EURASIAN PHYSICAL TECHNICAL JOURNAL

2024, Volume 21, No. 1 (47)

https://doi.org/10.31489/2024No1/124-137

Received: 26/01/2024 Revised: 22/02/2024 Accepted: 18/03/2024 Published online: 29/03/2024

Original Research Article

UDC: 530.145.61; 539.192; 539.194

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

Inyang E.P.[1,2], Ali N.R.[2,3], Endut R.[2,3], Aljunid S.A.[2,3]

[1] Department of Physics, National Open University of Nigeria, Jabi-Abuja, Nigeria
[2] Faculty of Electronic Engineering & Technology, Universiti Malaysia Perlis, Perlis, Malaysia
[3] Centre of Excellence Advanced Communication Engineering, Universiti Malaysia Perlis, Perlis, Malaysia
*Corresponding authors: etidophysics@gmail.com

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:

$$V\left(r_1\right)=-\frac{Z_I e^{-\vartheta_I r_1}}{1-e^{-\vartheta_I r_1}}-\frac{Z_{II} e^{-\vartheta_I r_1}}{r_1}+\frac{Z_{III} e^{-\vartheta_I r_1}}{r_1^2} \tag{1}$$

where Z_I is the PS the HP, ϑ_I 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.

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

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:

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

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

$$\psi_I(y)=y^{\lambda}\left(1-y\right)^{\nu} f(y) \tag{4}$$

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

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

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

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

and

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

Thus, it becomes

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

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

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

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

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

$$y^{\cdot}\left(1-y^{\cdot}\right)f''(y^{\cdot})+\left[c_I+\left(a_I+b_I+1\right)y^{\cdot}\right]f^{1}(y^{\cdot})-a_Ib_I\,f(y^{\cdot})=0 \tag{11}$$

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

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

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

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

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

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

$$p_3=\beta_I+2\lambda \tag{16}$$

3.The Schrodinger equation solutions using the HSKP

The SE reads [1]

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

where $\psi_n(r)$ is the Eigen functions, E_{nl} is the energy eigenvalues, The system's reduced mass is denoted by μ, 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 $\vartheta_I << 1$,

$$\frac{1}{r_1^2}\approx\frac{\vartheta_I{}^2}{\left(1-e^{-\vartheta_I r_1}\right)^2}. \tag{18}$$

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

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

Let, $y=e^{-\vartheta_I r_1}$ (20)

Equation (20) yields Eq. (21) as

$$\frac{d^2\psi_I(r)}{dr^2}=\vartheta_I{}^2y^2\frac{d^2\psi_I(y)}{dy^2}+\vartheta_I{}^2y\frac{d\psi_I(y)}{dy} \tag{21}$$

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

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

where

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

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

$$\left.\beta_I=\beta_{II}=\beta_{III}=1,\xi_I=\varepsilon+\eta_I,\xi_{II}=2\varepsilon+\eta_I-\eta_{II},\xi_{III}=\varepsilon+\gamma\right\} \tag{24}$$

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

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

.

$$v=\frac{1+\sqrt{1+4(\eta_{II}+\gamma)}}{2} \tag{26}$$

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

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

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

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

where,

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

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

$$p_3=1+2\sqrt{\varepsilon+\gamma}$$

(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 $Z_{II}=Z_{III}=0$.

$$V\left(r_1\right)=-\frac{Z_I e^{-\vartheta_I r_1}}{1-e^{-\vartheta_I r_1}} \tag{32}$$

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

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 $Z_I=0$.

$$V\left(r_1\right)=-\frac{Z_{II}e^{-\vartheta_I r_1}}{r_1}+\frac{Z_{III}e^{-\vartheta_I r_1}}{r_1^2} \tag{34}$$

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

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).

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

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

(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

$$\frac{\partial E_{nl}(q_I)}{\partial q_I}=\langle\psi_{nl}(q_I)\left|\frac{\partial\hat{H}(q_I)}{\partial q_I}\right|\psi_{nl}(q_I)\rangle \tag{38}$$

The effective Hamiltonian has the following form:

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

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:

$$\langle r_1^{-2}\rangle=\vartheta_I$$

$$-\frac{4\mu BV}{\hbar^2(2l+1)}\left[\frac{1}{2\sqrt{F}}-\frac{\left\{\left(n+\frac{1}{2}+\sqrt{F}\right)(2l+1)+\left(+\frac{2Z_1\mu}{\hbar^2\vartheta_I{}^2}+\frac{4\mu D_e r_e}{\hbar^2\vartheta_I}+l(l+1)\right)\frac{1}{2\sqrt{F}}\left(2l+1\right)\right\}}{\left(n+\frac{1}{2}+\sqrt{F}\right)^2}\right] \tag{40}$$

.

