Superstatistics of Diatomic Molecules with the Shifted Deng-Fan Potential Model

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Abstract: In this article, we discuss the thermodynamic properties of the shifted Deng-Fan potential for HCl, CrH, CuLi, and ScF diatomic molecules using the q-deformed superstatistics approach. The partition function is obtained with the help of the generalized Boltzmann factor from the modified Dirac delta distribution. In addition, thermodynamic functions such as entropy, specific heat capacity, free energy, and mean energy are obtained using the partition function. Our results are presented graphically, and the ordinary statistical quantities are recovered when the deformation parameter tends to zero. Our results may be useful in the study of thermal fluctuations in atomic and molecular systems involving short-range interactions.

Keywords: shifted Deng-Fan potential; diatomic molecules; superstatistics.

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1. Introduction

In recent times, investigations of diverse molecular potential models have gained the attention of many researchers [1-5]. This is because studies of the rotational motions of diatomic molecules within a given potential are a theme of enormous value in molecular physics[4,5]. In 1929, Philip Morse proposed an empirical potential with three parameters for studying atomic interaction in diatomic molecules[6]. This potential is given as[6];

\[ V(r) = D_e \left[ 1 - e^{\alpha(r-r_e)} \right]^2 \]  

(1)

where \( D_e \) is dissociation energy, \( r_e \) is the equilibrium internuclear distance, and \( \alpha \) is a parameter controlling the width of the potential, well commonly known as the screening parameter [7,8]. This progress was a remarkable one in quantum mechanics. It has application in physics and chemistry, particularly in areas of molecular spectroscopy and dynamics[9,10]. Because of its importance in the field of molecular physics[11], the Morse potential has been one of the most useful and convenient models [11,12]. As an empirical potential, this potential gives an exceptional description of the interaction between the two atoms. It is also very realistic to describe the interactions close to the surface [13-16].

In another development, Deng and Fan [17] modified the traditional Morse potential model as an improvement to describe diatomic molecule energy spectra and electromagnetic transitions. This potential reads as follows [17]:
where $r_e$ is the molecular bond length, $D_e$ is the dissociation energy, $r$ is the inter-nuclear distance, $\alpha$ the range of the potential well, and $0 < r < \infty$. The potential (2) has the correct physical boundary conditions at the origin and infinity, called a generalized Morse potential [17]. The discovery of this potential was another significant move and aroused the interest of several researchers for many years [18-21].

After discovering the highlighted molecular systems, many researchers have modified and or remodeled this potential with more parameters and wider scope of application. The recently developed potentials amongst many others include Manning-Rosen potential [22], Poschl-Teller potential [23], Rosen-Morse potential [24], and Tietz–Wei (STW) oscillator [25]. The aforementioned potentials have been modified and studied [26-28]. These modified and or improved molecular potentials have received remarkable attention. This is due to their various applications in many fields of Physics and Chemistry. Diatomic molecular potentials have been applied to simulate molecular potential energy curves[29], study bound state problems [30-33], predict thermochemical properties of diatomic molecules[34,35], calculations of molecular vibrational partition function [36,37], and prediction of enthalpy and entropy of gaseous dimers[38,39].

It is recognized that thermodynamics is an arm of physics that offers an analysis of macroscopic physical quantities at the molecular level [40]. It employs probability theory to investigate the activities of a system comprised of a large number of particles. The elucidation of the macroscopic theory of thermodynamics in terms of the more abstract microscopic statistical mechanics is one of the most important triumphs of physics in the early twentieth century [41, 42].

By way of generalizing thermodynamic studies, Beck and Cohen [43] presented the concept of superstatistics where non-equilibrium systems with complex dynamics in stationary states were considered. Superstatistics is defined as a superposition of two different statistics that describe non-equilibrium systems with a stationary state and parameter fluctuations[43,44]. In non-equilibrium statistical mechanics, $\beta = \frac{1}{k_B T}$ is not an inverse temperature, thus being seen as a random variable, but regarded as a constant parameter in the case of equilibrium statistical mechanics [4-47].

