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Energy eigenvalue and thermodynamic properties for Deng-Fan screening potential

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Abstract

This research aims to study energy eigenvalues and thermodynamic properties associated with the screening Deng-Fan potential in diatomic molecules. For this authors developed a theoretical model for energy eigenvalues and investigated the nature of energy eigenvalues for H_2*,* Cl_2*, and HCl, considering screening parameters and bond dissociation energy. The study involves detailed exploration, numerical simulations, and analysis to understand the relationship between screening parameters and energy levels. The bond dissociation energy affects the energy levels, providing insights into bond formation and breaking processes. The thermodynamic properties, partition function decreases exponentially within 0.005 screening range for* H_2*,* Cl_2*, and HCl. Entropy drops exponentially due to screening,* Cl_2 *has higher entropy due to electron density and screening effects. Mean free energy stays constant,* Cl_2 *is higher due to electron density and screening. Specific heat capacity is zero, indicating electrons lack measurable heat capacity unlike macroscopic objects. The findings are expected to contribute significantly to molecular physics and quantum mechanics, enhancing our understanding of molecular bonding and reactivity with potential applications in diverse physical systems and technologies.*

Keywords: Energy eigenvalue, thermodynamic properties, Deng-Fan Potential, diatomic molecules, screening parameter. .

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1 Introduction

The Eckart potential, which was first presented by Eckart in 1930, is a diatomic in nature molecular model that is crucial to both physics as well as chemical physics. Because of its importance, many academics have looked at bound condition solutions for the related wave equations. Because of its applicability in physics, analytical methods for resolving these bound state issues have attracted a lot of interest over time. These techniques make it easier to derive analytic eigen-solutions for relativistic as well as non-relativistic wave equations, which is essential for comprehending the behaviour of quantum mechanical systems. The Heun function approach, Laplace transformation, ansatz solution, super-symmetric quantum mechanics (SUSYQM), exact quantization methods, series expansion, Nikiforov-Uvarov method (NU) [1], Asymptotic iterative method (AIM) [2], and others are frequently used approaches. The latter is especially useful for studying solvable quantum systems that were previously unsolvable, such as the Konwent potential, rigid rotor problem, Mathieu potential, or sextic-type problem [3].

A quick and easy way to forecast how thermodynamic functions of a desired chemical process will change is to use the thermodynamic characteristics of gaseous compounds. In both the practical and theoretical aspects of material processing, however, understanding thermodynamic parameters such as enthalpy (H), entropy (S), as well as Gibbs free energy (G) for the chemical species is always the main goal. More research is currently being done on diatomic systems for a variety of uses in several domains, including phase transitions, adsorption, dissolution, and diverse chemical processes [4]. Partition functions are used to thermodynamic properties (total energy, free energy, entropy, specific heat capacity, entropy, etc.). The partition function is defined as

$$Z = \sum g_i e^{-\beta \epsilon_i} \quad \text{with} \quad \beta = \frac{1}{k_B T} \tag{1}$$

Numerous potential functions have been used to model interatomic interactions in diatomic molecular systems. Depending on the type of interaction occurring within the system, these possible functions change. The Deng-Fan potential, which is obtained by taking the Manning-Rosen function representing the vibration potential energy into consideration, is an improvement on the potential previously stated. Described by Deng and Fan, the Generalised Morse potential (GMP) is associated with the Manning-Rosen potential referred to as the Eckart potential by,

$$V(r) = D_e \left[1 - \frac{b}{e^{\eta r} - 1}\right]^2 \tag{2}$$

where r_e is the equilibrium bond length, $b = e^{\eta r_e} - 1$; $0 \leq r < \infty$, D_e is the dissociation energy, η is the screening parameter that determines the well's breadth, and r is the internuclear distance. These shortcomings inspired Deng and Fan to develop a brand-new, enhanced potential known as the Deng-Fan, or generalised Morse potential. Applying the Hulthen-Kratzer potential (HKP) model with magnetic as well as AB fields, Edet and Ikot investigated the N_2, I_2, CO, NO, and HCl diatomic molecules. Different approaches are presented [5] as well as utilised in quantum mechanics to solve the wave equations using a specific specified solvable potential in order to compute the energy eigenvalue. The power series definition of the hypergeometric function approach is applied for $|z| < 1$.

$$\begin{aligned} {}_2F_1(a,b;c;z) &= \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!} \\ &= 1 + \frac{ab}{c}\frac{z}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \dots \end{aligned} \tag{3}$$

Euler's Hypergeometric differential problem has a solution known as the Hypergeometric function [6].

$$z(z-1)\frac{d^2\omega}{dz^2} + [c - (a+b+1))]\frac{d\omega}{dz} - ab\omega = 0 \tag{4}$$

which has three regular singular points: 0,1 and ∞.

2 Literature Review

The Deng-Fan and Morse potentials to deal with the X-H expanding motion in tiny molecules. Similar to what happens to the Morse potential, the Deng-Fan potential displays the proper asymptotic behaviour when the interatomic distance approaches zero. The Deng-Fan potential does not perform considerably better than the Morse potential in forecasting observed energy levels as well as intensities in the examined cases, despite its accurate asymptotic behaviour [7]. The Nikiforov-Uvarov technique [8] was used to generate bound state solutions for the Deng-Fan molecular potential for diatomic molecule (HCl, LiH, H2, ScH, TiH, VH, CrH, CuLi, TiC, NiC, ScN, as well as ScF). Recently, Ekwevugbe [9] used the WKB approximation to obtain a nonrelativistic energy the spectrum corresponding to the Deng-Fan oscillator. It is well known that the Deng-Fan potential (DFP) is a very empirical method for accurately representing the electromagnetic transitions and energy spectrum of diatomic molecules (DM). Deng and Fan first proposed the DFP in 1957 as a way to take into consideration the conditions at the boundaries at both the origin and infinity of the ro-vibrational spectrum of DM, also known as the generalised Morse potential [10]. Moreover, this potential can be used to analyse and extract the energy spectra of diatomic molecular systems. Notably, Dong and Gu were able to solve the Schrödinger equation with the Deng-Fan molecular potential in 2008 [11].

