_1<r_2 \tag{16}$$

By replacing C_n in (14) by C_0 given in (12) and considering (3), we obtain the following result:

$$C_n = \frac{\hbar\sqrt{2mA}}{m}\left(n+\frac{1}{2}\right) - \frac{B^2}{4A} \tag{17}$$

Substituting eq. 8 into eq. 17, we obtain the energy eigen value

$$E_n = \frac{\hbar\sqrt{2m\left(\alpha^2V_0+\frac{1}{2}m\omega^2\right)}}{m}\left(n+\frac{1}{2}\right) - \frac{(\gamma-\alpha V_0)^2}{4\left(\alpha^2V_0+\frac{1}{2}m\omega^2\right)} + V_0 \tag{18}$$

For the sake of simplicity throughout this study, we let the following

$$\frac{\sqrt{2m\left(\alpha^2V_0+\frac{1}{2}m\omega^2\right)}}{m} = \varpi, \tag{19}$$

$$-\frac{(\gamma-\alpha V_0)^2}{4\left(\alpha^2V_0+\frac{1}{2}m\omega^2\right)} + V_0 = \varrho \tag{20}$$

$$E_n = \left(n+\frac{1}{2}\right)\hbar\varpi + \varrho \tag{21}$$

THERMODYNAMIC PROPERTIES OF THE SYSTEM

In other to consider the thermodynamic properties of the QMG+HO potential for s-wave state, we calculate first, the vibrational partition function

$$Q_1{}^{vib}(\beta) = \sum_{n=0}^{\infty} e^{-\beta E_n}, \tag{22}$$

$\beta = \frac{1}{kT}$, Where k is the Boltzmann constant. (23)

$$Q_1{}^{vib}(\beta) = \sum_{n=0}^{\infty} e^{-\beta\left[\left(n+\frac{1}{2}\right)\hbar\varpi+\varrho\right]} \tag{24}$$

$$Q_1{}^{vib}(\beta) = e^{-\frac{\beta\hbar\varpi}{2}-\beta\varrho}\sum_{n=0}^{\infty} e^{-\beta\hbar\varpi n} \tag{25}$$

$$Q_1{}^{vib}(\beta) = e^{-\beta\left(\frac{\hbar\varpi}{2}+\varrho\right)}\left(\frac{e^{\beta\hbar\varpi}}{e^{\beta\hbar\varpi}-1}\right) = e^{-\beta\varrho}\left(\frac{e^{\frac{\beta\hbar\varpi}{2}}}{e^{\beta\hbar\varpi}-1}\right) \tag{26}$$

$$Q_1{}^{vib}(\beta) = e^{-\beta\varrho}\left(2sinh\frac{\beta\hbar\varpi}{2}\right)^{-1} \tag{27}$$

The vibrational partition function with N-body interaction with no interaction inside is given by

$$Q_N{}^{vib}(\beta) = Q_1{}^{vib}(\beta)^N = e^{-N\beta\varrho}\left(2sinh\frac{\beta\hbar\varpi}{2}\right)^{-N} \tag{28}$$

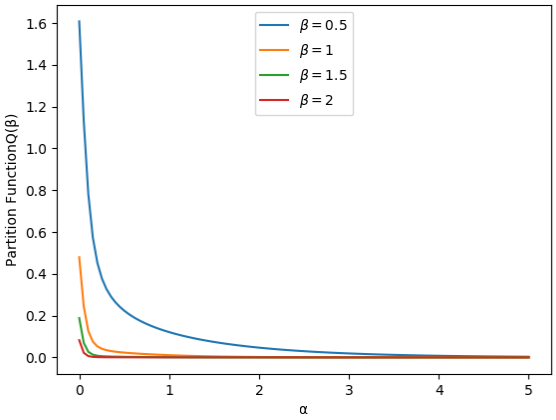

Figure 1 Vibrational partition function$Q_N{}^{vib}$ against α for different $\beta(0.5, 1, 1.5 \text{ and } 2)$

Taking natural log to both side of equation (28), we obtain

$$lnQ_N{}^{vib}(\beta) = Q_1{}^{vib}(\beta)^N = -N\beta\varrho - Nln\left(2sinh\frac{\beta\hbar\varpi}{2}\right) \tag{29}$$

The vibrational mean energy U($\boldsymbol{\beta}$)

