

Computational Analysis of the Energy States of the Hydrogen Molecule H_2 , and Lithium Hydride LiH

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Abstract: *This study investigates the rovibrational energy spectra of the hydrogen molecule and lithium hydride using Exact quantization rule (EQR) within the framework of the non-relativistic Schrödinger equation. The molecular interaction is modelled with a combined Kratzer plus generalized inverse quadratic Yukawa potential, which incorporates the long-range molecular interaction and short-range screening effects. The radial Schrödinger equation is formulated and solved analytically using EQR to obtain the bound-state energy eigenvalues and the corresponding eigenfunctions. The effects of the potential parameters, vibrational and rotational quantum numbers, on the energy spectra are examined. The spectroscopic constants are used to assess the suitability of the proposed potential in describing the molecular structure and vibrational behaviour of H_2 and LiH . The theoretical predictions are compared with available literature to establish the accuracy and reliability of the model. The study further provides insights into the applicability of the exact quantization rule to diatomic molecular systems and demonstrates the potential of the combined interaction model for investigating molecular vibrational spectra.*

Keywords: *Schrodinger equation, rotational, vibrational quantum numbers, Riccati equation, Exact quantization rule, Kratzer, Yukawa potential models*

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1.0 Introduction

The accurate determination of molecular energy spectra is a central problem in quantum mechanics, molecular physics, and quantum chemistry because molecular energy levels govern bond stability, vibrational and rotational transitions, dissociation behaviour, and spectroscopic properties. Under the Born–Oppenheimer approximation, the nuclear motion of a diatomic molecule is treated separately from its electronic motion and described using a radial Schrödinger equation containing an appropriate molecular potential-energy function. The reliability of the calculated energy eigenvalues therefore depends on both the suitability of the potential model and the effectiveness of the method used to solve the governing equation. Because many realistic molecular potentials do not permit straightforward analytical solutions, researchers have developed approximate and

analytical approaches that provide tractable expressions for molecular energy levels.

One such approach is the exact quantization rule (EQR) developed by Ma and Xu (2005a, 2005b). The method formulates the bound-state condition through a quantization relation comprising a contribution associated with the number of nodes in the wavefunction and a quantum-correction term. Subsequent studies have examined its relationship with semiclassical quantization, supersymmetric quantum mechanics, and related proper quantization methods, demonstrating its usefulness for obtaining energy spectra for a range of analytically solvable and molecularly relevant potentials (Dong *et al.*, 2007; Qiang & Dong, 2007, 2010; Qiang *et al.*, 2008; Serrano *et al.*, 2010). Applications to potentials such as the Morse, Hulthén, and Rosen–Morse models have further illustrated the method's potential for calculating bound-state energies without relying exclusively on direct numerical integration of the Schrödinger equation. These developments establish EQR as a useful framework for investigating molecular systems whose interaction potentials can be expressed in analytically manageable forms.

Among the potential models employed in molecular physics, the Kratzer potential is important because it represents diatomic interactions using parameters associated with the equilibrium bond length and dissociation energy. Its mathematical structure also makes it suitable for analytical investigations of

$$V(r) = D_e \left(\frac{r_e - r}{r} \right)^2 + V_0 \left(-a + \frac{b}{r} e^{-\theta r} \right)^2 = A - \frac{B}{r} - \frac{C e^{-\theta r}}{r} + \frac{F}{r^2} + \frac{G e^{-2\theta r}}{r^2} \quad (1)$$

where $A = D_e + V_0 a^2$, $B = 2D_e r_e$, $C = 2V_0 ab$, $D = D_e r_e^2$ and $F = V_0 b^2$ are the potential parameters. D_e is the dissociation energy, r_e is the equilibrium bond length, r is the inter-nuclear distance, θ is the screening parameter, V_0 is the potential depth and a and b are arbitrary potential fitting constant.

