Research article

Superstatistics of Schrödinger equation with pseudo-harmonic potential in external magnetic and Aharonov-Bohm fields

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ABSTRACT

In this work, the thermodynamic properties of pseudo-harmonic potential in the presence of external magnetic and Aharonov-Bohm fields are investigated. The effective Boltzmann factor in the superstatistics formalism was used to obtain the thermodynamic properties such as Helmholtz free energy, Internal energy, entropy and specific heat capacity of the system. In addition, the thermal properties of some selected diatomic molecules of $N_2$, $Cl_2$, $I_2$ and $CH$ using their experimental spectroscopic parameters and the effect of varying the deformation parameter of $q = 0.3$, $0.7$ were duly examined.

1. Introduction

The solution of the Schrödinger equation and its relativistic counterpart with diverse physical potential models plays a very imperative role in many sub-disciplines of physics and chemistry since it contains all the essential information for the description of a quantum mechanical system [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. Furthermore, this solution is very pertinent in particle, nuclear and chemical physics amongst many others. It has been used to study the mass spectra, binding energies, decay rates and transition properties, and thermodynamic functions for certain systems of interest [16, 17, 18].

In quantum mechanics, not many physical systems can be solved exactly in a closed form. For instance, the few that are exactly solvable are; the harmonic oscillator and Coulomb potential [19, 20], pseudo-harmonic and Kratzer potential [21, 22, 23] etc. The solutions of the Schrodinger in two dimension (2D) for a charged particles confined by an harmonic oscillator in the presence of magnetic and Aharonov-Bohm field have been studied by numerous authors [24, 25, 26, 27]. Also, other effects of an unvarying magnetic field on different physical systems have been investigated [28]. Kosick and Okopinska considered the pseudo-exact solutions for dual interrelating electrons using Coulomb force with restricted anisotropic harmonic oscillator in 2D anisotropic dot [29]. Aygun et al. [30] studied the effect of magnetic field on the energy spectra of a particle moving under the Kratzer potential using the asymptotic iteration method [31]. Also, Ikhdair and Hamzavi [32] studied the spectral properties of quantum dots in the non-relativistic regime with anharmonic potentials and superposition of pseudo-harmonic plus linear plus Coulomb potentials with magnetic and Aharonov-Bohm fields being present. The problem was solved using the well-known Nikiforov-Uvarov (NU) method [33]. Furthermore, Dirac equation in two dimension have been solved with anharmonic potential in the presence of magnetic and Aharonov-Bohm fields [34]. Subsequently, many Schrödinger-like equations with harmonic and anharmonic potentials with and without external magnetic and Aharonov-Bohm fields have been investigated [35, 36, 37].

In addition, studies on the thermal properties of gases and diatomic molecules over a wide range of temperature limits have attracted the attention of many researchers [38]. Yepes et al. [39] evaluated the heat capacity and magnetization for Gallium Arsenide (GaAs) quantum dot with asymmetric confinement. The thermodynamic and magnetic properties of electronic confinement have attracted significant interest such as electron-electron interaction on the energy spectrum [40] and electronic...
structure [41]. For instance, Atomyan et al. [42] studied the relativistic spin zero particles in a 2D cylindrical potential. Gumber et al. [43] studied a two dimensional cylindrical QD in the presence of external electric and magnetic fields. They went further to determine the canonical partition function and other statistical mechanical properties of the system. The first step in obtaining the thermal properties of a system is by evaluating the partition function of the system, after which other thermodynamic properties can be evaluated accordingly. The partition function which depends on temperature is often regarded as the Boltzmann distribution function in statistical mechanics which was first brought to limelight by Boltzmann in 1870 [44]. Other statistical mechanical representations besides Boltzmann had been proposed such as Gibbs [45], Einstein [46], Boltzmann-Gibbs (BG) [47], Tsallis [48] and the recently renown one which is the superstatistics [49, 50]. Superstatistics is a mishmash of two statistics, hence the name superstatistics, this statistics was originally formulated by Wilk and Wlodarczyk [49], thereafter Beck and Cohen [50] reformulated the concept into what is widely used and adopted today. This concept is used in the description of non-equilibrium system with steady state and intensive parameter fluctuations. Superstatistics has numerous applications in different fields of physics and chemistry such as cosmic rays [51], wind velocity fluctuations [52], hydrodynamic turbulence [53] among others.

