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Research Article

Mass spectra and thermal properties of deformed Schrödinger Equation for pseudoharmonic potential

E. E. Ibekwe[1] , E. P. Inyang[2*], J. B. Emah[1], A.O.Akpan[1] and O.J.Yawo[1]

[1] *Department of Physics, Akwa Ibom State University, Ikot Akpaden, P.M.B. 1167, Uyo, Nigeria*

[2] *Department of Physics, National open University of Nigeria, P.M.B. 581, Jabi, Abuja, Nigeria*

Abstract

In this research, non-relativistic Schrödinger Equation was solved and the related quantum mechanical properties were solved using the Nikiforov–Uvarov (NU) method. The energy spectrum and wave function of the pseudoharmonic potential model are obtained. We applied the energy eigenvalues to investigate the mass spectra (MS) of heavy mesons such as charmonium and bottomonium. In addition, the partition function is calculated in a closed-form and is used to obtain expressions for other thermal properties such as vibrational free energy, mean energy, vibrational entropy, and vibrational heat capacity. The MS was found to be in agreement with the experimental data and previously reported results of others.

Keywords: Deformed quantum mechanics; bound state; mass spectra; thermal properties

* Corresponding author: etidophysics@gmail.com OR einyang@noun.edu.ng

https://orcid.org/0000-0002-5031-3297

1. INTRODUCTION

In both relativistic and non-relativistic quantum mechanics, the solution to wave equations has contributed immensely to the study of quantum systems owing to their ability to give sufficient information about the system of consideration[1-2]. In non-relativistic quantum mechanics, researchers work mostly on the solutions of the Schrödinger equation (SE) [3-5]. Consequently, many researchers in this area make it their main aim to generate solutions for the SE with any available potential model [6-7]. Some of the potential models includes pseudoharmonic potential [8-10], Kratzer potential [11-12], Coulomb potential [13-15], and many more. In the recent time, these potential models are modified either by addition of screening parameter as in the case of screened Kratzer potential [16-17], screened Coulomb potential [18] or adding two or more potentials together as in the case of modified Kratzer plus screened Coulomb potential [19-20]. In solving the solutions, it is observed that very few of the potential can be solved exactly with the SE [21-22] while others can only be solved approximately through the use of approximation scheme such as Greene–Aldrich approximation Scheme [23] and Perkeris approximation [24].

Many approaches have been employed in solving for the solutions of the SE and some of the techniques in the available literatures include the series expansion method [25,26], factorization method [27-29], Nikiforov-Uvarov method (NU) [30-32], the asymptotic iteration method [33-35] and a few others. The solution of the SE has a wide area of applications in physics, chemistry and in quantum field theory [36]. Some of such applications include the investigation of thermal function of a system [37], the study of diatomic molecular interaction [38], examination of mass spectroscopy for heavy [39-44] and lighter quarks [45]. A pseudoharmonic potential (PP) is simply an extension of the harmonic oscillator potential, a combination of the harmonic oscillator potential with a centrifugal potential which takes the form [46-47].

$$V(X) = AX^2 + \frac{B}{X^2} + C, \tag{1}$$

where *A*,*B* and *C* are potential constants. If the constants *C* and *B* set to be zero, the potential reduces to harmonic oscillator potential. Maiz [48] and Ikot et. al.[49] describe the potential as a very important molecular potential of diatomic molecules. This potential has been in existence for decades but its value keeps increasing in worth. In the recent articles, Ikot et. al. [49] study the thermal properties of the PP in the presence of AB field, Onate et.al, [50] obtained the polynomial solution of the potential with SE. Onate et.al.[51] obtained the exact solution of SE with the PP. Song et al., under relativistic quantum mechanics, obtained the exact solution to Klein Gordon equation with PP.