Hydrogen molecule (H_2) is an important benchmark system for testing analytical molecular potentials because of its simple electronic structure and the extensive

vibrational and rotational energy levels. Kratzer-type and modified Kratzer potentials have consequently been applied to molecular spectral calculations and related quantum-mechanical problems. However, the conventional Kratzer potential does not explicitly include an exponential screening factor, which can limit its flexibility when screening effects need to be represented in the interaction model.

Yukawa-type potentials incorporate exponential screening and have been used in quantum-mechanical studies of screened interactions. The generalized inverse quadratic Yukawa potential extends this framework by combining screened interaction terms with inverse-distance and inverse-square contributions, allowing a broader range of potential behaviours to be investigated. Research on Yukawa-related and generalized screened potentials has examined their bound-state spectra and their application to different quantum systems. Composite models that combine Kratzer and Yukawa-type terms provide a further means of representing molecular interactions by incorporating features of both the Kratzer structure and exponential screening. Such models motivate the application of EQR to determine molecular energy spectra and investigate how potential parameters influence the resulting bound states.

The central Kratzer-Inversely quadratic Yukawa potential is given as

theoretical and computational research devoted to its bound states. High-accuracy calculations have established detailed descriptions of its potential-energy curve and molecular energy



levels, providing valuable reference data for evaluating approximate and analytical methods (Corongiu, 2010; Nakashima & Nakatsuji, 2018). Kratzer-type potentials have also been applied to describe molecular vibrational levels, including those of hydrogen, while exact quantization rule (EQR) methods have been used to obtain analytical energy spectra for Kratzer-type interactions and diatomic molecules (Ikhdair & Sever, 2009; Van Hooydonk, 2009). Lithium hydride (LiH), which differs from H₂ in its reduced mass, equilibrium bond length, dissociation characteristics, and electronic structure, provides a complementary test of the applicability of analytical molecular potentials. Investigating both molecules within a common potential framework therefore offers an opportunity to examine the consistency and flexibility of the model across distinct diatomic systems.

The EQR method provides a systematic approach to solving the radial Schrödinger equation by transforming it into a Riccati-type equation and deriving a quantization condition involving the classical momentum and a quantum correction (Ma & Xu, 2005a, 2005b). Subsequent studies have applied this approach to several molecular and quantum-mechanical potentials, including the Morse, Hulthén, Rosen–Morse, and Kratzer potentials (Dong *et al.*, 2007; Gu *et al.*, 2009; Qiang & Dong, 2007; Qiang *et al.*, 2008). Related investigations have also examined the proper quantization rule and its application to exactly solvable quantum systems (Qiang & Dong, 2010; Serrano *et al.*, 2010). In the context of molecular spectroscopy, the method has been used to obtain rotational and vibrational energy levels for Kratzer-type interactions, demonstrating its usefulness for analytical molecular modelling (Ikhdair & Sever, 2009). These developments provide a methodological foundation for investigating composite molecular potentials.

The modified Kratzer plus generalized inverse quadratic Yukawa potential combines the

molecular-binding characteristics of the Kratzer term with the screening flexibility of the Yukawa contribution. Research on generalized inverse quadratic Yukawa potentials has addressed their bound-state solutions and applications to quantum-mechanical systems (Oluwadare & Oyewumi, 2017; Okoi *et al.*, 2022; Inyang *et al.*, 2024). The composite potential has also been employed to investigate energy spectra and Shannon entropy measures for selected diatomic molecules (Inyang *et al.*, 2023). Related studies have explored ro-vibrational energies, expectation values, and thermodynamic properties using alternative potential models, including applications involving LiH (Inyang *et al.*, 2024; William *et al.*, 2022). Nevertheless, extending a common analytical framework to H₂ and LiH remains useful for assessing how the composite potential responds to differences in molecular parameters and spatial dimensionality. Comparisons with alternative analytical techniques, such as the asymptotic iteration method and the Nikiforov–Uvarov method, can further help establish the consistency of the calculated energy spectra (Bayrak *et al.*, 2007; Leite *et al.*, 2024).

