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## ENERGY SPECTRA, EXPECTATION VALUES, AND THERMODYNAMIC PROPERTIES OF HCl AND LiH DIATOMIC MOLECULES

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**Abstract.** The Schrödinger equation is solved by applying the Nikiforov-Uvarov-Functional Analysis method to the Hulthén plus screened Kratzer Potential. The Greene-Aldrich approximation is employed to determine the closed form expressions for the energy equation and the wave function. The Hellmann-Feynman theorem was employed to calculate the energy spectra and expectation values of various quantum states for diatomic molecules of HCl and LiH. Subsequently, we employed the energy equation that we had previously derived to compute the partition function, which in turn enabled us to determine the thermodynamic properties associated with the diatomic molecules. The partition function for the diatomic molecules of  $H_2$  and LiH was calculated at different temperatures. The results indicate that the partition function of the two diatomic molecules rose as the temperature increased. The findings we obtained align with the results documented in the literature.

**Keywords:** Greene-Aldrich approximation, Bound State; Hellmann-Feynman theorem; Thermodynamic properties.

### 1. Introduction

The partition function (PF) which is dependent on temperature, enables the investigation of the thermodynamic properties (TPs) of a system. The partition function, widely employed in molecular physics and statistical physics, facilitates the computation of various thermodynamic properties such as entropy, specific heat capacity, mean free energy, and others [1]. To analyze the behavior of non-relativistic particles in quantum mechanics, including the properties of the system's elementary particles and the mass distribution of mesons, the Schrodinger equation (SE) needs to be solved [2,3]. Several scholars [4–10] have examined these solutions, exploring a range of potential functionalities. The utilization of computational methods to solve the SE is of great significance in understanding the behavior of non-relativistic particles in the realm of quantum science. Consequently, numerous researchers have recognized the high importance of solving this equation. Utilizing these techniques is crucial for evaluating the thermodynamic properties of the entire structure, as well as the mass distribution of mesons and other related phenomena. To analyze the SE with different potentials, several methods have been employed, such as the asymptotic iteration method (AIM) [11], the Nikiforov-Uvarov Functional Analysis (NUFA) technique [12], and others [13, 14]. Lately, theorists have shown increasing interest in examining the energy of bound states in various diatomic molecules (DMs) using both a lone potential and collective potential functions [15–20]. For example, Inyang

et al. [21] investigated a small number of DMs by employing the Eckart and Hellmann potential model. In addition, Obogo et al. [22] examined several dynamical models with a q-deformed Hulthén potential combined with a quadratic exponential-type potential. Edet and Ikot [23] also analyzed a selected few DMs with the Deng-Fan (DF) potential. In addition, Edet et al. [24] calculated several diatomic molecules using the DF plus Eckart potential. We have utilized the Hulthén plus screened Kratzer potential (HSKP) to investigate the HCl and LiH diatomic molecules through the SE using the newly suggested NUFA method, taking into consideration the previous research conducted by certain scholars. To analyze the interaction between two particles, the Hulthén potential (HP) [25] is employed. The application of this concept extends to diverse fields including condensed matter, nuclear, particle, chemical, atomic, and molecular physics [26, 27]. Conversely, Ikot et al. [28] introduced the screened Kratzer potential (SKP), a model widely employed in molecular physics and used by several authors in the literature [29, 30]. The goal of this study is to solve the SE using the HSKP and applying the NUFA method. The purpose is to analyze the energy spectra, expectation values, and thermodynamic properties of diatomic molecules of HCl and LiH.

Utilizing two potential functions enhances the potential strength (PS) for improved outcomes [31]. The combined potential is as follows:

$$V(r_1) = -\frac{Z_I e^{-\vartheta_1 r_1}}{1 - e^{-\vartheta_1 r_1}} - \frac{Z_{II} e^{-\vartheta_1 r_1}}{r_1} + \frac{Z_{III} e^{-\vartheta_1 r_1}}{r_1^2} \quad (1)$$

where  $Z_I$  is the PS the HP,  $\vartheta_1$  is the screening parameter. The letter  $Z_{II} \equiv 2D_e r_e$  and  $Z_{III} \equiv D_e r_e^2$ . In this case, the equilibrium bond length is  $r_e$ , and the dissociation energy is  $D_e$ .

## 2. Review of the NUFA Technique

The NUFA technique is a work conducted by Ikot et al. [12] that presents a modern methodology for resolving a second-order differential equation. It is straightforward and refined. This technique combines the factorization, parametric NU, and NU approaches.

$$\psi_I''(y) + \frac{\tilde{\tau}_I(y)}{\sigma_I(y)} \psi_I'(y) + \frac{\tilde{\sigma}_I(y)}{\sigma_I^2(y)} \psi_I(y) = 0 \quad (2)$$

where  $\tilde{\sigma}_I(y)$  and  $\sigma_I(y)$  are quadratic polynomials, while  $\tilde{\tau}_I(y)$  is a linear polynomial. Tezcan and Sever [32] subsequently presented the parametric formulation of the NU technique as follows:

$$\psi_I'' + \frac{\beta_I - \beta_{II}y}{y(1 - \beta_{III}y)} \psi_I' + \frac{1}{y^2(1 - \beta_{III}y)^2} [-\xi_I y^2 + \xi_{II} y - \xi_{III}] \psi_I(y) = 0, \quad (3)$$

where  $\beta_i$  and  $\xi_i (i = I, II, III)$  are all parameters. We consider the wave function in the specified form (Eq. 4) due to the presence of two singularities at points  $y \rightarrow 0$  and  $y \rightarrow 1$  in the differential equation mentioned in Eq. (3).  $y \rightarrow 0$  and  $y \rightarrow 1$ .

