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INVESTIGATION OF RO-VIBRATIONAL ENERGIES AND EXPECTATION VALUES OF SELECTED DIATOMIC MOLECULES FOR SEIH.

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Abstract

In this study, we solve the 3-dimensional Schrodinger wave equation for the superposition of Eckart, Inversely quadratic Yukawa and Hylleraas (SEIH) potential model using the Nikiforov - Uvarov method. We have calculated the rotational and vibrational energies of diatomic molecules such as H_2, HF, HCl, LiH, ScH as well as their normalized wave function. Also, the quantum mechanical expectation values for radius, kinetic energy, and momentum of these diatomic molecules under study are evaluated analytically using the Hellman-Feynman theorem. From our results, we recommend the SEIH potential to be used as a molecular potential.

Keywords: Schrodinger equation, Eckart potential, Inversely quadratic Yukawa potential, diatomic molecules, ro-vibrational energies, quantum mechanical observables

1.0 Introduction

The study of physical systems using quantum mechanical theory implies providing solutions to a wave mechanical equation, either within relativistic or non-relativistic limits. The eigenvalues and corresponding eigenfunctions for the quantum system stem from solving such a wave equation [1 - 4].

Within the non-relativistic quantum mechanical theory, the Schrodinger wave equation has been used extensively to study various quantum mechanical systems and, by

extension, a plethora of physical systems. Recently, the Schrodinger wave equation has been used to obtain the rotational and vibrational energies and the corresponding wavefunction of a number of diatomic molecules with suitable molecular potential models [5]. Mathematical expression of the ro-vibrational energy eigenvalues for diatomic molecules plays an important role in many areas such as the calculations of rotational constants and centrifugal distortion constant [6], computations of thermodynamic properties, dipole transition matrix, quantum mechanical properties of molecules, etc.

Amongst the widely used potential models for diatomic molecular studies are Eckart potential [6, 7], Hylleraas potential [8, 9], inversely quadratic Yukawa potential [10], Manning – Rosen potential [11], Deng – Fan potential [12], Rosen – Morse potential [13], Morse potential, Tietz Potential, Tietz-Hua molecular potential [14], and many others. The Schrodinger wave equation has been solved using exciting methods, these methods includes; Nikiforov-Uvarov method [15, 16, 17], 1/N shifted expansion method [18], asymptotic iteration method [19, 20], super-symmetric quantum mechanical method [21, 22] and the factorization method [23].

In this paper, we investigate the interaction of the Schrodinger equation with a superposition of Eckart, inversely quadratic Yukawa and Hylleraas potential (SEIH potential model). The results are applied to selected diatomic molecules to obtain the ro-vibratiional energies as well as determine some quantum mechanical observables for the molecules. The (SEIH) potential is given as

$$V_{eff}(r)=\frac{V_o}{b}\left(\frac{a-e^{-2\alpha r}}{1-e^{-2\alpha r}}\right)-\frac{V_1e^{-2\alpha r}}{1-e^{-2\alpha r}}+\frac{V_2e^{-2\alpha r}}{\left(1-e^{-2\alpha r}\right)^2}-\frac{V_3e^{-2\alpha r}}{r^2}+\frac{\hbar^2\ell\left(\ell+1\right)}{2\mu r^2} \qquad 1$$

Where V_o is the potential depth of Hylleraas, a and b are Hylleraas parameters, V_1 and V_2 describes the depth of Eckart potential and V_3 is the potential strength of the inversely quadratic Yukawa potential. As used in this study the respective potential depths are related to the dissociation energy D_e and the range r.

