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## THERMODYNAMIC PROPERTIES OF YTTRIUM BARIUM COPPER OXIDE ( $YBa_2Cu_3O_{7-x}$ ) SUPERCONDUCTING QUANTUM WELL

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### ABSTRACT

In this work, we obtained analytical bound state solution of Schrodinger wave equation and thermodynamic properties with modified Hulthen plus generalized Coulomb Potential as applied to Yttrium Barium copper oxide ( $YBa_2Cu_3O_{7-x}$ ) superconductor using parametric Nikiforov-Uvarov method (NU). We obtained the energy eigenvalues for various screening parameter ( $\alpha = 0.2, 0.4, 0.6, 0.8, 1.0$ ) and the total normalized wave function expressed in terms of Jacobi polynomial. Thermodynamic properties of  $YBa_2Cu_2O_{7-x}$  such as the vibrational mean energy  $U(\beta)$ , vibrational heat capacity  $C(\beta)$ , vibrational entropy  $S(\beta)$  and vibrational free energy  $F(\beta)$  were obtained using partition function. The thermodynamic wave functions and probability density plots were also obtained. Yttrium Barium copper oxide can be used on an adjustment measure to obtain necessary inherent and band gap energies for the production and manufacturing of  $YBa_2Cu_2O_{7-x}$  technological devices.

**Keywords:** Schrödinger Equation; Thermodynamic properties, Nikiforov-Uvarov method; Modified Hulthen plus generalized Coulomb potential, Yttrium Barium copper oxide

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### Introduction

The high-temperature superconductor (HTS)  $YBa_2Cu_2O_{7-x}$  is one of the most promising materials for applications and hence it has been intensively investigated by many researches since its discovery in 1986. The important issue here is to improve the efficiency of current transmission for HTS  $YBa_2Cu_2O_{7-x}$  as well as making its superconducting properties more reliable robust and reproducible, which is associated with difficulty in fabrication for practical applications (Zhang, *et al.*, 2016). According to Ikot *et al.* (2021), a crucial and fascinating problem in physics is to study the thermal and magnetic properties of quantum systems, and some researchers have investigated in this direction. For example, Johan *et al.* (2019) scrutinized the effect of geometric and transport properties of a Gallium Arsenide (GaAs) quantum Dot (QD) using the power exponential potential model. There are several ways of classifying superconductors, either by their response to an external magnetic field, their materials constituents such as elements, alloys or ceramics and their critical temperature (low temperature or high temperature).

Type I superconductors comprises mainly of metals and has only one critical field while Type II superconductors comprise mainly of alloys and compound with two critical fields exhibiting perfect diamagnetism (Josephson, 1964). Studying thermodynamic properties of High temperature superconductor ( $YBa_2Cu_2O_{7-x}$ ) will reveal some hidden properties that enhance the development of several superconductor technological devices. Thermodynamic properties of quantum mechanical system is derived from exact partition function (Okon, *et al.*, 2015). The eigen functions obtained by solving schrodinger wave equation provide vital information and gives in-depth understanding of quantum mechanical systems (Greiner, 2001; Chen, 2004; Zhang *et al.*, 2010; Flugge, 1974 and Onate *et al.*, 2022). The

relativistic wave equations are Dirac and Klein-Gordon equations while Schrödinger wave equation is a non-relativistic wave equation (Antia *et al.*, 2022; Chalk, 1988; Okon, *et al.*, 2015; Isonguyo, *et al.*, 2014; Omugbe, *et al.*, 2020; Farout, *et al.*, 2021 and Edet, *et al.*, 2020).