$$\psi_I(y) = y^\lambda (1 - y)^\nu f(y) \quad (4)$$

Equation that results from substituting Eq. (4) into Eq. (3) is as follows:

$$\begin{aligned}
 & y(1 - \beta_{III}y) f''(y) + [\beta_I + 2\lambda - (2\lambda\beta_{III} + 2v\beta_{III} + \beta_{II})y] f'(y) \\
 & - \beta_{III} \left( \lambda + v + \frac{\beta_{II}}{\beta_{III}} - 1 + \sqrt{\left(\frac{\beta_{II}}{\beta_{III}} - 1\right)^2 + \frac{\xi_I}{\beta_{III}}} \right) \\
 & \left( \lambda + v + \frac{\beta_{II}}{\beta_{III}} - 1 + \sqrt{\left(\frac{\beta_{II}}{\beta_{III}} - 1\right)^2 + \frac{\xi_I}{\beta_{III}^2}} \right) f(y) \\
 & + \left[ \frac{\lambda(\lambda - 1) + \beta_I\lambda - \xi_{III}}{y} + \frac{\beta_{II}v - \beta_I\beta_{III}v + v(v - 1)\beta_{III} - \frac{\xi_I}{\beta_{III}} + \xi_{II} - \xi_{III}\beta_{III}}{(1 - \beta_{III}y)} \right] f(y) = 0.
 \end{aligned} \tag{5}$$

Equation (5) can be simplified to a Gauss hypergeometric equation if and only if the subsequent functions are removed:

$$\lambda(\lambda - 1) + \beta_I\lambda - \xi_{III} = 0, \tag{6}$$

and

$$\beta_{II}v - \beta_I\beta_{III}v + v(v - 1)\beta_{III} - \frac{\xi_I}{\beta_{III}} + \xi_{II} - \xi_{III}\beta_{III} = 0. \tag{7}$$

Thus, it becomes

$$\begin{aligned}
 & y(1 - \beta_Iy) f''(y) + [\beta_I + 2\lambda - (2\lambda\beta_{III} + 2v\beta_{III} + \beta_{II})y] f'(y) \\
 & - \beta_{III} \left( \lambda + v + \frac{\beta_{II}}{\beta_{III}} - 1 + \sqrt{\left(\frac{\beta_{II}}{\beta_{III}} - 1\right)^2 + \frac{\xi_I}{\beta_{III}}} \right) \left( \lambda + v + \frac{\beta_{II}}{\beta_{III}} - 1 + \sqrt{\left(\frac{\beta_{II}}{\beta_{III}} - 1\right)^2 + \frac{\xi_I}{\beta_{III}^2}} \right) f(y) = 0.
 \end{aligned} \tag{8}$$

Upon resolving equations (6) and (7), equations (9) and (10) are transformed into the following expressions:

$$\lambda = \frac{(1 - \beta_I)}{2} \pm \frac{1}{2} \sqrt{(1 - \beta_I)^2 + 4\xi_{III}} \tag{9}$$

$$v = \frac{(\beta_{III} + \beta_I\beta_{III} - \beta_{II}) \pm \sqrt{(\beta_{III} + \beta_I\beta_{III} - \beta_{II})^2 + \left(\frac{\xi_I}{\beta_{III}} + \beta_{III}\xi_{III} - \xi_{II}\right)}}{2} \tag{10}$$

Equation (8) features a hypergeometric equation in the form of a type

$$y(1 - y) f''(y) + [c_I + (a_I + b_I + 1)y] f'(y) - a_I b_I f(y) = 0 \tag{11}$$

Equations (4), (8), and (11), respectively, are used to obtain the energy equation and the associated wave equation for the NUFA technique:

$$\lambda^2 + 2\lambda \left( v + \frac{\beta_{II}}{\beta_{III}} - 1 + \frac{n}{\sqrt{\beta_{III}}} \right) + \left( v + \frac{\beta_{II}}{\beta_{III}} - 1 + \frac{n}{\sqrt{\beta_{III}}} \right)^2 - \left( \frac{\beta_{II}}{\beta_{III}} - 1 \right)^2 - \frac{\xi_I}{\beta_{III}^2} = 0, \tag{12}$$

$$\begin{aligned}
 \psi(y) = Ny & \frac{(1 - \beta_I) + \sqrt{(1 - \beta_I)^2 + 4\xi_{III}}}{2} \\
 & \frac{(\beta_{III} + \beta_I\beta_{III} - \beta_{II}) + \sqrt{(\beta_{III} + \beta_I\beta_{III} - \beta_{II})^2 + \left(\frac{\xi_I}{\beta_{III}} + \beta_{III}\xi_{III} - \xi_{II}\right)}}{2} {}_2F_1(p_1, p_2, p_3; y),
 \end{aligned} \tag{13}$$