Against this background, the present study applies the exact quantization rule to the Schrödinger equation with the combined modified Kratzer plus generalized inverse quadratic Yukawa potential to calculate the bound-state energy spectra of H₂ and LiH. It examines the influence of the vibrational and rotational quantum numbers, molecular parameters, potential strength, screening parameter, and spatial dimensionality on the resulting energy levels. The calculated spectra are compared with available theoretical results and established analytical treatments where the molecular systems, parameter definitions, and computational assumptions are consistent. By treating both molecules within the same formalism, the study seeks to evaluate the versatility of the composite potential, identify



parameter-dependent trends in the energy results for subsequent molecular modelling and spectra, and provide additional analytical numerical

2.0 Exact quantization rule

Generally, the D-dimensional Schrodinger equation is written as

$$\frac{d^2\chi_{nl}}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} - V(r) - \frac{\hbar^2 \kappa(\kappa+1)}{2\mu r^2} \right] \chi_{nl} = 0 \quad (2)$$

where E_{nl} is the energy spectra, $V(r)$ is the potential, χ_{nl} is the eign wave function, μ is the reduced mass, $\hbar$ is the reduced Planck constant, $\kappa = l + \frac{1}{2}(D - 3)$, r is the radial inter-nuclear distance and D is the dimension.

It is transformed into the Ricatti equation as

$$\frac{d\phi(r)}{dr} + (\phi(r))^2 + \frac{2\mu}{\hbar^2} [E_{nl} - V_{eff}(r)] = 0 \quad (3)$$

where $V_{eff}(r)$ is the effective potential, $\phi(r) = \chi'_{nl}(r)/\chi_{nl}(r)$ is the logarithmic derivative of the wave function $\chi_{nl}(r)$ which represents the phase angle of the Schrodinger equation. From the Ricatti equation, it is seen that as r increases across a node of wavefunction $\chi_{nl}(r)$, the logarithmic derivative $\phi(r)$ decreases $-\infty$ and jumps to $+\infty$ and then, decreases back again (Falaye *et al.*, 2015).

Ma and Xu (2005a,b) established that, the exact quantization condition is given as,

$$\int_{r_1}^{r_2} k(r) dr = N\pi + \int_{r_1}^{r_2} \phi(r) \left[\frac{dk(r)}{dr} \right] \left[\frac{d\phi(r)}{dr} \right]^{-1} dr \quad (4)$$

where $k(r) = \left[\frac{2\mu}{\hbar^2} [E_{nl} - V_{eff}(r)] \right]^{1/2}$ is the momentum, r_1 and r_2 are the turning points determined by the equilibrium condition that $E_{nl} - V_{eff}(r)$ with $N = n + 1$ number of nodes in the region. And the second term in the right-hand-side is the quantum correction term Q_c which has a property that it does not dependent on the number of nodes of the wavefunction and hence or otherwise, only the ground state is sufficient.

$$Q_c = \int_{r_1}^{r_2} k'_0(r) \cdot \frac{\phi_0(r)}{\phi'_0(r)} dr \quad (5)$$

3.0 Solution of Kratzer-Generalized inverse quadratic Yukawa potential

The D-dimensional Schrodinger equation, given that $\kappa = l + 1/2(D - 3)$ is written as

$$\frac{d^2\chi_{nl}}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} - V(r) - \frac{\hbar^2 \kappa(\kappa+1)}{2\mu r^2} \right] \chi_{nl} = 0 \quad (6)$$

Putting eq. (1) into eq. (6) gives

$$\frac{d^2\chi_{nl}}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} - \left\{ A - \frac{B}{r} - \frac{Ce^{-\theta r}}{r} + \frac{F}{r^2} + \frac{Ge^{-2\theta r}}{r^2} + \frac{\hbar^2 \kappa(\kappa+1)}{2\mu r^2} \right\} \right] \chi_{nl} = 0 \quad (7)$$

Employing the Greene and Aldrich approximation,

$$\frac{1}{r^2} \approx \frac{\theta^2 e^{2\theta r}}{(e^{\theta r} - 1)^2} \quad (8)$$

