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***RESEARCH ARTICLE***

# EIGENSOLUTIONS AND THERMODYNAMIC PROPERTIES OF THE ECKART PLUS HULTHÉN POTENTIAL AND A CLASS OF YUKAWA

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***Abstract***

In this paper, we present the bound-state solutions of the Schrödinger equation and analyze the thermodynamic properties of the Eckart plus Hulthén potential and a class of Yukawa potentials. The eigenvalues and eigenfunctions were determined using the Parametric Nikiforov-Uvarov Method (PNUM). The eigenenergies of HCl and ScH molecules were calculated for various values of n and ℓ. All calculated eigenenergies for these molecules are negative, unlike those in atomic units. For a given pair (n, ℓ), the energy of ScH is higher than that of HCl. Furthermore, for these molecules, at constant n, the energy increases with increasing ℓ; and at constant ℓ, the energy increases with increasing n. The obtained energy values were then used to calculate the partition function, which served as a basis to derive thermodynamic properties such as mean energy, specific heat capacity, entropy, and free energy. The study revealed that the system exhibits high disorder for small values of β, while increasing β leads to a significant reduction in disorder.



## Introduction: -

The study of statistical physics in general, and quantum statistics in particular, has over the years enabled the prediction and interpretation of various thermodynamic properties of different systems [1]. The self-energy obtained from the Schrödinger equation is used to calculate the partition function, which is the central parameter for studying thermodynamic properties such as mean energy, specific heat (heat capacity), entropy, and free energy. These thermodynamic properties are essential elements of quantum physics.

Recently, many researchers have shown interest in the study of thermodynamic properties because of their applications and unique characteristics [2]. For example, Dong and Cruz-Irisson calculated the thermodynamic properties of the modified Rosen-Morse potential [3]. Khordad and Sedehi [4], studied the different thermodynamic properties for a double ring-shaped potential. Inyang et al. [5], calculated the various thermodynamic properties of the Eckart-Hellman potential in one of the recent studies. Njoku et al. [6], in their work, obtained approximate solutions of the Schrödinger equation and corresponding thermodynamic properties. Demirci and Sever [7], calculated the

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nonrelativistic thermal properties of Eckart plus class of Yukawa potential. Ramantswana et al. [8], in their own study, determined the thermodynamic properties of CrH, NiC and CuLi diatomic molecules with the linear combination of Hulthén-type potential plus Yukawa potential. The thermodynamic properties of some diatomic molecules confined by an-harmonic oscillating system was also studied by Oluwadare et al. [9]. In ref [10], I. B. Okon et al. studied thermodynamic properties using hyperbolic Hulthén plus hyperbolic exponential inversely quadratic potential. Edet et al .[11], used Poisson summation approach to study thermal properties of Deng-fan Eckart potential model. Okorie et al. [12], calculated the thermodynamic properties of the modified Yukawa potential. U. S. Okorie et al. [13], studied thermodynamic properties with modified Mobius square potential (MMSP). Okon et al. [14], combined Mobius Square and Screened Kratzer Potential to obtained thermodynamic properties and bound State Solutions to Schrödinger equation. E. Omugbe et al. [15], studies Thermodynamic properties and Expectation Values of a mixed hyperbolic Poschl-Teller potential (MHPTP). Cecilia N. Isonguyo [16], studied eigensolutions and Thermodynamic Properties of Kratzer plus generalized Morse Potentiel. I. B. Okon et al. [17], obtained Eigen Solution and Thermodynamic Properties of Manning Rosen Plus Exponential Yukawa Potential. K. O. Emeje et al. [18], examined Eigensolution and Thermodynamic Properties of Standard Coulombic Potential. Recently, we obtained the Eigensolutions and thermodynamic properties of generalized hyperbolic Hulthen and Woods–Saxon potential [19].

It should be noted that the Schrödinger equation is only solvable for the angular momentum quantum number $\ell = 0$ for certain potential models. However, for states where $\ell \neq 0$, it is necessary to use approximations such as the Pekeris approximation to handle the centrifugal term or to solve it numerically [20]. The Eckart plus Hulthén potential is an interesting combined molecular and diatomic potential, widely used in several fields such as applied physics and chemical physics [21]. It is defined by [22]:

$$V_{EHP}(r) = \operatorname{cosech}^2(\alpha r) + \coth(\alpha r) + \frac{V_0}{1 - e^{-2\alpha r}} - \frac{V_1}{(1 - e^{-2\alpha r})^2}, \quad (1)$$

where $V_0$ and $V_1$ have the dimensions of energy, representing the depths of the potentials well, and $\alpha$ is the inverse of the potential range. A class of Yukawa potentials is given by the form [23]:

$$V_{CYP}(r) = -\frac{V_2 e^{-\delta r}}{r} - \frac{V_3 e^{-2\delta r}}{r^2}, \quad (2)$$

where $\delta$ is the screening parameter. The first and second parts of this potential represent, respectively, the pure Yukawa potential and the inversely quadratic Yukawa potential [24]. This potential is particularly significant in explaining the interaction between nucleons [23].