2. CLASSICAL OSCILLATOR ALGEBRA

The classical oscillator algebra is defined by the canonical commutation [1]

$$\begin{aligned} \left[a, a^{\dagger}\right] &= 1, \\ \left[N, a\right] &= -a, \\ \left[N, a\right] &= a^{\dagger}, \end{aligned} \tag{1a}$$

where the number operator is given by N and it is assumed to be Hermitian. The first deformation by following expressions Arik and Coon [40]:

$$\begin{aligned} aa^{\dagger} - qa^{\dagger}a &= 1, \\ \left[N, a^{\dagger}\right] &= a^{\dagger}, \\ \left[N, a\right] &= -a. \end{aligned} \tag{1b}$$

the number operator and step operators are related by the expression,

$$a^{\dagger}a = \left[N\right]_q, \tag{2}$$

where q-number is defined as

$$\left[X\right]_q = \frac{1-q^X}{1-q}. \tag{3}$$

The Jackson derivative is defined as follows [1, 52]:

$$\partial_x^q f\left(x\right) = \frac{f(x) - f(qx)}{(1-q)x}, \tag{4}$$

as $q \to 1$,equation(4) reduces to the ordinary derivative.

We can obtain the q-deformed SE of the form

$$\left[-\frac{\hbar^2}{2\mu}\left(\partial_x^q\right)^2 + U(x)\right]\psi(x) = E\psi(x), \tag{5}$$

if we introduce $\partial_q = \left(\hbar/i\right)\partial_x^q$.

In recent investigation, Tsallis [41] proposed another type of q-deformed theory appeared in statistical physics.

3. THE DEFORMED SCHRÖDINGER TIME-INDEPENDENT EQUATION

The time-independent SE in deformed mechanism is given by [1]

$$\left[-\frac{\hbar^2}{2\mu}D_x^2+V(x)\right]U(x)=EU(x), \tag{6}$$

where,

$$D_x=\left(1+q\left|x\right|\right)\frac{\partial}{\partial x}. \tag{7}$$

By using change of variable [1]

$$X=\frac{1}{q}\ln\left(1+q\left|x\right|\right), \tag{8}$$

equation (6) becomes

$$-\frac{\hbar^2}{2\mu}\frac{d^2U(X)}{dX^2}+V(X)U(X)=EU(X). \tag{9}$$

Now considering the pseudoharmonic potential [2, 42]

$$V(X)=AX^2+\frac{B}{X^2}+C. \tag{10}$$

Substituting equation (10) into equation (9) and applying the change of variable $s=X^2$ yields

$$\frac{d^2U(s)}{ds^2}+\frac{1}{2s}\frac{dU(s)}{ds}+\frac{1}{4s^2}\left(-\alpha s^2-\varepsilon s-\beta\right)U(s)=0, \tag{11}$$

with,

$$\alpha=\frac{-2\mu A}{\hbar^2},\ \beta=\frac{2\mu B}{\hbar^2},\quad -\varepsilon=\frac{2\mu\left(E-C\right)}{\hbar^2}. \tag{12}$$

Comparing Eq. (11) with the hypergeometric equation below

$$\psi''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s). \tag{13}$$

We obtain these parameters which are necessary for NU method

$$\begin{aligned}&\tilde{\tau}(s)=1,\\&\sigma(s)=2s,\\&\tilde{\sigma}(s)=\left(-\alpha s^2-\varepsilon s-\beta\right)\end{aligned} \tag{14}$$

One of the key parameters of NU method which is employed to solve the hypergeometric differential equation is $\pi(s)$ given by the expression [43-46]

$$\pi(s)=\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\pm\sqrt{\left(\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\right)^2-\tilde{\sigma}(s)+k\sigma(s)}. \quad (15)$$

Substituting equation (14) into equation (15) we obtain

$$\pi(s)=\frac{1}{2}\pm\sqrt{\alpha s^2+\left(\varepsilon+2k\right)s+\beta+\frac{1}{4}}. \quad (16)$$

Setting the discriminant of the quadratic term inside the square root to zero yields

$$k=-\frac{\varepsilon}{2}\pm\sqrt{\alpha\left(\beta+\frac{1}{4}\right)}. \quad (17)$$

Putting equation 17 into equation 16 results in

$$\pi(s)=\frac{1}{2}\pm\left(\sqrt{\alpha}s-\sqrt{\beta+\frac{1}{4}}\right). \quad (18)$$