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 μ, which implies $-\frac{1}{\mu}\langle T\rangle=-\frac{1}{\mu}\left(H-V\right)$. From the relation $T=\frac{p^2}{2\mu}$, we substitute for T in $-\frac{1}{\mu}\langle T\rangle=-\frac{1}{\mu}\left(H-V\right)$ which yields.

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

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

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

The PD of Eq. (27) with respect to μ gives

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

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

Hence,

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

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

Hence,

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

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]

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

where k_B, λ 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.

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

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

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

where

$$\Lambda = Q_0 + 2Q_1Q_2$$

$$\rho = n+\Delta$$

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

$$Q_1 = \frac{\vartheta_I{}^2 \mathrm{h}^2}{8\mu}$$

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

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

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

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

where

$$\Upsilon_0 = 4Q_0Q_1$$

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

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

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

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

(a)vibrational mean energy

$$U(\beta)=-\frac{\partial InZ(\beta)}{\partial\beta} \tag{50}$$

(b) Vibrational specific heat capacity

$$C(\beta)=k_B\beta^2\left(\frac{\partial^2 InZ(\beta)}{\partial^2\beta}\right) \tag{51}$$

(c) Vibrational free energy

$$F(\beta)=-k_B TInZ(\beta) \tag{52}$$

(d)Vibrational entropy

$$S(\beta)=k_B InZ(\beta)-k_B\beta\frac{\partial InZ(\beta)}{\partial\beta} \tag{53}$$