Motivated by the thermodynamic properties and applications offered by the Eckart plus Hulthén potentials, as well as the Yukawa potential, we propose a linear combination of the Eckart plus Hulthén potential and a class of Yukawa potentials (denoted as $(V_{EHCYP}(r))$ in this work. This combined potential can be useful in several theoretical and practical fields, such as materials physics, statistics, particle physics, atomic, molecular, nuclear, condensed matter.

The paper is organized as follows: In Section 2, we solve the Schrödinger equation with the Eckart plus Hulthén potential and a class of Yukawa potentials. In Section 3, we present the thermodynamic properties. Numerical results and discussions are provided in Section 4. Finally, our conclusions are presented in the last section.

**Bound State Solution of the Schrodinger Equation**

In spherical coordinates, the radial part of the Schrodinger wave equation, is given by [25]:

$$\frac{d^2\Psi_{n\ell}(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E_{n\ell} - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]\Psi_{n\ell}(r) = 0, \quad (3)$$

where $\Psi_{n\ell}(r)$ is the radial wave function, $E_{n\ell}$ is the energy spectrum, $\hbar$ is the reduced Planck constant, m is the reduced mass, $\frac{\ell(\ell+1)}{r^2}$ is the centrifugal barrier. This equation is solved using the Greene-Aldrich approximation scheme, which is a good approximation for $\alpha r << 1$, given by [26]:

$$\frac{1}{r^2} \approx 4\alpha \frac{e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}, \quad (4)$$

here, $\ell$ and n represent the angular momentum and principal quantum numbers, respectively, and $V(r)$ represents the Eckart plus Hulthén potential and a class of Yukawa denoted by $V_{EHCYP}(r)$, given by:

$$V_{EHCYP}(r)=\text{cosech}^2(\alpha r)+\coth^2(\alpha r)+\frac{V_0}{1-e^{-2\alpha r}}-\frac{V_1}{(1-e^{-2\alpha r})^2}-\frac{V_2e^{-\delta r}}{r}-\frac{V_3e^{-2\delta r}}{r^2}. \quad (5)$$

Using the Greene-Aldrich approximation scheme, hyperbolic transformations, and setting $s=e^{-2\delta r}$ (with α=δ), we obtain the following hypergemetric equation:

$$\Psi''(s)+\frac{1-s}{s(1-s)}\Psi'(s)+\frac{1}{[s(1-s)]^2}[-\varepsilon_1 s^2+\varepsilon_2 s-\varepsilon_3]\Psi(s)=0, \quad (6)$$

with

$$\varepsilon_1=-\frac{2m}{4\hbar^2\delta^2}[E_{n\ell}+2\delta(2V_3-V_2)+1], \qquad \varepsilon_2=\frac{2m}{4\hbar^2\delta^2}[-2E_{n\ell}+2\delta V_2+V_0+4]-\ell(\ell+1),$$

$$\varepsilon_3=\frac{2m}{4\hbar^2\delta^2}[E_{n\ell}+V_1-V_0-1].$$

According to the Parametric Nikiforov-Uvarov method [16, 23], we obtain the following parameters:

$$c_1=c_2=c_3=1, c_4=0, c_5=-\frac{1}{2}, c_6=\frac{1}{4}+\varepsilon_1, c_7=-\varepsilon_2, c_8=\varepsilon_3, c_9=\varepsilon_1-\varepsilon_2+\varepsilon_3+\frac{1}{4}, c_{10}=1+2\sqrt{\varepsilon_3}, c_{11}=2+2\left(\sqrt{\varepsilon_1-\varepsilon_2+\varepsilon_3+\frac{1}{4}}+\sqrt{\varepsilon_3}\right), c_{12}=\sqrt{\varepsilon_3} \text{ and } c_{13}=-\frac{1}{2}-\left(\sqrt{\varepsilon_1-\varepsilon_2+\varepsilon_3+\frac{1}{4}}+\sqrt{\varepsilon_3}\right). \quad (7)$$