The thermodynamic properties examined in this work are vibrational mean energy  $U(\beta)$ , vibrational heat capacity  $C(\beta)$ , Vibrational entropy  $S(\beta)$  and vibrational free energy  $U(\beta)$ . The proposed potential use in this work is modified Hulthen plus generalized Coulomb Potential. This potential has applications in several branches of physics such as high energy physics, particle physics, molecular physics and for modelling superconductors (Chalk, 1988; Ita, *et al.*, 2017; Falaye, *et al.*, 2013; Ahmadov, *et al.*, 2021; Ikhdair, 2011 and Landau, *et al.*, 1977). The proposed potential model is given as

$$V(r) = -\frac{Ve^{-2xr}}{1-e^{-2xr}} - \frac{Ze^{-2xr}}{r} \quad (1)$$

### Parametric Nikiforov – Uvarov Method

The parametric formalization of NU involves reducing the second order linear differential equation to a generalized equation of hyper-geometric-type. This method provides exact solutions in terms of special orthogonal functions as well as the corresponding energy equation. With appropriate coordinate transformation,  $s = s(x)$ , this equation can be written as (Nikiforov, 1988; Okon, *et al.*, 2017; Ikhdair, 2009 and Tezcan, *et al.*, 2009).

$$\psi''(s) + \frac{\bar{r}(s)}{\sigma(s)} \psi'(s) + \frac{\bar{q}(s)}{\sigma^2(s)} \psi(s) = 0 \quad (2)$$

where  $\bar{r}(s)$  is a polynomial of degree one,  $\sigma(s)$  and  $\bar{q}(s)$  are polynomials of at most degree two. Then the parametric NU differential equation is in the form (Okon, *et al.*, 2017).

$$\psi''(s) + \frac{c_1 - c_2 s}{s(1-c_3 s)} \psi'(s) + \frac{1}{s^2(1-c_3 s)^2} [-\xi_1 s^2 + \xi_2 s - \xi_3] \psi(s) = 0 \quad (3)$$

Other parametric constants can be obtained as

$$\left[ \begin{array}{l} c_1 = c_2 = c_3 = 1, c_4 = \frac{1}{2}(1 - c_1), c_5 = \frac{1}{2}(c_2 - 2c_3), \\ c_6 = c_5^2 + \xi_1, c_7 = 2c_4 c_5 - \xi_2, c_8 = c_4^2 + \xi_3, \\ c_8 = c_4^2 + \xi_3, c_9 = c_3 c_7 + c_3^2 c_8 + c_6, c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}, \\ c_{11} = c_2 - 2c_5 + 2(\sqrt{c_9} + c_3 \sqrt{c_8}), c_{12} = c_4 + \sqrt{c_8} \\ c_{13} = c_5 - (\sqrt{c_9} + c_3 \sqrt{c_8}) \end{array} \right] \quad (4)$$

The energy eigen equation is given as

$$c_2 n - (2n + 1)c_5 + (2n + 1)(\sqrt{c_9} + c_3 \sqrt{c_8}) + n(n - 1)c_3 + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0 \quad (5)$$

while corresponding wave function is given by

$$\psi(s) = \phi(s) \chi_n(s) = N_n s^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{(c_{10}-1, \frac{c_{11}}{c_3} - c_{10}-1)} (1 - 2c_3 s) \quad (6)$$

### Solution of Schrödinger Equation Using Modified Hulthen Plus Generalised Coulomb Potential

The radial solution of Schrödinger wave equation in the presence of orbital angular quantum number for varying quantum state. (Inyang, *et al.*, 2020; Pakdel, *et al.*, 2014; Bale, *et al.*, 2019; Ikot, *et al.*, 2016; Okon, *et al.*, 2018; Farout, *et al.*, 2021; Ikot, *et al.*, 2012; Sever, *et al.*, 2012; Ukewuihe, *et al.*, 2012 and Diao, *et al.*, 2009) is given as

$$\frac{d^2 R(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left\{ (E_{nl} - V(r)) - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right\} \psi(r) = 0 \quad (7)$$

where  $E_{nl}$  is the exact bound state energy eigenvalues,  $\psi(r)$  is the wave function,  $\mu$  represent the reduced mass.  $n$  and  $l$  are known as the quantum number and rotation quantum number. On substituting equation (1) into equation (7), the radial part of the Schrödinger equation for the Modified Hulthen Plus Generalised Coulomb potential is given as:

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

To deal with the present of the centrifugal barrier in equation (8) above, the Greene–Aldrich approximation scheme (Ikhdair, 2009) is employed:

$$\frac{1}{r^2} = \frac{\alpha^2}{(1 - e^{-\alpha r})^2} \Rightarrow \frac{1}{r} = \frac{\alpha}{(1 - e^{-\alpha r})} \quad (9)$$