In examining atomic interactions inside diatomic molecules, the Deng–Fan–Eckart potential assists the Morse potential by employing an enhanced Pekeris-type approximation to manage the centrifugal term, bound-state solution for the radial Schrödinger equation. The energy equation allows the Poisson summation method to be used to evaluate the thermodynamic properties of specific diatomic molecules (H_2, CO, ScN, and ScF). By modifying potential parameters, calculating numerical eigenvalues, and exhibiting outstanding agreement with alternative techniques, the accuracy is confirmed [12]. Using the ordinary differential technique and specific characteristics of Gaussian hypergeometric functions, precise analytical formulations for regular as well as irregular solution in all partial waves are constructed. For a few lower partial waves, the function derived from the irregular solution's near-origin behaviour is suitably employed to calculate scattering phase changes for the systems of protons and deuteron neutrons. Although we did not employ the screening effect, our findings are in good accord with the experimental data [13].

2.1 Research gap

For the purpose of describing diatomic molecular vibrations, Deng and Fan devised the molecular Deng-Fan potential, which is a modified version of their Morse potential. Despite its application in various contexts and its well-studied nature, there exists a research gap regarding the analysis of energy eigenvalues linked to the Deng-Fan screening potential. While extensive research has explored Deng-Fan potentials, including their theoretical framework and applications, the specific investigation into energy eigenvalues within the realm of Deng-Fan screening potential remains unexplored. The prevailing literature has focused on the effects of Deng-Fan potentials on interactions, scattering, and related phenomena. However, the crucial aspect of quantifying and analyzing energy eigenvalues resulting from the integration of Deng-Fan screening potential into quantum mechanical systems has not been adequately addressed. This research seeks to address this gap by delving into the energy eigenvalues linked to the Deng-Fan screening potential. Through a comprehensive theoretical and computational analysis, the study aims to provide insights into how the Deng-Fan screening potential influences energy levels within quantum mechanical systems. This analysis is vital for a broader understanding of the implications of Deng-Fan potentials and their effects on particle interactions and system dynamics.

2.2 Significant of work

This research holds significance by addressing a gap in the analysis of energy eigenvalues associated with the Deng-Fan screening potential. Despite the well-studied nature of Deng-Fan potentials, their specific impact on energy levels within quantum systems remains unexplored. This study's comprehensive exploration provides insights into this crucial aspect, enhancing our understanding of how the Deng-Fan screening potential influences particle behavior. By bridging this gap, the research contributes to a more comprehensive grasp of particle interactions, offering potential applications in diverse fields where accurate energy predictions are vital, from molecular dynamics to quantum chemistry.

3 Methods and Materials

3.1 Theoretical formulation

Using the aforementioned analytical techniques, the Schrödinger equation (SE) can be examined for various quantum-mechanical phenomena. The analytical solutions of this equation in the presence of a physical potential are crucial to our comprehension of the fundamentals of a quantum system. This is due to the fact that the eigenvalues as well as eigenfunctions provide important details about the quantum system that is being studied. Nonetheless, in certain situations—the Coulomb potential, for instance—it is possible to obtain the precise bound state solutions of the SE of several of these potentials. When the random angular momentum quantum number l does not correspond to equal to zero, the SE can be solved using an acceptable approximation approach such as Pekeris or Greene as well as Aldrich, among others, to achieve the approximate solutions [12]. The radial form of schrodinger wave equation (SE) is

$$\psi^{''}(r)+\frac{2m}{2}\left[E_{nl}-V(r)-\frac{l(l+1)^2}{2mr^2}\right]\psi(r)=0 \quad (5)$$

Here $\psi(r)$ is radial wave function, E_{nl} is energy eigen value, $V(r)$ is potential strength, m is reduce mass, l is orbital quantum number using centrifugal approximation to get rid of centrifugal approximation [14]; (Greene and Aldrich approximation)

$$\frac{1}{r^2}=\frac{\eta^2}{(1-e^{-\eta r})^2} \quad (6)$$

The Deng–Fan potential physically represents the realistic interaction between two atoms in a diatomic molecule, showing strong repulsion at short interatomic distances, stable bonding at the equilibrium distance, and a gradual weakening of attraction as the atoms move farther apart until the bond dissociates. It effectively captures the balance between attractive and repulsive forces, providing a more accurate description of molecular vibration and bond behavior than simpler potentials like the Morse potential. Now, using Deng- fan potential [15] by modified to Deng-fan potential as shown in equation (7) is given by

$$V(r)=D_e\left(1-\frac{b}{e^{\eta r}-1}\right)^2 e^{-\eta r} \quad (7)$$

D_e is energy of dissociation, η is screening parameter(width of well), $b = e^{\eta r} - 1$, r_e is equilibrium bond length , r is the inter-nuclear distance. The modification of the Deng–Fan potential, as given in equation (7), was necessary to include the effect of the screening parameter (η), which represents the influence of an external environment on the interaction between two atoms in a molecule. This modified form allows the potential to account for how the molecular bond and interaction energy change when an external screening field is introduced, such as in a plasma or thermally active medium. The original Deng–Fan potential does not consider such screening effects; therefore, this modification provides a more realistic description of the screened molecular interaction. Moreover, since no previous research has examined this specific screened form, it offers a novel approach to understanding the nature of molecular interactions under external screening conditions.

$$\psi''(z) + \frac{\psi'(z)}{z} + \Bigg[\frac{2mE_{nl}}{{}^2\eta^2 z^2} - \frac{2mD_e}{{}^2\eta^2 z} + \frac{4mbD_e}{{}^2\eta^2 z(1-z)} - \frac{2mb^2D_e}{{}^2\eta^2 z(1-z)^2} - \frac{l(l+1)}{z^2(1-z)^2}\Bigg]\psi(z) = 0 \tag{8}$$