The aim of the present work is to investigate the Schrödinger equation in 2D for a pseudo-harmonic oscillator in the presence of external and Aharonov-Bohm fields with applications to superstatistics. The pseudo-harmonic potential is one of the precisely solvable potentials in physics [54]. The pseudo-harmonic potential is defined as,

\[ V(r) = L^2 + \frac{M}{r^2} + N, \]  

(1)

where \( L, M \) and \( N \) are potential constants. As an application, we present the thermal properties of the system within the framework of superstatistics. The thermodynamic properties of some selected diatomic molecules of \( N_2, Cl_2, I_2 \) and \( CH \) within framework of superstatistics are also reported.

2. The parametric NU method

The parametric form of the NU method takes the form [56].

\[ \frac{d^2 \psi}{dr^2} + \frac{a_1 - a_2}{s(1 - a_3)} \frac{d\psi}{dr} + \frac{1}{s^2(1 - a_3^2)} \left\{ -\xi_1 s^2 + \xi_2 s - \xi_3 \right\} \psi(s) = 0 \]  

(2)

The energy eigenvalues equation and eigenfunctions respectively satisfy the following sets of equation,

\[ \alpha^2 n^2 - (2\alpha + 1)(\alpha + 1) + n(n - 1) - \alpha^2 \alpha_1 + 2 \alpha_1 \alpha_2 + 2 \alpha_2 \alpha_3 - \alpha_3 = 0, \]  

(3)

\[ \psi(s) = s^{\alpha_0}(1 - a_3 s)^{-\alpha_1} \frac{a_2 - a_0}{s^2} P_n^\alpha (1 - 2a_3 s), \]  

(4)

where

\[ a_1 = \frac{1}{2}(1 - a_1), a_2 = \frac{1}{2}(a_2 - 2a_1), a_3 = a_2 + \xi_1, \]  

(5)

\[ a_0 = 2a_2 a_3 - \xi_2, a_2 = a_2^2 + \xi_3, a_1 = a_1 + a_2^2 a_3 + a_2 \]  

and \( P_n^\alpha \) is the orthogonal Jacobi-polynomial which define as

\[ P_n^\alpha(x) = \frac{\Gamma(\alpha + n + 1)}{n!\Gamma(\alpha + n + 1)} \sum_{m=0}^{n} \binom{n}{m} \frac{\Gamma(\alpha + m + 1)}{\Gamma(\alpha + m + 1)} \left( x - 1 \right)^m \]  

(6)

3. Solutions of the Schrödinger equation in external magnetic and Aharonov-Bohm fields

The Schrödinger equation for charged particles moving in a magnetic and Aharonov-Bohm fields is [24, 25, 26, 27],

\[ \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right\} \psi(r, \phi) = E_n \psi(r, \phi), \]  

(7)

where \( \mu \) is the effective mass of the system, \( e \) is the electric charge, \( c \) is the speed of light, the vector potential \( \vec{A} \) can be expressed as \( \vec{A} = \vec{A}_1 + \vec{A}_2 \) in such a way that \( \vec{A} \times \vec{A}_1 = \vec{B} \) and \( \vec{A} \times \vec{A}_2 = 0 \) with \( \vec{B} = h \vec{E} \) being the applied magnetic field and \( \vec{A}_2 \) describing the additional magnetic flux \( \Phi_{AB} \) created by a uniform magnetic field [24, 25, 26, 27],

\[ \vec{A}_1 = \frac{1}{2} \left( \vec{B} \times r \right), \]  

(8)

\[ \vec{A}_2 = \frac{\vec{B} \times \vec{r}}{2} + \frac{\Phi_{AB}}{2\pi r}, \]  

(9)

where \( \Phi_{AB} = \frac{B}{2\pi} \) \( \alpha \).

Now substituting Eq. (1) into Eq. (7), we get

\[ \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right\} \psi(r, \phi), \]  

(10)

Inserting Eq. (8) into Eq. (9), we obtain

\[ \left\{ -\frac{\hbar^2}{2m} \left( \frac{\vec{B} \cdot \vec{r}}{2} + \frac{\Phi_{AB}}{2\pi r} \right) \right\} \psi(r, \phi), \]  

(11)

In order to find an exact solution of Eq. (10), we make the following choice for the wave function as,

\[ \psi(r, \phi) = e^{im\phi}, m = 0, \pm 1, \pm 2... \]  

(12)

and this transform Eq. (10) into the second-order Schrödinger equation as

\[ \frac{d^2 R(r)}{dr^2} + \left( \frac{2mE_n}{\hbar^2} - \frac{\vec{B} \cdot \vec{r}}{2m} \right) L^2 + \frac{M}{r^2} + N \right\} \frac{1}{r^2} \left( \frac{m^2 - \frac{1}{4} + 2mE_n}{4\hbar^2} + \frac{\Phi_{AB}^2}{2\pi \hbar^2} \right) \]  