Using the coordinate transformation  $s = e^{-\alpha r}$  and by substituting equation (9), into equation (8) with the help of equation 5, gives energy eigen equation as

$$E_{nl} = -\frac{\hbar^2 \alpha^2}{2\mu} \left\{ \frac{n^2 + n + \frac{1}{2} + (n + \frac{1}{2}) \sqrt{1 + 4l(l+1)} - \frac{\mu v}{2\hbar^2 \alpha^2} - \frac{Z e \mu}{\hbar^2 \alpha} + l(l+1)}{(2n+1) + 1 + 4l(l+1)} \right\}^2 \quad (10)$$

Equation (10) can be express in a closed and compact form as

$$E_{nl} = -\frac{\hbar^2 \alpha^2}{2\mu} \left\{ \left[ n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4l(l+1)} \right] + \frac{\left( \frac{-\mu v}{2\hbar^2 \alpha^2} - \frac{Z e \mu}{\hbar^2 \alpha} \right)^2}{\left[ n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4l(l+1)} \right]} \right\}^2 \quad (11)$$

Which can further be simplified as

$$E_{nl} = -Q_1 \left\{ (n + \delta) + \frac{Q_2}{(n + \delta)} \right\}^2 \quad (12)$$

Where

$$Q_1 = \frac{\hbar^2 \alpha^2}{2\mu}, Q_2 = \left( \frac{-\mu v}{2\hbar^2 \alpha^2} - \frac{Z e \mu}{\hbar^2 \alpha} \right), \delta = \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4l(l+1)} \quad (13)$$

The total wave function is obtained using equation (6) as

$$\Psi_n(r) = N_{nl} (e^{-2\alpha r})^\beta (1 - e^{-2\alpha r})^\zeta P_n^{[2\beta, (2\zeta-1)]} (1 - 2e^{-2\alpha r}) \quad (14)$$

$$\beta = \sqrt{\frac{-\mu E_{nl}}{2\hbar^2 \alpha^2}}, \zeta = \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4l(l+1)} \quad (15)$$

### Thermodynamic Properties for the proposed potential.

The thermodynamic properties of quantum systems can be obtained from the exact partition function given as:

$$Z(\beta) = \sum_{n=0}^{\lambda} e^{-\beta E_n} \quad (16)$$

Where,  $\lambda$  an upper bound of the vibrational quantum number obtain from the numerical solution of  $\frac{dE_n}{dn} = 0$ ,  $\beta = \frac{1}{kT}$ ,  $K$  and  $T$  are Boltzmann constant and absolute temperature respectively. In classical limit, the summation in equation (16) can be replaced with the integral:

$$Z(\beta) = \int_0^{\lambda} e^{-\beta E_n} dn \quad (17)$$

By inserting equation (10) into (13) and simplifying gives the partition function as

$$Z(\beta) = e^{2\beta Q_1 Q_2} \int_{\delta}^{\lambda} e^{\beta \left( Q_1 \rho^2 + \frac{Q_1 Q_2}{\rho^2} \right)} d\rho \quad (18)$$

$$\text{Where } \rho = n + \delta \quad (19)$$

The solution of equation (18) Using Mathematica software is given as:

$$Z(\beta) = \frac{1}{4\sqrt{-\beta Q_1}} e^{2\beta Q_1 Q_2} \sqrt{\pi} \left\{ \begin{array}{l} e^{-2\sqrt{-\beta Q_1} \sqrt{\beta Q_1 Q_2^2}} \left[ 1 + \operatorname{erf} \left( \lambda \sqrt{-\beta Q_1} - \frac{\sqrt{\beta Q_1 Q_2^2}}{\lambda} \right) \right] \\ + e^{2\sqrt{-\beta Q_1} \sqrt{\beta Q_1 Q_2^2}} \left[ -1 + \operatorname{erf} \left( \lambda \sqrt{-\beta Q_1} + \frac{\sqrt{\beta Q_1 Q_2^2}}{\lambda} \right) \right] \end{array} \right\} \quad (20)$$