Let, $z = e^{-\eta r}$ and hence $z = \frac{1}{e^{\eta r}} => e^{\eta r} = \frac{1}{z}$, So, $\frac{\partial z}{\partial r} = \frac{\partial\left(e^{-\eta r}\right)}{\partial r} = -\eta e^{-\eta r} = -\eta z$, $\frac{\partial \psi(r)}{\partial r} = \frac{\partial \psi(z)}{\partial z}\frac{\partial z}{\partial r} = \frac{\partial \psi(z)}{\partial z}\left(-\eta e^{-\eta r}\right) = -\psi'(z)\eta e^{-\eta r} = -\eta\psi'(z)z$, $\psi^{''}(r) = \eta^2 z^2 \psi^{''}(z) + \eta^2 z\psi'(z)$ and on substituting the value of exponential in term of z from equation (**??**) and solving we get

$$\psi''(z) + \frac{\psi'(z)}{z} + \Bigg[\frac{2mE_{nl}}{{}^2\eta^2 z^2} - \frac{2mD_e}{{}^2\eta^2 z} + \frac{4mbD_e}{{}^2\eta^2 z(1-z)} - \frac{2mb^2D_e}{{}^2\eta^2 z(1-z)^2} - \frac{l(l+1)}{z^2(1-z)^2}\Bigg]\psi(z) = 0 \tag{9}$$

Now multiply by $z(1-z)$ on both side of equation (9) we get,

$$\psi''(z)z(1-z) + \psi'(z)(1-z) + \Bigg[\frac{2mE_{nl}(1-z)}{{}^2\eta^2 z} - \frac{2mD_e(1-z)}{{}^2\eta^2} + \frac{4mbD_e}{{}^2\eta^2} - \frac{2mb^2D_e}{{}^2\eta^2(1-z)} - \frac{l(l+1)}{z(1-z)}\Bigg]\psi(z) \tag{10}$$

Assuming, $\frac{2mE_{nl}}{{}^2\eta^2} = -\epsilon^2$, $\frac{2mD_e}{{}^2\eta^2} = \sigma$, $\frac{4mbD_e}{{}^2\eta^2} = \delta$, $\frac{2mb^2D_e}{{}^2\eta^2} = \alpha$, $l(l+1) = \lambda$ and putting this assumption of equation (10) we get,

$$\psi^{''}(z)z(1-z) + \psi'(z)(1-z) + \Bigg[\frac{-\epsilon^2(1-z)}{z} - \sigma(1-z) + \delta - \frac{\alpha}{(1-z)} - \frac{\lambda}{z(1-z)}\Bigg]\psi(z) = 0 \tag{11}$$

The behavior of equation (11) asymptotically at $r \to \infty$ ($z \to 0$) and $r \to 0$ ($z \to 1$) is now shown. The newly developed function $f(z)$ will now be introduced as

$$\psi(z) = z^{\mu}(1-z)^{\phi} f(z) \tag{12}$$

Differentiating equation (10) we have $\psi'(z) = \mu z^{\mu-1}(1-z)^{\phi} f(z) - z^{\mu}\phi(1-z)^{\phi-1} f(z) + z^{\mu}(1-z)^{\phi} f'(z)$ and $\psi^{''}(z) = z^{\mu}(1-z)^{\phi} f^{''}(z) + 2\mu z^{\mu-1}(1-z)^{\phi} f'(z) - 2\phi z^{\mu}(1-z)^{\phi-1} f'(z) - 2\phi\mu z^{\mu-1}(1-z)^{\phi-1} f(z) + \phi z^{\mu}(\phi-1)(1-z)^{\phi-2} f(z) + \mu(\mu-1)z^{\mu-2}(1-z)^{\phi} f(z)$ on substituting these value with the help of equation (12) in (11) we get on solving,

$$\begin{aligned} z(1-z)f''(z) &+ \left[(1+2\mu) - (2\mu+2\phi+1)z\right] f'(z) \\ &- \left[2\mu\phi - \frac{\phi^2 z}{1-z} + \frac{\phi z}{1-z} - \frac{\mu^2}{z} + \mu^2 + \phi\right] f(z) \\ &+ \left[-\frac{\epsilon^2(1-z)}{z} - \sigma(1-z) + \delta - \frac{\alpha z^2}{1-z} - \frac{\lambda}{z(1-z)}\right] f(z) = 0 \end{aligned} \tag{13}$$

Multiplying by minus sign in second last term,

$$\begin{aligned} z(1-z)f''(z) &+ \left[(1+2\mu) - (2\mu+2\phi+1)z\right] f'(z) \\ &+ \left[-2\mu\phi + \frac{\phi^2 z}{1-z} - \frac{\phi z}{1-z} + \frac{\mu^2}{z} - \mu^2 - \phi\right] f(z) \\ &+ \left[-\frac{\epsilon^2(1-z)}{z} - \sigma(1-z) + \delta - \frac{\alpha z^2}{1-z} - \frac{\lambda}{z(1-z)}\right] f(z) = 0 \end{aligned} \tag{14}$$

Arranging two last term, $\frac{\phi^2 z}{(1-z)} - \frac{\phi^2}{(1-z)} = \frac{\phi^2 z - \phi^2}{(1-z)} = \frac{\phi^2(z-1)}{(1-z)} = -\frac{\phi^2(1-z)}{(1-z)} = -\phi^2 => \frac{\phi^2 z}{(1-z)} = -\phi^2 + \frac{\phi^2}{(1-z)}$ of equation (14) and solving we get

$$\begin{aligned} z(1-z)f''(z) &+ \left[(1+2\mu) - (2\mu+2\phi+1)z\right] f'(z) \\ &- \left[(\mu+\phi)^2 + (\mu+\phi) + \lambda\right] f(z) \\ &+ \Bigg[\frac{\epsilon^2}{z} + \epsilon^2 - \sigma + \sigma z + \delta - \frac{\alpha z^2}{1-z} - \\ &\frac{\lambda}{z} - \frac{\lambda}{1-z} + \frac{\phi^2}{1-z} + \frac{\mu^2}{z} + \phi \\ &- \frac{\phi}{1-z} + \lambda + \mu\Bigg] f(z) = 0 \end{aligned} \tag{15}$$