The Vibrational mean energy for the QMGHOP model is obtained as

$$U(\beta) = -\frac{\partial}{\partial\beta} lnQ_N{}^{vib}(\beta) \tag{30}$$

$$U(\beta) = -\frac{\partial}{\partial\beta}\left(-N\beta\varrho - Nln\left(2sinh\frac{\beta\hbar\varpi}{2}\right)\right) \tag{31}$$

$$U(\beta) = N\left(\varrho + \frac{\hbar\varpi}{2} coth\frac{\beta\hbar\varpi}{2}\right) \tag{32}$$

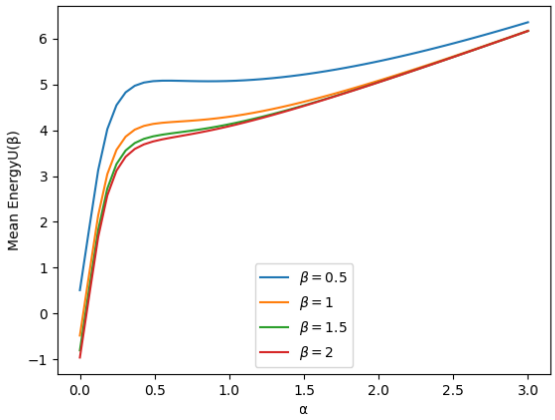

Figure 2 Vibrational Mean Energy U against α for different $\beta(0.5, 1, 1.5 \text{ and } 2)$

The vibrational mean free energy $\boldsymbol{F(\beta)}$:

$$F(\beta) = -\frac{1}{\beta} lnQ_N{}^{vib}(\beta) \tag{33}$$

$$F(\beta) = -\frac{1}{\beta}\left[-N\beta\varrho - Nln\left(2sinh\frac{\beta\hbar\varpi}{2}\right)\right] \tag{34}$$

$$F(\beta) = \left[N\varrho + \frac{N}{\beta} ln\left(2sinh\frac{\beta\hbar\varpi}{2}\right)\right] \tag{35}$$

$$F(\beta) = \left[N\varrho + NkTln\left(2sinh\frac{\hbar\varpi}{2kT}\right)\right] \quad (36)$$

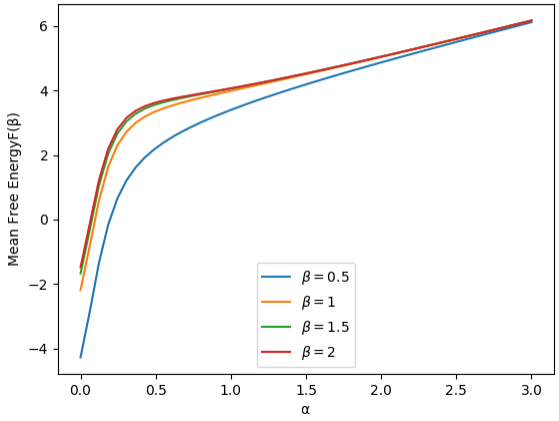

Figure 3 Vibrational Mean Free Energy F against α for different $\beta(0.5, 1, 1.5 \text{ and } 2)$

The Chemical potential$\mu(N)$

$$\mu = \frac{\partial F}{\partial N} = \frac{\partial}{\partial N}\left[N\varrho + NkTln\left(2sinh\frac{\hbar\varpi}{2kT}\right)\right] \quad (37)$$

$$\mu = \left[\varrho + kTln\left(2sinh\frac{\hbar\varpi}{2kT}\right)\right] \quad (38)$$

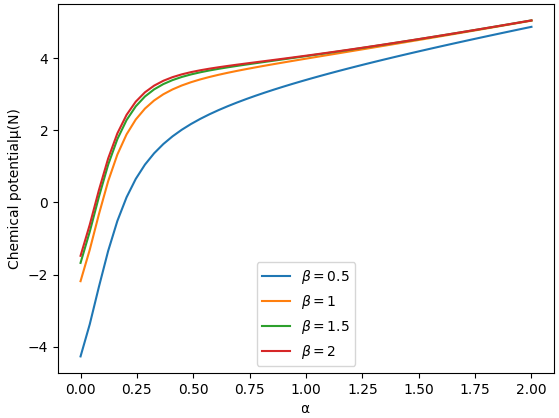

Figure 4 Chemical potential $\mu(N)$ against α for different $\beta(0.5, 1, 1.5 \text{ and } 2)$