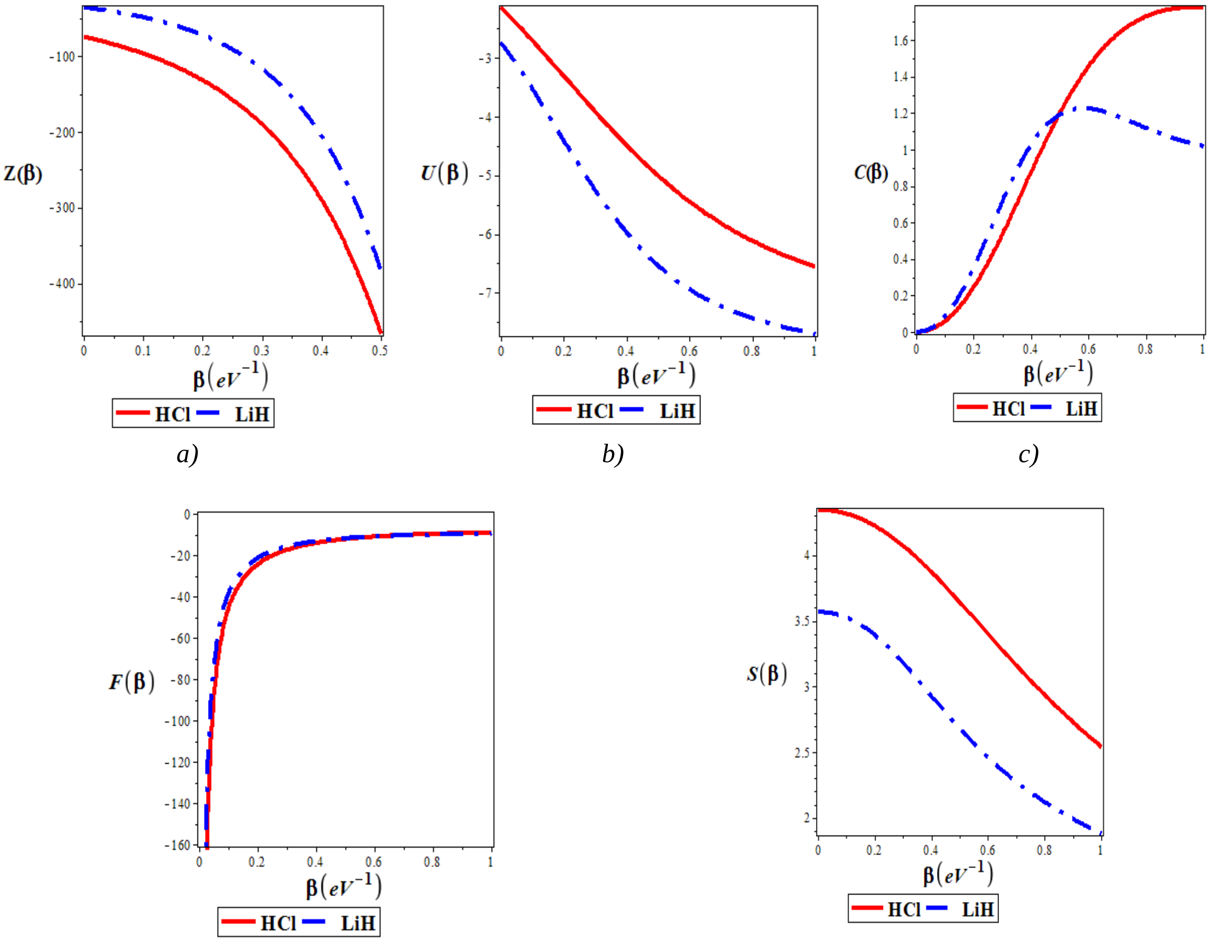
6.Results and Discussion

The experimental results from Ref. [1,5], which are shown in Table 1, were applied using Eq. (27), together with the conversion $\hbar c=1973.29\ \mathrm{eV\,\mathring{A}}$ [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_2 and LiH diatomic molecules. The partition function of the two diatomic molecules increases with temperature. Engineers can use this prediction because hydrogen (H_2) is a vital gas with many industrial and technological uses.

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

Molecules	$D_e(eV)$	$\alpha=\vartheta\left(\mathring{A}^{-1}\right)$	$r_e(\mathring{A})$	$\mu(MeV)$
HCl	4.6190309050	1.86770	1.2746	0.09129614886
LiH	2.5152672118	1.12800	1.5956	0.08198284801
H_2	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 (β). As β is raised, it can be seen in (a) that the PF of the diatomic molecules decreases. The internal energy of the molecules with β is displayed in (b), as can be observed. In this instance, when β is raised, the molecules' internal energy drops. The molecules' specific heat capacity is seen in (c). Each molecule of specific heat capacity rises as β is raised. The plot of the free energy's behavior as a function of β are shown in (d). For each diatomic molecule, we observed that the free energy rises with a rise in β and converges at a particular point. We display a graph of the diatomic molecules ' entropy as a function of β as is seen in (e). It has been shown that as β is raised, each diatomic molecules entropy reduces.



a) *b)* *c)*

d) *e)*

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.

Funding

This research was carried out under the 2017-2022 merged TETFUND INSTITUTION BASED RESEARCH (IBR) with grant number NOUN/DRA/TETFUNDAW/VOL I.

This research was also carried out under LRGS Grant LRGS/1/2020/UM/01/5/2 (9012-00009) Fault-tolerant Photonic Quantum States for Quantum Key Distribution provided by Ministry of Higher Education of Malaysia (MOHE).

Acknowledgements.

Inyang, E.P. acknowledges the Tertiary Education Trust Fund (TETFUND) of Nigeria for funding this research through the National Open University of Nigeria (Nigeria)-Tertiary Education Trust Fund-Institutional Based Research Grant (TETFUND-IBR) scheme with grant number NOUN/DRA/TETFUNDAW/VOL I. N. Ali and Inyang, E.P. acknowledges the support from the UniMAP Special Research Grant-International Postdoctoral with grant number: 9004-00100.