Another important parameter for the determination of the energy eigenvalues is given by the expression,

$$\tau(s)=\tilde{\tau}(s)+2\pi(s). \quad (19)$$

Plugging equations (14) and (18) into (19) yields

$$\tau(s)=2-2\sqrt{\alpha}s+2\sqrt{\beta+\frac{1}{4}}. \quad (20)$$

The energy parameter is given as

$$\lambda=k+\pi'(s). \quad (21)$$

$$\lambda=-\frac{\varepsilon}{2}-\sqrt{\alpha\left(\beta+\frac{1}{4}\right)}-\sqrt{\alpha}. \quad (22)$$

λ_n is another useful parameter given by the expression,

$$\lambda_n=-n\tau'(s)-\frac{n\left(n-1\right)}{2}\sigma''(s). \quad (23)$$

Evaluating Eq. (23) yields

$$\lambda_n=2n\sqrt{\alpha}. \quad (24)$$

Linking Eqs. (22) and (24) yields the eigenvalues expression as

$$E_n=\frac{\hbar^2}{\mu}\left(2n+1+\sqrt{\frac{1}{4}+\frac{2\mu B}{\hbar^2}}\right)\sqrt{\frac{2\mu A}{\hbar^2}}+C. \quad (25)$$

The unnormalized wave function is given as

$$\psi(s)=B_n s^{\left(1/2+\sqrt{\beta+1/4}\right)}e^{-\sqrt{\alpha}s/2}L_n^{\sqrt{\beta+1/4}}(s). \quad (26)$$

where, B_n is the normalization constant.

4. MASS SPECTRA

To determine the mass spectra of charmonium and bottomonium we use the following relation [54-61].

$$M = 2m_b + E_{nl}. \tag{27}$$

where, m_b is the mass of the particle under investigation and E_{nl} is the derived energy eigenvalues. Putting equation (25) into equation (27) we obtain

$$M = 2m + \frac{\hbar^2}{\mu}\left(2n+1+\sqrt{\frac{1}{4}+\frac{2\mu B}{\hbar^2}}\right)\sqrt{\frac{2\mu A}{\hbar^2}} + C. \tag{28}$$

5. THERMAL PROPERTIES

In this section, the partition function and other thermal properties are obtained.
The Partition function is given from the relation [47-50]

$$Z(\beta) = \sum_0^\infty e^{-E\beta}. \tag{29}$$

where, $\beta = \frac{1}{k_B T}$, k_B is Boltzmann constant and T is the absolute temperature.

Replacing Eq. (25) into Eq. (29) gives

$$Z(\beta) = \sum_0^\infty e^{-\beta\left[\frac{\hbar^2}{\mu}\left(2n+1+\sqrt{\frac{1}{4}+\frac{2\mu B}{\hbar^2}}\right)\sqrt{\frac{2\mu A}{\hbar^2}}+C\right]} \tag{30}$$

$$Z(\beta) = \frac{e^{-\frac{1}{2}\beta\left(\sqrt{2}\sqrt{\frac{\hbar^2 A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}-2\sqrt{2}\sqrt{\frac{\hbar^2 A}{\mu}}+2C\right)}}{e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2 A}{\mu}}}-1} \tag{31}$$

The mean energy is given as

$$U(\beta) = \frac{-\partial \ln Z(\beta)}{\partial \beta}. \tag{32}$$

Substituting Eq. (31) in Eq.(32) yields

$$U(\beta)=\frac{1}{2}\frac{1}{e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}-1}\left(\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}\right.$$
$$-\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}+2\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}} \tag{33}$$
$$\left.+2Ce^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}+2\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}-2C\right)$$

The vibrational free energy is given by the expression

$$F=\frac{-1}{\beta}\ln Z(\beta). \tag{34}$$

Substituting equation eqn (31) into Eq. (34) yields

$$F(\beta)=-\frac{1}{\beta}\ln\left(\frac{e^{-\frac{1}{2}\beta\left(\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}-2\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}+2C\right)}}{e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}-1}\right) \tag{35}$$

