Thermodynamic functions for boron nitride with q-deformed exponential-type potential

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ABSTRACT

Within the framework of the supersymmetric quantum mechanics, the energy spectrum of the six-parameter exponential-type potential model was obtained. The partition function for this energy has been calculated in a closed and compact form and was used to obtain an expression for the ro-vibrational mean free energy $F(T)$, mean free energy $U(T)$, entropy $S(T)$, and the specific heat capacity $C(T)$. The thermodynamic functions obtained were then applied to study the behaviour of the zinc-blende BN crystal structure and the results obtained show fair agreement with reported experimental data for the specific heat capacity.

Introduction

There has been a growing interest in investigating the analytical solutions of wave equations for some typical potential models in the area of quantum mechanics. This could be because the analytical solution has some useful information that can describe any quantum system under consideration. A quantum system under nonrelativistic wave equation in a strong potential field is usually described by the Schrödinger wave equation. Over the years, various physical potential models have been studied with the Schrödinger wave equation by different researchers. For instance, Falaye et al. [1], studied bound state solution of the Schrödinger equation with Manning-Rosen potential, Hassanabadi et al. [2], obtained approximate analytical solutions to the generalized-Pöschl-Teller potential in D-Dimensions, Gu et al. [3], obtained energy spectra for modified Rosen-Morse potential solved by the exact quantization rule, Ikhdair and Abu-Hasna [4], in their study deduced quantization rule solution to the Hulthèn potential in arbitrary dimension with a new approximation scheme for the centrifugal term, Bayrak et al. [5], studied exact analytical solutions to the Kratzer potential by the asymptotic iteration method. Gao [6], in his studies, obtained solutions of the Schrödinger equation for an attractive potential. Onate et al [7] studied the approximate solutions of the Schrödinger equation with hyperbolical potential in the framework of supersymmetric quantum mechanics approach, Scott and Shertzer [8], studied the solution of logarithmic Schrödinger equation with a Coulomb potential. The analytical bound states solution of the five-

parameter exponential-type potential model was proposed by Jia et al. [9]. The results obtained by using the five-parameter potential model gave rise to other useful potentials of interest that can be applied to diverse areas of physics. Recently, these potential models have found useful applications to molecular physics [10–15]. For example, owing to the simplicity of this exponential-type potential, Jia and co-workers obtained the thermodynamic properties of the lithium and sodium dimer molecules respectively by using the improved Manning-Rosen potential mode [10,11]. Also, the improved Pöschl–Teller potential energy model for diatomic molecules has also been studied by Jia et al. [13]. The expression for the partition function in this case have been used by various authors to describe the detail vibrational mean energy, vibrational specific heat capacity, vibrational mean free energy, and vibrational entropy for various diatomic molecular systems [10–20].

Motivated by the usefulness and the simplicity of the multiple parameter exponential-type potential, we proposed a q-deformed six-parameter exponential-type potential model for applications in molecular and condensed matter physics. The q-deformed six-parameter exponential-type potential model proposed is of the form

$$V(r) = Q_1 - \frac{Q_2}{1 - qe^{-2\alpha r}} + \frac{Q_3 e^{-2\alpha r}}{1 - qe^{-2\alpha r}} - \frac{Q_4 e^{-4\alpha r}}{(1 - qe^{-2\alpha r})^2}, \tag{1}$$

where Q_i, $i = 1, 2, 3$, and 4, are the adjustable potential parameters. In this work, the deformed parameter will be taken as unity in all the computation of numerical results. The results of this potential can produce the result for constant potential, Coulomb potential, Hulthén

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potential, Yukawa potential, inversely quadratic Yukawa potential, Hellmann potential and others as we will see in the special cases later.

The Ro-vibrational energy spectrum for q-deformed six-parameter exponential-type potential

To obtain the solution of the Schrödinger equation in the presence of the q-deformed six-parameter exponential-type potential given in Eq. (1), we first consider the original Schrödinger equation given by

$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\psi(r)$$
$$= (E_{n\ell} - V(r))\psi(r). \tag{2}$$

Setting the wave function $\psi(r) = \frac{R_{n\ell}Y_{m\ell}(\theta,\phi)}{r}$ and then consider the radial part of the Schrödinger equation, Eq. (2) reduces to the form

$$-\frac{\hbar^2}{2\mu}\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}R_{n\ell}(r) = (E_{n\ell} - V(r))R_{n\ell}(r), \tag{3}$$