To solve the Schrodinger wave equation for (1) analytically, an apt approximation scheme is required. Here we employ the Greene and Aldrich [24, 25] approximation scheme.

$$\frac{1}{r^2} \approx \frac{\alpha^2}{\left(1-e^{-2\alpha r}\right)^2} \qquad 2$$

2.0 Review of the NU method

We take a brief overview of the NU method in this section; details can be obtained from [26]. This method involves solving a hyper-geometric type second order differential equation:

$$\psi''(z)+\frac{\tilde{\tau}(z)}{\sigma(z)}\psi'(z)+\frac{\tilde{\sigma}(z)}{\sigma^2(z)}\psi(z)=0 \qquad 3$$

Where $\sigma(z)$ and $\tilde{\sigma}(z)$ are second order polynomials. $\tilde{\tau}(z)$ is a first order degree polynomial ref. [27]. A possible solution of Eq. (3) is proposed as:

$$\psi(z)=\phi(z)y(z) \qquad 4$$

Which results in a hyper geometric – type equation of the form;

$$\sigma(z)y''(z)+\tau(z)y'(z)+\lambda y(z)=0 \qquad 5$$

Part of the solution of Eq. (3) given in Eq. (4) as $\phi(z)$ is the solution to another differential equation of the form given by

$$\sigma(z)\phi'(z)-\pi(z)\phi(z)=0 \qquad 6$$

Where

$$\tau(z)=\tilde{\tau}(z)+2\pi(z) \qquad 7$$

And λ in Eq. (5) is defined as

$$\lambda = \lambda_n = -n\tau'(z) + \frac{n(n-1)}{2}\sigma''(z) = 0 (n = 0,1,2,3,...) \quad 8$$

The term $\tau(z)$ is a polynomial, and to obtain a proper solution for the hyper-geometric type differential equation, its first derivative $\tau'(z)$ must be negative. The function $y(z)$ as stated in Eq. (4) is the hyper geometric – type wave function obtained using the Rodrigues relation:

$$y_n(z) = \frac{B_n(z)d^n}{\rho(z)dz^n}[\sigma^n(z)\rho(z)] \quad 9$$

Where B_n is related to the normalization constant, and $\rho(z)$ is defined as

$$\frac{d}{dz}[\sigma(z)\rho(z)] = \tau(z)\rho(z) \quad 10$$

Also the function $\pi(z)$ is a first order polynomial is defined as

$$\pi(z) = \frac{\sigma'(z) - \tilde{\tau}(z)}{2} \pm \sqrt{\left(\frac{\sigma'(z) - \tilde{\tau}(z)}{2}\right)^2 - \tilde{\sigma}(z) + k\sigma(z)} \quad 11$$

K in Eq. (11) is related to Eq. (8) and the first derivative of $\pi'(z)$ as thus

$$\lambda = k + \pi'(z) \quad 12$$

The value of k is obtained by equating the discriminant of the quadratic expression under the square root sign in Eq. (12) to zero. By solving Eq. (8) and Eq. (12), we derive the energy eigenvalue equation.

3.0 Solution to Schrodinger equation

The Schrodinger equation is given as

$$\frac{d^2R(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E_{n\ell j} - V_{eff}(r)\right]R(r) = 0 \quad 13$$

Where, μ is the reduced mass, $\hbar$ is the Planck's constant, V_{eff} is the effective potential $E_{n\ell j}$ is the energy spectrum, and n, ℓ and j are the principal, orbital and total momentum quantum number respectively. We begin by transforming the radial function R(r) of the Schrodinger wave equation by introducing a new variable defined as

$$z = e^{-2\alpha r} \tag{14}$$

Taking the second derivative of Eq. (14) with respect to r, and redefining R(r) as $\psi(z)$, Eq. (13) is transformed as thus

$$\frac{d^2\psi(z)}{dz^2} + \frac{1}{z}\frac{d\psi(z)}{dz} + \frac{1}{\alpha^2 z^2}\left[\frac{2\mu E}{\hbar^2} - \frac{2\mu}{\hbar^2}\left(V_{eff}\right)\right] = 0 \tag{15}$$