where  $p_1, p_2,$  and  $p_3$  are given as follows;

$$p_1 = \sqrt{\beta_{III}} \left( \lambda + \nu + \frac{\beta_{II}}{\beta_{III}} - 1 + \sqrt{\left( \frac{\beta_{II}}{\beta_{III}} - 1 \right)^2 + \frac{\xi_I}{\beta_{III}}} \right) \quad (14)$$

$$p_2 = \sqrt{\beta_{III}} \left( \lambda + \nu + \frac{\beta_{II}}{\beta_{III}} - 1 - \sqrt{\left( \frac{\beta_{II}}{\beta_{III}} - 1 \right)^2 + \frac{\xi_I}{\beta_{III}}} \right) \quad (15)$$

$$p_3 = \beta_I + 2\lambda \quad (16)$$

### 3. The Schrodinger equation solutions using the HSKP

The SE reads [1]

$$\frac{d^2 \psi_l(r_1)}{dr_1^2} + \left[ \frac{2\mu}{\hbar^2} (E_{nl} - V(r_1)) - \frac{l(l+1)}{r_1^2} \right] \psi_l(r_1) = 0, \quad (17)$$

where  $\psi_n(r)$  is the Eigen functions,  $E_n$  is the energy eigenvalues, The system's reduced mass is denoted by  $\mu$ , the reduced Planck's constant by  $\hbar$ , and the radial distance by  $r_1$ .

Equation (17) is solved using the Greene-Aldrich approximation (GAA) [33] in order to get past the centrifugal barrier. This GAA, which is expressed as follows, is a better approximation to the centrifugal barrier and is valid for  $\vartheta_l \ll 1$ ,

$$\frac{1}{r_1^2} \approx \frac{\vartheta_l^2}{(1 - e^{-\vartheta_l r_1})^2}. \quad (18)$$

Equations. (1) and (18) are substituted into Eq. (17) to obtain Eq. (19).

$$\frac{d^2 \psi_l(r_1)}{dr_1^2} + \left[ \frac{2\mu E_{nl}}{\hbar^2} + \frac{2\mu Z_I e^{-\vartheta_l r_1}}{\hbar^2 (1 - e^{-\vartheta_l r_1})} + \frac{2\mu Z_{II} \vartheta_l e^{-\vartheta_l r_1}}{\hbar^2 (1 - e^{-\vartheta_l r_1})} - \frac{2\mu Z_{III} \vartheta_l^2 e^{-\vartheta_l r_1}}{\hbar^2 (1 - e^{-\vartheta_l r_1})^2} - \frac{\vartheta_l^2 l(l+1)}{(1 - e^{-\vartheta_l r_1})^2} \right] \psi_l(r_1) = 0 \quad (19)$$

$$\text{Let, } y = e^{-\vartheta_l r_1} \quad (20)$$

Equation (20) yields Eq. (21) as

$$\frac{d^2 \psi_l(r)}{dr^2} = \vartheta_l^2 y^2 \frac{d^2 \psi_l(y)}{dy^2} + \vartheta_l^2 y \frac{d\psi_l(y)}{dy} \quad (21)$$

Following a number of simplifications and the integration of Eqs. (20) and (21) into Eq. (19), we obtain:

$$\frac{d^2 \psi_l(y)}{dy^2} + \frac{1-y}{y(1-y)} \frac{d\psi_l(y)}{dy} + \frac{1}{y^2(1-y)^2} \left[ -(\varepsilon + \eta_I) y^2 + (2\varepsilon + \eta_I - \eta_{II}) y - (\varepsilon + \gamma) \right] \psi_l(y) = 0, \quad (22)$$

where

$$-\varepsilon = \frac{2\mu E_{nl}}{\vartheta_l^2 \hbar^2}, \quad \eta_I = \frac{2\mu Z_I}{\vartheta_l^2 \hbar^2} + \frac{2\mu Z_{II}}{\vartheta_l \hbar^2}, \quad \eta_{II} = \frac{2\mu Z_{III}}{\hbar^2}, \quad \gamma = l(l+1) \quad (23)$$

Combining Eqs. (22) and (3) yields the following:

$$\beta_I = \beta_{II} = \beta_{III} = 1, \quad \xi_I = \varepsilon + \eta_I, \quad \xi_{II} = 2\varepsilon + \eta_I - \eta_{II}, \quad \xi_{III} = \varepsilon + \gamma \quad (24)$$

Equation (24) is inserted into equations (9) and (10) to produce

$$\lambda = \frac{1}{2} \sqrt{4(\varepsilon + \gamma)} \quad (25)$$

$$y = \frac{1 + \sqrt{1 + 4(\eta_{II} + \gamma)}}{2}$$

(26)

Furthermore, the HSKP energy equation is obtained as follows when Eq. (12) is substituted with Eqs. (23), (24), (25), and (26).