Also using relation $\frac{\lambda}{z}+\frac{\lambda}{(1-z)}=\frac{\lambda-\lambda z+\lambda z}{z(1-z)}=\frac{\lambda}{z(1-z)}$ and $\phi-\frac{\phi}{(1-z)}=\frac{\phi(1-z)-\phi}{(1-z)}=\frac{\phi-\phi z-\phi}{(1-z)}=-\frac{\phi z}{(1-z)}$ in equation (15) and solving we get,

$$\begin{aligned} z(1-z)f^{''}(z)+\left[(1+2\mu)-(2\mu+2\phi+1)z\right]f'(z) \\ -\left[(\mu+\phi)^2+(\mu+\phi)+\lambda\right]f(z) \\ +\left[\left(\frac{-\epsilon^2+\mu^2-\lambda}{z}\right)+\sigma z+(\epsilon^2\right. \\ -\sigma+\delta+\phi+\lambda+\mu) \\ \left.+\left(\frac{-\alpha z^2+\phi^2-\phi}{(1-z)}\right)\right]=0 \end{aligned} \tag{16}$$

Equation (16) is gaussian hypergeometric differential equation [6] when square term bracket is equal to zero. On equating to zero the square bracket term, we can also obtained the required value as $\sigma=0$, $-\epsilon^2+\mu^2 \Rightarrow \epsilon^2=\mu^2$, $\epsilon^2-\sigma+\delta+\phi+\lambda+\mu=0 \Rightarrow \mu^2+\delta+\phi+\lambda+\mu=0$ and $\mu^2+\delta+\phi+\lambda+\mu=0 \Rightarrow \phi=-(\mu^2+\delta+\lambda)$. Also, as third term of equation (16) can be written as,

$$\begin{aligned} &(\mu+\phi)^2+(\mu+\phi)+\lambda \\ &=\mu^2+\phi^2+2\mu\phi+\mu+\phi+\lambda \\ &=\mu^2+\phi^2+\frac{1}{4}+2\mu\phi+\phi+\mu-\frac{1}{4}+\lambda \\ &=\left(\mu+\phi+\frac{1}{2}\right)^2-\left(\sqrt{\frac{1}{4}-\lambda}\right)^2 \\ &=\left(\mu+\phi+\frac{1}{2}+\sqrt{\frac{1}{4}-\lambda}\right)\times \\ &\left(\mu+\phi+\frac{1}{2}-\sqrt{\frac{1}{4}-\lambda}\right) \end{aligned} \tag{17}$$

Now the from equation (17) and equation (16), the equation (16) become

$$\begin{aligned} z(1-z)f^{''}(z)+\left[(1+2\mu)-(2\mu+2\phi+1)z\right]f'(z) \\ -\left[\left(\mu+\phi+\frac{1}{2}+\sqrt{\frac{1}{4}-\lambda}\right)\right. \\ \left.\left(\mu+\phi+\frac{1}{2}-\sqrt{\frac{1}{4}-\lambda}\right)\right]f(z)=0 \end{aligned} \tag{18}$$

Now comparing equation (18) and (4) we have, $a=\left(\mu+\phi+\frac{1}{2}+\sqrt{\frac{1}{4}-\lambda}\right)$, $b=\left(\mu+\phi+\frac{1}{2}-\sqrt{\frac{1}{4}-\lambda}\right)$ and $c=1+2\mu$. Now, by replacing the given value of f(z) in equation (12) with these parameters, we obtain

$$\begin{aligned} \psi(z)=z^{\mu}(1-z)^{\phi}\,{}_2F_1\left[\mu+\phi+\frac{1}{2}+\sqrt{\frac{1}{4}-\lambda},\right. \\ \left.\mu+\phi+\frac{1}{2}-\sqrt{\frac{1}{4}-\lambda};1+2\mu;z\right] \end{aligned} \tag{19}$$

A polynomial equation with $n=0,1,2,3,\ldots,n_{\max}$ integer will be formed from the hypergeometric function $f(Z)$ if a, b, and c are equal to the negative of the integer (n). Quantum condition application [?] $a=-n$, we have,

$$\mu+\phi+\frac{1}{2}+\sqrt{\frac{1}{4}-\lambda}=-n \tag{20}$$

Assuming $\frac{1}{2}+\sqrt{\frac{1}{4}-\lambda}=\xi$, we obtained, $\mu=-n-\phi-\xi$, also we have $\phi=-(\mu^2+\delta+\lambda)$. Therefore, on similifcation we get $\mu^2-\mu+\delta+\lambda-\xi-n=0$ and comparing with quadratic Equation, $a_1x^2+b_1x+c_1=0$. we get $a_1=1$, $b_1=-1$, $c_1=\delta+\lambda-\xi-n$, and solving for root we get $\mu=\frac{1\pm\sqrt{1-4(\delta+\lambda-\xi-n)}}{2}$. The Equation is valid only when $(1-4(\delta+\lambda-\xi-n))$ is perfect square .i.e. $1-4(\delta+\lambda-\xi-n)=\chi^2$. And hence $\mu=\frac{1\pm\chi}{2}$. On taking positive and negative, we get $\mu_+=\frac{1+\chi}{2}$ and, $\mu_-=\frac{1-\chi}{2}$. Squaring both side we get, $\mu_+^2=\frac{1+2\chi+\chi^2}{4}$ and, $\mu_+^2=\frac{1-2\chi+\chi^2}{4}$. Since we have $\epsilon^2=\mu^2$, and now substituting value of μ in above we get

$$\begin{aligned} \epsilon^2=\frac{1}{4}\Big[1+2\left\{1-4(\delta+\lambda-\xi-n)\right\}+ \\ \left\{1-4(\delta+\lambda-\xi-n)\right\}^2\Big] \end{aligned} \tag{21}$$

Substituting the value in $\frac{2mE_{nl}}{{}^2\eta^2}=-\epsilon^2$ we have from equation (19) as

$$\begin{aligned} E_{nl}=-\frac{{}^2\eta^2}{8m}\Big[1+2\left\{1-4(\delta+\lambda-\xi-n)\right\}+ \\ \left\{1-4(\delta+\lambda-\xi-n)\right\}^2\Big] \end{aligned} \tag{22}$$

3.2 Thermodynamic Properties

For this work we take positive value and hence thermodynamic Properties [?] is obtained as

$$Z_{vibration}=\sum_{n=0}^{n}e^{\beta\frac{{}^2\eta^2}{8m}\left[1+2\{1-4(\delta+\lambda-\xi-n)\}+\{1-4(\delta+\lambda-\xi-n)\}^2\right]} \tag{23}$$