References

1 Inyang E.P., Ayedun F., Ibanga E.A., Lawal K.M., Okon I. B., William E.S., Ekwevugbe O., Onate C.A., Antia A. D., Obisung E. O. Analytical Solutions of the N-Dimensional Schrödinger equation with modified screened Kratzer plus Inversely Quadratic Yukawa potential and Thermodynamic Properties of selected Diatomic Molecules**.** *Results in Physics,* 2022, Vol.43, 106075. https://doi.org/10.1016/j.rinp.2022.106075

2 Edet C.O., Mahmoud S., Inyang E.P., Ali N., Aljunid A., Endut R., IkotA.N., Asjad M. Non-Relativistic Treatment of the 2D Electron System Interacting via Varshni-Shukla Potential Using the Asymptoptic Iteration Method. *Mathematics.*2022, Vol.10, pp. 2812-2824. https://doi.org/10.3390/math10152824

3 Inyang E.P., Obisung E.O., Iwuji P.C., Ntibi J.E., Amajama J., William E.S. Masses and thermal properties of a charmonium and Bottomonium mesons. *Recent Advances in Applications of Potential Models*, 2022, Vol.4, pp.875-884. https://doi.org/10.46481/jnsps.2022.884

4 Bayrak O., Kocak G., Boztosun I. Any l-state solutions of the Hulth´en potential by the asymptotic iteration method. *Journal of Physics A*, 2006, Vol.39, pp.11510-11521. https://doi.org/10.1088/0305-4470/39/37/012

5 Oluwadere O. J., Oyewumi K. J. Energy spectra and the expectation values of diatomic molecules confined by the shifted Deng-Fan potential. *European Physical Journal plus*, 2018, Vol.133, pp.410-422. https://doi.org/10.1140/epjp/i2018-12210-0

6 Ibekwe E.E., Okorie U.S., Emah J.B., Inyang E.P., Ekong S.A. Mass spectrum of heavy quarkonium for screened Kratzer potential (SKP) using series expansion method. *European Physical Journal Plus*, 2021, Vol.87, pp.1-11. https://doi.org/10.1140/epjp/s13360-021-01090-y

7 Inyang E.P., Inyang E.P., Ntibi J. E., Ibekwe E. E., William E. S. Approximate solutions of D-dimensional Klein-Gordon equation with Yukawa potential via Nikiforov-Uvarov method**.** *Indian Journal of Physics,* 2021, Vol.95, pp.2733-2739. https://doi.org/10.1007/s12648-020-01933-x

8 Omugbe E., Osafile O.E., Inyang E.P., Jahanshir A. Bound state solutions of the hyper-radial Klein-Gordon equation under the Deng-Fan potential by WKB and SWKB methods. *Physica Scripta,* 2021, Vol. 96, pp. 125408. https://doi.org/10.1088/1402-4896/ac38d4

9 Omugbe E., Osafile O.E., Okon I.B., Inyang E.P., William E.S., Jahanshir A. Any L-state energy of the spinless Salpeter equation under the Cornell potential by the WKB Approximation method: An Application to mass spectra of mesons. *Few-Body Systems*, 2022,Vol. 63, pp 1-7. https://doi.org/10.1007/s00601-021-01705-1

10 Inyang E.P., William E.S., Omugbe E., Inyang E.P., Ibanga E.A., Ayedun F., Akpan I.O., Ntibi J.E. Application of Eckart-Hellmann potential to study selected diatomic molecules using Nikiforov-Uvarov-Functional analysis method. *Revista Mexicana de Fisica. 2022,* Vol. 68, pp.1-14. https://doi.org/10.31349/revmexfis.68.020401

11 Ciftci H., Kisoglu H.F. Nonrelativistic-Arbitrary l-states of quarkonium through Asymptotic Iteration method. *Advances in High Energy Physics*, 2018, 4549705. https://doi.org/10.1155/2018/4549705

12 Ikot A.N., Okorie U.S., Amadi P.O., Edet C.O., Rampho G.J., Sever R. The Nikiforov-Uvarov –Functional Analysis (NUFA) Method: A new approach for solving exponential – Type potentials. *Few-Body System*, 2021, Vol.62**,** pp.1-9. https://doi.org/10.1007/s00601-021-021-01593-5

13 Ibekwe E.E., Emah J.B., Inyang E.P. Akpan A. O. MASS Spectrum of Heavy Quarkonium for Combined Potentials (Modified Kratzer Plus Screened Coulomb Potential). *Iranian Journal of Science and Technology,* 2022, Vol.46, pp.1741-1748. https://doi.org/10.1007/s40995-022-01377-4

14 Inyang E.P., Inyang E.P., Ntibi J.E., William E.S. Analytical solutions of Schrodinger equation with Kratzer-screened Coulomb potential for a Quarkonium system. *Bulletin of Pure and Applied Sciences*, 2021, Vol.40, pp.1-12. https://doi.org/10.5958/2320-3218.2021.0002.6