$$E_{nl} = \frac{\vartheta_l^2 \hbar^2 l(l+1)}{2\mu} - \frac{\vartheta_l^2 \hbar^2}{8\mu} \left[ \frac{\left( n + \frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2 - \frac{2\mu Z_I}{\vartheta_l^2 \hbar^2} + \frac{4\mu D_e r_e}{\hbar^2 \vartheta_l} + l(l+1)}{n + \frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}} \right]^2. \quad (27)$$

To obtain the appropriate unnormalized wave function, Eq. (13) is substituted with Eq. (24) and the result is given as

$$\psi_l(y) = N \frac{\sqrt{4(\varepsilon + \gamma)}}{2} \times (1-y)^{\frac{1 + \sqrt{1 + \eta_{II} + \gamma}}{2}} {}_2F_1(p_1, p_2, p_3; y) \quad (28)$$

where,

$$p_1 = \sqrt{\varepsilon + \gamma} + \frac{1 + \sqrt{1 + \eta_{II} + \gamma}}{2} + \sqrt{\varepsilon + \eta_I} \quad (29)$$

$$p_2 = \sqrt{\varepsilon + \gamma} + \frac{1 + \sqrt{1 + \eta_{II} + \gamma}}{2} - \sqrt{\varepsilon + \eta_I} \quad (30)$$

$$p_3 = 1 + 2\sqrt{\varepsilon + \gamma} \quad (31)$$

### 3.1 Special cases of the HSKP

1. We possess the HP described in Equation (32) and its corresponding energy equation as stated in Equation (33) for the case  $Z_{II} = Z_{III} = 0$ .

$$V(r_1) = -\frac{Z_I e^{-\vartheta_l r_1}}{1 - e^{-\vartheta_l r_1}} \quad (32)$$

$$E_{nl} = \frac{\vartheta_l^2 \hbar^2 l(l+1)}{2\mu} - \frac{\vartheta_l^2 \hbar^2}{8\mu} \left[ \frac{(n+l+1)^2 - \frac{2\mu Z_I}{\vartheta_l^2 \hbar^2} + l(l+1)}{n+l+1} \right]^2. \quad (33)$$

Equation (33) and Equation (32) of [4] agree.

2. We possess the SKP described in Equation (34) and its corresponding energy equation as stated in Equation (35) for the case  $Z_I = 0$ .

$$V(r_1) = -\frac{Z_{II} e^{-\vartheta_l r_1}}{r_1} + \frac{Z_{III} e^{-\vartheta_l r_1}}{r_1^2} \quad (34)$$

$$E_{nl} = \frac{\vartheta_l^2 \hbar^2 l(l+1)}{2\mu} - \frac{\vartheta_l^2 \hbar^2}{8\mu} \left[ \frac{\left( n + \frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2 + \frac{4\mu D_e r_e}{\hbar^2 \vartheta_l} + l(l+1)}{n + \frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}} \right]^2. \quad (35)$$

The results of Equation (35) and Eq. (29) of [28] agree.

3. When setting  $Z_I = \vartheta_I = 0$  is used, the Kratzer potential (KP) is represented by Equation (36), and the energy equation for the KP is given by Equation (37).

$$V(r_1) = -\frac{Z_{II}}{r_1} + \frac{Z_{III}}{r_1^2} \quad (36)$$

$$E_{nl} = -\frac{2\mu D_e^2 r_e^2}{\hbar^2 \left( n + \frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right)^2} \quad (37)$$

Equation (37) and Eq. (46) of [28] are identical;

#### 4. The expectation values of HSKP via the Hellmann-Feynman theorem

The expectation values of different quantum systems are derived by utilizing the Hellmann-Feynman Theorem (HFT) [5,17,21]. Suppose that the Hamiltonian of a specific quantum system is dependent on a parameter. Let the eigenvalues and eigenfunctions of the Hamiltonian  $\hat{H}(q_I)$  be  $E(q_I)$  and  $\Psi(q_I)$ , respectively. The HFT states that

$$\frac{\partial E_{nl}(q_I)}{\partial q_I} = \langle \Psi_{nl}(q_I) | \frac{\partial \hat{H}(q_I)}{\partial q_I} | \Psi_{nl}(q_I) \rangle \quad (38)$$

The effective Hamiltonian has the following form:

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr_1^2} - \frac{\hbar^2}{\mu r_1} \frac{d}{dr_1} + \frac{\hbar^2}{2\mu r_1^2} l(l+1) - \frac{Z_I e^{-\vartheta_I r_1}}{1 - e^{-\vartheta_I r_1}} - \frac{Z_{II} e^{-\vartheta_I r_1}}{r_1} + \frac{Z_{III} e^{-\vartheta_I r_1}}{r_1^2} \quad (39)$$