The vibrational entropy is given by the expression

$$S=K\ln Z(\beta)-K\beta\frac{\partial}{\partial\beta}\ln Z(\beta). \tag{36}$$

Substituting Eq.(31) in Eq.(36) yields

$$S(\beta)=\frac{1}{2}\frac{1}{e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}-1}\left(\left(\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}\beta\right.\right.$$
$$-\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}\beta+2\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}\beta$$
$$\left.+2Ce^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}\beta+2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}-2C\beta\right)$$
$$+2\ln\left(\frac{e^{-\frac{1}{2}\beta\left(\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}-2\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}+2C\right)}}{e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}-1}\right)e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}} \tag{37}$$
$$\left.-2\ln\left(\frac{e^{-\frac{1}{2}\beta\left(\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}\sqrt{\frac{8B\mu+\hbar^2}{\hbar^2}}-2\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}+2C\right)}}{e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}-1}\right)K\right)$$

The vibrational heat capacity (C) is obtained by the expression

$$C(\beta)=K\beta^2\frac{\partial^2}{\partial\beta^2}\ln Z(\beta). \tag{38}$$

Substituting Eq.(31) into Eq.(38) yields

$$C(\beta)=\frac{8K\beta^2A\mu^2e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}}{\mu\left(e^{2\beta\sqrt{2}\sqrt{\frac{\hbar^2A}{\mu}}}-1\right)^2}. \tag{39}$$

6. RESULTS AND DISCUSSION

In this work, the bound state solutions of the deformed SE has been obtained and applied to study the mass spectra (MS) and thermal properties of a quarkonium system. The expression for MS has been applied to investigate two heavy quarks (charmonium and bottomonium). The numerical result of the MS for the system in comparison with other investigations and the experimental data (ED) are presented in Tables 1 and 2 for charmonium and bottomonium, respectively.

Table 1. Mass spectra of Charmonium

$m_c=1.209GeV, A=0.01683411603$ GeV, $B=1.818933600\,GeV and\ C=$ -0.3993298767 GeV.

State	Present work	Ref.[58]	Ref.[53]	Ref.[54]	Exp.[60]
1s	3.095999999	3.0961	3.0959	3.098	3.096
2s	3.567999999	3.6862	3.6858	3.689	3.686
3s	4.040000001	4.0403	4.3228	4.041	4.040
4s	4.512000001	4.3411	4.9894	4.266	4.263
5s	4.984000001	-	-	-	4.421

Table 2. Mass spectra of Bottomonium

$m_b=4.68GeV, A=0.03224051994$ GeV, $B=0.9245003269$ GeV $and\ C=$ -0.522 GeV

State	Present work	Ref.[58]	Ref. [53]	Ref. [54]	Exp.[60]
1s	9.69112601	9.4607	9.5151	9.461	9.460
2s	10.02312601	10.0240	10.0180	10.023	10.023
3s	10.35512601	10.3563	10.4414	10.365	10.355
4s	10.68712601	10.6196	10.8577	10.588	10.580
5s	11.01912601	-	-	-	

The ED is taken from [60]. From the tables, it is observed that the masses increase with increase in quantum states and that the results agree with the theoretical results of similar investigations. Figures 1 to 3 are the variation of the MS of charmonium with the potential parameters *A*, *B* and *C*.

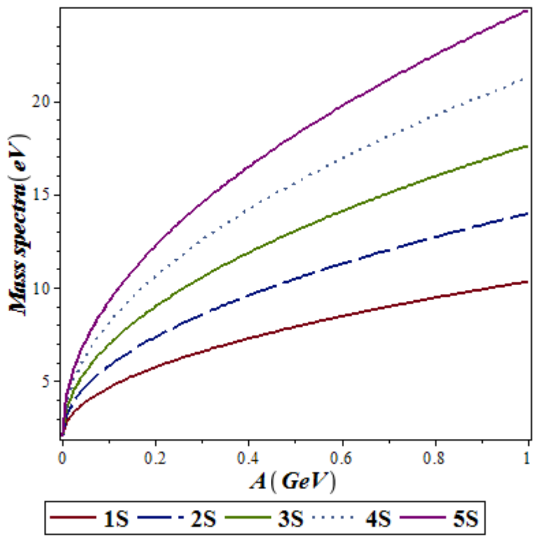

Fig.1: The plot of the mass spectra of charmonium against potential parameter *A* for different quantum mechanical states