It is noted that Eq. (3) cannot be solved for $\ell \neq 0$ due to the presence of the centrifugal term. To address this issue, we must approximate the centrifugal term. For short potential range, the following formula is suitable for the approximation of the centrifugal term

$$\frac{\ell(\ell+1)}{r^2} \approx \frac{\ell(\ell+1)\alpha^2}{(1-e^{-\alpha r})^2} \tag{4}$$

Substituting Eqs. (1) and (4) into Eq. (3), we have a second-order differential equation of the form

$$\frac{d^2R_{n\ell}(r)}{dr^2} = V_{T_0}R_{n\ell}(r) + \frac{V_{T_1}e^{-2\alpha r}}{1-qe^{-2\alpha r}}R_{n\ell}(r) + \frac{V_{T_2}e^{-2\alpha r}+V_{T_3}e^{-4\alpha r}}{(1-qe^{-2\alpha r})^2}R_{n\ell}(r), \tag{5}$$

where

$$V_{T_0} = \ell(\ell+1)\alpha^2 + \frac{2\mu(Q_1 - Q_2 - E_{n\ell})}{\hbar^2}, \tag{6}$$

$$V_{T_1} = \ell(\ell+1)\alpha^2 q - \frac{2\mu qQ_2}{\hbar^2} + \frac{2\mu Q_3}{\hbar^2}, \tag{7}$$

$$V_{T_3} = \ell(\ell+1)\alpha^2 q, \tag{8}$$

$$V_{T_3} = \frac{2\mu Q_4}{\hbar^2}. \tag{9}$$

To solve Eq. (5) using the elegant supersymmetric approach [21], we propose a superpotential function of the form

$$W(r) = \omega_0 + \frac{\omega_1}{1-qe^{-2\alpha r}}, \tag{10}$$

whose ground state wave function is written as

$$R_{0,\ell}(r) = \exp\left(-\int W(r)dr\right). \tag{11}$$

Eq. (10) is a solution to the differential equation of Eq. (5). But the manifestation of its reality can been seen only if the values of the two parameters ω_0 and ω_1 are known. However, in this bound state solution, the radial part of the wave function must satisfy the boundary conditions that $R_{n,\ell}(r)/r$ becomes zero as $r \to \infty$, and $R_{n,\ell}(r)/r$ is finite at $r \to 0$. Proceeding further, the non-linear Riccati equation relates to the solution of Eq. (5) as

$$V_{T_0}R_{n\ell}(r) + \frac{V_{T_1}e^{-2\alpha r}}{1-qe^{-2\alpha r}}R_{n\ell}(r) + \frac{V_{T_2}e^{-2\alpha r}+V_{T_3}e^{-4\alpha r}}{(1-qe^{-2\alpha r})^2}R_{n\ell}(r)$$
$$= W^2(r) - \frac{dW(r)}{dr}. \tag{12}$$

Comparing Eq. (12) to Eq. (5), we have the values of the parameters in Eq. (10) as follows:

$$\omega_0^2 = \frac{2\mu(Q_1 - Q_2 - E_{n\ell})}{\hbar^2} + \ell(\ell+1)\alpha^2, \tag{13}$$

$$\omega_1 = \alpha(\ell+1)q, \tag{14}$$

$$\omega_0 = \frac{\frac{2\mu(Q_5 - Q_3 + qQ_2)}{\hbar^2} - \ell(\ell+1)\alpha^2 q - \omega_1^2}{2\omega_1}. \tag{15}$$

Using the superpotential function given in Eq. (10), we can now construct a pair of partner potentials $V_\pm(r)$ in the form

$$V_+(r) = W^2(r) + \frac{dW(r)}{dr} = \omega_0^2 + \frac{\omega_1(\omega_1+2\omega_0)}{1-qe^{-2\alpha r}} + \frac{q\omega_1(\omega_1-2\alpha)e^{-2\alpha r}}{(1-qe^{-2\alpha r})^2}, \tag{16}$$

$$V_-(r) = W^2(r) - \frac{dW(r)}{dr} = \omega_0^2 + \frac{\omega_1(\omega_1+2\omega_0)}{1-qe^{-2\alpha r}} + \frac{q\omega_1(\omega_1+2\alpha)e^{-2\alpha r}}{(1-qe^{-2\alpha r})^2}. \tag{17}$$