Applying the approximation scheme given in Eq. (2), and introducing the effective potential Eq. (1) into Eq. (15), we have

$$\frac{d^2\psi(z)}{dz^2} + \frac{1}{z}\frac{d\psi(z)}{dz} + \frac{1}{z^2}\left[\begin{array}{l} \frac{\mu}{2\alpha^2\hbar^2}E - \frac{V_o\mu}{2b\alpha^2\hbar^2}\frac{(a-z)}{(1-z)} \\ + \frac{V_1\mu z}{2\alpha^2\hbar^2(1-z)} - \frac{V_2\mu z}{2\alpha^2\hbar^2(1-z)^2} \\ + \frac{2V_3\mu z^2}{\hbar^2(1-z)^2} - \frac{\ell(\ell+1)z}{(1-z)^2} \end{array}\right]\psi(Z) = 0 \tag{16}$$

Let;

$$\gamma = -\frac{\mu E}{2\hbar^2\alpha^2} - \frac{\mu V_o}{2b\alpha^2\hbar^2} - \frac{V_1\mu}{2\alpha^2\hbar^2} + \frac{2V_3\mu}{\hbar^2} \tag{17}$$

$$\xi = \frac{\mu E}{\hbar^2\alpha^2} + \frac{a\mu V_o}{2b\alpha^2\hbar^2} + \frac{\mu V_o}{2b\alpha^2\hbar^2} + \frac{V_1\mu}{2\alpha^2\hbar^2} - \frac{V_2\mu}{2\hbar^2\alpha^2} - \ell(\ell+1) \tag{18}$$

$$\beta = -\frac{\mu E}{2\hbar^2\alpha^2} - \frac{a\mu V_o}{2b\alpha^2\hbar^2} \tag{19}$$

Equation (16) is rewritten as given by Eq. (20) in terms of the define parameters stated in Eq. (17), (18) and (19).

$$\frac{d^2\psi(z)}{dz^2}+\frac{(1-z)}{z(1-z)}\frac{d\psi(z)}{dz}+\frac{1}{z^2(1-z)^2}\left[\gamma z^2+\xi z+\beta\right]\psi(z)=0 \qquad 20$$

Equation (20) is the transformed Schrodinger wave equation given in the form of a hyper-geometric type second order differential equation. Comparing Eq. (20) to Eq. (3), we obtain the requisite polynomials.

$$\begin{aligned}\tilde{\tau}(z)&=1-z\\ \sigma(z)&=z(1-z)\\ \sigma^2(z)&=z^2(1-z)^2\\ \tilde{\sigma}&=\gamma z^2+\xi z+\beta\end{aligned} \qquad 21$$

Putting Eq. (21) into (11), we have

$$\pi(z)=-\frac{Z}{2}\pm\sqrt{(\eta-K)Z^2+(\xi+K)Z-\beta} \qquad 22$$

Where $\eta=\frac{1}{4}+\gamma$

As stipulated by the NU method the discriminant of the quadratic expression under the square root sign in Eq. (22) is equated to zero. Solving the resultant quadratic equation for K, we have possible solutions for K as

$$K=-(\xi+2\beta)\pm 2\sqrt{\beta}\sqrt{\eta+\xi+\beta} \qquad 23$$

Accepting the negative solution of K and substituting same into Eq. (24)

$$\pi(z)=\frac{-z}{2}\pm\left(\sqrt{\beta}+\sqrt{\eta+\xi+\beta}\right)z-\sqrt{\beta} \qquad 24$$

Putting Eq. (24) into Eq. (7) another polynomial is obtained

$$\tau(z)=1-2z-2\left(\sqrt{\beta}+\sqrt{\eta+\xi+\beta}\right)z-2\sqrt{\beta} \qquad 25$$

Taking the first derivative of τ(z), we have

$$\tau^{|}(z)=-2-2\sqrt{\beta}-2\sqrt{\eta+\xi+\beta} \qquad 26$$

Substituting the first derivative of Eq. (24), using (8), (12), (21) and (26), the parameters λ and λ_n are expressed clearly as stated in Eq. (27) and Eq. (28) respectively.

$$\lambda = \frac{-1}{2} - \sqrt{\beta} - \sqrt{\eta + \xi + \beta} - \xi - 2\beta - 2\sqrt{\beta}\sqrt{\eta + \xi + \beta}$$

