Energy Eigenvalue and Thermodynamic Properties of $q$-deformed Hulthen Potential

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ABSTRACT
The objective of this work is to calculate the energy eigenvalue for $q$-deformed Hulthen potential using a Gaussian hypergeometric function with centrifugal approximation factor and related thermodynamical properties. For this, we develop a mathematical model using the Schrodinger wave equation to find the energy eigenvalue. In addition, the thermodynamic parameters were also calculated for $q$-deformed Hulthen potential using the partition function. The energy eigenvalue for quantum numbers $n=1$ to $n=5$ was observed for screening parameters 0.1, 0.5, and 1. In between, 0.1 to 1 and $n=1$ to $n=2$ the energy eigenvalue ranges from -1.048 to -208.572. The energy eigenvalue for considering potential shows that decrease with increasing the quantum number which means electron are loosely bounded nucleus in an atom. Also, the vibrational mean energy, vibrational mean free energy, vibrational specific heat capacity, and vibrational entropy are obtained but due to complexity, the further development of the equation is the limitation of this work.

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1. Introduction

Deformation Hulthen Potential (HP) with q-deformation is well-defined as
\[ V(r) = -\frac{V_0 e^{-2ar}}{1 - q e^{-2ar}} \]
Here \( V_0 = Ze^2 \) is known as coupling strength, and \( z \) is the screening parameter [1-5]. HP has introduced to study the detail of deuterons and has extensive applications in physics like Nuclear physics, particle physics, Atomic physics, Condensed Matter Physics, etc. HP is one of the short-range potentials like Yukawa potential, which behaves as a Coulomb potential at a small distance and exponentially decreases with increasing the distance from the nucleus. For spin-zero particles, Klein-Gordon HP for their equation to solve as
\[ V(r) = Za \frac{\exp(-zr)}{1-\exp(-zr)} \quad \text{or} \quad V(r) = -Z e^2 \delta \frac{e^{-br}}{1-e^{-br}} \]

Different methods like the asymptotic iteration method, supersymmetry method, shift 31 expression, factorization method, Nikiforov-Uvarov, etc., are used to calculate energy eigenvalue for further potential. The q-deformed HP and modified inversely quadratic Yukawa (qDHMIQY) potential can be represented as,
\[ V(r) = \frac{V_0 e^{-2ar}}{1 - q e^{-2ar}} - \frac{V_1 e^{-2ar}}{r} \]
Here \( V_0 \), \( V_1 \), and \( q \) are coupling strength and deformation parameters, respectively. Such potential is used to describe different interactions such as nucleon-nucleon interactions, meson-meson interactions, the various field of nuclear physics, and quantum chemistry (Hulthen, 1942 and Tencan & Sever, 2009).

1.1. Different method to calculate energy eigenvalue

1.1.1. Asymptotic iteration method

This method is used to solve homogenous linear second-order differential equations defined as,
\[ y^{(n+1)} + \lambda \phi^{(n)} + \phi = 0 \]
here \( \lambda \) and \( \phi \) are function in \( C_0(a, b) \). On taking \((n+1)\)th and \((n+2)\)th derivative, we get
\[ y^{(n+1)} = \lambda y^{(n)} + s_{n-1}(x)y \quad \text{and} \quad y^{(n+2)} = \lambda y^{(n)} + s_n(x)y \]
Here \( \lambda_n = \lambda_{n-1} + s_{n-1} + \phi \lambda_{n-1} \) and \( s_n = s_{n-1} + \phi s_{n-1} \). On taking the ratio of \((n+2)\)th and \((n+1)\)th and applying the asymptotic condition \( \frac{s_n}{\lambda_n} = \gamma_n = \alpha \), the condition gives the eigenvalue of the considered equation, and we obtained
\[ y^{(n+1)}(x) = C_1 \lambda_n \exp \left( \int (\alpha + \lambda) dt \right) \]
This equation yields the solution of the asymptotic consider equation as
\[ y(x) = C_2 + C_1 \int \exp \left( \int (\lambda(r) + 2a(r)) dt \right) \]

1.1.2. Nikiforov-Uvarov

This method is used to solve the solution of an equation (e.g., Schrodinger) by transformation as \( \psi''(s) + \frac{\Gamma(2)}{\sigma(3)} \psi(s) + \frac{\delta(s)}{\sigma(2)} \psi(0) = 0 \). Here \( \Gamma(s) \) is polynomial of degree at most one, \( \sigma(s) \) and \( \delta(s) \) are second-degree polynomials. On applying the condition of \( \lambda = \lambda_0 \) one can obtain the energy eigenvalue. Here \( \lambda = k + \pi(s) \) and \( \lambda_0 = -\pi(s) - \frac{n(n-1)e^\pi(s)}{2} \), \( \pi(s) \) is also polynomial with four values obtained by comparing the standard equation.