3.2.1 Mean energy

$$U(\beta) = \frac{\partial}{\partial\beta}\left(\ln Z_{vib}(\beta)\right)$$
$$= \frac{\partial}{\partial\beta}\Bigg[ln$$
$$\left\{e^{\beta\frac{{}^2\eta^2}{8m}\left[1+2\{1-4(\delta+\lambda-\xi-n)\}+\{1-4(\delta+\lambda-\xi-n)\}^2\right]}\right\}\Bigg] \tag{24}$$

3.2.2 Mean free energy

$$F(\beta) = -k_BT\ \ln\left(Z_{vib}(\beta)\right)$$
$$= -k_BT\times$$
$$\ln\left\{e^{\beta\frac{{}^2\eta^2}{8m}\left[1+2\{1-4(\delta+\lambda-\xi-n)\}+\{1-4(\delta+\lambda-\xi-n)\}^2\right]}\right\} \tag{25}$$

3.2.3 Specific heat capacity

$$C_s(\beta) = k_B\ \beta^2\frac{\partial^2}{\partial\beta^2}\left(\ln Z_{vib}(\beta)\right)$$
$$= k_B\ \beta^2\frac{\partial^2}{\partial\beta^2}$$
$$\ln\left\{e^{\beta\frac{{}^2\eta^2}{8m}\left[1+2\{1-4(\delta+\lambda-\xi-n)\}+\{1-4(\delta+\lambda-\xi-n)\}^2\right]}\right\} \tag{26}$$

3.2.4 Entropy

$$S = k_B\left(\ln Z_{vib}(\beta)\right) - k_BT\frac{\partial}{\partial\beta}\left(\ln Z_{vib}(\beta)\right)$$
$$=\ k_B\times$$
$$\ln\left\{e^{\beta\frac{{}^2\eta^2}{8m}\left[1+2\{1-4(\delta+\lambda-\xi-n)\}+\{1-4(\delta+\lambda-\xi-n)\}^2\right]}\right\}$$
$$-\ k_BT\times$$
$$\frac{\partial}{\partial\beta}\ln\left\{e^{\beta\frac{{}^2\eta^2}{8m}\left[1+2\{1-4(\delta+\lambda-\xi-n)\}+\{1-4(\delta+\lambda-\xi-n)\}^2\right]}\right\} \tag{27}$$

4 Results and Discussion

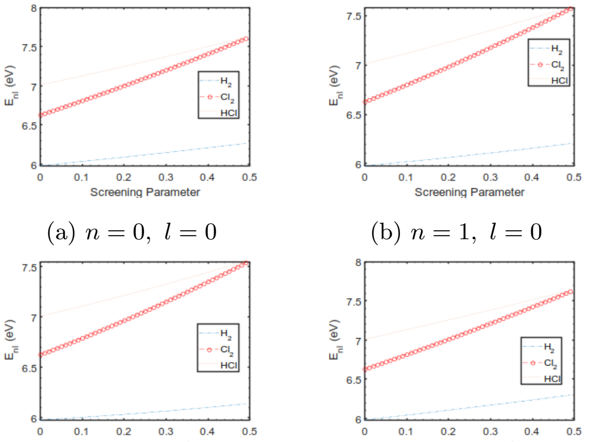
To study the nature of eigen value of screening parameters is used between 0.001 to 0.5, $n = 0$ to 2 and $l = 0$ to 1 for H_2, Cl_2 and HCl. The Dissociation energy of H_2, CL_2 and HCl is 4.738 eV, 2.514 eV and 4.618 eV respectively; and equilibrium bond distance is taken 0.74 , 1.93 and 1.27 , respectively [16–18].

4.1 Energy eigenvalue of H_2, Cl_2 and HCl with screening parameter

The computations were carried out using an atomic screening parameter of 0.9, with both the Planck constant and reduce electron mass normalized to 1 atomic unit. The molecular parameters used in the calculations include equilibrium bond lengths of 0.74 Å for H_2, 1.93 Å for Cl_2, and 1.27 Å for HCl. The corresponding dissociation energies considered were 5.938 eV for H_2, 2.514 eV for Cl_2, and 4.618 eV for HCl. The results indicate that the energy eigenvalues increase with the screening parameter, and tend to converge around 0.5 for quantum states $n = 0 - 2$ and $l = 0 - 1$. For the ground state ($n = l = 0$), the energy eigenvalues were found to range from 6.6 eV to 7.6 eV for Cl_2, and from 7.0 eV to 7.6 eV for HCl. Notably, at approximately 7.6 eV, the eigenvalues of Cl_2 and HCl become nearly identical, indicating energetic coincidence between the two molecules. In contrast, H_2 exhibits a lower energy eigenvalue of about 6.25 eV, showing a relatively linear behavior with respect to screening variation.

Furthermore, the energy eigenvalues for $n = l = 0$ are observed to be higher than those for $n = 1$ and $l = 0$, while for $n = 2$, the values corresponding to $l = 0$ are lower than those for $l = 1$. This demonstrates the influence of both principal and orbital quantum numbers on molecular energy states under screened conditions.

The energy eigen value of H_2, Cl_2 and HCl with screening parameters is shown in figure 1. The nature found that with increasing the screening parameters energy eigenvalue also increase. The energy eigenvalue with quantum number $n = 0$ to $n = 2$ and $l = 0$ to $l = 1$ shows, HCl has higher energy eigenvalue, for Dang-Fan screening potential. The increase in energy eigenvalues with screening parameters is a characteristic feature observed in some physical systems, especially when dealing with screened potentials. In quantum mechanics, screening refers to the shielding effect experienced by charged particles (such as electrons) when they are influenced by external electric fields, typically due to other charged particles in the vicinity. The screening effect weakens the interaction between the external field and the particle, leading to a reduction in the effective potential experienced by the particle. The results of the solution of the equation developed by Schrödinger for the provided potential are what define the energy levels when talking about the energy eigenvalue of the particle in a potential well as well as potential barrier (such as the Dang-Fan screening potential). When screening parameters are increased, it means that the screening effect becomes stronger. In the context of screening potentials, this typically implies that the potential experienced by the particle is further reduced due to increased shielding. As a result, the energy levels of the particle, represented by the energy eigenvalues, will increase. The increase in energy eigenvalues with stronger screening parameters can be understood intuitively as the particle experiencing less confinement or barrier height due to the reduction in the effective potential. This effect can have important implications for various physical systems, including atoms, molecules, and condensed matter systems, where screening plays a significant role. Keep in mind that the specific behavior of the energy eigenvalues with respect to screening parameters depends on the exact form of the potential and the particular system under consideration. It is essential to analyze the potential and solve the corresponding Schrödinger equation to determine the precise relationship between energy eigenvalues and screening parameters in a given physical context.