##### 4.1 Expectation value of $\langle r_1^{-2} \rangle$

The expectation value (EV) of  $\langle r_1^{-2} \rangle$  is obtain when replacing  $q_I = l$  in Eq. (38) and by taking the partial derivative (PD) of Eq. (27) with respect to  $l$ , then equating the resulting equations yields the EV of  $\langle r_1^{-2} \rangle$  as:

$$\langle r_1^{-2} \rangle = \vartheta_l \left[ \frac{4\mu BV}{\hbar^2 (2l+1)} \frac{1}{2\sqrt{F}} - \frac{\left\{ \left( n + \frac{1}{2} + \sqrt{F} \right) (2l+1) + \left( + \frac{2Z_I \mu}{\hbar^2 \vartheta_l^2} + \frac{4\mu D_e r_e}{\hbar^2 \vartheta_l} + l(l+1) \right) \frac{1}{2\sqrt{F}} (2l+1) \right\}}{\left( n + \frac{1}{2} + \sqrt{F} \right)^2} \right] \quad (40)$$

#### 4.2 Expectation values for $\langle T \rangle$ and $\langle \hat{P}^2 \rangle$

The EV of  $\langle T \rangle$  and  $\langle \hat{P}^2 \rangle$  are obtain when replacing  $q = \mu$  in Eq. (38) and by taking the PD of Eq. (39) with respect to  $\mu$ , which implies  $-\frac{1}{\mu}\langle T \rangle = -\frac{1}{\mu}(H - V)$ . From the relation  $T = \frac{P^2}{2\mu}$ , we substitute for  $T$  in  $-\frac{1}{\mu}\langle T \rangle = -\frac{1}{\mu}(H - V)$  which yields

$$\langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle = -\frac{1}{\mu} \langle T \rangle \quad (41)$$

Putting  $-\frac{1}{\mu}\langle T \rangle = -\frac{1}{2\mu^2}\langle \hat{P}^2 \rangle$  into Eq. (41) yields

$$\langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle = -\frac{1}{2\mu^2} \langle \hat{P}^2 \rangle \quad (42)$$

The PD of Eq. (27) with respect to  $\mu$  gives

$$\frac{\partial E_{nl}(\mu)}{\partial \mu} = -\frac{\vartheta_l \hbar^2 l(l+1)}{2\mu^2} + 2BV \left[ \frac{\frac{D_e r_e^2}{\hbar^2 \sqrt{F}} - \left\{ \left( n + \frac{1}{2} + \sqrt{F} \left( \frac{2Z_1}{\vartheta_l^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta_l} \right) \right) - \left( \frac{2Z_1}{\vartheta_l^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta_l} + l(l+1) \right) \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} \right\}}{\left( n + \frac{1}{2} + \sqrt{F} \right)^2} \right] \quad (43)$$

Eqs. (41) and (43) must be solved to obtain the EV of  $\langle T \rangle$ .

Hence,

$$\langle T \rangle = \frac{\vartheta_l \hbar^2 l(l+1)}{2\mu} - \frac{\hbar^2 \vartheta_l^2 \mu}{4\mu^2} V \left[ \frac{\frac{D_e r_e^2}{\hbar^2 \sqrt{F}} - \left\{ \left( n + \frac{1}{2} + \sqrt{F} \left( \frac{2Z_1}{\vartheta_l^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta_l} \right) \right) - \left( \frac{2Z_1}{\vartheta_l^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta_l} + l(l+1) \right) \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} \right\}}{\left( n + \frac{1}{2} + \sqrt{F} \right)^2} \right] \quad (44)$$

Also, Eqs. (42) and (43) must be solved to obtain the EV of  $\langle \hat{P}^2 \rangle$ .

Hence,

$$\langle \hat{P}^2 \rangle = \vartheta_l \hbar^2 l(l+1) - \frac{\hbar^2 \vartheta_l^2}{2} V \left[ \frac{\frac{D_e r_e^2}{\hbar^2 \sqrt{F}} - \left\{ \left( n + \frac{1}{2} + \sqrt{F} \left( \frac{2Z_1}{\vartheta_l^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta_l} \right) \right) - \left( \frac{2Z_1}{\vartheta_l^2 \hbar^2} + \frac{4D_e r_e}{\hbar^2 \vartheta_l} + l(l+1) \right) \frac{D_e r_e^2}{\hbar^2 \sqrt{F}} \right\}}{\left( n + \frac{1}{2} + \sqrt{F} \right)^2} \right] \quad (45)$$

### 5. Thermodynamic properties

An essential thermodynamic variable that enables the calculation of additional thermal properties for the system is the partition function (PF). The Boltzmann-Gibbs partition function reads [1]

$$Z(\beta) = \sum_{n=0}^{\lambda} e^{-\beta E_n} \quad \beta = \frac{1}{k_B T} \quad (46)$$

where  $k_B$ ,  $\lambda$  and  $T$  are the respective Boltzmann constant, maximum vibrational and the absolute temperature.