So, the effective potential $V_{eff}(r)$ obtained from eq. (7) becomes

$$V_{eff}(r) = A - \frac{Be^{\theta r}}{e^{\theta r} - 1} - \frac{C\theta}{e^{\theta r} - 1} + \frac{F\theta^2 e^{2\theta r}}{(e^{\theta r} - 1)^2} + \frac{G\theta^2}{(e^{\theta r} - 1)^2} + \frac{\hbar^2 \kappa(\kappa+1)\theta^2 e^{2\theta r}}{2\mu (e^{\theta r} - 1)^2} \quad (9)$$

Let us transform the coordinate as

Let $\xi = \frac{1}{e^{\theta r} - 1}$ and so, $e^{\theta r} = \frac{1+\xi}{\xi}$

So, the effective potential then becomes a quadratic equation in terms of ξ



$$V_{eff}(\xi) = (A - B\theta + F\theta^2 + \kappa) + (-B\theta - C\theta + 2F\theta^2 + 2\kappa)\xi + (F\theta^2 + G\theta^2 + \kappa)\xi^2 = E_{nl} \quad (10)$$

Using the ansatz that,

$$\begin{cases} \sigma_1 = A - B\theta + F\theta^2 + \kappa \\ \sigma_2 = -B\theta - C\theta + 2F\theta^2 + 2\kappa \\ \sigma_3 = F\theta^2 + G\theta^2 + \kappa \end{cases} \quad (11)$$

Then, eq. (10) becomes

$$\sigma_1 + \sigma_2\xi + \sigma_3\xi^2 - E_{nl} = 0 \quad (12)$$

The solution of the eq. (12) is

$$\xi = \frac{-\sigma_2 \pm \sqrt{\sigma_2^2 - 4\sigma_3(\sigma_1 - E_{nl})}}{2\sigma_3} \quad (13)$$

$$\xi_- + \xi_+ = -\frac{\sigma_2}{2\sigma_3} - \frac{\sqrt{\sigma_2^2 - 4\sigma_3(\sigma_1 - E_{nl})}}{2\sigma_3} - \frac{\sigma_2}{2\sigma_3} + \frac{\sqrt{\sigma_2^2 - 4\sigma_3(\sigma_1 - E_{nl})}}{2\sigma_3} = -\frac{\sigma_2}{\sigma_3} \quad (14)$$

$$\text{and } \xi_- \xi_+ = \left(-\frac{\sigma_2}{2\sigma_3} - \frac{\sqrt{\sigma_2^2 - 4\sigma_3(\sigma_1 - E_{nl})}}{2\sigma_3} \right) \left(-\frac{\sigma_2}{2\sigma_3} + \frac{\sqrt{\sigma_2^2 - 4\sigma_3(\sigma_1 - E_{nl})}}{2\sigma_3} \right) = \frac{\sigma_1 - E_{nl}}{\sigma_3} \quad (15)$$

$$k(\xi) = \sqrt{\frac{2\mu}{\hbar^2}} \sqrt{E_{nl} - V_{eff}(\xi)} = \sqrt{\frac{2\mu}{\hbar^2}} (-1)\sigma_3 \left[\frac{\sigma_1 - E_{nl}}{\sigma_3} + \frac{\sigma_2}{\sigma_3}\xi + \xi^2 \right] = \sqrt{\frac{2\mu}{\hbar^2}} (-1) \sqrt{[\xi^2 - (\xi_- + \xi_+)\xi + \xi_+\xi_-]} = \sqrt{\frac{2\mu}{\hbar^2}} \sqrt{(-1)[(\xi - \xi_-)(\xi - \xi_+)]} \quad (16)$$

From eq. (), we see that, $\frac{d\xi}{dr} = -\theta\xi(1 + \xi)$, But $\phi(r) = \frac{\chi'_{nl}(r)}{\chi_{nl}(r)}$, and then, the Ricatti equation is

$$\frac{d\phi(r)}{dr} = -\frac{2\mu}{\hbar^2} [E_{nl} - V_{eff}(r)] - (\phi(r))^2 \quad (17)$$