(a) $n = 0,\ l = 0$ (b) $n = 1,\ l = 0$

(c) $n = 2,\ l = 0$ (d) $n = 2,\ l = 1$

Figure 1: Energy eigenvalue with screening potential.

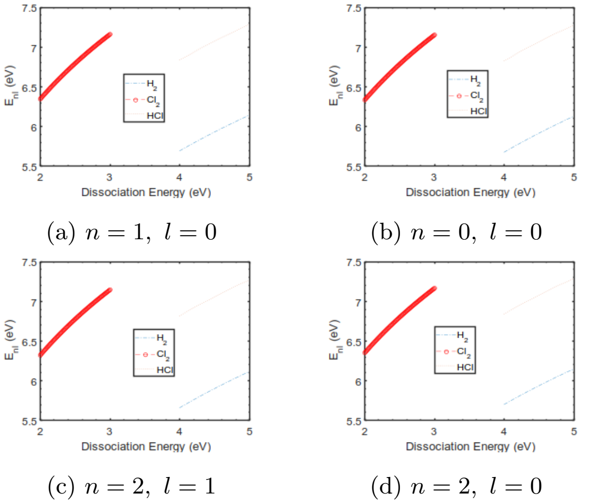
Edet et al. (2020) [12] studied the thermal properties of the Deng–Fan–Eckart potential model using the Poisson summation approach for molecules such as H_2, CO, ScN, and ScF. They found that the energy eigenvalue for the lower orbital quantum state (2p) was positive, and that these positive energy values increased with the rise in screening parameters across all quantum states.

4.2 Energy eigen value of H_2, Cl_2 and HCl with dissociation energy in screening Dang-Fan Potential

The increase in energy eigenvalue of H_2, Cl_2, and HCl with bond dissociation energy can be understood by considering the relationship between molecular bonding and potential energy. The computations were performed with an atomic screening parameter of 0.9, taking the Planck constant and reduced electron mass equal to 1 in atomic units. The molecular parameters used in the analysis include equilibrium bond lengths of 0.74 Å for H_2, 1.93 Å for Cl_2, and 1.27 Å for HCl. The dissociation energies considered were 5.938 eV for H_2, 2.514 eV for Cl_2, and 4.618 eV for HCl. In the case of H_2, Cl_2, and HCl, when these molecules are bonded, they are in a relatively stable state with a certain potential energy associated with the bond. The equation developed by Schrödinger, which incorporates both the potential energy resulting from interactions between particles and the energy generated by the motion of the particles (nuclei and electrons), describes the overall energy of a molecular system in quantum mechanics. The solutions to the Schrödinger equation yield the energy eigenvalues, which represent the quantized energy levels of the system. The increase in energy eigenvalues with bond dissociation energy is a fundamental feature of molecular systems and is crucial for understanding the thermodynamics and kinetics of chemical reactions. It provides insights into the energy changes associated with breaking and forming bonds in molecules, which are central to many chemical and biological processes. The nature of eigen value with dissociation energy for $n = 0$ to $n = 2$ and $l = 0$ to $l = 1$ is shown in figure 2.

The energy eigenvalues were found to vary depending on the molecular species and the quantum states considered. For the Cl_2 molecule, the eigenenergy ranges from 6.3 eV to 7.2 eV, while for HCl, it lies between 6.7 eV and 7.3 eV. In contrast, the H_2 molecule exhibits a lower energy range, from 5.7 eV to 6.1 eV, for the quantum state defined by $n = 0$ and $l = 0$. When the principal quantum number increases to $n = 1$ with $l = 0$, the corresponding energy eigenvalues of all three molecules are observed to decrease, indicating a reduction in bound-state energy with higher quantum excitation. Furthermore, for $n = 2$, the energy eigenvalues for $l = 0$ are lower than those for $l = 1$, showing the influence of orbital angular momentum on the total molecular energy.

The bond in H_2 is a simple covalent bond, where two hydrogen atoms share electrons to form a molecule. Hydrogen is the lightest element with relatively low electronegativity. The bonding electrons are held less tightly, resulting in a weaker bond. The bond in Cl_2 is also a covalent bond, but chlorine is a heavier element compared to hydrogen with higher electronegativity. The increased size and higher electronegativity lead to stronger bonding between chlorine atoms compared to hydrogen. HCl has a polar covalent bond between hydrogen and chlorine. Chlorine is significantly more electronegative than hydrogen, causing the bonding electrons to be shifted closer to the chlorine atom. The results of this study show a similar trend to those reported by Edet et al. (2020) [12]; however, the obtained E_{nl} values are higher than those in their work. Moreover, the behavior of the dissociation energy observed here aligns with the findings of Edet et al. [12], who investigated the thermal properties of the Deng–Fan–Eckart potential model using the Poisson summation approach.



(a) $n = 1,\ l = 0$ (b) $n = 0,\ l = 0$

(c) $n = 2,\ l = 1$ (d) $n = 2,\ l = 0$

Figure 2: Energy eigenvalue with dissociation energy

4.3 Thermodynamic properties

4.3.1 Partition function with beta

The partition function decreases sharply for screening parameters below 0.002, shows a moderate decrease between 0.002 and 0.005, and remains nearly constant above 0.005. The most significant change occurs in the 0–0.04 region. Calculations were performed using an atomic screening factor of 0.9, with reduce electron mass and Planck's constant set to 1, quantum number 2, and orbital number 1. Molecular parameters include bond lengths: H_2 (0.74 Å), Cl_2 (1.93 Å), HCl (1.27 Å), and dissociation energies: H_2 (5.938 eV), Cl_2 (2.514 eV), HCl (4.618 eV).The behavior of the partition function concerning the screening parameter is illustrated in Figure 4. It reveals an exponential decay within the screening region of 0.005 for H_2, Cl_2, and HCl. Moreover, the partition function for hydrogen surpasses that of HCl and Cl_2. The depicted exponential decline highlights the influence of the screening parameter on partition functions, offering insights into how this parameter impacts the energetic properties of diatomic molecules.