In the classical limit, the PF may be expressed as an integral at high temperatures.

$$Z(\beta) = \int_0^{\lambda} e^{-\beta E_n} dn \quad (47)$$

Further simplification of the energy equation in Eq.(27) is as follows:

$$E_n = Q_0 - Q_1 \left( n + \Delta + \frac{Q_2}{n + \Delta} \right)^2 = \Lambda - \left( Q_1 \rho^2 + \frac{Q_1 Q_2^2}{\rho^2} \right) \quad (48)$$

where

$$\Lambda = Q_0 + 2Q_1 Q_2$$

$$\rho = n + \Delta$$

$$Q_0 = \frac{\vartheta_l^2 \hbar^2 l(l+1)}{2\mu}$$

$$Q_1 = \frac{\vartheta_l^2 \hbar^2}{8\mu}$$

$$Q_2 = \frac{2\mu Z_l}{\vartheta_l^2 \hbar^2} - \frac{4\mu D_e r_e}{\vartheta_l \hbar^2} - l(l+1)$$

$$\Delta = \frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}$$

The maximum vibration principal quantum number is obtained as  $\lambda = -\Delta + \sqrt{Q_2}$

Inserting Eq. (48) into (47) and performing the integration with MAPLE software yields the PF

$$Z(\beta) = \frac{e^{-\beta Q_0} \sqrt{\pi}}{\Upsilon_3 \sqrt{\beta}} \left( e^{\Upsilon_0 \beta} \left( \operatorname{erf}(\Upsilon_1 \sqrt{\beta}) - 1 \right) + \operatorname{erf}(\Upsilon_2 \sqrt{\beta}) + 1 \right) \quad (49)$$

where

$$\Upsilon_0 = 4Q_0 Q_1$$

$$\Upsilon_1 = \sqrt{-Q_1} \left( \rho + \frac{Q_2}{\rho} \right), \Delta < \rho < \sqrt{Q_2}$$

$$\Upsilon_2 = \sqrt{-Q_1} \left( \rho - \frac{Q_2}{\rho} \right), \Delta < \rho < \sqrt{Q_2}$$

$$\Upsilon_3 = \sqrt{-Q_1}$$

Using Eq. (49) other thermodynamic relations are found as follows:

(a) vibrational mean energy

$$U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta} \quad (50)$$

(b) Vibrational specific heat capacity

$$C(\beta) = k_B \beta^2 \left( \frac{\partial^2 \ln Z(\beta)}{\partial^2 \beta} \right) \quad (51)$$

(c) Vibrational free energy

$$F(\beta) = -k_B T \ln Z(\beta) \quad (52)$$

(d) Vibrational entropy

$$S(\beta) = k_B \ln Z(\beta) - k_B \beta \frac{\partial \ln Z(\beta)}{\partial \beta} \quad (53)$$