Using the energy spectrum equation [16, 23] and (7), we obtain the following expression of the energy eigenvalue:

$$E_{n\ell}=V-\frac{\hbar^2\delta^2}{2m}\left(\frac{\frac{2m}{4\hbar^2\delta^2}V'+\left[n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{2m}{4\hbar^2\delta^2}\left(4-V_1-4\delta^2V_3\right)+\ell(\ell+1)}\right]^2}{\left[n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{2m}{4\hbar^2\delta^2}\left(4-V_1-4\delta^2V_3\right)+\ell(\ell+1)}\right]}\right)^2, (8)$$

with

$$V=(1+V_0-V_1), \frac{1}{4}+\frac{2m}{4\hbar^2\delta^2}\left(4-V_1-4\delta^2V_3\right)+\ell(\ell+1)\geq 0, V'=\left(2+V_0+4\delta^2V_3-2\delta V_2-V_1\right).$$

The total wave function is given by:

$$\Psi_{n\ell}(s)=C_{n\ell}s^{\sqrt{\varepsilon_3}}(1-s)^{\frac{1}{2}+\sqrt{\varepsilon_1-\varepsilon_2+\varepsilon_3+\frac{1}{4}}}P_n^{\left(2\sqrt{\varepsilon_3},2\sqrt{\varepsilon_1-\varepsilon_2+\varepsilon_3+\frac{1}{4}}\right)}(1-2s), (9)$$

with $s=e^{-2\delta r}$, $C_{n\ell}$ the normalization constant and $P_n^{\left(2\sqrt{\varepsilon_3},2\sqrt{\varepsilon_1-\varepsilon_2+\varepsilon_3+\frac{1}{4}}\right)}$ are the Jacobi polynomial.

**Non-relativistic thermodynamics properties**

Several thermodynamic properties can be studied from the partition function, which is defined as:

$$Z(\beta)=\sum_{n=0}^{\lambda}\exp\left(-\beta E_{n\ell}\right), \quad (10)$$

where λ is the largest value of the vibrational quantum number obtained from the numerical solution [16]: $\frac{dE_{n\ell}}{dn}=0$, and $\beta=\frac{1}{T}$, where k is the Boltzmann constant and T is the absolute temperature. In the classical limit the summation in equation (10) can be replaced by an integral:

$$Z(\beta)=\int_0^{\lambda}e^{-\beta E_{n\ell}}\,dn. \quad (11)$$

The energy expression from equation (8) can be rewritten as:

$$E_{n\ell}=V-q[\frac{p}{n+Q}+(n+Q)]^2, \quad (12)$$

where:

$$V = (1 + V_0 - V_1), q = \frac{\hbar^2\delta^2}{2m}, p = \frac{2mV'}{4\hbar^2\delta^2}, Q = \frac{1}{2}\sqrt{\frac{1}{4} + \frac{2m}{4\hbar^2\delta^2}(4 - V_0 - 4\delta^2 V_3) + \ell(\ell+1)}. \quad (13)$$

Substituting this equation into equation (11), we obtain:

$$Z(\beta) = \int_0^\lambda e^{-\beta(V - q[\frac{p}{n+Q} + (n+Q)]^2)}\, dn. \quad (14)$$

Equation (14) was integrated using mathematica, and we obtain:

$$Z(\beta) = \frac{1}{4\sqrt{-q\beta}} e^{\left(2pq\beta - V\beta - 2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{\pi}\left(-\mathrm{Erf}\left[Q\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{Q}\right] - e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q}\right] + \mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{Q+\lambda}\right] + e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q+\lambda}\right]\right), \quad (15)$$

with (q $< 0$, $Q \neq 0$, $\lambda \neq 0$, $\mathrm{Re}\left[\frac{Q}{\lambda}\right] \geq 0$ and $\mathrm{Erfi}(z) = -i\mathrm{Erf}(iz) = \sqrt{\frac{4}{\pi}}\int_0^z e^{u^2} du$ [27].