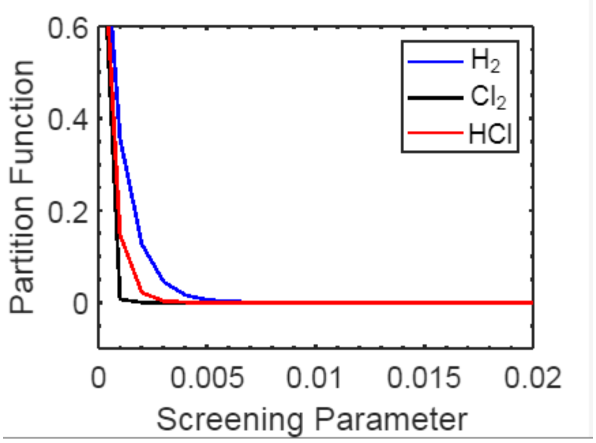


Figure 3: Partition function with screening parameter.

4.3.2 Entropy

The computations were performed considering an atomic screening factor of 0.9, with the reduce electron mass and Planck's constant normalized to 1. The principal quantum number was set to 2, while the orbital quantum number was 1. Molecular parameters used in the calculations include the equilibrium bond lengths: H_2 at 0.74 Å, Cl_2 at 1.93 Å, and HCl at 1.27 Å. The corresponding dissociation energies were taken as 5.938 eV/K for H_2, 2.514 eV/K for Cl_2, and 4.618 eV/K for HCl. These results indicate that the entropy behavior is strongly influenced by both the screening parameter and the intrinsic molecular properties, with the most significant changes occurring at low screening values. The entropy of the system exhibits a strong dependence on the screening parameter. Specifically, the entropy decreases sharply for screening parameters below 0.01, shows a moderate decrease in the range of 0.01 to 0.03, and remains nearly constant for values above 0.04. Notably, the rate of decrease in entropy is more pronounced in the 0–0.01 region, indicating higher sensitivity in this low-screening regime. Figure 5 displays an exponential decay in entropy with the screening parameter. Cl_2 entropy surpasses that of H_2 and HCl due to screening, attributed to higher density between Cl atoms, allowing electrons greater freedom. The higher electron density in Cl atoms compared to HCl and H_2 contributes to this effect. Similarly, the lower electron density in H atoms leads to lower entropy for bounded atoms (HCl and Cl_2). The observed entropy trend aligns with Edet et al. (2020) [12], but in this case, it's higher due to the presence of screening effects between diatomic molecules. This emphasizes the role of screening in shaping entropy behaviors, providing a deeper understanding of molecular energetics.

4.3.3 Mean free Energy

The mean free energy of the molecules under consideration was evaluated with atomic screening set at 0.9. For chlorine (Cl_2), the mean free energy remains approximately constant at 5400 eV. In comparison, hydrogen chloride (HCl) exhibits a mean free energy of around 2100 eV, while molecular hydrogen (H_2) shows a lower value of about 1100 eV, as illustrated in Figure 6. The computations also accounted for the equilibrium bond lengths of the respective molecules. For HCl, the equilibrium bond length is 1.27 Å, while H_2 has an equilibrium bond length of 0.74 Å, and Cl_2 exhibits a bond length of 1.93 Å. Furthermore, the dissociation energies of these molecules were determined. H_2 requires 5.938 eV for dissociation, Cl_2 requires 2.514 eV, and HCl requires 4.618 eV. These values are consistent with the molecular stability and bonding characteristics of each species. The mean free energy of a bounded electron within a given atom remains constant, as indicated by Figure 6. However, the mean free energy of Cl_2 surpasses that of HCl and H_2, attributed to electron density and screening influences. Notably, a consistent straight line depicts uniform screening effects across H_2, Cl_2, and HCl. This observation underscores the pivotal role that electron density and screening mechanisms play in shaping the mean free energy behaviors across different molecular species, revealing insights into their distinct energetic characteristics.

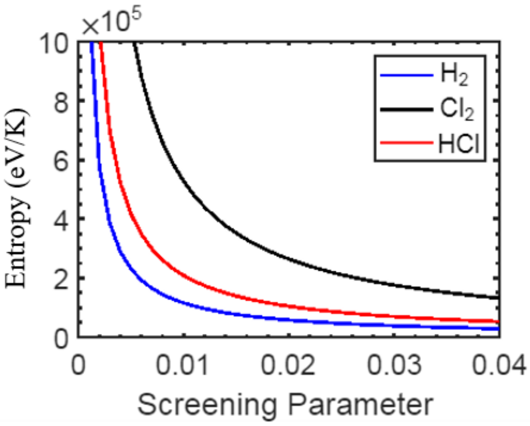


Figure 4: Entropy vs screening parameter.

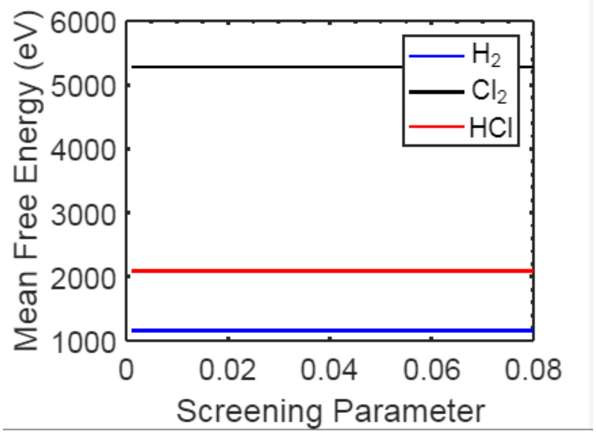


Figure 5: Mean free energy vs Screening parameters

4.3.4 Specific heat capacity

The absence of a measurable specific heat capacity for electrons, denoted as zero, holds intriguing implications. This signifies that electrons, as fundamental particles, differ from macroscopic objects in their heat capacity behavior. Unlike objects with discernible heat capacities, electrons exhibit a unique trait, challenging conventional expectations. This resonates deeply with the fundamental nature of particles at the quantum level, where traditional concepts of heat capacity may not apply in the same manner. This observation underscores the distinct behaviors and characteristics that arise when transitioning from macroscopic to quantum realms, prompting a reevaluation of heat-related properties at the quantum level. Edet et al. (2020) [14] studied and found that specific heat capacity constant as zero when they study the specific heat capacity of I_2 with ratio of magnetic flux and flux quantum.