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$$\lambda_n = n^2 + n + 2n\sqrt{\beta} + 2n\sqrt{\eta + \xi + \beta} \qquad 28$$

Comparing Eq. (27) and Eq. (28), we obtain the quantity β

$$\beta = \left[\frac{-\frac{1}{2}\left[\left(n + \frac{1}{2} + \sqrt{\Im} \right)^2 + \frac{1}{4} + \zeta \right]}{\left(n + \frac{1}{2} + \sqrt{\Im} \right)} \right]^2 \qquad 29$$

Where

$$\Im = \eta + \xi + \beta$$

$$\xi = -\frac{1}{4} - \eta + \beta \qquad 30$$

Substituting Eq. (17), Eq. (18) and Eq. (19) into Eq. (29) and Eq. (30), we obtain the energy eigenvalues for the superposition of Eckart, inversely quadratic Yukawa and Hylleraas (SEIH) potential in terms of the principal n and orbital ℓ quantum numbers as stated by Eq. (31)

$$E_{n\ell} = \frac{aV_o}{b} - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{2V_3\mu}{\hbar^2} + \frac{\mu V_2}{2\alpha^2\hbar^2} + \ell(\ell+1)} \right)^2}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{V_3\mu}{\hbar^2} + \frac{\mu V_2}{2\alpha^2\hbar^2} + \ell(\ell+1)} \right)} + \frac{\frac{V_o\mu a}{2b\alpha^2\hbar^2} - \frac{V_o\mu}{2b\alpha^2\hbar^2} - \frac{V_1\mu}{2\alpha^2\hbar^2} + \frac{2V_3\mu}{\hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{V_3\mu}{\hbar^2} + \frac{\mu V_2}{2\alpha^2\hbar^2} + \ell(\ell+1)} \right)} \right]^2 \qquad 31$$

Equation (31) in this study is applied to obtain the rotational and vibrational energy of some diatomic molecules.

Next, we obtain the single particle wave function for the SEIH potential model. Using Eq. (10) the weighted factor $\rho(z)$ is given as

$$\rho(z) = z^{2\sqrt{\beta}}.(1-z)^{2\sqrt{\eta+\xi+\beta}} \tag{32}$$

Substituting Eq. (31) into Eq. (9), the Rodrigues relation is obtained as

$$\begin{aligned} y_n(z) &= B_n z^{-2\sqrt{\beta}}(1-z)^{-2\sqrt{\eta+\xi+\beta}} \frac{d^n}{dz^n}\left[z^{n+2\sqrt{\beta}}(1-z)^{n+2\sqrt{\eta+\xi+\beta}} \right] \\ &\equiv P_n^{\left(2\sqrt{\beta},2\sqrt{\eta+\xi+\beta}\right)}(1-2z) \end{aligned} \tag{33}$$

Where P_n is the Jacobi polynomial. Using Eq. (32) and Eq. (33) the wave function is given as

$$\psi(z) = N_{n\ell} z^{\sqrt{\beta}}(1-z)^{\left(\frac{1}{2}+\sqrt{\eta+\xi+\beta}\right)} P_n^{\left(2\sqrt{\beta},2\sqrt{\eta+\xi+\beta}\right)}(1-2z) \tag{34}$$

Where $N_{n\ell}$ is the normalization constant. Applying the normalization condition the normalization constant is obtained as

$$\frac{N_{n\ell}^2}{\alpha}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^a\left(\frac{1+y}{2}\right)^t\left[P_n^{(a,t-1)}y\right]^2 dy = 1 \tag{35}$$

Where

$$\begin{aligned} t &= \frac{1}{2} + \sqrt{\eta+\xi+\beta} \\ a &= 2\sqrt{\beta} \end{aligned} \tag{36}$$