Much research has been conducted on the concept of superstatistics both in the equilibrium and non-equilibrium statistical mechanics regime [48-52]. Most recently, Sargolzaeipor et al. [46] introduced superstatistics in quantum mechanics and obtained thermodynamic properties of q-deformed Morse potential using this formalism. Okorie et al. [53] discussed the thermodynamic properties of modified Rosen-Morse potential via the q-deformed superstatistics approaches. In another consideration, Sargolzaeipor et al. [54] used superstatistics to study four important physics problems, and the system's thermodynamic properties were evaluated. $q$-deformed superstatistics of the Schrödinger equation in the commutative and non-commutative spaces with the magnetic field was examined by Sargolzaeipor et al. [55]. Sobhani et al. [56] studied the effects of cosmic-string parameters on the thermodynamic properties of a harmonic oscillator within the framework of ordinary
statistics and the \( q \)-deformed superstatistics approaches. An innate comprehension of superstatistics of systems involving short-range (exponential-type potential) interactions is required; hence further investigations into the thermodynamics of such systems are still necessary. The aim of this work is to extend the studies carried out by Oyewumi \textit{et al}. [57] on thermodynamic properties of a shifted Deng-Fan potential to the superstatistics scheme. These results may be useful to studies of thermal fluctuations in atomic and molecular systems involving short-range interactions. It is interesting to note that no study has been carried in this direction with an exponential-type potential.

2. The Shifted Deng-Fan Oscillator

Sequel to the discovery of the new generalized Morse potential, Hamzavi \textit{et al}.[58] proposed an improved expression for the Deng-Fan oscillator potential[17], it was found out that the shifted Deng-Fan was more Morse-like when compared on a plot than the original Deng-Fan oscillator(see. Fig.1 of Ref[58]).

\[
V(r) = D_1 \left(1 - \frac{b}{\left(e^{a'r} - 1\right)}\right)^2 - D_2
\]

where \( D_e = D_1 = D_2 \). The Morse and the sDF potentials are very close to each other for large values of \( r \) in the regions \( r \approx r_c \) and \( r > r_c \), but they are very different at \( r = 0 \). Further, if the two potentials are deep \( D_2 \downarrow 1 \), they could be well approximated by a harmonic oscillator in the region \( r \approx r_c \) [58]. This behavior encourages us to apply rotation-vibrational energy level expressions derived in the previous work [57] to calculate the partition function and investigate thermodynamic properties for \( HCl, CrH, CuLi \) and ScF using superstatistical mechanics.

This potential has been studied by some authors. Some of which include; Hamzavi \textit{et al}. [58], in a maiden consideration, obtained the energy spectra and wave function of the shifted Deng–Fan oscillator potential of a few diatomic molecules using the Nikiforov-Uvarov method [59] by employing Pekeris-type approximation [60] to deal with the centrifugal term. It was noted that their results were found to be in good agreement with those ones previously obtained by the Morse potential. Oyewumi \textit{et al}. [57] used the Pekeris-type approximation [60] to deal with the centrifugal term. The energy eigenvalues and the shifted Deng–Fan molecular potential wave functions were obtained using the asymptotic iteration method [62,63]. Rotational–vibrational energy eigenvalues were presented as follows [57].

\[
E_{\text{ef}} = \frac{\alpha^2 \hbar^2}{2m} \left[ \frac{2mD_1}{\alpha^2 \hbar^2} (b+1)^2 + \frac{2mD_2}{\alpha^2 \hbar^2} \left( \dfrac{(b+1)}{2} \right)^2 - 1 \right] + \frac{2mD_1}{\alpha^2 \hbar^2} \left( \dfrac{\ell + 1}{2} \right)^2 + \frac{2mb^2D_1}{\alpha^2 \hbar^2} + \frac{2n+1}{2} \right)^2 - 2 \left( \dfrac{\ell + 1}{2} \right)^2 + \frac{2mb^2D_1}{\alpha^2 \hbar^2} + \frac{2n+1}{2} \right) \right) - D_2
\]

where \( n = 0,1,2,3,...,n_{\text{max}} \), \( m \) is the reduced mass of a diatomic molecule, \( \hbar \) denotes the reduced Planck constant, \( n \) and \( \ell \) are the principal and angular momentum quantum numbers, respectively.