**a. Average energy**

Average energy is given by:

$$U(\beta) = -\frac{\partial \mathrm{Ln}(Z(\beta))}{\partial\beta} = \frac{\Lambda_1}{\Lambda_2}, \quad (16)$$

With $\Lambda_1 = \left(-\mathrm{Erf}\left[Q\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{Q}\right] - e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q}\right] + \frac{1}{\sqrt{\pi}} 4e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{-q\beta}\left(e^{\frac{q(p^2+Q^4)\beta}{Q^2}}Q - e^{\frac{q(p^2+(Q+\lambda)^4)\beta}{(Q+\lambda)^2}}(Q+\lambda) + 2\sqrt{\pi}e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{-p^2q\beta}\mathrm{Erf}\left[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q}\right] - 2\sqrt{\pi}e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{-p^2q\beta}\mathrm{Erf}\left[\frac{(Q+\lambda)^2\sqrt{-q\beta} + \sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right) + \mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right] + e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right] - 2\beta\left(2pq - V + \frac{2q\sqrt{-p^2q\beta}}{\sqrt{-q\beta}}\right)\left(-\mathrm{Erf}\left[Q\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{Q}\right] - e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q}\right] + \mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right] + e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right)\right),$

and

$$\Lambda_2 = \sqrt{\pi}\left(-\mathrm{Erf}\left[Q\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{Q}\right] - e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q}\right] + \mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right] + e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right).$$

b. **Specific heat capacity**

Specific heat capacity is given by:

$$C(\beta) = -k\beta^2 \frac{\partial^2 \mathrm{Ln}(Z(\beta))}{\partial\beta^2} = -k\beta^2 \frac{\partial \mathrm{Ln}(U(\beta))}{\partial\beta} = \frac{\wedge_3}{\wedge_4}, \qquad (17)$$

with $\wedge_3 = -k(\beta(-\mathrm{Erf}[Q\sqrt{-q\beta} - \frac{\sqrt{-p^2q\beta}}{Q}] - e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}\mathrm{Erf}[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2q\beta}}{Q} + \mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta} -$

$\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] + e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}])(\frac{e^{-\left(Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}\right)^2}\left(-Q^2\sqrt{-q\beta}+\sqrt{-p^2q\beta}\right)}{\sqrt{\pi}Q\beta} +$

$\frac{e^{\left(-\frac{p^2q\beta}{Q^2}+qQ^2\beta+2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)} q\left(p^2\sqrt{-q\beta}+Q^2\sqrt{-p^2q\beta}\right)}{Q\sqrt{\pi}\sqrt{-q\beta}\sqrt{-p^2q\beta}} + \frac{1}{\sqrt{\pi}} e^{-\left((Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right)^2} q\left(-\frac{(Q+\lambda)}{\sqrt{-q\beta}}+\frac{p^2}{(Q+\lambda)\sqrt{-p^2q\beta}}\right) -$

$\frac{e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}+\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}\right)} q\left(p^2\sqrt{-q\beta}+(Q+\lambda)^2\sqrt{-p^2q\beta}\right)}{(Q+\lambda)\sqrt{\pi}\sqrt{-q\beta}\sqrt{-p^2q\beta}} + \frac{4e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}q\sqrt{-p^2q\beta}\,\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]}{\sqrt{-q\beta}} +$

$\frac{1}{\sqrt{\pi}}4e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{-q\beta}(\frac{e^{\frac{q\beta(p^2+Q^4)}{Q^2}}q(p^2+Q^4)}{Q} - \frac{2e^{\frac{q\beta(p^2+Q^4)}{Q^2}}q(p^2\sqrt{-q\beta}+Q^2\sqrt{-p^2q\beta})}{Q\sqrt{-q\beta}} +$

$\frac{2e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}}q(p^2\sqrt{-q\beta}+(Q+\lambda)^2\sqrt{-p^2q\beta})}{(Q+\lambda)\sqrt{-q\beta}} - \frac{e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}}q(Q+\lambda)(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2} -$

$4e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}p^2q\sqrt{\pi}\sqrt{-q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] + \frac{1}{\beta}e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] +$

$4e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}p^2q\sqrt{\pi}\sqrt{-q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] + \frac{1}{\sqrt{-p^2q\beta}}e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}p^2q\sqrt{\pi}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+$

$\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] - \frac{1}{\sqrt{\pi}\sqrt{-q\beta}}2qe^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}} - (Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}} +$

$2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] - 2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+$

$\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}]) - \frac{1}{\sqrt{\pi}}8qe^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{-p^2q\beta}(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}} - (Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}} +$

$2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] - 2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+$

$\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}]) + \frac{1}{\sqrt{\pi}}4e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}((2pq-V)\sqrt{-q\beta}+2q\sqrt{-p^2q\beta})(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}} - (Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}} +$

$2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] - 2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+$

$\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}]) - \frac{1}{\sqrt{-q\beta}}4e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}q\sqrt{-p^2q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] - 2(2pq - V +$

$\frac{2q\sqrt{-p^2q\beta}}{\sqrt{-q\beta}})(-\mathrm{Erf}[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}] - e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] + \mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] +$