Other thermodynamic properties are obtained using the partition function as follows:

(a) Vibrational mean energy  

$$U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta} \quad (21)$$

(b) Vibrational entropy  

$$S(\beta) = K \ln Z(\beta) - K\beta \frac{\partial \ln Z(\beta)}{\partial \beta} \quad (22)$$

(c) Vibrational Free Energy  

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta) \quad (23)$$

(d) Vibrational Heat Capacity  

$$C(\beta) = K\beta^2 \left( \frac{\partial^2 \ln Z(\beta)}{\partial \beta^2} \right) \quad (24)$$

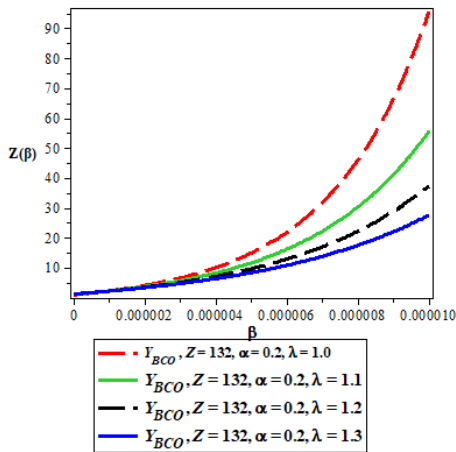


Figure 1: Variation of Thermodynamic Partition function with respect to inverse temperature parameter ( $\beta$ ).  
 Source: Researcher (2023)

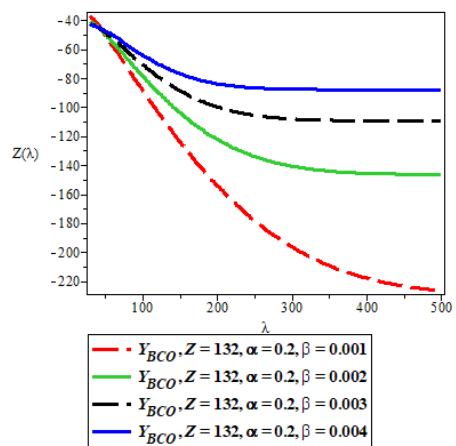


Figure 2: Variation of Thermodynamic Partition function with respect to maximum vibrational quantum number parameter ( $\lambda$ ).

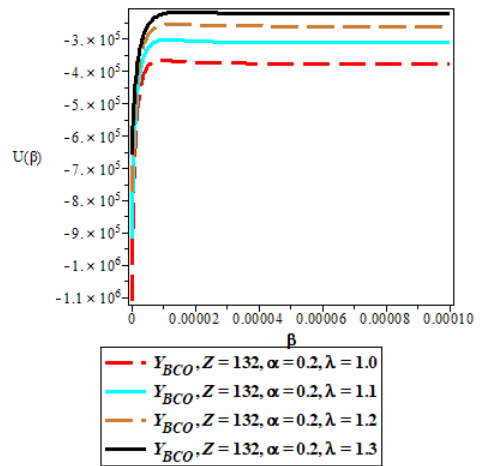


Figure 3: Variation of Thermodynamic vibrational mean energy with respect to inverse temperature parameter ( $\beta$ ).

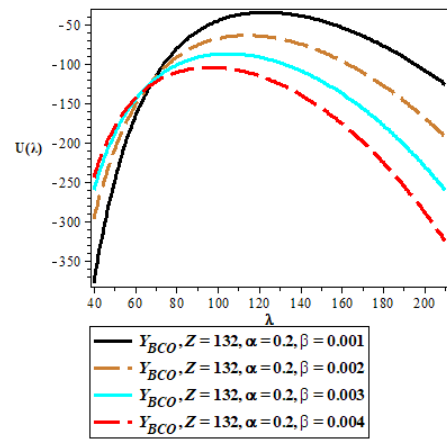


Figure 4. Variation of Thermodynamic vibrational mean energy with respect to maximum vibrational quantum number parameter ( $\lambda$ ).