Eq.(4) is written in close form as follows;
\[ E_n = \frac{\alpha^2 \hbar^2}{2m} \left\{ A - \frac{B}{2(n+C)} + \frac{n+C}{2} \right\}^2 \]  \hspace{1cm} (5)

\[ A = \frac{2m}{\alpha^2 \hbar^2} \left[ D_1 (b+1)^2 - D_2 \right], \quad B = \frac{2mdD_1}{\alpha^2 \hbar^2} \left[ (b+1)^2 - 1 \right] \]

\[ C = \frac{1}{2} \left[ 1 + \sqrt{1 + 4 \left( \frac{2mb^2 D_1}{\alpha^2 \hbar^2} \right)} \right] \]  \hspace{1cm} (6)

Furthermore, thermodynamic properties such as the vibrational mean \( U \), specific heat \( C \), free energy \( F \), and entropy \( S \) for the pure vibrational state in the classical limit for these energy eigenvalues were also scrutinized. In the present consideration, we evaluate the thermodynamic quantities of this potential in superstatistics in the next sections. Beck and Cohen[43] have proposed various superstatistics models based on different generalizations of the Boltzmann factor. They also demonstrated that all these models display a universal behavior at low energies or low fluctuations [44]. Consequently, in this paper, we focus only on the modified Dirac delta superstatistics, which is a particular model of superstatistics.

3. Thermodynamic Functions for Modified Dirac Delta Distribution

In this section, we introduce the necessary conditions of superstatistics. Superstatistics is a combination of manifold differing statistical models, which scrutinizes the non-linear and non-equilibrium systems. It is noted that this name is chosen because the new statistics represent a kind of "superposition of varying statistics". Superposition of statistical factors can be considered a new attempt to reformulate statistical mechanics [47, 48]. The effective Boltzmann factor of the system can be written as [46, 53]:

\[ B(E) = \int_0^{\infty} e^{-\beta E} f(\beta', \beta) \, d\beta' \]  \hspace{1cm} (7)

where \( f(\beta', \beta) = \delta(\beta' - \beta) \) is a probability density around the global equilibrium inverse temperature \( \beta \). For the random variable \( \beta' \), we assume that the average of these random variables is the same as the global equilibrium inverse temperature, indeed \( \langle \beta' \rangle = \beta \). The generalized Boltzmann factor of superstatistics is given by the Laplace transform of the probability density \( f(\beta', \beta) \). There are infinitely many possibilities for choosing the probability density [53].

As a final point, different choices of \( f(\beta', \beta) \) yield various effective Boltzmann factors \( B(E) \). Sargolzaeipor et al. [54] elucidated some of the well-known distributions such as uniform, two-level, Gamma, lognormal distribution, and F-distribution.

The generalized Boltzmann factor in q-deformed superstatistics is given as[53]:

\[ B_q(E) = e^{-\beta E} \left( 1 + \frac{q}{2} \beta^2 E^2 \right) \]  \hspace{1cm} (9)

where \( q \) is the deformation parameter. Details of Eq. (9) can be found in Appendix A of ref.[64] and references therein.

The Superstatistical partition function is written as[46]
\[ Z = \sum_{n=0}^{\infty} B(E) \]  

(10)

then, the extension of Eq. (8) is written in q-deformed superstatistic as follows [53]:

\[ f(\beta', \beta) = a\delta(\beta' - \beta) + b\beta' \frac{\partial}{\partial \beta'} \left[ \delta(\beta' - \beta) \right] + c\beta'^2 \frac{\partial^2}{\partial \beta'^2} \delta(\beta' - \beta). \]  

(11)

where \( a, b \) and \( c \) are constants determined by requiring \( f(\beta', \beta) \) to conform to certain physical conditions [46]. Such conditions lead to the values

\[ a = 1 + q, \quad b = 2q \quad \text{and} \quad c = \frac{1}{2} q \]  

(12)

for the constants, where \( q \) is a deformation parameter.