$e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}])) + \frac{1}{\sqrt{\pi}}2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{-q\beta}(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}} - (Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}} +$

$2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] - 2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+$

$\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}])\ (-\mathrm{Erf}[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}] - e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] +$

$\frac{1}{\sqrt{\pi}}4e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{-q\beta}(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}} - (Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}} + 2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[Q\sqrt{-q\beta}+$

$\frac{\sqrt{-p^2q\beta}}{Q}] - 2e^{(2\sqrt{-q\beta}\sqrt{-p^2q\beta})}\sqrt{\pi}\sqrt{-p^2q\beta}\,\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}]) + \mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] +$

$e^{(4\sqrt{-q\beta}\sqrt{-p^2q\beta})}\mathrm{Erf}[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}] - 2\beta(2pq - V + \frac{2q\sqrt{-p^2q\beta}}{\sqrt{-q\beta}})(-\mathrm{Erf}[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}] -$

$e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]+\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right])) - (-\mathrm{Erf}\left[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}\right]-e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]+\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right])) (-\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]-e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right] + \frac{1}{\sqrt{\pi}}4e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{-q\beta}\left(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}}-(Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}}+2e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{\pi}\sqrt{-p^2q\beta}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]-2e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{\pi}\sqrt{-p^2q\beta}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right)+\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right])) - 2(2pq-V+\frac{2q\sqrt{-p^2q\beta}}{\sqrt{-q\beta}})(-\mathrm{Erf}[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}]-e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}] + \mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right])))),$

$$\wedge_4 = (2(\mathrm{Erf}\left[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]-\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right] - e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right])^2).$$

**c. Free energy**

Free energy is given by:

$$F(\beta) = -\frac{1}{\beta}\mathrm{Ln}\big(Z(\beta)\big). \tag{18}$$

d. **Entropy**

Entropy is given by

$$S(\beta) = k\mathrm{Ln}\big(Z(\beta)\big) - k\beta\frac{\partial \mathrm{Ln}\big(Z(\beta)\big)}{\partial\beta} = k\beta^2\frac{\partial F(\beta)}{\partial\beta} = k\frac{\wedge_5}{\wedge_6}, \tag{19}$$

with

$\wedge_5 = \Bigg(-\mathrm{Erf}\left[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}\right]-e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]+\frac{1}{\sqrt{\pi}}4e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{-q\beta}\left(Qe^{\frac{q\beta(p^2+Q^4)}{Q^2}}-(Q+\lambda)e^{\frac{q\beta(p^2+(Q+\lambda)^4)}{(Q+\lambda)^2}}+2e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{\pi}\sqrt{-p^2q\beta}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]-2e^{\left(2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{\pi}\sqrt{-p^2q\beta}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right)+\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]-2\beta\left(2pq-V+\frac{2q\sqrt{-p^2q\beta}}{\sqrt{-q\beta}}\right)\left(-\mathrm{Erf}\left[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}\right]-e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]+\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right)\Bigg),$

and $\wedge_6 = 2\left(-\mathrm{Erf}\left[Q\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{Q}\right]-e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{Q}\right]+\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}-\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]+e^{\left(4\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta}+\frac{\sqrt{-p^2q\beta}}{(Q+\lambda)}\right]\right)+\mathrm{Ln}\left[\frac{1}{4\sqrt{-q\beta}}e^{\left(2pq\beta-V\beta-2\sqrt{-q\beta}\sqrt{-p^2q\beta}\right)}\sqrt{\pi}\left(-\mathrm{Erf}\left[Q\sqrt{-q\beta}-\right.\right.\right.$

$\left.\frac{\sqrt{-p^2 q\beta}}{Q}\right] - e^{\left(4\sqrt{-q\beta}\sqrt{-p^2 q\beta}\right)}\mathrm{Erf}\left[Q\sqrt{-q\beta} + \frac{\sqrt{-p^2 q\beta}}{Q}\right] + \mathrm{Erf}\left[(Q+\lambda)\sqrt{-q\beta} - \frac{\sqrt{-p^2 q\beta}}{(Q+\lambda)}\right] + e^{\left(4\sqrt{-q\beta}\sqrt{-p^2 q\beta}\right)}\mathrm{Erf}\left[(Q +\right.$
$\left.\left.\left.\lambda)\sqrt{-q\beta} + \frac{\sqrt{-p^2 q\beta}}{(Q+\lambda[])}\right]\right)\right].$