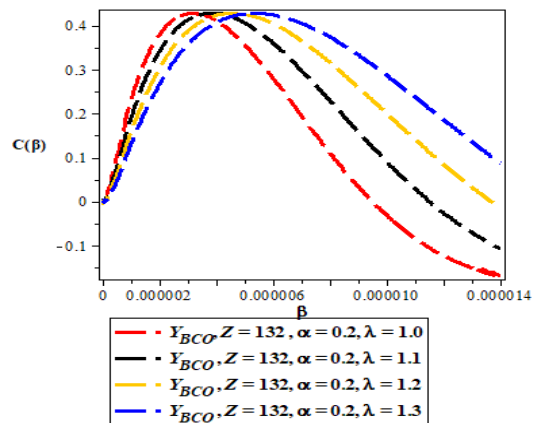


Figure 5: Variation of Thermodynamic vibrational heat capacity with respect to inverse temperature parameter ( $\beta$ ). Source: Researcher (2023)

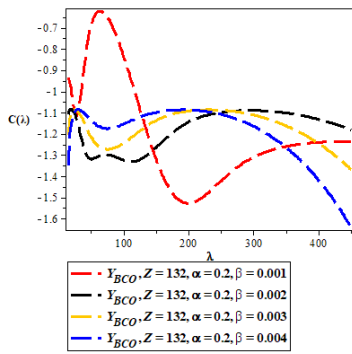


Figure 6 Variation of Thermodynamic vibrational heat capacity with respect to maximum vibrational quantum number parameter ( $\lambda$ ).

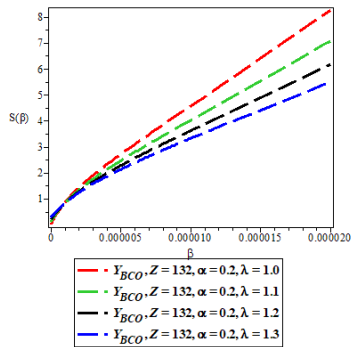


Figure 7: Variation of Thermodynamic entropy with respect to inverse temperature parameter ( $\beta$ ).

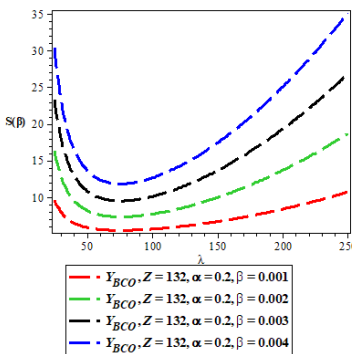


Figure 8: Variation of Thermodynamic entropy with respect to maximum vibrational quantum number parameter ( $\lambda$ ).

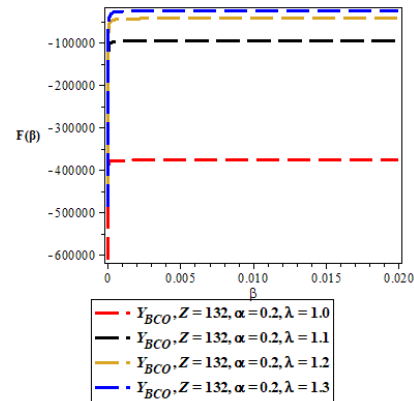


Figure 9. Variation of Thermodynamic vibrational free energy with respect to inverse temperature parameter ( $\beta$ ).

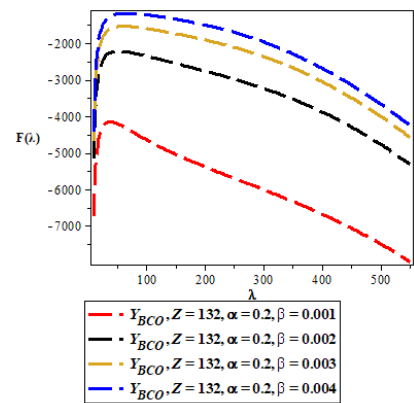


Figure 10: Variation of Thermodynamic free energy with respect to maximum vibrational quantum number parameter ( $\lambda$ ).