The partition function for the modified Dirac delta distribution has the following form [53]:

\[ Z_q = \int_{0}^{\infty} B_q(E) \, dn \]  

(13)

On substituting eq.(5) into eq.(13), the partition function \( Z_q \) in q-deformed superstatistics for the shifted Deng-Fan potential (3) is given by;

\[ Z_q = \int_{0}^{\infty} \left[ e^{-\frac{\alpha^2h^2}{2m} \left( A - \frac{B}{n+C} + \frac{n+C}{2} \right)^2} \right] \left[ 1 + \frac{q}{2} \beta^2 \left( A - \frac{B}{n+C} + \frac{n+C}{2} \right) \right]^2 \, dn \]  

(14)

Eq.(14) is rewritten as;

\[ Z_q = \int_{0}^{\infty} e^{-\frac{\alpha^2h^2}{2m} \left( \lambda A - \lambda \beta^2 \right)^2} \left[ 1 + \frac{q}{2} \beta^2 \left( \lambda A - \lambda \beta^2 \right) \right] \left[ 1 + \frac{y}{\sqrt{y^2 - B}} \right] \, dy \]  

(15)

where \( \lambda = \frac{\alpha^2h^2}{2m} \), \( y = \frac{B}{2(n+C)} + \frac{n+C}{2} \) and \( y_1 = \frac{B}{2C} + \frac{C}{2} \)  

(16)

The integral in the right-hand side of Eq. (15) is thereafter evaluated with Mathematica software. Thus, we obtain the following expression of the vibrational partition function for a diatomic molecule represented by the shifted Deng-Fan potential energy model,

\[ \frac{1}{16(-\beta \lambda)^{\frac{3}{2}}} e^{-A\beta \lambda} \beta^{\frac{3}{2}} \lambda^{\frac{3}{2}} \left( \sqrt{\beta} \sqrt{\lambda} - 2e^{\gamma_{\beta \lambda}} \sqrt{-\beta \lambda} \left( 2y_1\lambda + 2y_1^3\Omega + 3 + 4A\beta \lambda \right) + \Omega \left( 3 + 2(-2A + B) \beta \lambda \right) \right) \]  

(17)

where

\[ \Xi = 8 + q \left( 3 + 4\lambda (A - B) \beta \lambda (1 + (A - B) \beta \lambda) \right) \]

\[ \Sigma = 8 + q \left( 3 + 4A\beta \lambda (1 + A \beta \lambda) \right) \]

\[ \Omega = \sqrt{B + y_1^2} \]  

(18)
Other thermodynamic functions such as Helmholtz free energy, \( F_S(\beta) \), entropy, \( S_S(\beta) \), internal energy, \( U_S(\beta) \), and specific heat, \( C_S(\beta) \), functions can be obtained from the partition function(17) with the aid of the following expressions[34]

\[
F_S(\beta) = -\frac{1}{\beta} \ln Z(\beta)
\]

\[
S_S(\beta) = -k_\beta \frac{\partial F(\beta)}{\partial \beta}
\]

\[
U_S(\beta) = -\frac{\partial (\ln Z(\beta))}{\partial \beta}
\]

\[
C_S = k_\beta \frac{\partial U(\beta)}{\partial \beta}
\]

We have obtained the thermodynamic properties via the q-deformed superstatistics approach in terms of two mathematical functions, namely: the Dawson function and the imaginary error function. The Dawson function or Dawson integral in mathematics is denoted as [65]

\[
F(x) = e^{-x^2} \int_0^x e^{x^2} dy = \frac{\sqrt{\pi}}{2} e^{-x^2} \text{erfi}(x).
\]

Thus the Dawson's integral is implemented in Mathematica as \( \text{DawsonF}(x) \). On the other hand, the imaginary error function is an entire function defined by

\[
\text{Erfi}(x) = i \text{Erf}(ix)
\]

where \( \text{erf} \) denotes the error function (also called the Gauss error function) is a special function (non-elementary) of sigmoid shape, which occurs in probability, statistics, and partial differential equations. In mathematics, the error function can be denoted as [65]

\[
\text{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2} dt.
\]

The imaginary error function is implemented in Mathematica as \( \text{Erfi}(x) \).

4. Results and Discussion

In our calculations, we have used spectroscopic parameters shown in Table 1 and the conversions: 1 \( \text{amu} = 931.494028 \text{ MeV}/c^2 \), 1 \( \text{cm}^{-1} = 1.239841875 \times 10^{-4} \text{ eV} \) and

\[
f_c = 1973.29 \text{ eV} \text{Å} [30,32].
\]