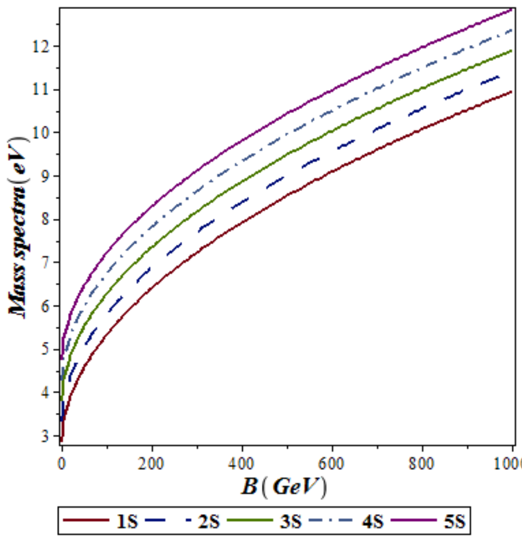

Fig.2: The plot of the mass spectra of Charmonium against potential parameter *B* for different quantum mechanical states

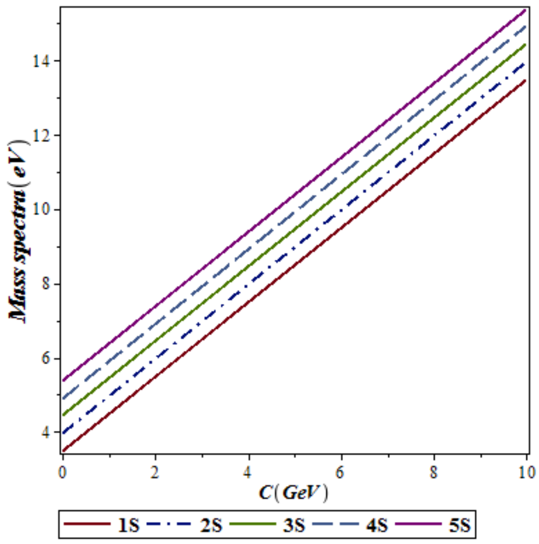

Fig.3: The plot of the mass spectra of charmonium against potential parameter C for different quantum mechanical states

Figures 4 to 6 present the variation of the MS of bottomonium with the potential parameters *A*, *B* and *C*. For potential parameter A, for the two systems, the curves for all the quantum states emanated from the origin and spread out, for different quantum state. Potential parameter *C* portrays a very linear relationship with the masses for all the quantum states which agrees with the ED. The masses increase as the potential parameter increases for the two systems.

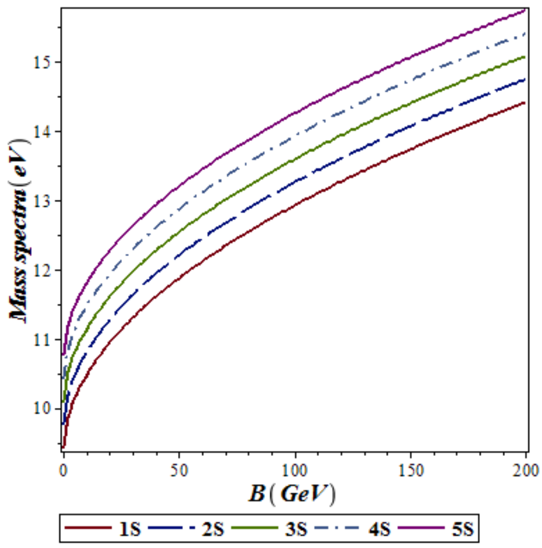

Fig.4: The variation of the mass spectra of bottomonium against potential parameter B for different quantum mechanical states