15 Inyang E.P., Inyang E.P., William E.S., Ntibi J.E., Ibanga E.A. Bound State Solutions of the Schrödinger equation with Frost-Musulin potential using the Nikiforov-Uvarov-Functional Analysis (NUFA) method. *Bulgarian Journal of Physics*, 2022, Vol.20, pp. 1-11. https://doi.org/10.55318/bgjp.2022.49.4.329

16 William E. S., Inyang E. P., Thompson E. A. Arbitrary ℓ-solutions of the Schrödinger equation interacting with Hulthén-Hellmann potential model. *Revista Mexicana Fisica*, 2020, Vol. 66, pp.730-741. https://doi.org/10.31349/RevMexFis.66.730.

17 Okoi P.O., Edet C.O., Magu T.O. Inyang E.P. Eigensolution and Expectation values of the Hulthén and Generalized Inverse Quadratic Yukawa potential. *Jordan Journal of Physics*, 2022, 15, pp.137-148. https://doi.org/10.47011/15.2.4

18 Inyang E.P., Obisung E.O., Amajama J., Bassey D.E., William E.S., Okon I.B. The Effect of Topological Defect on The Mass Spectra of Heavy and Heavy-Light Quarkonia. *Eurasian Physical Technical Journal*, 2022, Vol. 9, 4(42), pp. 78 – 87. https://doi.org/10.31489/2022No4/78-87

19 Ikot A.N., Obagboye L.F., Okorie U.S., Inyang E.P., Amadi P.O., Abdel-Aty A. Solutions of Schrodinger equation with generalized Cornell potential (GCP) and its applications to diatomic molecular systems in D-dimensions using Extended Nikiforov–Uvarov (ENU) formalism. *The European Physical Journal Plus*, 2022, Vol.137, pp.1370 https://doi.org/10.1140/epjp/s13360-022-03590-x

20 William E.S., Inyang E.P., Akpan I.O., Obu J.A., Nwachukwu A.N., Inyang E.P. Ro-vibrational energies and expectation values of selected diatomic molecules via Varshni plus modified Kratzer potential model. *Indian Journal of Physics*, 2022, Vol.96,pp.3461-3476. https://doi.org/10.1007/s12648-0222-02308-0

21 Inyang E.P., William E.S., Obu J.O., Ita B. I., Inyang E.P., Akpan I.O. Energy spectra and expectation values of selected diatomic molecules through the solutions of Klein-Gordon equation with Eckart-Hellmann potential model. *Molecular Physics*, 2021, Vol.119, pp. e1956615 https://doi.org/10.1080/00268976.2021.1956615

22 Obogo U.P., Ubi O.E., Edet C.O., Ikot, A.N. Effect of the deformation parameter on the nonrelativistic energy spectra of the q-deformed Hulthen-quadratic exponential-type potential. *Ecletica Quimica Journal*, 2021, Vol. 46, pp.63-73. https://doi.org/10.26850/1678-4618eqj.v46.4.2021.p60-73

23 Edet C.O., Ikot A.N., Superstatistics of Diatomic molecules with the shifted Deng-Fan potential model. *Biointerface Research in Applied Chemistry*. 2022, Vol.**12**, pp.4128-4139. https://doi.org/10.33263/BRIAC123.41264139

24 Edet C.O., Okorie U.S., Osobonye G., Ikot A.N., Rampho G.J., Sever R. Thermal properties of Deng-Fan-Eckart potential model using Poisson summation approach. *Journal Mathematical Chemistry*, 2020, Vol.10, pp.12-25. https://doi.org/10.1007/s10910-020-01107-4

25 Inyang E.P., William E.S., Obu J.O Eigensolutions of the N-dimensional Schro¨dinger equation interacting with Varshni-Hulthen potential model. *Revista Mexicana Fisica*, 2021, Vol**.** 67, pp. 193-205. https://doi.org/10.31349/RevMexFis.67.193.