Table 4.6: The Numerical Bound State Solution for Screening Parameter  $\alpha = 0.2$

n	$E_{nl}(\alpha = 0.2), l = 0$	$E_{nl}(\alpha = 0.2), l = 1$	$E_{nl}(\alpha = 0.2), l = 2$	$E_{nl}(\alpha = 0.2), l = 3$
0	-15022.23291	-3735.80153	-1645.77310	-914.32394
1	-3735.80153	-1645.77310	-914.32394	-575.83416
2	-1645.77310	-914.32394	-575.83416	-392.03393
3	-914.32394	-575.83416	-392.03393	-281.28192
4	-575.83416	-392.03393	-281.28192	-209.47558
5	-392.03393	-281.28192	-209.47558	-160.32316
6	-281.28192	-209.47558	-160.32316	-125.24392
7	-209.47558	-160.32316	-125.24392	-99.36962
8	-160.32316	-125.24392	-99.36962	-79.77148

Table 2: The Numerical Bound State Solution for Screening Parameter  $\alpha = 0.4$

n	$E_{nl}(\alpha = 0.4), l = 0$	$E_{nl}(\alpha = 0.4), l = 1$	$E_{nl}(\alpha = 0.4), l = 2$	$E_{nl}(\alpha = 0.4), l = 3$
0	-15022.23291	-3735.80153	-1645.77310	-914.32394
1	-3735.80153	-1645.77310	-914.32394	-575.83416
2	-1645.77310	-914.32394	-575.83416	-392.03393
3	-914.32394	-575.83416	-392.03393	-281.28192
4	-575.83416	-392.03393	-281.28192	-209.47558
5	-392.03393	-281.28192	-209.47558	-160.32316
6	-281.28192	-209.47558	-160.32316	-125.24392
7	-209.47558	-160.32316	-125.24392	-99.36962
8	-160.32316	-125.24392	-99.36962	-79.77148

Table 3: The Numerical Bound State Solution for Screening Parameter  $\alpha = 0.6$

n	$E_{nl}(\alpha = 0.6), l = 0$	$E_{nl}(\alpha = 0.6), l = 1$	$E_{nl}(\alpha = 0.6), l = 2$	$E_{nl}(\alpha = 0.6), l = 3$
0	-15022.23291	-3735.80153	-1645.77310	-914.32394
1	-3735.80153	-1645.77310	-914.32394	-575.83416
2	-1645.77310	-914.32394	-575.83416	-392.03393
3	-914.32394	-575.83416	-392.03393	-281.28192
4	-575.83416	-392.03393	-281.28192	-209.47558
5	-392.03393	-281.28192	-209.47558	-160.32316
6	-281.28192	-209.47558	-160.32316	-125.24392
7	-209.47558	-160.32316	-125.24392	-99.36962
8	-160.32316	-125.24392	-99.36962	-79.77148

Table 4. The Numerical Bound State Solution for Screening Parameter  $\alpha = 0.8$

n	$E_{nl}(\alpha = 0.8), l = 0$	$E_{nl}(\alpha = 0.8), l = 1$	$E_{nl}(\alpha = 0.8), l = 2$	$E_{nl}(\alpha = 0.8), l = 3$
0	-14954.65958	-3660.12889	-1569.37250	-838.58037
1	-3660.12889	-1569.37250	-838.58037	-501.39510
2	-1569.37250	-838.58037	-501.39510	-319.36485
3	-838.58037	-501.39510	-319.36485	-210.78596
4	-501.39510	-319.36485	-210.78596	-141.52984
5	-319.36485	-210.78596	-141.52984	-95.29227
6	-210.78596	-141.52984	-95.29227	-63.48597
7	-141.52984	-95.29227	-63.48597	-41.23899
8	-95.29227	-63.48597	-41.23899	-25.62029