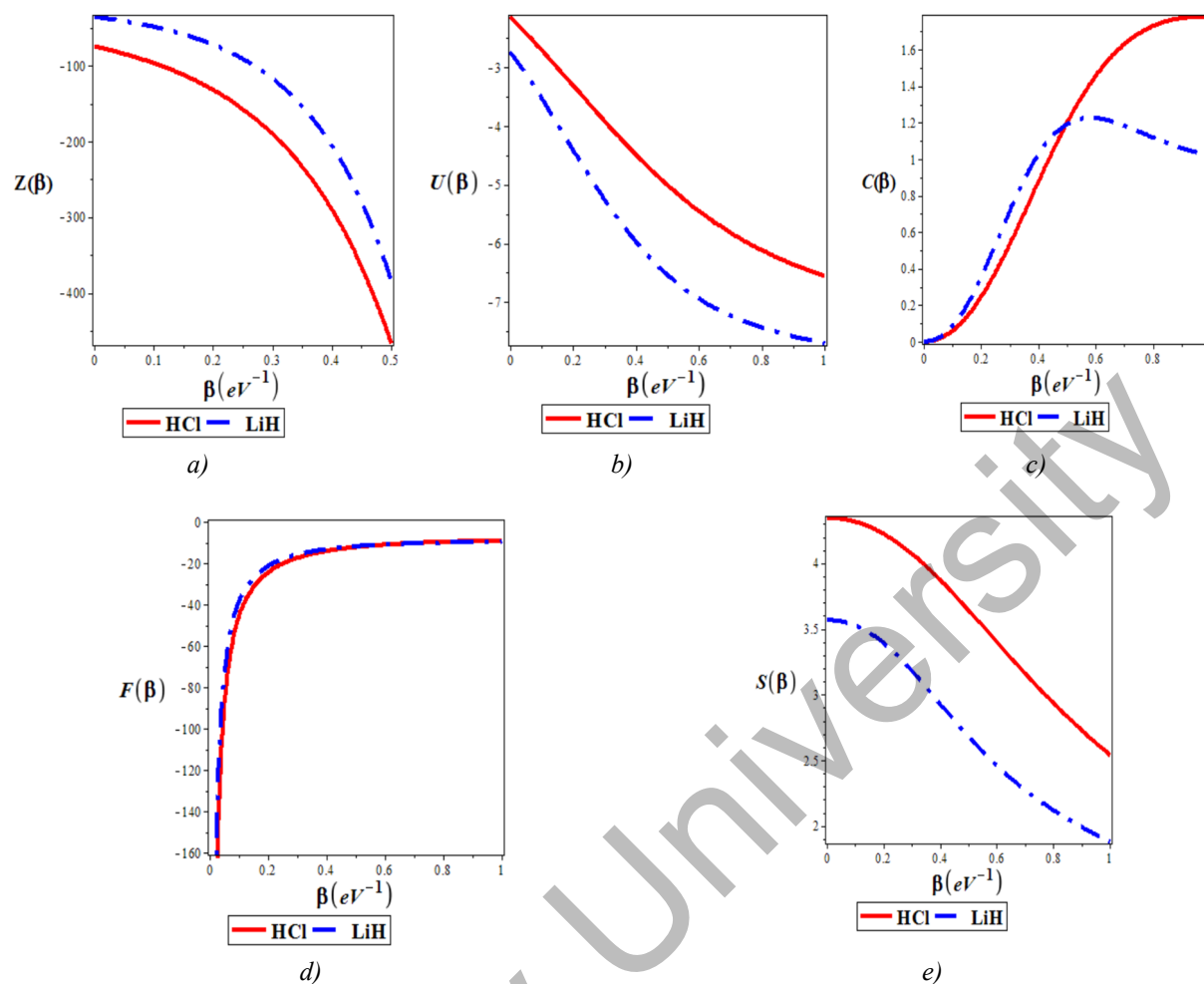
## 6. Results and Discussion

The experimental results from Ref. [1,5], which are shown in Table 1, were applied using Eq. (27), together with the conversion  $\hbar c = 1973.29 \text{ eV \AA}$  [5]. As shown in Tables 2 and 3, we calculated the energy spectra of the HSKP for HCl and LiH diatomic molecules. For each vibrational quantum number, it has been found that, for each of the diatomic molecules, the vibrational energies rise in proportion to the increase in the rotational quantum number. In addition, the HFT technique was employed to analyze the expectation value (EV) of  $\langle r_1^{-2} \rangle$ ,  $\langle T \rangle$  and  $\langle \hat{P}^2 \rangle$ . The resulting numerical calculations for the selected diatomic molecules are presented in Tables 2 and 3. The results indicate that the expectation value of  $\langle r_1^{-2} \rangle$  decreases as the vibrational quantum number increases. Additionally, for the chosen diatomic molecules, the expectation value of  $\langle T \rangle$  and  $\langle \hat{P}^2 \rangle$  rise as the rotational quantum number rises for each vibrational quantum number. Table 4 shows how temperature affects partition function for H<sub>2</sub> and LiH diatomic molecules. The partition function of the two diatomic molecules increases with temperature. Engineers can use this prediction because hydrogen (H<sub>2</sub>) is a vital gas with many industrial and technological uses.

**Table 1.** Parameters of selected diatomic molecules [1,5]

Molecules	$D_e \text{ (eV)}$	$\alpha = v \text{ (\AA}^{-1}\text{)}$	$r_e \text{ (\AA)}$	$\mu \text{ (MeV)}$
HCl	4.6190309050	1.86770	1.2746	0.09129614886
LiH	2.5152672118	1.12800	1.5956	0.08198284801
H <sub>2</sub>	4.7446000000	1.94260	0.7416	0.503910

The plots of thermodynamic properties for HCl and LiH molecules are shown in Figure 1 (a–e) as a function of the thermodynamic parameter ( $\beta$ ). As  $\beta$  is raised, it can be seen in (a) that the PF of the diatomic molecules decreases. The internal energy of the molecules with  $\beta$  is displayed in (b), as can be observed. In this instance, when  $\beta$  is raised, the molecules' internal energy drops. The molecules' specific heat capacity is seen in (c). Each molecule of specific heat capacity rises as  $\beta$  is raised. The plot of the free energy's behavior as a function of  $\beta$  are shown in (d). For each diatomic molecule, we observed that the free energy rises with a rise in  $\beta$  and converges at a particular point. We display a graph of the diatomic molecules' entropy as a function of  $\beta$  as is seen in (e). It has been shown that as  $\beta$  is raised, each diatomic molecules entropy reduces.



**Fig.1 (a-e).** Thermodynamic properties as a function of thermodynamic beta parameter for HCl and LiH molecules. Red line (-) represent HCl and blue line (-) represent LiH.

## 7. Conclusion

The HSKP was used to study the energy eigenvalues and expectation value of LiH and HCl diatomic molecules. The NUFA methodology and HFT were employed, along with the Greene-Aldrich approximation. The findings demonstrated a positive correlation between the quantum numbers and the elevation of energy eigenvalues and expectation value. This suggests that quantum numbers exert a substantial influence on the energy levels of these molecules. In addition, the PF of the system was calculated, followed by the determination of other thermodynamic properties. Our findings align with the results of previous studies. Additional investigation in this field can yield valuable knowledge about diverse physical systems, encompassing atoms, molecules, and condensed matter systems. We calculated the partition function for two diatomic molecules ( $H_2$  and LiH) at different temperatures. With increasing temperature, the partition function of the two diatomic molecules increases. Because hydrogen ( $H_2$ ) is a vital gas with many industrial and technological uses, this prediction can help engineers.

### Conflict of interest statement

The authors declare that they have **no conflict of interest** in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

### CRedit author statement

Inyang E. P.: Conceptualization, Methodology, Writing- Original draft preparation, Funding acquisition; Ali N.: Software, Data curation, Funding acquisition; Endut R.: Visualization, Investigation; Aljunid S.A.: Validation, Supervision, Writing- Reviewing and Editing. The final manuscript was read and approved by all authors.