But $\frac{d\phi(r)}{dr} = \frac{d\phi(r)}{d\xi} \frac{d\xi}{dr}$, so, substituting into the Ricatti equation gives,

$$-\theta\xi(1 + \xi) \frac{d\phi_0(\xi)}{d\xi} + (\phi_0(\xi))^2 = -\frac{2\mu}{\hbar^2} [E_0 - \sigma_1 - \sigma_2\xi - \sigma_3\xi^2] \quad (18)$$

Letting $\phi_0(\xi) = \alpha + \beta\xi$, then, $(\phi_0(\xi))^2 = \alpha^2 + 2\alpha\beta\xi + \beta^2\xi^2$, and the eq. (18) becomes

$$\alpha^2 + (2\alpha\beta - \theta\beta)\xi + (\beta^2 - \theta\beta)\xi^2 = \frac{2\mu}{\hbar^2} [\sigma_1 - E_0 + \sigma_2\xi + \sigma_3\xi^2] \quad (19)$$

And by equating coefficients of indices of ξ , we obtain

$$\begin{cases} \alpha^2 = \frac{2\mu}{\hbar^2} (\sigma_1 - E_0) \\ 2\alpha\beta - \theta\beta = \frac{2\mu}{\hbar^2} \sigma_2 \\ \beta^2 - \theta\beta = \frac{2\mu}{\hbar^2} \sigma_3 \end{cases} \quad (20)$$

Therefore, by solving third quadratic equation in the bracket yields, $\beta = \frac{\theta \pm \sqrt{\theta^2 + \frac{8\mu\sigma_3}{\hbar^2}}}{2}$, where the positive is the only acceptable physical solution

Then,



$$\int_{r_1}^{r_2} k(r) dr = \int_{\xi_-}^{\xi_+} k(\xi) d\xi = -\frac{1}{\theta} \int_{\xi_-}^{\xi_+} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \left[\frac{\sqrt{(-1)[(\xi-\xi_-)(\xi-\xi_+)]}}{\xi(1-\xi)} \right] d\xi \quad (21)$$

But

$$\int_{\xi_-}^{\xi_+} \left[\frac{\sqrt{(-1)[(\xi-\xi_-)(\xi-\xi_+)]}}{\xi(1-\xi)} \right] d\xi = \pi \left[\sqrt{(\xi_-+1)(\xi_++1)} - 1 - \sqrt{\xi_- \xi_+} \right] \quad (22)$$

So, eq. (21) becomes

$$\int_{\xi_-}^{\xi_+} k(\xi) d\xi = -\frac{\pi}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \left[\sqrt{(\xi_-+1)(\xi_++1)} - 1 - \sqrt{\xi_- \xi_+} \right] = -\frac{\pi}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \left[\sqrt{\frac{\sigma_1-E_{nl}-\sigma_2+\sigma_3}{\sigma_3}} - 1 - \sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}} \right] \quad (23)$$

For the quantum correction, Q_c is given as

$$Q_c = \int_{r_1}^{r_2} k'_0(r) \cdot \frac{\phi_0(r)}{\phi'_0(r)} dr = \frac{1}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \int_{\xi_-}^{\xi_+} \left[\frac{(\xi-\frac{\xi_-+\xi_+}{2})(\frac{\alpha}{\beta}+\xi)}{\xi(1+\xi)\sqrt{(-1)[(\xi-\xi_-)(\xi-\xi_+)]}} \right] d\xi$$

$$= \frac{1}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \int_{\xi_-}^{\xi_+} \left[\frac{(1+\frac{\xi_-+\xi_+}{2})(\frac{\alpha}{\beta}-1) - \frac{\alpha}{\beta}(\frac{\xi_-+\xi_+}{2})(1+\xi)+\xi(1+\xi)}{\xi(1+\xi)\sqrt{(-1)[(\xi-\xi_-)(\xi-\xi_+)]}} \right] d\xi \quad (24)$$