Eqs. (16) and (17) are shape-invariant via mapping of $\omega_1 \to \omega_1 + 2\alpha$ as $a_1 = f(a_0) = a_0 + 2\alpha$, where $a_0 = \omega_1$. Here, a_0 is an old set of parameters and a_1 is a new set of parameters uniquely determined from a_0. Establishing a recurrence relation for these two sets of parameters, we have: $a_2 = a_0 + 4\alpha$, $a_3 = a_0 + 6\alpha$, $a_4 = a_0 + 8\alpha$ and consequently, $a_n = a_0 + 2n\alpha$. The two-partner potentials are related by a simple formula

$$V_+(a_0, r) = V_-(a_1, r) + R(a_1), \tag{18}$$

where $R(a_1)$ is a remainder term that is independent of the variable r. In terms of the parameters of the system, Eq. (18) can be recast in the following forms

$$R(a_1) = \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_0^2}{2a_0}\right)^2 - \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_1^2}{2a_1}\right)^2, \tag{19}$$

$$R(a_2) = \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_1^2}{2a_1}\right)^2 - \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_2^2}{2a_2}\right)^2, \tag{20}$$

$$R(a_3) = \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_2^2}{2a_2}\right)^2 - \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_3^2}{2a_3}\right)^2, \tag{21}$$

$$R(a_n) = \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_{n-1}^2}{2a_{n-1}}\right)^2 - \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_n^2}{2a_n}\right)^2. \tag{22}$$

The energy eigenvalue equation can now be written as

$$E_{n\ell} = \sum_{k=1} R(a_k) = \left(\frac{V_{T_3} - V_{T_2} - V_{T_1} - a_{n-1}^2}{2a_{n-1}}\right)^2. \tag{23}$$

This finally gives a complete non-relativistic energy equation for the six-parameter exponential-type potential for arbitrary value of the ro-vibrational quantum numbers n and ℓ as

$$E_{n,\ell} = P_1 - \frac{\hbar^2}{2\mu}\left(\frac{P_2}{2(n+\delta)} - \frac{(n+\delta)}{2}\right)^2, \tag{24}$$

where,

$n = 0, 1, 2, \ldots, n_{max}, \delta = q(\ell+1)$, with ℓ being the rotational quantum number,

$$P_1 = Q_1 - Q_2 + \frac{\ell(\ell+1)\alpha^2\hbar^2}{2\mu}, \quad P_2 = \frac{2\mu\alpha(Q_4 - Q_3 + qQ_2)}{\hbar^2} - l\delta. \tag{24b}$$

Partition function and thermodynamic properties

The contribution of the energy to the ro-vibrational partition function for a diatomic molecule at a temperature T is given by

$$Z(\beta) = \sum_{n=0}^{n_{\max}} e^{-\beta E_{n,l}}, \tag{25}$$

where $\beta = \frac{1}{kT}$ with k as the Botzmann constant and $E_{n,\ell}$ is the ro-vibrational energy spectrum for the system. Substitution Eq. (24) into Eq. (25), we obtain

$$Z(\beta) = \sum_{n=0}^{n_{\max}} e^{-\beta\left(P_1 - \frac{\hbar^2}{2\mu}\left(\frac{P_2}{2(n+\delta)} - \frac{(n+\delta)}{2}\right)^2\right)} \tag{26}$$

where

$$n_{\max} = \sqrt{P_2} - q(l+1) \tag{27}$$

To evaluate Eq. (26) we use the Poison summation formula given by [11,22–26]

$$\sum_{n=0}^{n_{\max}} f(n) = \frac{1}{2}[f(0) - f(n_{max}+1)] + \sum_{m=-\infty}^{\infty} \partial \int_0^{n_{\max}+1} f(x)e^{-i2\pi mx}dx. \tag{28}$$

For a lower order approximation, Eq. (28) reduces to [16–19]

$$\sum_{n=0}^{n_{\max}} f(n) = \frac{1}{2}[f(0) - f(n_{max}+1)] + \int_0^{n_{\max}+1} f(x)dx. \tag{29}$$

By using Eq. (29) we can write Eq. (26) as

$$Z(\beta) = \frac{1}{2}\left[e^{-\beta(P_1 - P_2 P_3^2)} - e^{-\beta(P_1 - P_2 P_4^2)} + \int_0^{v+1} e^{-\beta a - \frac{\beta b}{\rho^2} - \beta c\rho^2}d\rho\right], \tag{30}$$

$$P_3 = \frac{Q_1}{2n_{max}} + \frac{n_{max}}{4}, \quad P_4 = \frac{Q_1}{2(n_{max}+\delta+1)} + \frac{n_{max}+\delta+1}{2(n_{max}+\delta+1)}. \tag{}$$

where $\rho = n + \delta$, $a = P_1 - \frac{\hbar^2 P_2}{4\mu}$, $b = \frac{\hbar^2 P_2^2}{8\mu}$ and $c = \frac{\hbar^2}{8\mu}$. On evaluating the integral of Eq. (30), we obtained the ro-vibrational partition function for the molecular q-deformed six-parameter exponential-type potential model as follows