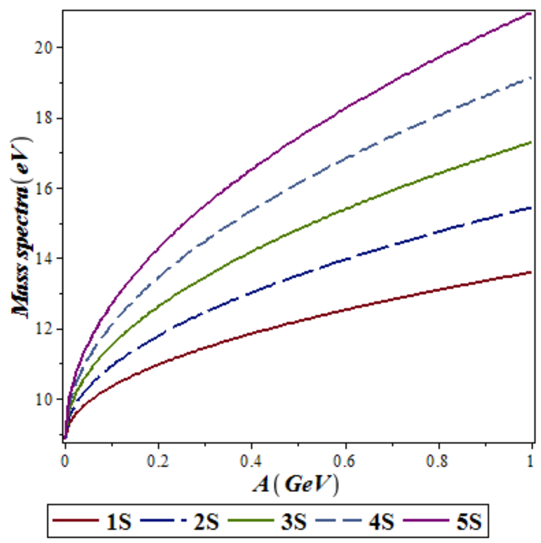

Fig.5: The variation of the mass spectra of bottomonium against potential parameter B for different quantum mechanical states

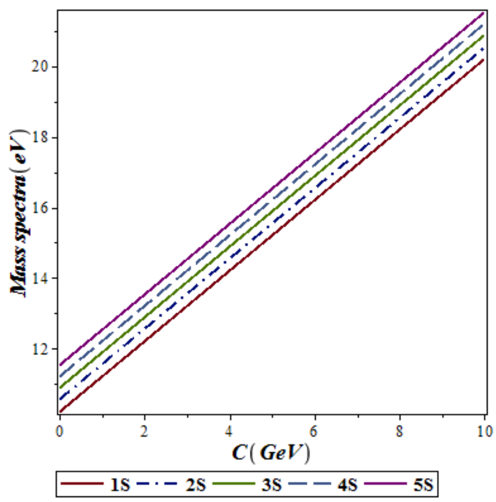

Fig.6: The variation of the mass spectra of bottomonium against potential parameter C for different quantum mechanical states

The plots of the thermal properties are presented in Figs.7 to 11. In Fig. 7 the partition function $Z(\beta)$ was noticed to decrease exponentially with increasing temperature (β) for different values of potential parameter (A). In Fig. 8 the mean energy $U(\beta)$ decreases as the temperature increases with diverse values of A. Figure 9 reveals that free energy $F(\beta)$ increases with an increase in temperature. The variation of entropy $S(\beta)$ as a function of temperature β and the A is shown in Fig. 10. Upward shift in the entropy $S(\beta)$ as the temperature increases was observed. Figure 11 depicts a decrease in specific heat as temperature increases.