(13)

where \( m \) is the magnetic quantum number. We can express Eq. (12) as,

\[ \frac{d^2 R(r)}{dr^2} + \left( -ar^2 + \frac{r}{r^2} \right) R(r) = 0, \]  

(14)

where,
\[ \epsilon^2 = \frac{2\mu}{h^2}(E_{\text{tot}} - N), \quad \alpha = \left(\frac{2\mu L}{h^2} - \frac{e^2 B^2}{4\hbar^2 c^2}\right). \quad (14) \]

To get the solution of Eq. (13), we introduce a coordinate transformation of the form \( s = r^2 \) and Eq. (13) becomes,

\[ \frac{d^2 R(s)}{ds^2} + \frac{1}{2s} \frac{dR(s)}{ds} + \left(\frac{\alpha}{4} - e^2 s + \frac{\gamma}{4}\right) R(s) = 0. \quad (15) \]

Eq. (15) is be solved by the parametric Nikiforov-Uvarov (pNU) method [56] (details is given in section 2) and the energy spectrum is obtained as,

\[ E_{\text{tot}} = \frac{h^2}{\mu} \left(2\mu L - \frac{e^2 B^2}{4\hbar^2 c^2}(2n + 1 + \frac{1}{16} - \frac{\gamma}{4}) + N\right). \quad (16) \]

4. Boltzmann factor in the superstatistics

The q-deformed superstatistics is a combination of two different statistical models [11, 12, 13, 14, 15] with myriad applications in physics. The effective Boltzmann factor is obtained as [11, 12, 13, 14, 15],

\[ B(E_{\text{tot}}) = e^{-\beta E_{\text{tot}}^q} \left(1 + \frac{q}{2} E_{\text{tot}}^q\right), \quad (17) \]

where \( q \) is the deformation parameter that lies between \( 0 \leq q \leq 1 \), \( \beta = \frac{1}{k_B T} \), \( T \) is the temperature, \( k_B \) is the Boltzmann constant and \( E_{\text{tot}} \) is the energy of the quantum system. It should be noted that Dirac-delta distribution function was used in obtaining Eq. (17) as reported in Ref. [11, 12, 13, 14, 15]. Consequently, one can obtain the ordinary statistical mechanics when \( q = 0 \) [15]. It is worthy to note that the thermodynamic properties of the system within the superstatistics framework are valid for all values of \( q \) and depends on the energy of the system.

5. Thermodynamic properties with pseudo-harmonic potential in the presence of an external magnetic field

The partition function in the superstatistics framework is defined as [11, 12, 13, 14, 15],

\[ Z(\beta) = \int_0^\infty B(E_{\text{tot}}) \, d\eta \quad \text{(18)} \]

By substituting Eqs. (16) and (17) into Eq. (18), we obtain an expression for the partition function within the superstatistics framework as,

\[ Z(\beta) = \frac{1}{4\beta^2} \left\{2e^{-\beta^2 Q^2 + N + \zeta^2} q + 2\eta e^{-\beta^2 Q^2 + N + \zeta^2} q + N^2 \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q\right\} \]

\[ + \frac{1}{4\beta^2} \left\{2N^2 \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q + N^2 \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q + 2e^{-\beta^2 Q^2 + N + \zeta^2} q\right\} \]

\[ + \frac{1}{4\beta^2} \left\{4\zeta^2 Q^2 \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q + 4\zeta^2 Q^2 \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q\right\} \]

\[ + \frac{1}{4\beta^2} \left\{2N \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q\right\} \]

\[ + \frac{1}{4\beta^2} \left\{4\zeta Q^2 \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q + 4N \beta^2 e^{-\beta^2 Q^2 + N + \zeta^2} q\right\}, \quad (19) \]

where,

\[ \zeta = \frac{h^2}{\mu} \left(2\mu L - \frac{e^2 B^2}{4\hbar^2 c^2}\right) \quad \text{(20)} \]

Other thermodynamic functions like Helmholtz free energy \( F(\beta) \), mean energy \( U(\beta) \), entropy \( S(\beta) \) and specific heat capacity at constant volume \( C_v(\beta) \) can be obtained from the partition function of Eq. (19) using the following relations

\[ F(\beta) = -\frac{1}{\beta} \ln Z(\beta); \quad (22) \]

\[ U(\beta) = -\frac{\beta}{\partial Z(\beta)}; \quad (23) \]

\[ S(\beta) = k_B \ln Z(\beta) - k_B \beta \frac{\partial \ln Z(\beta)}{\partial \beta}; \quad (24) \]

\[ C_v(\beta) = k_B \beta^2 \frac{\partial^2 \ln Z(\beta)}{\partial \beta^2}. \quad (25) \]

Equations (22) – (25) gives the expressions that will aid in our study of these thermal properties of the system.