$$Z(\beta) = \frac{1}{2}[e^{-\beta(P_1 - P_2 P_3^2)} - e^{-\beta(P_1 - P_2 P_4^2)} + e^{-\beta a - \beta c\rho^2}\sqrt{\beta b}\,(\Gamma_1)], \tag{31}$$

where

$$\Gamma_1 = \frac{2(n_{\max}+1)e^{-\frac{\beta b}{(n_{\max}+1)^2}}}{\sqrt{\beta b}} + 2\sqrt{\pi}\, erf\left(\frac{\sqrt{\beta b}}{(n_{\max}+1)}\right) - 2\sqrt{\pi}, \tag{32}$$

and the error function ($erf(x)$) is the imaginary error function which is of the sigmoid shape given by [11,22–26].

$$erf(x) = -ierf(ix) = \frac{2}{\sqrt{\pi}}\int_0^x e^{t^2}dt. \tag{33}$$

From the solution obtained for the vibrational partition function of Eq. (31), other thermodynamic properties of interest can now be computed as follows

a. The vibrational mean energy U

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

$$= \frac{1}{2}\left\{((\Gamma_2 - \Gamma_3\sqrt{\beta b}\,(\Gamma_1)) + \frac{1}{4}\frac{\Gamma_4}{\sqrt{\beta b}}b - \frac{1}{2}\frac{\Gamma_4\Gamma_5}{\Gamma_1\beta}\right)\right\}X\left(\frac{1}{2}(\Gamma_6 + \Gamma_4\sqrt{\beta b})\right)^{-1} \tag{34}$$

where

$$\left.\begin{aligned}
\Gamma_2 &= (P_1 - P_2 P_3^2)e^{-\beta(P_1 - P_2 P_3^2)} - (P_1 - P_2 P_4^2)e^{-\beta(P_1 - P_2 P_4^2)},\\
\Gamma_3 &= (-a - c\rho^2)e^{-\beta a - \beta c\rho^2},\\
\Gamma_4 &= e^{-\beta a - \beta c\rho^2}\Gamma_1, \quad \Gamma_5 = (n_{\max}+1)e^{-\frac{\beta b}{(n_{\max}+1)^2}},\\
\Gamma_6 &= e^{-\beta(P_1 - P_2 P_3^2)} - e^{-\beta(P_1 - P_2 P_4^2)}
\end{aligned}\right\} \tag{35}$$

b. Vibrational mean free energy F

$$F = -KT\ln(Z) = \frac{1}{\beta}\ln(Z) = -\frac{1}{\beta}\ln\left[\frac{1}{2}\left(\Gamma_6 + \frac{\Gamma_4}{\Gamma_1}\sqrt{\beta b}\,(\Gamma_1)\right)\right]. \tag{36}$$

c. Vibrational specific heat capacity C

$$\begin{aligned}
C(\beta) &= \frac{\partial}{\partial T}U = -k\beta^2\frac{\partial}{\partial\beta}U = -k\beta^2\left\{\left(\left(\frac{1}{2}\left(\Gamma_7 + \Gamma_8\Gamma_1\sqrt{\beta b} + \frac{\Gamma_9\Gamma_1 b}{\sqrt{\beta b}}\right)\right.\right.\right.\\
&\quad \left.\left.-\frac{\Gamma_9\Gamma_5}{b} - \frac{\Gamma_4 b^2}{8(\sqrt{\beta b})^3} + \frac{\Gamma_4\Gamma_5}{4\beta^2} + \frac{\Gamma_{10} b}{\beta(v_{\max}+1)}\right)\right)X\left(\frac{1}{2}(\Gamma_6 + \Gamma_{11}\Gamma_1)\right)^{-1}\\
&\quad -\left(\frac{1}{2}(\Gamma_2 - \Gamma_9\sqrt{\beta b}\,(\Gamma_1)\right.\\
&\quad \left.\left.-\frac{\Gamma_{11}\Gamma_1 b}{\beta b} + \frac{\Gamma_{10}}{\beta}^2\right)X\left(\frac{1}{2}\left(\Gamma_6 + \Gamma_{11}\left(\frac{2\Gamma_5}{\sqrt{\beta b}} + \Gamma_1\right)\right)\right)^{-2}\right\},
\end{aligned} \tag{37}$$