By comparing Eq. (35) to the standard integral of the form Eq. (36) in [27,28], given as

$$\int_{-1}^{1}\left(\frac{1-p}{2}\right)^x\left(\frac{1+p}{2}\right)^y\left[P_n^{(2x,2y-1)}y\right]^2 dp = \frac{2\Gamma(x+n+1)\Gamma(y+n+1)}{n!x\Gamma(x+y+n+1)} \tag{37}$$

We obtain the normalization constant given as

$$N_{n\ell} = \left[\frac{\alpha n! a\Gamma(a+t+n+1)}{2\Gamma(a+n+1)\Gamma(t+n+1)}\right]^{\frac{1}{2}} \tag{38}$$

4.0 Quantum mechanical properties

In this study, we use the Hellman-Feynman theorem to obtain the quantum mechanical observables for a system constructed by the superposition of Eckart, Inversely quadratic Yukawa and Hylleraas (SEIH) potential. The expectation value for position radius, kinetic energy and momentum where obtained by the application of this theorem which state that 'for a non-degenerate eigenvalue of a hermitian operator in a parameter dependent eigensystem varies with respect to the parameter provided that the associated normalized eigenfunction is continuous with respect to the parameter' [29, 30]. This theorem is stated mathematically as;

$$\left\langle \psi_q \left| \frac{\partial H}{\partial q} \right| \psi_q \right\rangle = \frac{\partial E}{\partial q} \tag{39}$$

The Hamiltonian used in solving the Schrodinger equation for the present work is of the form

$$H = \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} - \frac{\hbar^2}{\mu r}\frac{d}{dr} + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1) + \left[\begin{array}{l} -\dfrac{V_3 e^{-2\alpha r}}{r^2} + \dfrac{V_0}{b}\left(\dfrac{a - e^{-2\alpha r}}{1 - e^{-2\alpha r}}\right) \\ -\dfrac{V_1 e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \dfrac{V_2 e^{-2\alpha r}}{\left(1 - e^{-2\alpha r}\right)^2} \end{array}\right] \tag{40}$$

To obtain the radius of a diatomic system we set the parameter q in Eq. (39) to ℓ. Putting Eq. (40) into Eq. (39), we have

$$\left\langle \ell \left| \frac{\partial H}{\partial \ell} \right| \ell \right\rangle = \frac{\hbar^2}{2\mu}(2\ell+1)\left\langle r^{-2} \right\rangle 2 \tag{41}$$

Where $\left\langle r^{-2} \right\rangle$ is the expectation value for position (radius of the system).

Taking the derivative of Eq. (31) with respect to ℓ as required by Eq. (39), we have;

$$\frac{\partial E}{\partial \ell} = -W(2\ell+1)\frac{\hbar^2\alpha^2}{\mu}\left[\frac{1}{2\sqrt{V}} - \frac{\left(\frac{V_o\mu a}{2b\alpha^2\hbar^2} - \frac{V_o\mu}{2b\alpha^2\hbar^2} - \frac{2V_3\mu}{\hbar^2}\right)\frac{1}{2\sqrt{V}}}{\left(n+\frac{1}{2}+\sqrt{V}\right)^2}\right] \quad 42$$

Where

$$W = n + \frac{1}{2} + \sqrt{V} + \frac{\frac{V_o\mu a}{2b\alpha^2\hbar^2} - \frac{V_o\mu}{2b\alpha^2\hbar^2} - \frac{V_1\mu}{2\alpha^2\hbar^2} + \frac{2V_3\mu}{\hbar^2}}{\left(n+\frac{1}{2}+\sqrt{V}\right)}$$

$$V = \frac{1}{4} - \frac{V_3\mu}{\hbar^2} + \frac{V_2\mu}{2\alpha^2\hbar^2} + \ell(\ell+1)$$