## Numerical Results and Discussions: -

We consider the diatomic molecules HCl and ScH with spectroscopic parameters as indicated in Table 1. These parameters have been applied to equation (8) to calculate the numerical values of the eigenenergies, as shown in Table 2, for arbitrary quantum numbers n and angular momenta $\ell$. In Table 2, all the calculated eigenenergies for both molecules are negative. For each pair (n, $\ell$), the energy of ScH is higher than that of HCl. For these molecules, at a constant n, the energy E increases with increasing $\ell$, and for a constant $\ell$, E increases with increasing n. Table 3 shows the numerical values obtained from equation (8) in atomic units. In this case, the energy spectrum is positive and increases with increasing n+ $\ell$. If n+$\ell$ remains constant, the energy is quasi-degenerate (approximately equal across different states), which is in agreement with aligns with the physical properties of quantum systems where states with the same sum n+$\ell$ often exhibit very similar energies.

We also used the parameters from Table 1 to plot Figure 1, which shows the variations in energy of the HCl and ScH molecules as a function of the quantum number n. From Figure 1, both curves (HCl and ScH) decrease as n increases. Initially, the two curves converge, but they diverge as n continues to increase. After diverging, the HCl curve decreases more rapidly than the ScH curve. For $\ell$ = 0,1,2,3,4,5, all the curves show a decrease in energy with increasing n. Moreover, the lower the value of $\ell$, the higher the energy. The gap between the respective curves is more pronounced for the HCl molecule.

Note that in thermodynamic contexts, with $\beta = \frac{1}{kT}$, for Z(β), U(β), C(β), F(β) and S(β) to be plotted, q would need to be strictly negative, as these functions involve terms like $\sqrt{-q\beta}$. However, according to equation (13), $q = \frac{\hbar^2\delta^2}{2m}$, and there is no molecule with a negative mass based on the current state of scientific knowledge. Therefore, q is positive, regardless of m. Since both β and q are positive, the thermodynamic properties cannot be plotted using the parameters from Table 1. Instead, we have plotted some properties using arbitrary values for $p, q, Q, V, \lambda$ and k. Figure 2 illustrates the variations of the partition function Z(β), average (mean) energy U(β), free energy F(β) and entropy S(β). The partition function Z(β) decreases exponentially as β increases. Both U(β) and F(β) decrease with increasing β, with U(β) decreasing more rapidly than F(β). The entropy curve shows high entropy at small β, followed by a rapid drop as β increases, and then a slower rate of decrease. This behavior indicates that the system's disorder is high at small β, and as β increases, the disorder significantly decreases.

**Table 1:-** Model parameters for some selected molecules in this study [28].

| Molecules | $\delta(\text{Å}^{-1})$ | m(amu) |
|---|---|---|
| HCl | 1.8677 | 0.9801045 |
| ScH | 1.41113 | 0.986040 |