where

$$\left.\begin{aligned}
\Gamma_7 &= (P_1 - P_2 P_3^2)^2 e^{-\beta(P_1 - P_2 P_3^2)} - (P_1 - P_2 P_4^2)^2 e^{-\beta(P_1 - P_2 P_4^2)},\\
\Gamma_8 &= (-ba - c\rho^2)^2 e^{-\beta ba - \beta c\rho^2},\\
\Gamma_9 &= (-ba - c\rho^2)e^{-\beta ba - \beta c\rho^2}, \quad \Gamma_{10} = (n_{\max}+1)e^{-\beta ba - \beta c\rho^2}e^{-\frac{\beta b}{(n_{\max}+1)^2}},\\
\Gamma_{11} &= e^{-\beta ba - \beta c\rho^2}\sqrt{\beta b}
\end{aligned}\right\} \tag{38}$$

d. Vibrational entropy S

$$S = k\ln Z(\beta) - k\beta\, U(Z). \tag{39}$$

Discussion

The six-parameter exponential-type potential model has been obtained in the non-relativistic regime. The following parameters $q_1 = Q_2 = 1$, $Q_1 = Q_3 = 2$, $Q_4 = 3$, have been chosen arbitrary for the computation of the ro-vibrational energy spectrum. As we can see from the plot of the deformed parameter against the energy, it clearly shows the attractive nature of the potential (Figs. 1 and 2). There is a
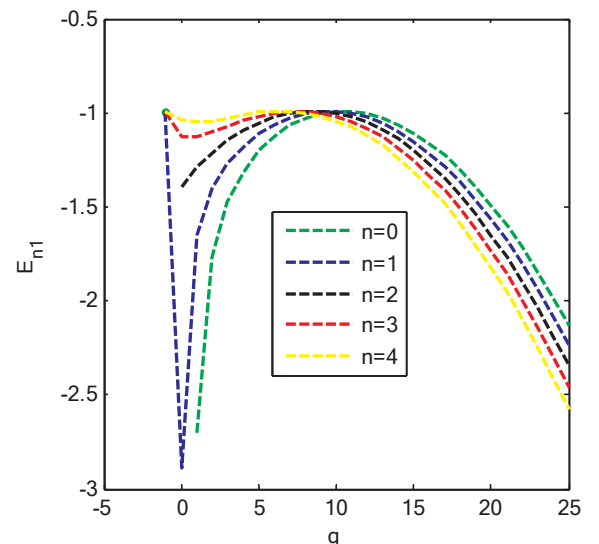

Fig. 1. The ro-vibrational energy spectrum for the six-parameter exponential-type potential against the deformed parameter.
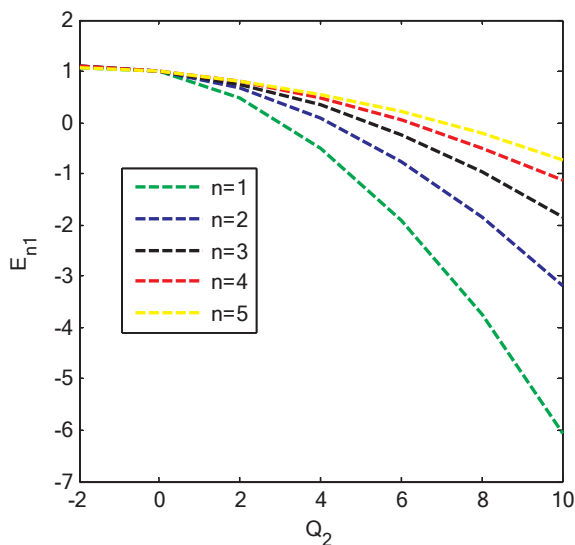
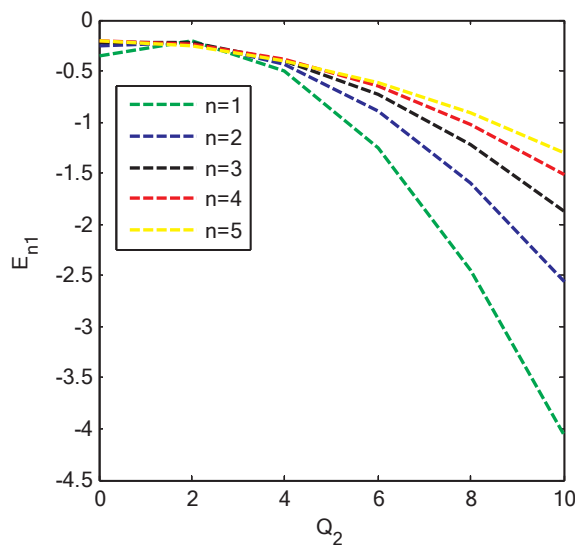**Fig. 2.** The ro-vibrational energy spectrum against Q2 for the six-parameter exponential-type potential model.