1.1.3. Supersymmetry method

To calculate the energy eigenvalue, this method assumes a particular type of wave function \( \psi_\alpha = \exp[\int W_\alpha \exp(r dr + \beta(r)] \phi_\alpha(r) \), here \( W_\alpha \) is supersymmetry in quantum mechanics assumed as Witten superpotential. \( \phi_\alpha(r) \) is a new function, and \( \beta(r) \) is also a wave function that leads to correct asymptotic value. As we knew Schrodinger equation is used to obtain the energy Eigenvalue by replacing the general wave function by \( \psi_\alpha \) and solving similar to the conventional method, we get energy eigenvalue for any potential.

1.1.4. Factorization method

In this method, the wave function for a particular coordinate system (example, Schrodinger equation spherical coordinate system) contains angular and coordinate system, and this method separates the angular and radial part by factorization method known as separation of variables in general like \( \Psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi) \) after separating the angular and radial parts. The radial part is defined as \( R(r) = U(r)\mathcal{U}(r) \). Here \( \mathcal{U}(r) \) is related to potential and \( L(r) \) is associated with Laguerre differential equation. The angular part is defined as \( \Theta(x) = U(x)P(x) \), here \( x = \cos\theta \), \( P(x) \) related to the Jacobi function.

2. Theoretical Formulation

We have radial form part of SE is
\[ \psi''(r) + \frac{2m}{\hbar^2} \left[ E_{nl} - V(r) - \frac{(l + 1)\hbar^2}{2mr^2} \right] \psi(r) = 0 \]
Using centrifugal approximation \( 1 = \frac{4\alpha^2 e^{-2ar}}{(1-e^{-2ar})^2} \), a radical form of SE become
\[ \psi''(r) + \frac{2m}{\hbar^2} \left[ E_{nl} + \frac{V_0 e^{-2ar}}{1 - q e^{-2ar}} - \frac{l(l + 1)\hbar^2}{2m} \right] \psi(r) = 0 \]
Let us consider \( Z = \frac{1}{1-e^{-2ar}} \) then the radial form of the equation become
\[ \psi''(r) + \frac{2m}{\hbar^2} E_{nl} + \frac{V_0 e^{-2ar}}{1 - q e^{-2ar}} - \frac{l(l + 1)\hbar^2}{2m} Z^2 4\alpha^2 \psi(Z - 1) = 0 \]
On solving equation (1), we get
\[ \psi''(Z) (Z - 1) + \psi'(Z) (Z - 2) - \frac{m\hbar^2}{2k^2} \left[ e^\pi Z \left( l(n+1) \right) \right] + \frac{mV_0}{2k^2} \frac{1}{Z^2} Z^2 \frac{(l+1)\hbar^2}{2m} \psi(Z) = 0 \]
Now again suppose \( \frac{mV_0}{2k^2} \frac{1}{Z^2} \) as \( -\epsilon/\delta \), \( \epsilon = \frac{mV_0}{2k^2}, \delta = l(l + 1) \), therefore equation (2) becomes
\[ \psi''(Z) (Z - 1) + \psi'(Z) (1 - 2Z) \]
\[ + \frac{m\hbar^2}{2k^2} \psi(Z) = 0 \]
(3)
Now asymptotic behavior of equation (3), at \( r \to 0 \) \( Z \to 0 \) and \( r \to \infty \) \( Z \to 0 \), Let us introduce a new function \( f(Z) \) as
\[ \psi(Z) = Z^n (1 - Z) \psi f(Z) \]
Combining equations (4) and (3), we get a new equation of the form
\[ \left[ Z(1 - Z) f''(Z) + (1 + 2\mu - (2\mu - 2\phi - Z)f'(Z) \right] \]
\[ - \left[ (\mu + \phi)^2 + (\mu + \phi + \gamma) \right] f(Z) \]
\[ + \left[ -\epsilon - \delta + \mu + \phi \right] f(Z) \]
\[ = 0 \]
Now equation (5) becomes the Gauss hypergeometric equation when the square bracket term equal to zero
\[ -\epsilon - \delta + \mu + \phi = 0 \]
\[ \phi = \mu - \delta = 0 \]
Therefore, equation (5) is written as
\[ Z(1 - Z)f''(Z) + [1 + 2\mu - (2\mu - 2\phi - 2)Z]f'(Z) \]
\[ = \left( \frac{\mu + \phi + \frac{1}{2} - \frac{1}{\sqrt{4 - \xi}}}{\sqrt{4 - \xi}} \right) \times \left( \frac{\mu + \phi + \frac{1}{2} - \frac{1}{\sqrt{4 - \xi}}}{\sqrt{4 - \xi}} \right) f(Z) \]
\[ = 0 \]  
(6)