5 Conclusion

The energy eigenvalues of H_2, Cl_2, and HCl were studied with screening parameters and bond dissociation energy. The results showed that increasing the screening parameters led to an increase in energy eigenvalues, indicating that the screening potential has a significant impact on the energy levels of these molecules. Furthermore, when investigating the energy eigenvalues for specific quantum numbers ($n = 0$ to $n = 2$) and angular momentum quantum numbers ($l = 0$ to $l = 1$), it was found that HCl exhibited the highest energy eigenvalue, followed by Cl_2 and H_2. Partition function decreases exponentially (0.005 screening range) for H_2, Cl_2, HCl. Hydrogen's exceeds HCl, Cl_2. Entropy decays exponentially due to screening; Cl_2 has higher entropy (electron density, screening). Mean free energy remains steady; Cl_2 has higher due to density, screening. Electrons lack measurable heat capacity (zero specific heat capacity) unlike macroscopic objects. Further research in this area can provide valuable insights into various physical systems, including atoms, molecules, and condensed matter systems, where these factors play a significant role in their behavior and properties.

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References

[1] E. P. Inyang, I. O. Akpan, J. E. Ntibi, and E. S. William. Masses and thermodynamic properties of a quarkonium system. *Canadian Journal of Physics*, 99:982, 2021. doi:https://doi.org/10.1139/cjp-2020-0578.

[2] R. Rani, S. B. Bhardwaj, and F. Chand. Mass spectra of heavy and light mesons using asymptotic iteration method. *Communications in Theoretical Physics*, 70(2):179, 2018. doi:https://doi.org/10.1088/0253-6102/70/2/179.

[3] M. Abu-Shady and A. N. Ikot. Analytic solution of multidimensional Schrödinger equation in hot and dense QCD media using the SUSYQM method. *The European Physical Journal Plus*, 134:321, 2019. doi:https://doi.org/10.1140/epjp/i2019-12685-y.

[4] A. Hesam, H. Nikoofard, and M. Sargolzaei. Prediction of thermodynamic properties of formation of HCl at temperatures 200-1000 K. *Chemical Physics Letters*, 764:138276, 2021. doi:10.1016/j.cplett.2020.138276.

[5] B. Karki, S. H. Dhobi, J. J. Nakarmi, and K. Yadav. Energy eigenvalue and thermodynamic properties of q-deformed Hulthen potential. *BIBECHANA*, 19(1-2):165–169, 2022. doi:10.3126/bibechana.v19i1-2.46416.

[6] R. Vidunas. Transformations of algebraic gauss hypergeometric functions. *arXiv preprint*, 2008. arXiv:0807.4808.

[7] Z. Rong, H. G. Kjaergaard, and M. L. Sage. Comparison of the Morse and Deng-Fan potentials for X-H bonds in small molecules. *Molecular Physics*, 101(14):2285–2294, 2003.

[8] K. J. Oyewumi, O. J. Oluwadare, K. D. Sen, and O. A. Babalola. Bound state solutions of the Deng-Fan molecular potential with the Pekeris-type approximation using the Nikiforov-Uvarov (N-U) method. *Journal of Mathematical Chemistry*, 51:976, 2012. doi:https://doi.org/10.1007/s10910-012-0123-6.

[9] E. Omugbe. Non-relativistic energy spectrum of the Deng-Fan oscillator via the WKB approximation method. *Asian Journal of Physical and Chemical Sciences*, 8(1):26, 2020. doi:https://doi.org/10.9734/ajopacs/2020/v8i130107.

[10] M. Abu-Shady, E. M. Khokha, and T. A. Abdel-Karim. The generalized fractional NU method for the diatomic molecules in the Deng-Fan model. *The European Physical Journal D*, 76:159, 2022. doi:https://doi.org/10.1140/epjd/s10053-022-00480-w.

[11] A. Maireche. Diatomic molecules and fermionic particles with improved Hellmann-generalized Morse potential through the solutions of the deformed Klein-Gordon, Dirac and Schrödinger equations in extended relativistic quantum mechanics and extended nonrelativistic quantum mechanics symmetries. *Revista Mexicana de Física*, 68(2):020801, 2022.

[12] C. O. Edet, U. S. Okorie, G. Osobonye, et al. Thermal properties of Deng-Fan-Eckart potential model using poisson summation approach. *Journal of Mathematical Chemistry*, 58:989–1013, 2020. doi:https://doi.org/10.1007/s10910-020-01107-4.

[13] B. Khirali, A. K. Behera, J. Bhoi, and U. Laha. Scattering with Manning-Rosen potential in all partial waves. *Annals of Physics*, 412:168044, 2020. doi:10.1016/j.aop.2019.168044.

[14] C. O. Edet and A. N. Ikot. Analysis of the impact of external fields on the energy spectra and thermo-magnetic properties of N2, I2, CO, NO, and HCl diatomic molecules. *Molecular Physics*, 119(16):e1957170, 2021. doi:https://doi.org/10.1080/00268976.2021.1957170.

[15] I. J. Njoku, E. Onyeocha, P. Nwaokafor, and M. Onuoha. Energy eigenvalues of diatomic molecules with the shifted Deng-Fan potential using a recently introduced approximation

scheme. *Chemical Physics Impact*, 5:100096, 2022.

[16] K. P. Huber and G. Herzberg. *Molecular Spectra and Molecular Structure IV. Constants of Diatomic Molecules*. Van Nostrand Reinhold, New York, 1979.

[17] A. E. Douglas and A. R. Hoy. The resonance fluorescence spectrum of C12 in the vacuum ultraviolet. *Canadian Journal of Physics*, 53(18):1965–1975, 1975.

[18] P. G. Hajigeorgiou. An extended Lennard-Jones potential energy function for diatomic molecules: Application to ground electronic states. *Journal of Molecular Spectroscopy*, 263(2):101–110, 2010.