$$Q_c = \frac{1}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \int_{\xi_-}^{\xi_+} \left[\frac{(\frac{\alpha}{\beta}-1)(1+\frac{\xi_-+\xi_+}{2})}{(1+\xi)\sqrt{(-1)(\xi-\xi_-)(\xi-\xi_+)}} - \frac{\frac{\alpha}{\beta}(\frac{\xi_-+\xi_+}{2})}{\xi\sqrt{(-1)(\xi-\xi_-)(\xi-\xi_+)}} + \frac{1}{\sqrt{(-1)(\xi-\xi_-)(\xi-\xi_+)}} \right] d\xi \quad (25)$$

$$Q_c = \frac{1}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \left[\frac{(\frac{\alpha}{\beta}-1)(1-\frac{\sigma_2}{2\sigma_3})\pi}{\sqrt{\frac{\sigma_1-E_{nl}-\sigma_2+\sigma_3}{\sigma_3}}} - \frac{\frac{\alpha}{\beta}(-\frac{\sigma_2}{2\sigma_3})\pi}{\sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}}} + \pi \right] \quad (26)$$

Taking that $\sqrt{\frac{\sigma_1-E_{nl}-\sigma_2+\sigma_3}{\sigma_3}} = \sqrt{\frac{\hbar^2}{2\mu\sigma_3}}(\alpha-\beta)$ and $\sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}} = \sqrt{\frac{\hbar^2}{2\mu\sigma_3}}\alpha$, then,

$$Q_c = \frac{\pi}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \left[\frac{1}{\beta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} + 1 \right] = \frac{\pi}{\theta} \left[\frac{1}{\beta} (\beta^2 - \theta\beta) + \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \right] = \pi \left[\frac{\beta}{\alpha} - 1 + \frac{1}{\alpha} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \right] \quad (27)$$

For the condition for exact quantization rule is,

$$\int_{r_1}^{r_2} k(r) dr = N\pi + \int_{r_1}^{r_2} \phi(r) \left[\frac{dK(r)}{dr} \right] \left[\frac{d\phi(r)}{dr} \right]^{-1} \quad (28)$$

$$-\frac{\pi}{\theta} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \left[\sqrt{\frac{\sigma_1-E_{nl}-\sigma_2+\sigma_3}{\sigma_3}} - 1 - \sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}} \right] = N\pi + \pi \left[\frac{\beta}{\alpha} - 1 + \frac{1}{\alpha} \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} \right]$$

$$- \left[\sqrt{\frac{\sigma_1-E_{nl}-\sigma_2+\sigma_3}{\sigma_3}} - 1 - \sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}} \right] = \sqrt{\frac{2\mu\sigma_3}{\hbar^2}} (\beta + \theta n) + 1 \quad (29)$$

$$\frac{\sigma_1-E_{nl}-\sigma_2+\sigma_3}{\sigma_3} = \left(-\sqrt{\frac{2\mu\sigma_3}{\hbar^2}} (\beta + \theta n) + \sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}} \right)^2 \quad (30)$$

$$-2\sqrt{\frac{2\mu\sigma_3}{\hbar^2}} (\beta + \theta n) \sqrt{\frac{\sigma_1-E_{nl}}{\sigma_3}} = \frac{\sigma_3-\sigma_2}{\sigma_3} - \left(\sqrt{\frac{2\mu\sigma_3}{\hbar^2}} (\beta + \theta n) \right)^2 \quad (31)$$

$$E_{nl} = \sigma_1 - \frac{\sigma_3}{4 \left(\sqrt{\frac{2\mu\sigma_3}{\hbar^2}} (\beta + \theta n) \right)^2} \left[\frac{\sigma_3-\sigma_2}{\sigma_3} - \left(\sqrt{\frac{2\mu\sigma_3}{\hbar^2}} (\beta + \theta n) \right)^2 \right]^2 \quad (32)$$

$$E_{nl} = \sigma_1 - \frac{\hbar^2}{8\mu} \left[\frac{2\mu(\sigma_3-\sigma_2)}{\hbar^2 (\beta + \theta n)} - (\beta + \theta n) \right]^2 \quad (33)$$