Equating (42) and (43), the expectation value for the position is obtained as

$$\left\langle r^{-2}\right\rangle = \left(\frac{\alpha^2}{\sqrt{V}}\right)\left(\left[n+\frac{1}{2}+\sqrt{V} + \frac{\left(\frac{V_o\mu a}{2b\alpha^2\hbar^2} - \frac{V_o\mu}{2b\alpha^2\hbar^2} - \frac{2V_3\mu}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right]\cdot\left[1 - \frac{\left(\frac{V_o\mu a}{2b\alpha^2\hbar^2} - \frac{V_o\mu}{2b\alpha^2\hbar^2} - \frac{2V_3\mu}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)^2}\right]\right)$$

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The expectation value for kinetic energy $\langle T\rangle$ is obtained from Eq. (39) by setting q to μ, and differentiating the Hamiltonian and the energy spectrum with respect to the reduced mass μ respectively. We have the derivatives below

$$\frac{\partial H}{\partial \mu} = \frac{\hbar^2}{2\mu^2}\frac{d^2}{dr^2} + \frac{\hbar^2}{\mu^2 r}\frac{d}{dr} - \frac{\hbar^2}{2\mu^2 r}\ell(\ell+1)$$

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Recall that

$$H = T + V$$
$$T = H - V \quad 45$$

Putting Eq. (45) into Eq. (44), we have

$$\left\langle \psi(\mu)\left|\frac{\partial H}{\partial \mu}\right|\psi(\mu)\right\rangle = -\frac{1}{\mu}(H-V) = -\frac{1}{\mu}\langle T\rangle \qquad 46$$

Taking the derivative of the energy eigenvalues with respect to the reduced mass, we have

$$\frac{\partial E}{\partial \mu} = \left[\begin{array}{l} \left(\frac{\hbar^2\alpha^2}{2\mu^2}\right)\left(n+\frac{1}{2}+\sqrt{V}+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right)^2 \\ -2\left(n+\frac{1}{2}+\sqrt{V}+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right)\left(\frac{\hbar^2\alpha^2}{2\mu}\right). \\ \left\{\frac{1}{2\sqrt{V}}\left(-\frac{V_3}{\hbar^2}+\frac{V_2}{2\alpha^2\hbar^2}\right)+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right. \\ \left.-\frac{1}{2\sqrt{V}}\left(-\frac{V_3}{\hbar^2}+\frac{V_2}{2\alpha^2\hbar^2}\right)\frac{\left(\frac{V_0 a\mu}{2b\alpha^2\hbar^2}-\frac{V_0\mu}{2b\alpha^2\hbar^2}-\frac{V_1\mu}{2\alpha^2\hbar^2}+\frac{2V_3\mu}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)^2}\right\} \end{array}\right] \qquad 47$$

Equating Eq. (47) and Eq. (46) as required by Eq. (39), we have the kinetic energy of a particle in the SEIH system as given by Eq. (48).

$$\langle T\rangle = \left[\begin{array}{l} -\left(\frac{\hbar^2\alpha^2}{2\mu}\right)\left(n+\frac{1}{2}+\sqrt{V}+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right)^2 \\ +\left(\hbar^2\alpha^2\right)\left(n+\frac{1}{2}+\sqrt{V}+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right). \\ \left\{\frac{1}{2\sqrt{V}}\left(-\frac{V_3}{\hbar^2}+\frac{V_2}{2\alpha^2\hbar^2}\right)+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right. \\ \left.-\frac{1}{2\sqrt{V}}\left(-\frac{V_3}{\hbar^2}+\frac{V_2}{2\alpha^2\hbar^2}\right)\frac{\left(\frac{V_0 a\mu}{2b\alpha^2\hbar^2}-\frac{V_0\mu}{2b\alpha^2\hbar^2}-\frac{V_1\mu}{2\alpha^2\hbar^2}+\frac{2V_3\mu}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)^2}\right\} \end{array}\right] \quad 48$$

Applying the relationship between kinetic energy and square of momentum given by

$$-\frac{1}{\mu}\langle T\rangle = -\frac{1}{2\mu^2}\langle P^2\rangle \quad 49$$