| Molecules | \( D_e (\text{eV}) = D_1 = D_2 \) | \( r_e (\text{Å}) \) | \( \alpha (\text{Å}^{-1}) \) | \( \mu (\text{a.m.u}) \) |
|-----------|---------------------------------|----------------|----------------|-----------------|
| HCl [57]  | 4.619031                        | 1.2746         | 1.8677         | 0.980105        |
| CrH [57]  | 2.13                            | 1.694          | 1.52179        | 0.988976        |
| CuLi [57] | 1.74                            | 2.31           | 1.00818        | 6.259494        |
| ScF [57]  | 5.85                            | 1.794          | 1.46102        | 13.35894        |
The variation of the thermodynamic functions with $\beta$ the modified Dirac delta distribution and different diatomic molecules are shown in Figures 1-5. We first obtained a high-temperature partition function and then obtained thermodynamic functions, such as free energy $F(\beta)$, mean vibrational energy $U(\beta)$, specific heat capacity $C(\beta)$, and entropy $S(\beta)$ with the application to some recognized diatomic molecules (for HCl, CrH, CuLi and ScF).

4.1. Partition function.

From the variation of the thermodynamic properties obtained, we discovered that in Fig. 1, for all the diatomic molecules except CuLi, $Z(\beta)$ monotonically decreases with increasing $\beta$ for $q = 0, 0.4, 0.8$ and 1. In the case of CuLi, $Z(\beta)$ increases with increasing $\beta$.

![Graphs showing the variation of the thermodynamic functions with $\beta$ for different molecules.]

**Figure 1.** Vibrational partition function $Z$ of HCl, CrH, CuLi and ScF diatomic molecules as a function of $\beta$ for different $q$.

4.2. Free energy.

In Figure 2, we examine the behavior of the mean free energy as it varies in the region $0 < \beta < 0.08$. It is observed that $F(\beta)$ it decreases monotonically as $\beta$ it increases but increases as the deformation ($q$) increases for all diatomic molecules considered.
Figure 2. Vibrational mean free energy $F(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$.

Figure 3. Vibrational entropy $S(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$. 
4.3. Entropy.

Figure 3 shows the variation of the vibrational entropy $S(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$. It is clearly revealed that entropy $S(\beta)$ of molecules considered at the start decrease with $\beta$ and lastly increases monotonically with increasing $\beta$ except when $q = 0$. We observed a continuous monotonic decrease. The curves for different deformation values show a uniform convergence in the region of low $\beta$ but diverges as $\beta$ increases. More so, it was noted that the entropy of the system increased as the deformation parameter increases. It could be physically said that the deformation increases the disorderliness in the quantum system.

4.4. Vibrational mean energy.

Figure 4 explicitly shows the mean vibrational energy $U(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$. We examined the variation of the mean energy in the region $0 < \beta < 0.05$. In Fig. 4, we found that $U(\beta)$ monotonically increases with $\beta$ for $HCl$ and $ScF$ but linearly increases with $\beta$ for $CuLi$ and $CrH$. However, in Fig. 4, it is also noted that $U(\beta)$ increases with increasing value of the deformation parameter.

Figure 4: Vibrational mean energy $U(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$.
4.5. Vibrational specific heat capacity.

Figure 5 shows the variation of the vibrational specific heat capacity $C(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$. The specific heat increases monotonically with increasing $\beta$ and $q$. We state here that ordinary statistical quantities are recovered when the deformation parameter tends to zero.

![Figure 5: Vibrational specific heat capacity $C(\beta)$ of $HCl$, $CrH$, $CuLi$ and $ScF$ diatomic molecules as a function of $\beta$ for different $q$.](image)

5. Conclusions

In this study, the energy spectra obtained for shifted Deng-Fan potential have been adopted to calculate the partition function with the help of the generalized Boltzmann factor for the modified Dirac delta distribution. Other thermodynamic functions such as free energy $F(\beta)$, mean energy $U(\beta)$, entropy $S(\beta)$, and specific heat capacity $C(\beta)$ have been obtained via the superstatistics approach. The variations of these thermodynamic functions with $\beta$ and $q$ in the absence and presence of the deformation parameters have been displayed graphically and discussed extensively for selected diatomic molecules. Specifically, interesting demonstrations are observed in the presence of the deformation parameter. Also, our results agree with the ordinary statistics in the absence of the deformation parameter ($q = 0$).

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Collins Edet dedicates this work to his late father (Mr. Okon Edet Udo).

Conflicts of Interest

The authors declare no conflict of interest.

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