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## Appendix A

**Table 2.** Energy spectra and expectation values of the HSKP for HCl molecule

$n$	$l$	$E_{nl}$ (eV)	$\langle r_1^{-2} \rangle (\text{\AA})^{-2}$	$\langle T \rangle$ (eV)	$\langle P^2 \rangle (\text{eV}/c)^2$
0	0	-22.17032494	1.4461305900	-1.527357607	-0.2430954250
0	1	-22.17022128	0.4934942126	-1.527879485	-0.2365343415
0	2	-22.17001432	0.3089006158	-1.528850921	-0.2230060212
0	3	-22.16970474	0.2328634781	-1.530131019	-0.2018428796
0	4	-22.16929354	0.1919356503	-1.531517495	-0.1723326932
0	5	-22.16878209	0.1661204903	-1.532756774	-0.1339118832
1	0	-22.24690799	1.5187697310	-1.512273934	-0.2397598466
1	1	-22.24679078	0.5157465898	-1.512585935	-0.2328013301
1	2	-22.24655670	0.3200992442	-1.513146168	-0.2185951989
1	3	-22.24620649	0.2388704404	-1.513830364	-0.1966640774
1	4	-22.24574126	0.1949209917	-1.514459993	-0.1664947819
1	5	-22.24516244	0.1672300249	-1.514811074	-0.1276768573
2	0	-22.33432382	1.5676664310	-1.499019961	-0.2380244021
2	1	-22.33419477	0.5306022009	-1.499146722	-0.2307718818
2	2	-22.33393705	0.3274233022	-1.499343883	-0.2160599846
2	3	-22.33355145	0.2426244599	-1.499501576	-0.1935463559
2	4	-22.33303911	0.1965821729	-1.499461878	-0.1628618456
2	5	-22.33240157	0.1675873809	-1.499026507	-0.1237106879
3	0	-22.43212310	1.6000110030	-1.487438213	-0.2375700761
3	1	-22.43198398	0.5402950041	-1.487400766	-0.2300928725
3	2	-22.43198398	0.3320371224	-1.487275955	-0.2149910763
3	3	-22.43129039	0.2447983109	-1.486966448	-0.1920208669

**Table 3.** Energy spectra and expectation values of the HSKP for LiH molecule

$n$	$l$	$E_{nl}$ (eV)	$\langle r_1^{-2} \rangle \left( \frac{\text{\AA}}{\text{\AA}} \right)^{-2}$	$\langle T \rangle$ (eV)	$\langle P^2 \rangle (\text{eV}/c)^2$
0	0	-9.044861721	0.48384419100	-1.529859845	-2.733360767
0	1	-9.044847651	0.16604146380	-1.531954979	-2.742387859
0	2	-9.044819582	0.10527772010	-1.536098894	-2.751403066
0	3	-9.044777634	0.08115099160	-1.542199980	-2.764720459
0	4	-9.044722014	0.06914333150	-1.550123565	-2.782099026
0	5	-9.044652964	0.06254753050	-1.559695049	-2.803226301
1	0	-9.033844252	0.60792631400	-1.518791268	-2.718030441
1	1	-9.033836790	0.20701468020	-1.520693254	-2.722233863
1	2	-9.033821914	0.12940273500	-1.524454369	-2.730564012
1	3	-9.033799708	0.09790208600	-1.529989917	-2.742869320
1	4	-9.033770284	0.08168807260	-1.537175349	-2.758926885
1	5	-9.033733821	0.07233546910	-1.545849125	-2.778447621
2	0	-9.029306244	0.71587103800	-1.508675050	-2.699926444
2	1	-9.029304880	0.24265837200	-1.510399495	-2.703812140
2	2	-9.029302176	0.15038870280	-1.513808697	-2.711512506
2	3	-9.029298171	0.11247235160	-1.518824211	-2.722887159
2	4	-9.029292928	0.09259811150	-1.525330645	-2.737729591
2	5	-9.029286529	0.08084615000	-1.525330645	-2.755771878
3	0	-9.030892408	0.81001512100	-1.499451470	-2.683419916
3	1	-9.030896786	0.27374373700	-1.501012381	-2.687012953
3	2	-9.030905540	0.16868922100	-1.504097390	-2.694133144
3	3	-9.030918685	0.12517627150	-1.508633721	-2.704650248

**Table 4:** The partition function of the H<sub>2</sub> and LiH Diatomic Molecules

T(K)	LiH (Our work)	LiH [34]
2000	47.3888750	47.38997454
2100	48.3713842	48.37247223
2300	49.3314884	49.33159274
2400	50.2688135	50.26893405
2500	51.1858283	51.18591962
2600	52.9638837	52.96379383
2700	53.8269754	53.82686513
2800	54.6748887	54.67397768
T(K)	H <sub>2</sub> (Our work)	H <sub>2</sub> [34]
300	20.9471874	20.94709840
400	23.3731582	23.37304905
500	25.4964598	25.49634848
600	27.4086363	27.40872531
700	29.1632280	29.16311708
800	30.7934865	30.79338849
900	32.3228778	32.32276890
1000	33.7681845	33.76801939