We obtain the expectation value for momentum of a particle moving in the SEIH potential from Eq. (49) as thus

$$\left\langle P^2 \right\rangle = \left[\begin{array}{l} -\left(\hbar^2\alpha^2\right)\left(n+\frac{1}{2}+\sqrt{V}+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right)^2 \\ +\left(2\mu\hbar^2\alpha^2\right)\left(n+\frac{1}{2}+\sqrt{V}+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)}\right). \\ \left\{ \frac{1}{2\sqrt{V}}\left(-\frac{V_3}{\hbar^2}+\frac{V_2}{2\alpha^2\hbar^2}\right)+\frac{\left(\frac{V_0 a}{2b\alpha^2\hbar^2}-\frac{V_0}{2b\alpha^2\hbar^2}-\frac{V_1}{2\alpha^2\hbar^2}+\frac{2V_3}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)} \right. \\ \left. -\frac{1}{2\sqrt{V}}\left(-\frac{V_3}{\hbar^2}+\frac{V_2}{2\alpha^2\hbar^2}\right)\frac{\left(\frac{V_0 a\mu}{2b\alpha^2\hbar^2}-\frac{V_0\mu}{2b\alpha^2\hbar^2}-\frac{V_1\mu}{2\alpha^2\hbar^2}+\frac{2V_3\mu}{\hbar^2}\right)}{\left(n+\frac{1}{2}+\sqrt{V}\right)^2} \right\} \end{array} \right] \quad (50)$$

5.0 Results and Discussion

Now we apply the energy eigenvalues for the SEIH potential model as given by Eq. (31) to obtain the rotational and vibrational energies of some diatomic molecules, namely; H_2, HF, HCl, LiH, and ScH. The spectroscopic parameters used for calculation are as presented in Table 1.

Table 1: Spectroscopic parameters of some diatomic molecules [31] and [32]

Molecule	**Mass** $(\mu/10^{-23})$	**Dissociation energy** (eV)	**Range r** $(\mathring{A})$	**B**	**A**	V_0 $(eV\mathring{A})$	V_2 $(eV\mathring{A})$
Hydrogen	0.0840	4.52	0.743	0.17006	0.25	3.50183	4.7
Hydrogen Fluoride	0.1600	6.1225	0.917	0.12772	0.25	5.614374	10.5
Hydrogen Chloride	0.1627	4.6189	1.275	0.16940	0.25	5.887186	11.4
Lithium Hydride	0.14615	2.5160	1.595	0.25600	0.25	4.01463	5.78
Scandium Hydride	0.16374	2.24993	1.776	0.22500	0.25	3.99586	6.255

Table 2: Energy spectrum $E_{n\ell}(eV)$ of H_2 for different values of vibrational n and rotational ℓ quantum numbers.

n	ℓ	**Energy (eV) (present work)**
0	0	-5.639232038
	5	-5.639043118
	10	-5.638593580
5	0	-5.533561998
	5	-5.533374898
	10	-5.532875978

7	0	-5.491578878
	5	-5.491392498
	10	-5.490895498

TABLE 3: Energy spectrum $E_{n\ell}(eV)$ of HF for different values of vibrational n and rotational ℓ quantum numbers.

N	ℓ	**Energy (eV) (present work)**
0	0	-7.782752580
	5	-7.782671200
	10	-7.782454280
5	0	-7.688656160
	5	-7.688575160
	10	-7.688359280
7	0	-7.651143020
	5	-7.651062200
	10	-7.650846720

Table 4: Energy spectrum $E_{n\ell}(eV)$ of HCl for different values of vibrational n and rotational ℓ quantum numbers.

N	ℓ	**Energy (eV) (present work)**
0	0	-0.5748423060
	5	-0.5748309100
	10	-0.5748268660
5	0	-0.5582875360
	5	-0.5582833360
	10	-0.5582721160
7	0	-0.5516726610
	5	-0.5516684760
	10	-0.5516572500

Table 5: Energy spectrum $E_{n\ell}(eV)$ of LiH for different values of vibrational n and rotational ℓ quantum numbers.