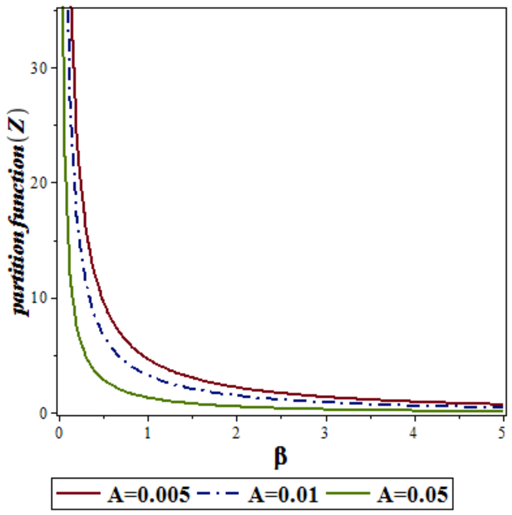

Fig. 7: Vibrational partition function (Z) against temperature

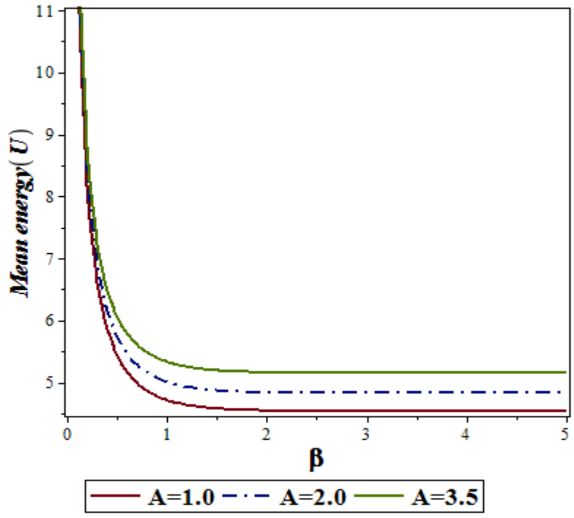

Fig. 8: Variation of vibrational mean energy (*U*) with temperature

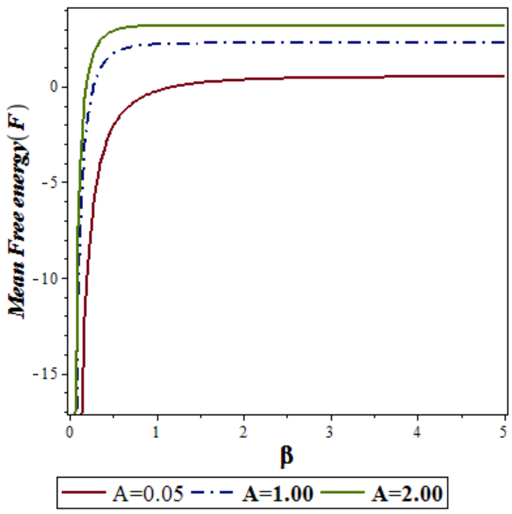

Fig. 9: Variation of vibrational free energy (F) with temperature

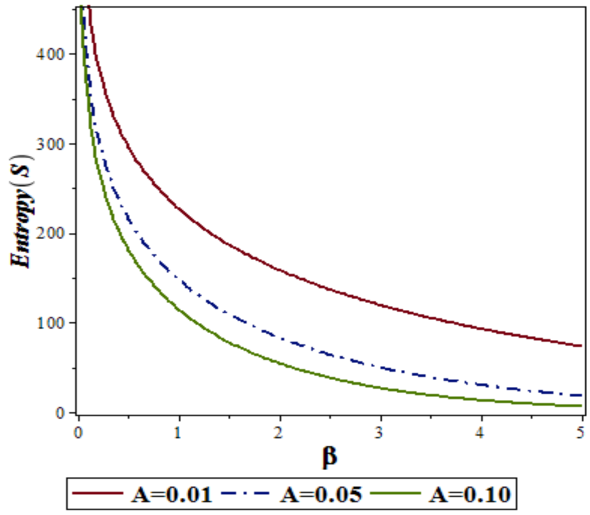

Fig. 10: Vibrational Entropy (S) with temperature

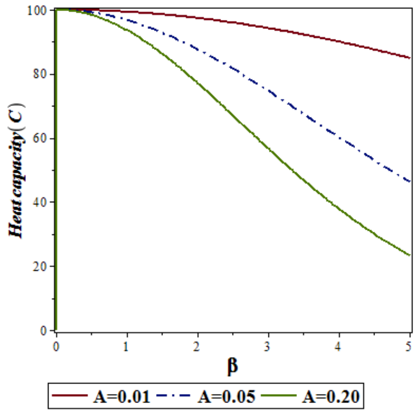

Fig. 11: Variation of vibrational heat capacity (*C*) with temperature

6. CONCLUSION

In this article, we adopted the q-deformation quantum mechanics. Within the framework of such formalism of quantum mechanics, we obtained the bound state energy spectrum of pseudoharmonic potential using the well-known NU method. The energy spectrum was used to determine the MS of heavy mesons such as charmonium and bottomonium. Also, the vibrational partition functions Z(β) was obtained from the energy equation, followed by other TPs such as vibrational mean energy U(β), vibrational entropy S(β), vibrational heat capacity and vibrational mean free energy F(β). The variation of MS with various potential parameters and plots of TPs were discussed. The determined MS agreed with ED and other theoretical determination reported in literature.

AVAILABILITY OF DATA AND MATERIALS
All data generated during this study are included in the references in the paper.

COMPETING INTERESTS
The authors declare that they have no competing interests.

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