6. Applications

In this section, we evaluate the thermodynamic properties for different diatomic molecules of \( \text{N}_2 \), \( \text{Cl}_2 \), \( \text{I}_2 \) and \( \text{CH} \) using their experimental values with a deformation parameter of \( q = 0.3 \) in the presence and absence of the external magnetic fields. These molecules are selected based on availability of spectroscopic data and their wide usage in many industrial applications. The second application is carried out by evaluating the thermodynamic properties for different deformation parameter of \( q = 0.3 \), \( 0.7 \) and \( 1 \) in the presence of the external magnetic fields.

6.1. Applications to diatomic molecules

Here, we consider the pseudoharmonic oscillator of the form [55],

\[ V(r) = D_s \left(\frac{r}{r_e} - \frac{r}{r}\right)^2, \quad (26) \]

where \( D_s \) is the dissociation energy (i.e. the energy required to break every chemical bond in a molecule and completely separate all its atoms) [55], \( r_e \) is the equilibrium bond length (i.e. the distance between two atoms when they are bonded to each other) [55] and \( r \) is the radial distance to the particle.

On comparing Eqs. (1) and (26) gives the values of \( L, M \) and \( N \) as \( L = D_s r_e^2 \), \( M = D_s r_i^2 \) and \( N = -2D_s \) [55].

We also take \( \theta = 37^\circ \), \( m = 1 \), \( \Phi_{AB} = 1 \), \( \hbar c = 1973.29 \) eV, 1 amu = 931.494028 \( \times 10^6 \text{eVc}^{-2} \) and \( c = e = 1 \) in the presence of the magnetic fields and zero otherwise. The experimental values of some selected diatomic molecules of \( \text{N}_2 \), \( \text{Cl}_2 \), \( \text{I}_2 \) and \( \text{CH} \) are taken from Ref. [55] as shown in Table 1.

By using these experimental data, we plot the partition function \( Z(\beta) \) for \( \text{N}_2 \), \( \text{Cl}_2 \), \( \text{I}_2 \) and \( \text{CH} \) in the presence and absence of the magnetic field \( B \) in Figure 1a and b within the framework of superstatistics at \( q = 0.3 \). As shown in Figure 1a and b, the partition functions in the presence and absence of the magnetic fields decreased monotonically as the inverse temperature \( \beta \) is increased. The plots of the Helmholtz free energy \( F(\beta) \) for both cases are also shown in Figure 2a and b. Figure 2a and b show the behaviour of the Helmholtz free energy versus \( B \). It is observed in Figure 2a and b that the Helmholtz free energy increases as parameter \( \beta \) is increased. Figure 3a and b show the internal energy of the diatomic molecules within the superstatistics formulation. As shown in Figure 3a and b, the internal energy \( U(\beta) \) of the diatomic molecules...
decreased with increasing $\beta$ in the presence of the external magnetic fields $\vec{B}$ and $\Phi$. The variations of the entropy $S(\beta)$ with inverse temperature $\beta$ are shown in Figure 4a and b for the three diatomic molecules. Here, the entropy decreases with increasing $\beta$ in the presence and absence of the magnetic field. In Figure 5a and b, the variations of the heat capacity $C_v(\beta)$ as a function of inverse temperature are shown. Figure 5a shows that the specific heat peaked at unity and decreased with increasing $\beta$ for different diatomic molecules in the presence of the external magnetic field. Nevertheless, in the absence of the magnetic field, a similar trend is observed but this occurs in the region of very high

Table 1. Spectroscopic Parameters of the selected Diatomic Molecules [55].

| Molecule | $r_e$ (Å) | $\mu$ (amu) | $d_0$ (cm$^{-1}$) |
|----------|-----------|-------------|------------------|
| $N_2$    | 1.0940    | 7.00335     | 98288.03528      |
| $Cl_2$   | 1.9872    | 17.4844     | 20276.440        |
| $I_2$    | 2.6664    | 63.452235   | 12547.300        |
| $CH$     | 1.1198    | 0.929931    | 31838.08149      |

Figure 1. (a) Partition function as a function of $\beta$ for various diatomic molecules in the presence of the magnetic field $\vec{B}$ and $\Phi$. (b) Partition function as a function of $\beta$ for various diatomic molecules in the absence of the magnetic fields.