The Vibrational specific heat capacity $C_v(\beta)$

$$C_v(\beta) = \frac{\partial U(\beta)}{\partial T} = -k\beta^2\frac{\partial U(\beta)}{\partial \beta} \quad (39)$$

$$C_v(\beta) = -k\beta^2\frac{\partial}{\partial \beta}\left[N\left(\varrho + \frac{\hbar\varpi}{2}coth\frac{\beta\hbar\varpi}{2}\right)\right] \quad (40)$$

$$C_v(\beta) = \frac{Nk\beta^2\hbar^2\varpi^2}{4}\left(sinh^2\left(\frac{\beta\hbar\varpi}{2}\right)\right)^{-1} \quad (41)$$

$$C_v(\beta) = \frac{N\hbar^2\varpi^2}{4kT^2}\left(sinh^2\left(\frac{\hbar\varpi}{2kT}\right)\right)^{-1} \quad (42)$$

$$C_v(\beta) = Nk\beta^2\hbar^2\varpi^2\frac{e^{-\beta\hbar\varpi}}{(1-e^{-\beta\hbar\varpi})^2} \quad (43)$$

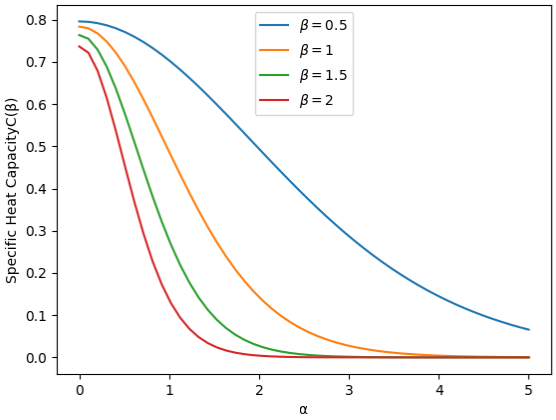

Figure 5 Vibrational Specific heat capacity C_v against α for different $\beta(0.5, 1, 1.5 \text{ and } 2)$

The Vibrational entropy$S(\beta)$

$$S(\beta) = klnQ_N{}^{vib}(\beta) - k\beta\frac{\partial}{\partial\beta}lnQ_N{}^{vib}(\beta) \tag{44}$$

$$S(\beta) = k\left(-N\beta\varrho - Nln\left(2sinh\frac{\beta\hbar\varpi}{2}\right)\right) - k\beta\left(-N\left(\varrho + \frac{\hbar\varpi}{2}coth\frac{\beta\hbar\varpi}{2}\right)\right) \tag{45}$$

$$S(\beta) = -Nkln\left(2sinh\frac{\beta\hbar\varpi}{2}\right) + Nk\beta\frac{\hbar\varpi}{2}coth\frac{\beta\hbar\varpi}{2} \tag{46}$$

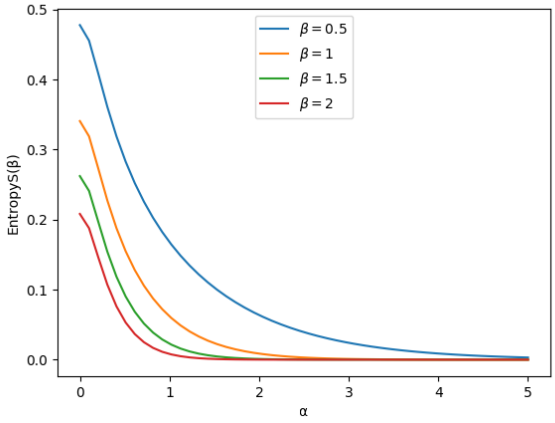

Figure 5 Vibrational Entropy S against α for different $\beta(0.5, 1, 1.5 \text{ and } 2)$

If we let $\beta = V_0 = 0$, then we obtain the energy spectrum of the harmonic oscillator potential.

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

CONCLUSION

In this study, we obtained by using the proper quantization rule, the analytical solutions of the Schrödinger equation for the Deformed Harmonic Oscillator potential. Furthermore, we study the thermodynamic properties of this model potential. From a high temperature partition function obtained, thermodynamic functions, such as vibrational mean energy U, specific heat C, free energy F and vibrational entropy S are derived. It is found that in the classical limit, the vibrational entropy S converges to a point for all the diatomic molecules at a different range of β. Also, we have conducted the numerical analysis by calculating the bound state energies in terms of the thermodynamic functions.

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