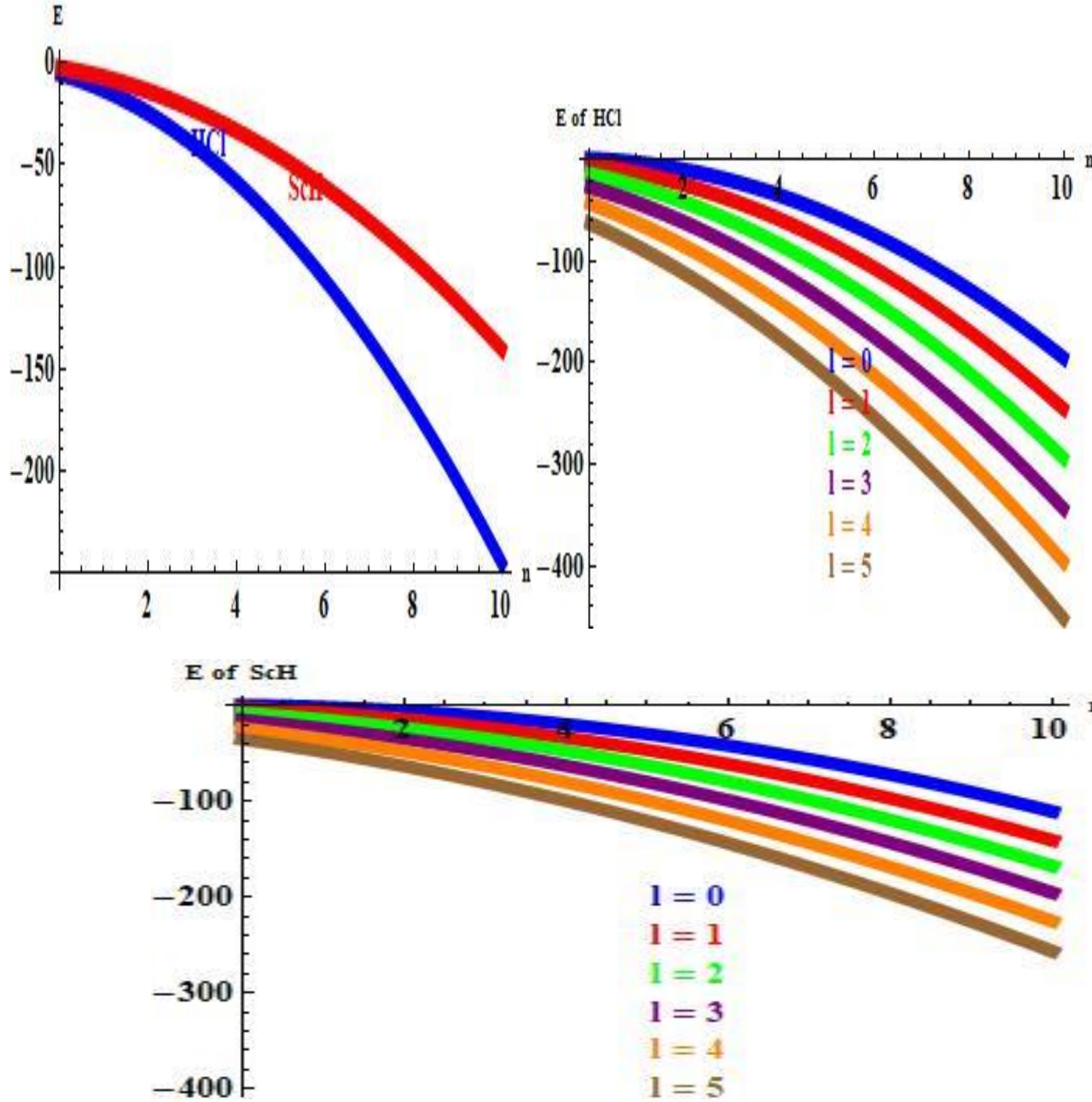
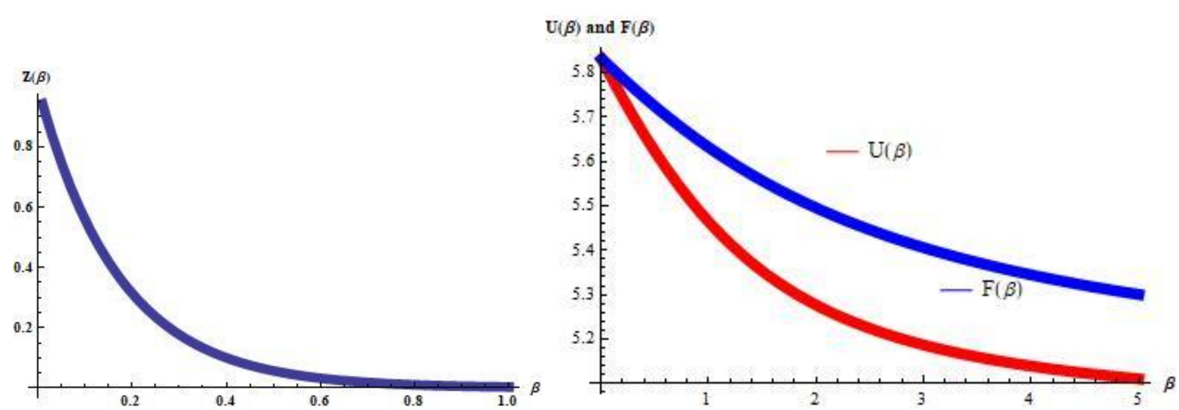