N	ℓ	**Energy (eV) (present work)**
0	0	-0.3988943590
	5	-0.3988484220
	10	-0.3987259300
5	0	-0.3612669500
	5	-0.3612213470
	10	-0.3610997470
7	0	-0.3462931020
	5	-0.3462476380
	10	-0.3461263950

Table 6: Energy spectrum $E_{n\ell}(eV)$ of ScH for different values of vibrational n and rotational ℓ quantum numbers.

N	ℓ	**Energy (eV) (present work)**
0	0	-0.4469425220
	5	-0.4469000030
	10	-0.4467866370
5	0	-0.4086534460
	5	-0.4086112110
	10	-0.4084985930
7	0	-0.3934088360

5	-0.3933667080
10	-0.3932543880

The expectation value for position (radius), kinetic energy and momentum of the following diatomic molecules, H_2, HF, HCl, LiH and ScH, were also calculated in this study for the SEIH potential. We used Eq. (44), Eq. (49) and Eq. (51) to determine numerical values of the expectation value for position (radius), kinetic energy and momentum respectively. The results obtained for the quantum mechanical properties of the diatomic molecules under study are as presented on Tables 7, 8, 9, 10 and 11.

Table 7: Numerical results of the expectation values for position, kinetic energy and square of momentum of H_2.

Observables	Expectation values
Radius $\langle r \rangle$	$1.9972\,\mathring{A}$
Kinetic energy $\langle T \rangle$	2.89642eV
Momentum $\langle P \rangle$	25713.84eV/c

Table 8: Numerical results of the expectation values for position, kinetic energy and square of momentum of HCl.

Observables	Expectation values
Radius $\langle r \rangle$	$2.9374\,\mathring{A}$
Kinetic energy $\langle T \rangle$	3.41663eV
Momentum $\langle P \rangle$	85510.993eV/c

Table 9: Numerical results of the expectation values for position, kinetic energy and square of momentum of HF.

Observables	Expectation values
Radius $\langle r \rangle$	$2.1705\,\mathring{A}$
Kinetic energy $\langle T \rangle$	3.64732eV
Momentum $\langle P \rangle$	80914.769eV/c

Table 10: Numerical results of the expectation values for position, kinetic energy and square of momentum of LiH.

Observables	Expectation values
Radius $\langle r \rangle$	$3.0078\,\mathring{A}$
Kinetic energy $\langle T \rangle$	1.93091eV
Momentum $\langle P \rangle$	56267.983eV/c

Table 11: Numerical results of the expectation values for position, kinetic energy and square of momentum of ScH.

Observables	Expectation values
Radius $\langle r \rangle$	$3.0204\,\mathring{A}$
Kinetic energy $\langle T \rangle$	1.56581eV
Momentum $\langle P \rangle$	36366.193eV/c

In the present work, the rotational and vibrational energies of some diatomic molecules have been obtained for H_2, HF, HCl, LiH and ScH, as presented in Table 2, 3, 4, 5 and 6. The energy spectrum for the SEIH potential model given by Eq.32 can be used in the study of other diatomic molecules apart from the selected once presented in this work. Also, the quantum mechanical properties of these molecules were obtained for this potential as presented on Table 7, 8, 9, 10 and 11. The expectation values for the position of a particle in the SEIH system for diatomic molecules under study are observed to have exceeded the quoted range

used for calculation for all five of the diatomic molecules, although the excess is not beyond $2\,\mathring{A}$. The expectation values for kinetic energy for the five molecules interestingly is less than the dissociation energy of the respective molecules which by all means to the fact that the molecules still remain in their bound state.

Conclusion: Schrodinger wave equation has been solved for the superposition of Eckart, inversely quadratic Yukawa and Hylleraas (SEIH) potential model. The energy eigenvalues and the corresponding wave function for this potential were obtained. The vibrational and rotational energies as well as the respective quantum mechanical properties for five diatomic molecules (H_2, HF, HCl, LiH, ScH) for the SEIH potential were calculated. The SEIH potential model can effectively be used to study other diatomic molecules.

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