26 Hassanabadi H., Ghominejad M., Zarrinkamar S., The Yukawa potential in semi relativistic formulation via supersymmetry quantum mechanics. *Chinese Physics B*, 2013, Vol.22, pp.060303. https://doi.org/10.1088/1674-1056/22/6/060303

27 Okon I.B, Omugbe E., Antia A.D., Onate C.A., Akpabio L.E., Osafile O.E. Spin and pseudospin solutions to Dirac equation and its thermodynamic properties using hyperbolic Hulthen plus hyperbolic exponential inversely quadratic potential. *Scientific Reports*, 2021, Vol. 11, pp.9- 21. https://doi.org/10.1038/s41598-020-77756-x

28 Ikot A.N., Okorie U.S., Sever R., Rampho G.J. Eigensolution, expectation values and thermodynamic properties of the screened Kratzer potential. *European Physical Journal Plus*, 2019, Vol. 134, pp 386. https://doi.org/10.1140/epjp/i2019-12783-x

29 Inyang E.P., Obisung E.O. The study of electronic states of NI and ScI molecules with screened Kratzer Potential. *East European Journal of Physics*, 2022, Vol. 3, pp.32-38. https://doi.org/10.26565/2312-4334-2022-3-04

30 Ikot A.N., Edet C.O., Amadi P.O., Okorie U.S., Rampho G.J., Abdullah H.Y. Thermodynamic properties of Aharanov-Bohm (AB) and magnetic fields with screened Kratzer potential. *European Physical Journal D*, 2020, Vol.74, pp.1-13. https://doi.org/10.1140/epjd/e2020-10084-9

31 Inyang E.P., Inyang E.P., Akpan I.O., Ntibi J.E., William E.S. Masses and thermodynamic properties of a Quarkonium system. *Canadian Journal Physics*, 2021, Vol. 99, pp.982-990. https://doi.org/10.1139/cjp-2020-0578

32 Tezcan C., Sever R. A general approach for the exact solution of the Schrodinger equation. *International Journal of Theoretical Physics*, 2009, Vol. 48, pp.328-337. https://doi.org/10.1007/s10773-008-9806-y

33 Greene R.L., Aldrich C. Variational wave functions for a screened Coulomb potential. *Physical Review A., 1976, Vol.* 14, pp. 2363-2374. https://doi.org/10.1103/PhysRevA.14.2363

34 Servatkhah M., Khordad R., Ghanbari A. Accurate prediction of thermodynamic functions of H2 and LiH using theoretical Calculations. *International Journal of Thermophysics,* 2020, Vol. 41, pp.30-37. https://doi.org/10.1009/s10775-020-2616-0

AUTHORS' INFORMATION

Inyang, Etido P. – Dr. (Sci.), Professor, Department of Physics, National Open University of Nigeria, Victoria Island, Lagos, Nigeria; Nigeria Institute of Physics, Nigeria; ORCID iD: 0000-0002-5031-3297; etidophysics@gmail.com

.

Ali, **Norshamsuri R.** – Dr. (Sci.), Professor, Faculty of Electronic Engineering & Technology, University Malaysia Perlis, Perlis, Malaysia; Centre of Excellence Advanced Communication Engineering (ACE), University Malaysia Perlis, Perlis, Malaysia; ORCID iD: 0000-0002-9348-0714; norshamsuri@unimap.edu.my

Endut, R. – Dr. (Sci.), Professor, Faculty of Electronic Engineering & Technology, University Malaysia Perlis, Perlis, Malaysia; Centre of Excellence Advanced Communication Engineering (ACE), University Malaysia Perlis, Perlis, Malaysia; ORCID iD: 0000-0003-3659-9740; rosdisham@unimap.edu.my

Aljunid, S.A. – Dr. (Sci.), Professor, Faculty of Electronic Engineering & Technology, University Malaysia Perlis, Perlis, Malaysia; Centre of Excellence Advanced Communication Engineering (ACE), University Malaysia Perlis, Perlis, Malaysia; ORCID iD: 0000-0003-2739-6220; syedalwee@unimap.edu.my

Appendix A

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

n	l	$E_{nl}\,(\mathrm{eV})$	$\langle r_1^{-2}\rangle\,(\mathring{\mathrm{A}})^{-2}$	$\langle T\rangle(\mathrm{eV})$	$\langle P^2\rangle(\mathrm{eV}/c)^2$
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	$E_{nl}\,(\mathrm{eV})$	$\langle r_1^{-2}\rangle\,(\mathring{A})^{-2}$	$\langle T\rangle\,(\mathrm{eV})$	$\langle P^2\rangle\,(\mathrm{eV}/c)^2$
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_2 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_2 (Our work)	H_2 [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

.