The Gaussian hypergeometric function (GHF), \( \mathcal{F}(a; b; c; z) \) can be expressed as infinite series for \( |z| < 1 \) as,
\[ \mathcal{F}(a; b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n} \frac{z^n}{n!} = 1 + \frac{ab z}{c} + \frac{a(a+1)b(b+1)z^2}{c(c+1)} + \cdots \]

Here \( (a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} \), \( (b)_n = \frac{\Gamma(b+n)}{\Gamma(b)} \), \( (c)_n = \frac{\Gamma(c+n)}{\Gamma(c)} \) putting these in the above equation and simplifying we get,
\[ f(Z) = \mathcal{F}(a_1,b_1,c_1, Z) = \frac{\Gamma(c_1)}{\Gamma(a_1)} \Gamma(b_1) \]

Here we consider \( a_1, b_1 \) and \( c_1 \) as unknown parameters whose values are expressed as \( a_1 = \left( \mu + \phi + \frac{1}{2} + \frac{1}{\sqrt{4 - \xi}}, b_1 = \left( \mu + \phi + \frac{1}{2} - \frac{1}{\sqrt{4 - \xi}}, c_1 = 1 + 2\mu \right) \) . Now substituting the value of \( f(Z) \) with these parameters in \( \psi(Z) = Z^\mu(1 - Z)^\phi f(Z) \) in this, we get
\[ \psi(Z) = Z^\mu(1 - Z)^\phi \]

If \( a_1, b_1 \), and \( c_1 \) is equal to the negative of integer (n) then hypergeometric function \( f(Z) \) will become a polynomial with \( n = 0, 1, 2, 3, \ldots, n_{\text{max}} \) integer, applying quantum condition we have, \( a_1 = -n \) and \( b_1 = -n \). Now using \( \phi^2 - \mu^2 + \delta = 0 \) to calculate the value of \( \phi \) and \( \mu \) from the above suitable value we get
\[ \phi = \left( \frac{\omega n}{2} - \frac{\delta}{2(\omega n)} \right) \text{ and } \mu = \left( \frac{\omega n}{2} - \frac{\delta}{2(\omega n)} \right) \text{ where } \omega = \frac{1}{\sqrt{4 - \xi}} - \frac{1}{\omega} \]

Now to calculate the energy we have from \( -\delta + \mu^2 + \mu^2 = 0 \) and \( \phi^2 - \mu^2 + \delta = 0 \) is \( e = \phi^2 \). Since we have \( m_{\text{el}} = \frac{mE_{\text{el}}}{2\hbar^2a^2} \), therefore we have,
\[ E_{\text{el}} = -\frac{2\hbar^2a^2}{m} \left( \frac{\omega n}{2} - \frac{\delta}{2(\omega n)} \right) \]
\[ + \left( \frac{1}{\sqrt{4 - \xi}} - \frac{1}{\omega} \right) \quad (7) \]

Substituting the value of \( \delta, \omega, \xi \) in equation (7) we get,
\[ E_{\text{el}} = -\frac{2\hbar^2a^2}{m} \left( \frac{1}{\sqrt{4 - l(l+1) - \frac{1}{2} - n}} \right) + \left( \frac{mV_0}{2\hbar^2a^2} \right) \left( \frac{1}{\sqrt{4 - l(l+1) - \frac{1}{2} - n}} \right)^2 \]

(8)

This equation is dependent upon the quantum number and screening parameters. It is a non-relativistic energy spectrum that was calculated using HP, which is short-range potential.

