**Super-statistical description of thermodynamic properties of Diatomic molecules with Deng-Fan-Eckart Oscillator**

**C. O. EDET\* and A. N. IKOT**

 ***Theoretical Physics Group, Department of Physics, University of Port Harcourt.***

*Corresponding author e-mail address:* [*collinsokonedet@gmail.com*](collinsokonedet%40gmail.com)

**Abstract**

In this study, we carry out a superstatistical analysis of diatomic molecules using the Deng-Fan-Eckart Oscillator with the Dirac-delta distribution. The energy equation of the system is first obtained by solving the Schrodinger equation via the exact quantisation rule (EQR) and the numerical eigenvalue compared with literature for validity. With the analytic energy expression and some algebraic manipulations, the partition function is obtained. The partition function is then used to obtain other thermodynamic functions in terms of the deformation parameter “q”. By way of showing application, we extend this concept to the case of diatomic molecules.

**Keywords**: Schrodinger equation (SE); Exact Quantisation Rule (EQR); Deng-Fan-Eckart potential; Dirac-Delta distribution function; partition function; superstatistics; diatomic molecules

**1. Introduction**

The Deng-Fan-Eckart potential is a newly proposed model for studying atomic interactions in diatomic molecules [1]. This model suites very well for the simplified description of diatomic molecules because it behaves exactly in the same fashion like the traditional Morse potential [2]. This potential result from an attempt to simulate the interaction in two-atom molecules. Two-atom molecules have been subject of major research interest in the last ten years [3-6]. This potential model is given as;

 (1)

where  is the molecular bond length, is the dissociation energy,  is the inter-nuclear distance, the range of the potential well, and  are the potential strengths .

A good grasp of the macroscopic theory of thermodynamics in terms abstract microscopic statistical mechanics is one of the most crucial accomplishments of physics in the twentieth century [3]. In a bid to take a broad view of thermodynamic studies, the concept of superstatistics was presented by Beck and Cohen [4] to study “non-equilibrium” systems with complex dynamics in stationary states. This generalized thermal description of a system can take account of the fluctuations in temperature and several other intensive observables and thus, the conventional Boltzmann-Gibbs formulation (BGF) cannot be used. However, this requires that an all-encompassing formalism to describe situations out of the thermodynamic equilibrium is employed. Its applications in several fields need not be overemphasized.

The major goal of this paper is to convey this superstatistics concept to the case of two-atom molecules, we will calculate the superstatistical properties of the Deng-Fan-Eckart oscillator. The inspiration behind this action are in two-folds: to the best of our, this study has not been well treated and discussed in the literature. Moreover, superstatistics of systems involving short range (exponential-type potential) interactions is required since it lacks greatly in literature and the application to selected homonuclear and heteronuclear has not been treated: this encourages us to extend our study to the case of diatomic molecules, it should be noted here that the molecules are selected based on their wide range of applications (details will be shown in the subsequent section)

**2. Results**

The partition function is obtained as follows;

 (2)

This partition function is then used to obtain the specific heat capacity, free energy, entropy and internal energy of the diatomic molecules.

Several interesting results have been obtained. However, the specific heat capacity revealed a very interesting behavior even when Boltzmann-Gibbs statistics is recovered.

Fig. 1 shows the variation of the specific heat capacity  of and  diatomic molecules as a function of  for different . The specific heat increases with increasing  and  for . For and  a wave-like variation pattern is observed as  increases. We state here that ordinary statistical quantities is recovered when the deformation parameter  tends to zero. In the functional form, translational and rotational parts of the specific heat capacity of these molecules are usually considered but the present study, we are only considering the vibrational partition function which was used to calculate vibrational specific heat capacity. The peaks observed can be attributed to anomaly which makes it deviate from Dulong Petit law and Schokky anomaly is observed [5]. The temperature-dependence of the rotational contribution to the heat capacity of the molecules shows a *Schottky anomaly*: whereas for many systems the heat capacity can be expected to increase with increasing temperature, for these molecules there is a temperature range within which it reaches a maximum before *decreasing*. Only at higher temperatures it may revert to "conventional" behaviour.



**Figure 1**: Vibrational specific heat capacity of and  diatomic molecules as a function of  for different.

**3. References**

[1] C. O. Edet, U. S. Okorie, G. Osobonye, A. N. Ikot, G. J. Rampho and R. Sever. J. Math. Chem. **58** (2020) 989

[2] P. M. Morse, Phys. Rev. **34** (1929) 57.

[3] P.T. Landsberg, Thermodynamics and Statistical Mechanics, Dover, New York (1991).

[4] C. Beck, E. G. D. Cohen, Physica A **322** (2003) 267.

[5] J. D. Castano-Yepes, C. F. Ramirez-Gutierrez H. , Correa-Gallego, & E. A. Gómez. Physica E **103** (2018) 464-470.