Figure 2. (a) Free energy as a function of $\beta$ for various diatomic molecules in the presence of magnetic field $\vec{B}$ and $\Phi$. 2(b): Free energy as a function of $\beta$ for various diatomic molecules in the absence of the magnetic field $\vec{B}$ and $\Phi$. 
temperature, this is in contrast to that of the presence of the magnetic field which occurs in the low temperature region as shown in Figure 5a and b.

### 6.2. Deformation parameter

Similarly, taking $B = 3$, $m = 1$, $\Phi_{AB} = 1$ and $\hbar = c = e = 1$, we investigated the behaviour of the partition function $Z(\beta)$, Helmholtz free energy $F(\beta)$, internal energy $U(\beta)$, entropy $S(\beta)$ and specific heat capacity $C_v(\beta)$ for different superstatistics parameters $q = 0.3, 0.5, 0.7$ and $1.0$. In Figure 6a, we plot the behaviour of the partition function versus $\beta$ for different values of the deformation parameter, $q$. As can be seen in Figure 6a, by increasing $\beta$, the partition function decreases monotonically. Also, in Figure 6b, the behaviour of the Helmholtz free energy is plotted as a function of the inverse temperature $\beta$. The Helmholtz free energy increases with increasing $\beta$ to a maximum value for different values of $q$. Figure 6c shows the behaviour of internal energy as a function of $\beta$ within the superstatistics formulation for different $q$ values. As it is observed in Figure 6c, the internal energy decreased with increasing $\beta$ in the presence of the magnetic field $B$ and $\Phi$. The variation of the entropy with inverse temperature $\beta$ is shown in Figure 6d. The entropy decreases with increasing $\beta$ in the presence of the magnetic field. In Figure 6e, the variation of the heat capacity as a function of inverse temperature is shown. Figure 6e shows that the specific heat peaked at unity and decreased with increasing $\beta$ for different deformation parameter $q$ in the presence of the external magnetic field.

It is worthy to note that Sargolzaeipor et al. [11] studied the thermodynamic properties and $q$-deformed superstatistics in commutative and noncommutative spaces with external magnetic field. The results obtained with different deformation parameters of the system agree with the behaviour of the results in our work. In another development, the cornell potential in the presence of an Aharonov-Bohm magnetic field...
was employed to solve the Klein-Gorden equation \cite{57}. The energy relation obtained was further used to evaluate the superstatistics of the system within the modified Dirac delta distribution formalism. The behaviour of the thermodynamic properties here with different values of the deformation parameters agrees with our results discussed above.

Recently, Okorie and his collaborators \cite{58} studied the superstatistics of modified Rosen-Morse potential with Dirac delta and uniform distribution formalisms. The graphical variation of the thermodynamic properties with the inverse temperature parameter here agrees with the variation obtained in our results. It is worthy to mention here that no

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**Figure 5.** (a) Specific heat capacity as a function of $\beta$ for various diatomic molecules in the presence of the magnetic field $B$ and $\Phi$. (b) Specific heat capacity as a function of $\beta$ for various diatomic molecules in the absence of the magnetic field $B$ and $\Phi$.

**Figure 6.** (a) Partition function as a function of $\beta$ for different deformation parameters. (b) Helmholtz free energy as a function of $\beta$ for different deformation parameters. (c) Mean energy as a function of $\beta$ for different deformation parameters. (d) Entropy as a function of $\beta$ for different deformation parameters. (e) Specific heat capacity as a function of $\beta$ for different deformation parameters.
literatures exist on the concept of superstatistics with diatomic molecules to be best of our knowledge. As such, it is difficult for us to make comparison. We therefore hope that these results will be useful for further studies.

7. Conclusions

In this work, we have studied the thermodynamic properties of pseudoharmonic potential in the presence of external magnetic and Aharonov-Bohm fields. We obtained in closed-form the energy spectrum of the system and calculated the partition function of the system within the framework of superstatistics using the modified Dirac delta distribution. With the partition function, we determine other thermodynamic properties such as Helmholtz free energy, mean energy, entropy and the specific heat capacity. We applied the result to study the thermodynamic properties of some selected diatomic molecules of N$_2$, Cl$_2$, I$_2$ and CH within the framework of superstatistics.

Declarations

Author contribution statement

A. N. Ikot, U. S. Okorie: Conceived and designed the analysis; Analyzed and interpreted the data; Wrote the paper.

G. Osobonye, P. O. Amadi, C. O. Edet, M. J. Sitbole, G. J. Rampho, R. Sever: Analyzed and interpreted the data; Wrote the paper.

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