**Table 1: Energy eigenvalue of q-deformed HP**

| Quantum Number | Energy eigenvalue \( (E_{\text{el}}) \) |
|---------------|----------------------------------------|
| n l = 1        | \( V_0 = 1, \alpha = 1, \alpha = 1, \alpha = 0.5, \alpha = 0.1, \alpha = 1 \) |
| 0 1            | 2.20977 -2.20977 1.511428 1.0479577 -0.373922 |
| 1 -3.09095 165 927 -0.21685 |
| 0 2            | 6.78920 1.15 437 457 -0.20085 |
| 3 1            | 7.95751 1.65 927 -0.21685 |
| 2 1            | 6.78920 1.15 437 457 -0.20085 |
| 3 1            | 7.95751 1.65 927 -0.21685 |
| 2 2            | 6.78920 1.15 437 457 -0.20085 |
| 3 2            | 6.78920 1.15 437 457 -0.20085 |
| 4 1            | 6.78920 1.15 437 457 -0.20085 |
| 3 2            | 6.78920 1.15 437 457 -0.20085 |
| 4 2            | 6.78920 1.15 437 457 -0.20085 |
| 5 1            | 6.78920 1.15 437 457 -0.20085 |
| 4 2            | 6.78920 1.15 437 457 -0.20085 |
| 5 2            | 6.78920 1.15 437 457 -0.20085 |

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2.1. Thermodynamic Properties

HP is also used to explain the electronic properties of some alkali halides, study the bound state and scattering properties, etc. Moreover, statistical physics and quantum statistical mechanics help predict, interpret, analyze, etc., different thermodynamic properties such as vibrational and rotational energy levels of various molecules [6]. Thermodynamics properties of HP are also studied for statistical quantum chromodynamics (QCD), nuclear matter, a color deconfinement partonic phase, and the quark-gluon plasma (QGP) at sufficiently high temperature/density [7].

Now to calculate the thermodynamic properties for HP, now we develop (8) equation to study the thermodynamic properties; we use the vibrational partition function for this we summarized \( E_{nf} \) as,

\[
E_{nf} = \frac{\hbar^2 \alpha^2}{2m} \frac{p}{(\sigma + n)}^2 - (\sigma + n)^2
\]

From this equation, the vibrational partition function is defined as

\[
Z_{vib}(\beta) = \sum_{n=0}^{\eta} e^{-\beta E_{nf}} = \frac{1}{kT}
\]

Therefore, substituting the value of \( E_{nf} \) in \( Z_{vib} \) HP with partition function modified as,

\[
Z_{vib}(\beta) = \sum_{n=0}^{\eta} e^{-\beta \sqrt{\frac{\hbar^2 a^2}{2m} \left( \frac{p}{(\sigma + n)^2} - (\sigma + n)^2 \right)}}
\]

Replacing the sum by an integral in the classical limit of equation (10), we have

\[
\int_0^{\eta} e^{-\beta \sqrt{\frac{\hbar^2 a^2}{2m} \left( \frac{p}{(\sigma + n)^2} - (\sigma + n)^2 \right)}} d\sigma = \frac{1}{kT}
\]

Supposing \( \sigma + n = \rho \), equation (becomes) become [8]

\[
Z_{vib}(\beta) = \int_0^{\eta} e^{-\beta \sqrt{\frac{\hbar^2 a^2}{2m} \frac{p}{(\sigma + n)^2} - (\sigma + n)^2}} d\rho
\]

(12)

Here \( a = \frac{\hbar^2 a^2}{2m} \), \( b = \frac{\hbar^2 a^2}{2m} \), \( c = -\frac{\hbar^2 a^2}{m} \), now equation (12) becomes

\[
e^{-\beta \left[ \sqrt{\frac{\hbar^2 a^2}{2m} \left( \frac{p}{(\sigma + n)^2} - (\sigma + n)^2 \right)} \right] + \beta \alpha p + \beta \alpha p + \beta \alpha p + \beta \alpha p}
\]

(13)

2.2. Energy eigenvalue of q-deformed HP

The energy eigenvalue is represented in atom unit with \( m = \hbar = 1 \), \( V_0 = 0.5 \), 1 and \( \sigma = 0.5 \), 1. The energy eigenvalue is developed of q-deformed HP. It is beneficial to calculate the thermodynamic properties of physics fields like quantum chromodynamics, meson-meson interaction, nuclear matter color chromodynamics, etc. The nature of energy eigenvalue with quantum number is shown in figure 1, which shows that with an increased quantum number the electron bounded energy decreases which means the electron goes loosely bounded with the nucleus in an atom.