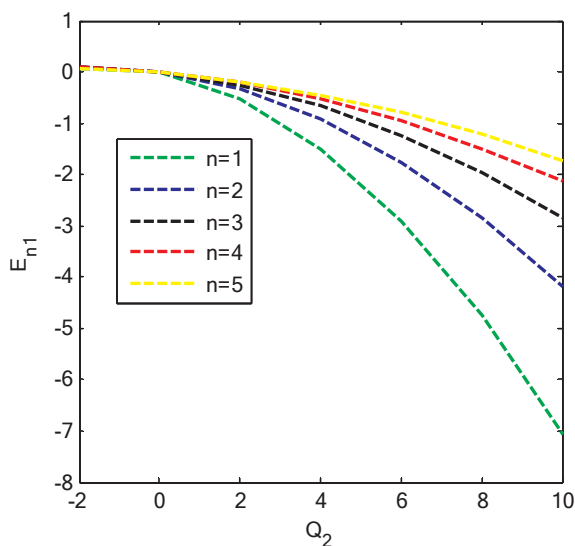**Fig. 4.** Hellman potential obtained from the potential parameter when $Q_1 = Q_4 = 0$.

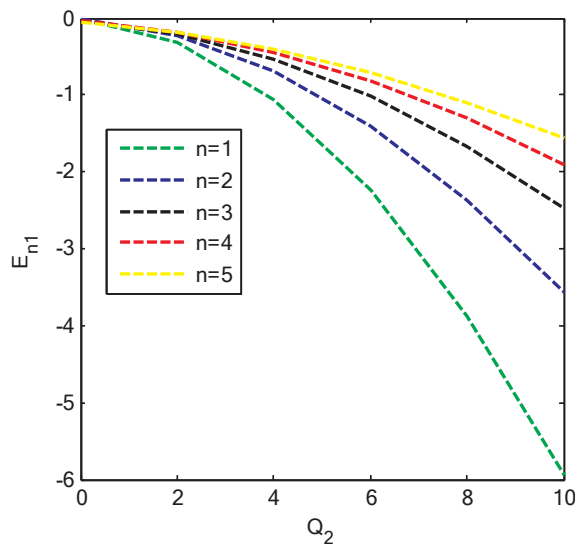**Fig. 3.** The class of Yukawa potential obtained from the potential parameter when $Q_1 = 0$.

Fig. 5. The Yukawa potential obtained from the potential parameter when $Q_1 = Q_4 = Q_2 = 0$.

formation of bands between the energy levels at various quantum states. Other molecular exponential-type potentials have also been obtained. For instance, if $Q_1 = 0$, a class of the Yukawa potential is obtained as we can see in Fig. 3. Also in Fig. 4, if $Q_1 = Q_4 = 0$, we obtained Hellman potential, $Q_1 = Q_2 = Q_4 = 0$, we obtained Yukawa potential, $Q_1 = Q_4 = Q_3 = 0$, we obtained Coulomb potential, and $Q_1 = Q_2 = Q_3 = 0$, the inverse quadratic Yukawa potential is also obtained as we can see in Figs. 5–7 respectively.

Furthermore, the thermodynamics properties of the Zinc-Blende crystal structure were also computed using Maple 16. For brevity we have used the effective mass listed for the zinc-blende boron nitride (BN) on ref. [27] as $\mu = 0.752m_0$, where m_0 is the mass of free electron. The results obtained for the partition function (Fig. 8) shows convergence at $T = 2K$ before increasing gradually with an increase in the temperature, similar behaviour was also obtained for the harmonic oscillator [28]. At high temperature, more energy levels are expected to be populated with a higher value of the upper bound vibrational quantum number n_{max}. The rotational contribution to the partition function $Z(T)$ shows peak at a particular value of n_{max} and then a slight

increase as the value of $Z(T)$ converges at about 47 K. A monotonic decrease in the free energy with temperature is seen in Fig. 9. As we can see from the plot, the vibrational quantum numbers show some level of dissociation starting at the point T = 0.08 K. A monotonic decrease in the mean energy $U(T)$ with an increase in T is also noticed in Fig. 10. At a temperature of about 0.2 K, there is a strong dissociation as the temperature and the ro-vibrational quantum numbers decreases. In Fig. 11, the entropy obtained shows a disordered decrease with an increasing parameter T. The range of values obtained for the specific heat capacity at a low temperature range shows a monotonic increase with an increasing temperature. The values obtained in our research are at variance with the $0.6Jg^{-1}k^{-1}$ reported in the experimental observation in ref. [27]. The internal energy at this point is being contributed by the maximum vibrational quantum number n_{max} and gave rise to the specific heat capacity of the crystal as shown in Fig. 12.