Table 5: The Numerical Bound State Solution for Screening Parameter  $\alpha = 1.0$

n	$E_{nl}(\alpha = 1.0), l = 0$	$E_{nl}(\alpha = 1.0), l = 1$	$E_{nl}(\alpha = 1.0), l = 2$	$E_{nl}(\alpha = 1.0), l = 3$
0	-14939.43785	-3636.86996	-1545.08834	-814.48447
1	-3636.86996	-1545.08834	-814.48447	-477.98657
2	-1545.08834	-814.48447	-477.98657	-296.96654
3	-814.48447	-477.98657	-296.96654	-189.66029
4	-477.98657	-296.96654	-189.66029	-121.91403
5	-296.96654	-189.66029	-121.91403	-77.41148
6	-189.66029	-121.91403	-77.41148	-47.55901
7	-121.91403	-77.41148	-47.55901	-27.48107
8	-77.41148	-47.55901	-27.48107	-14.24444

## RESULTS AND DISCUSSION

Figure 1 is the variation of the thermodynamic partition function with respect to inverse temperature parameter ( $\beta$ ). Here the partition function increases exponentially with increasing value of inverse temperature parameter. Figure 2 is the variation of thermodynamic partition function with respect to maximum vibrational quantum number parameter ( $\lambda$ ). Here, the partition function decreases exponentially in

a converging manner from the negative y-axis before splitting into a unique spectral curve in an increasing value of maximum vibrational quantum number.

Figure 3 is the variation of thermodynamic vibrational mean energy with respect to inverse temperature parameter ( $\beta$ ). Here, the vibrational mean energy increases monotonically from the origin in a converging manner before splitting into different spectral curve with unique equal spacing. Figure 4

is the variation of thermodynamic vibrational mean energy with respect to maximum vibrational quantum number parameter ( $\lambda$ ). Here, vibrational mean energy is a parabolic curve with unique intersection before sloping into unique spectral lines increasing value of maximum vibrational quantum number.

Figure 5 is the variation of thermodynamic vibrational heat capacity with respect to inverse temperature parameter ( $\beta$ ). In this plot the specific heat capacity follows a unique symmetrical plot with different maximum points before decreasing into various spectral curves with an increasing value of inverse temperature parameter.

Figure 6 is the variation of thermodynamic vibrational heat capacity with respect to maximum vibrational quantum number parameter ( $\lambda$ ). This curve intertwines like sinusoidal curves with local maximum and minimum points before increasing with increasing value of maximum vibrational quantum number. Figure 7 is the plot of variation of thermodynamic entropy with respect to inverse temperature parameter ( $\beta$ ). This is a linear graph that increases monotonically from the origin before splitting into different spectral curves which diverges in an increasing value of inverse temperature parameter.

Figure 8 is the variation of thermodynamic entropy with respect to maximum vibrational quantum number parameter ( $\lambda$ ). This plot showcases parabolic plots that concaves upward with an increasing value of maximum vibrational quantum number.

Figure 9 is the variation of thermodynamic vibrational free energy with respect to inverse temperature parameter ( $\beta$ ).

This is a monotonic plot that increases asymptotically into a unique spectral quantized curve with unequal spacing. Figure 10 is the variation of thermodynamic free energy with respect to maximum vibrational quantum number parameter ( $\lambda$ ). This plot showcases semi parabolic curves that increases with an increase in maximum temperature parameter. The thermodynamic plots agrees with work of Chen *et al.*, (2022), Okon *et al.*, (2021) and Horchani *et al.*, (2022). Tables 1-5 are numerical bound state solutions of the modified Hulthen Plus generalized Coulomb potential for various screening parameters  $\alpha = 0.2, 0.4, 0.6, 0.8$  and  $1.0$ . for varying orbital angular quantum number  $l = 0, 1, 2$  and  $3$ . Tables 1 -5 shows negative energy eigenvalues which is the necessary and sufficient condition for bound state solutions. Also, the numerical eigenvalues of tables 1-5 increases with an increase in quantum state.

## CONCLUSION

In this work, we solve Schrodinger wave equation with modified Hulthen plus Coulomb potential Using parametric Nikiforov-Uvarov method and use it to model Yttrium Barium copper oxide superconductor. The total wave function and eigen energy equation were obtained. The energy equation was put in a closed and compact form and used to study partition function and other thermodynamic properties. The trend of thermodynamic plots agrees with work of an existing literature. Numerical bound state

solutions were also obtained for various screening parameter and with varying orbital angular quantum number.

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