**Figure 1:-**Variation of E(n) of HCl and ScH for $V_0=V_1=V_2=2$ and $V_3=0.5$.



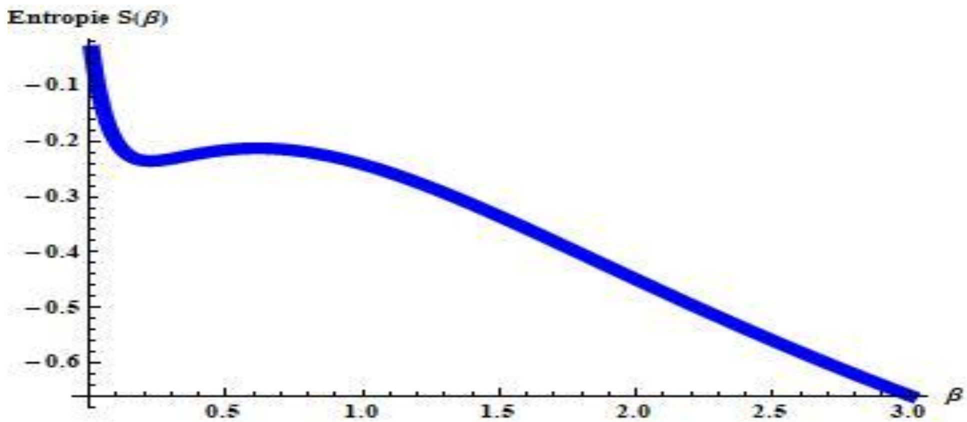



**Figure 2:-** Variation of Z(β), U(β), F(β) and S(β) for q=-1 and q=Q=V=k=λ=1

**Table 2**:- Energy spectrum -E(eV) of HCl, ScH, for n and ℓ arbitrary, $\hbar c$=1973.29 eVÅ, $V_0=V_1=V_2=2$ and $V_3$ = 0.5.

| n | ℓ | HCl | ScH |
|---|---|---|---|
| 0 | 0 | 7438.36181 | 4220.04498 |
| 1 | 0 | 7438.07812 | 4219.98152 |
| 1 | 1 | 7438.02566 | 4219.96978 |
| 2 | 0 | 7438.02570 | 4219.96978 |
| 2 | 1 | 7438.00735 | 4219.96567 |
| 2 | 2 | 7437.99888 | 4219.96377 |
| 3 | 0 | 7438.00737 | 4219.96567 |
| 3 | 1 | 7437.99888 | 4219.96377 |
| 3 | 2 | 7437.99427 | 4219.96273 |
| 3 | 3 | 7437.99150 | 4219.96211 |
| 4 | 0 | 7437.99889 | 4219.96377 |
| 4 | 1 | 7437.99428 | 4219.96273 |
| 4 | 2 | 7437.99150 | 4219.96211 |
| 4 | 3 | 7437.98970 | 4219.96171 |
| 4 | 4 | 7437.98846 | 4219.96143 |
| 5 | 0 | 7437.99428 | 4219.96273 |
| 5 | 1 | 7437.99150 | 4219.96211 |
| 5 | 2 | 7437.98970 | 4219.96171 |
| 5 | 3 | 7437.98846 | 4219.96143 |
| 5 | 4 | 7437.98758 | 4219.96123 |
| 5 | 5 | 7437.98693 | 4219.96108 |

**Table 3:-** Energy spectrum E(eV) for arbitrary n and ℓ, for the atomic unit ($\hbar$=m=1), δ=0.5, $V_0=V_1=V_2$ = 2 and $V_3$ = 0.5.

| N | ℓ | E(eV) |
|---|---|---|
| 0 | 0 | 0.54974 |
| 1 | 0 | 0.88622 |
| 1 | 1 | 0.94864 |
| 2 | 0 | 0.94869 |
| 2 | 1 | 0.97056 |
| 2 | 2 | 0.98070 |
| 3 | 0 | 0.97058 |
| 3 | 1 | 0.98071 |
| 3 | 2 | 0.98622 |
| 3 | 3 | 0.98954 |
| 4 | 0 | 0.98072 |

| | | |
|---|---|---|
| 4 | 1 | 0.98622 |
| 4 | 2 | 0.98954 |
| 4 | 3 | 0.99170 |
| 4 | 4 | 0.99318 |
| 5 | 0 | 0.98623 |
| 5 | 1 | 0.98954 |
| 5 | 2 | 0.99170 |
| 5 | 3 | 0.99318 |
| 5 | 4 | 0.99424 |
| 5 | 5 | 0.99502 |

## Conclusion:-

In the present study, we solved the Schrodinger equation with the Eckart plus Hulthén potential and a class of Yukawa using the Parametric Nikiforov-Uvarov method. The eigenenergies and the corresponding wave functions were obtained. The calculated energy allowed us to compute the partition function. From this, thermodynamic properties such as the average energy U(β), specific heat C(β), free energy F(β), and entropy S(β) were determined. It was found that, in thermodynamic contexts, these properties are not applicable to molecules. As a result, disorder is high for small values of β, and increasing β leads to a significant decrease in disorder in the system.

**Data Availability Statement**:
No Data associated in the manuscript.

**Author Contribution Statement:**
All authors contributed equally to this work. They actively participated in the study design, data analysis, manuscript writing, and revision. This equal contribution also includes the validation of results and final approval of the version submitted for publication.

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