![Figure 1: Energy eigenvalue of deformed Hulthen Potential](image)

2.3. Thermodynamic properties of q-deformed HP

2.3.1. Vibrational mean energy of q-deformed HP

(VMEqHP)

The mean vibrational energy for the HP model is defined as

\[
\langle E \rangle = \frac{1}{kT} \left( \eta \int_0^{\eta} e^{-\beta \sqrt{\frac{\hbar^2 a^2}{2m} \left( \frac{p}{(\sigma + n)^2} - (\sigma + n)^2 \right)}} d\sigma \right)
\]

(14)

By solving this equation, we get

\[
\langle E \rangle = \frac{1}{kT} \left( \frac{\eta}{\sqrt{\beta \hbar^2 a^2}} + \frac{d}{d\beta} \left[ \ln(\beta + \frac{1}{\beta}) \right] \right)
\]

(15)

2.3.2. Vibrational mean free energy of q-deformed HP

(VMEqFHP)

The vibrational mean free energy is obtained as

\[
F(\beta) = -kT \ln(Z_{vib}(\beta))
\]

(16)

\[
F(\beta) = -kT \ln \left( \frac{1}{\sqrt{\beta \hbar^2 a^2}} \left( \sqrt{\frac{1}{\beta} + \frac{d}{d\beta} \left[ \ln(\beta + \frac{1}{\beta}) \right]} \right) \right)
\]

Where \( \Gamma_1 = \sqrt{\frac{-b\beta}{\sigma}} \), \( \Gamma_2 = \sqrt{1-a\beta} \), \( \Omega_1 = \sqrt{1-a\beta} \), \( \Omega_2 = \sqrt{\frac{-b\beta}{\Omega + \sigma}} \), and \( Z = \text{erf}[\Omega_1 + \Gamma_2 - \Omega_2] \) and the error function well-defined as

\[
\text{erf}(Z) = \frac{2}{\sqrt{\pi}} \int_0^Z e^{t^2} dt
\]

Equation (13) plays an integral equation used to describe the thermodynamic properties of q-deformed HP. This equation described vibrational mean and free energy, vibrational entropy, and specific heat capacity. The Integrals error function \( \text{erf}(Z) \) has essential applications in atomic physics, astrophysics, statistical analysis, etc. [9]
2.3.3. Vibrational specific heat capacity of q-deformed HP (VSqHP)

The vibrational specific heat capacity \( C_v \) is given as

\[
C_v(\beta) = k\beta^2 \frac{\partial^2}{\partial \beta^2} \ln(Z_{\text{vib}}(\beta))
\]

\[
C_v(\beta) = k\beta^2 \frac{\partial^2}{\partial \beta^2} \ln\left(\frac{\Gamma(\beta - 1) + e^{\beta - 2} \Gamma(\beta) \text{erf}(\beta) - e^{-\beta} \Gamma(\beta + 1) + e^{-\beta} \Gamma(\beta + 2) - e^{-2\beta} \Gamma(\beta + 3) + e^{-2\beta} \Gamma(\beta + 4)}{4\beta} \right)
\]

2.3.4. Vibrational entropy of q-deformed HP (VEqHP)

The vibrational entropy is obtained as

\[
S(\beta) = k\ln(Z_{\text{vib}}(\beta)) + kT \frac{\partial}{\partial \beta} \ln(Z_{\text{vib}}(\beta))
\]

\[
S(\beta) = k\ln\left(\frac{\Gamma(\beta - 1) + e^{\beta - 2} \Gamma(\beta) \text{erf}(\beta) - e^{-\beta} \Gamma(\beta + 1) + e^{-\beta} \Gamma(\beta + 2) - e^{-2\beta} \Gamma(\beta + 3) + e^{-2\beta} \Gamma(\beta + 4)}{4\beta} \right)
\]

Thermodynamical properties have error functions with different parameters and in literature [9] authors discuss its multiuse use. Therefore, studying the thermodynamic properties for consideration in this paper has equal importance as discussed in the literature [8, 9]. The thermodynamic properties of the electron in considering potential is obtained in equation (14), (15), (16), and (17) showing that the thermodynamic properties depend upon quantum number also. Therefore, the thermodynamic properties for considering potential depend upon quantum number as well as temperature.

3. Conclusion

The development of energy eigenvalue for q-deformation HP potential develops in equation (8) with the help of this energy vibrational thermodynamical properties are calculated. The development of a mathematical model for thermodynamic properties for the electron in q-deformation potential is completely new. In addition, the thermodynamic properties also depend upon the quantum number which means vary with the quantum number. For example, the thermodynamic properties of the electron in the n=1 orbit are different from the thermodynamic properties of the electron in the n=2 orbit and so on. This is because the thermodynamic properties depend upon the energy eigenvalue of the electron and the energy eigenvalue of the electron depends upon the quantum number. The developed mathematical model is based on a Gaussian hypergeometric function with a partition function. To study the more detailed thermodynamic properties of an electron in considering potential one may extend the development theory due to the complexity of mathematical derivation authors consider the limitations of their work.

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