Concluding remarks

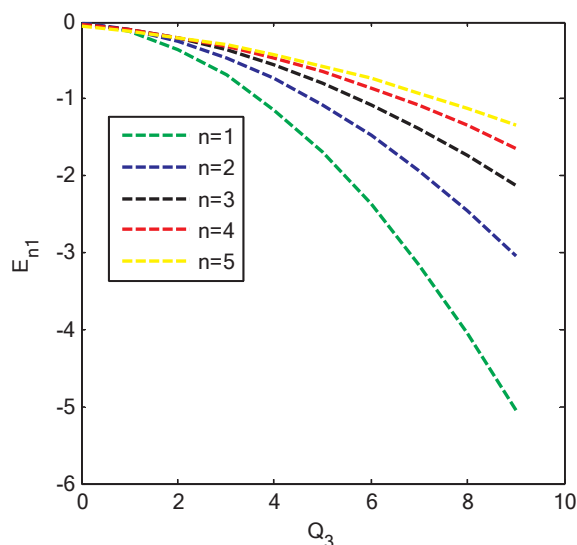The ro-vibrational energy spectrum of the six-parameter

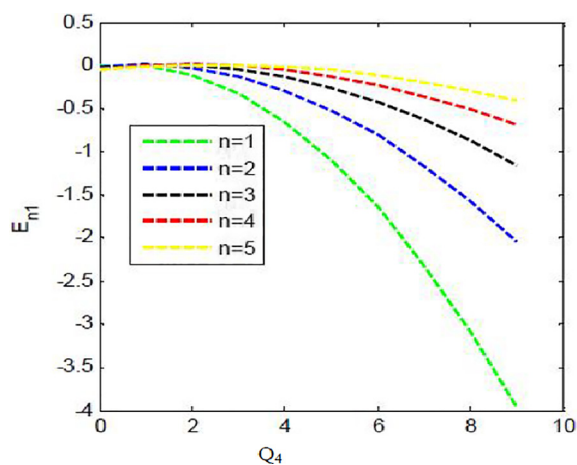**Fig. 6.** Coulomb potential obtained from the potential parameter when $Q_1 = Q_4 = Q_3 = 0$.

Fig. 7. The Inversely Quadratic Yukawa potential obtained from the potential parameter when $Q_1 = Q_2 = Q_3 = 0$.
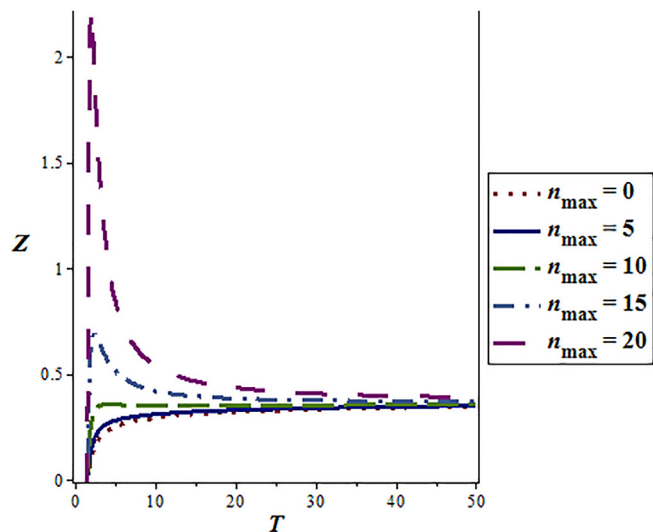

Fig. 8. The ro-vibrational partition function against temperature for zinc-blende BN using Eq. (31).
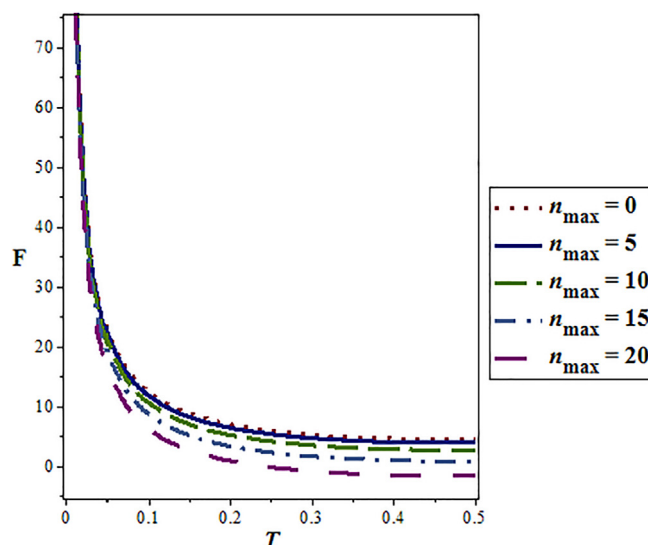

Fig. 9. The ro-vibrational free energy against temperature for zinc-blende BN using Eq. (36).
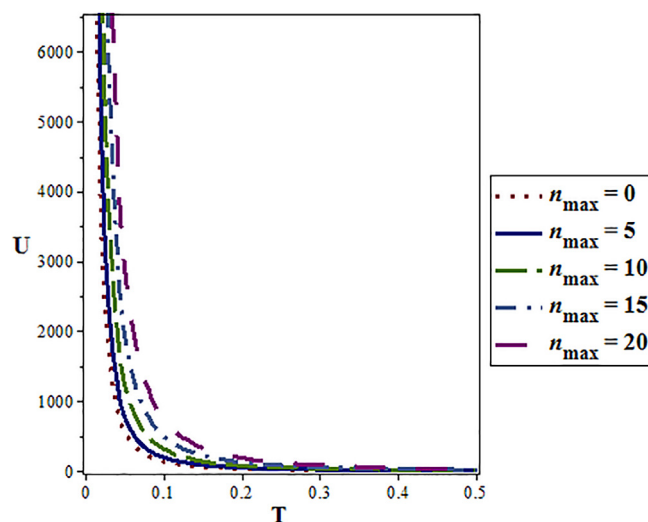

Fig. 10. The ro-vibrational mean energy against temperature for zinc-blende BN using Eq. (34).

exponential-type molecular potential has been obtained using the supersymmetric quantum mechanics approach. The potential clearly shows attractive nature as results of other molecular potentials have also be deduced from the potential parameters. The partition function in a closed form has also been obtained and applied to calculate the thermodynamic properties of the ro-vibrational mean free energy $F(T)$, mean free energy $U(T)$, entropy $S(T)$, and the specific heat capacity $C(T)$. We have plotted also the thermodynamic function against the temperature T at the upper bound vibrational quantum number n_{max} for the BN zinc-blende crystal structure. The result obtained for the specific heat capacity is in fair agreement with the experimental data reported on ref. [27] for the same crystalline BN. This study has many applications in the synthesis of materials [29].

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
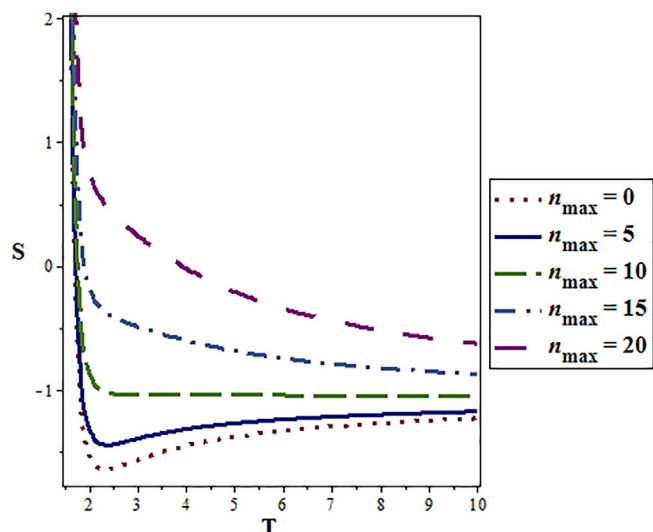
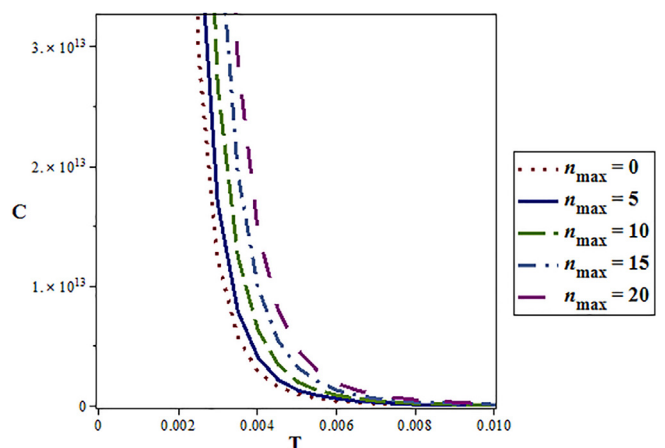**Fig. 11.** The ro-vibrational entropy against temperature for zinc-blende BN using Eq. (39).

Fig. 12. The ro-vibrational specific heat capacity against temperature for zinc-blende BN using Eq. (37).

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