Where $\sigma_3 - \sigma_2 = B\theta + C\theta - F\theta^2 + G\theta^2 - \kappa$ and $\beta = \frac{\theta}{2} + \sqrt{\frac{\theta^2}{4} + \frac{2\mu\sigma_3}{\hbar^2}}$

The Wave function is obtained from parametric Nikiforov-Uvarov technique

$$\chi_{nl}(\nu) = N_n \nu^{\sqrt{\eta_1}} (1 - \nu)^{\frac{1}{2} + \sqrt{\frac{1}{2} + \eta_1 - \eta_2 + \eta_3}} P_n^{(2\sqrt{\eta_1}, 2 + 2\sqrt{\frac{1}{2} + \eta_1 - \eta_2 + \eta_3})} (1 - 2\nu) \quad (34)$$

Where $e^{\theta r} = \frac{1+\xi}{\xi} = \nu$ and N_n is the normalization constant given as

$$N_n = \left[\frac{n! \theta (\lambda - 1) \Gamma(\lambda + \gamma + n - 1)}{\Gamma(\lambda + n) \Gamma(\gamma + n)} \right]^{1/2} \quad (35)$$

$$\left\{ \begin{array}{l} \eta_1 = \frac{2\mu}{\hbar^2} (E_{nl} - A) + \frac{2\mu}{\hbar^2} C\theta + \frac{2\mu}{\hbar^2} G\theta^2 \\ \eta_2 = \frac{4\mu}{\hbar^2} (E_{nl} - A) - \frac{2\mu}{\hbar^2} B\theta + \frac{2\mu}{\hbar^2} C\theta \\ \eta_3 = \frac{2\mu}{\hbar^2} (E_{nl} - A) - \frac{2\mu}{\hbar^2} B\theta - \frac{2\mu}{\hbar^2} F\theta^2 - 2\kappa(\kappa + 1)\theta^2 \\ \lambda = 2\sqrt{\eta_3} \\ \gamma = -2 + 2\sqrt{\frac{1}{2} + \eta_1 - \eta_2 + \eta_3} \end{array} \right\} \quad (36)$$

4.0 Discussion

In Tables 1 and 2, we present comparative results for the inverse quadratic Yukawa potential with the results obtained from the Nikiforov-Uvarov (NU) by Edet *et al* (2019) and Proper Quantization Rule (PQR) by Oluwadare and Oyewumi (2017) for validation. It is observed that our results are in excellent agreement with the literature.

Tables 3 and 4 present the investigation of the nature of the states of the ro-vibrational energy spectra for the Kratzer – inverse quadratic Yukawa potential model in 2D, 3D and 4D for H₂ and LiH, respectively. The results for various vibrational n and

rotational l angular momentum quantum numbers for the diatomic molecules are obtained from the spectroscopic constants presented in Table 5. Where we have used $\hbar c = 1973.29 \text{ eVÅ}$, $1 \text{ amu} = 931.494028 \text{ MeV}/c^2$ and $1 \text{ cm}^{-1} = 1.24 \times 10^{-4} \text{ eV}$. We observe that the ro-vibrational energy states increase slowly for increasing dimension, but decrease for increasing n, l states for both H₂ and LiH. The ro-vibrational energy spectra are also seen to increase as the potential depth V_0 increases for H₂, whereas the reverse is the case for LiH.



Table 1: Energy spectra of the Inverse quadratic Yukawa potential model in 3D, $D_e = r_e = 0$, $a = -1$, $b = 1$, $D = 3$, $\theta = 0.001$, $\hbar = \mu = 1$

$\backslash(n)$	$\backslash(l)$	Present $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	NU	PQR	Present $\backslash(E_{nl})$, $\backslash(V_0=1)$	NU	PQR
0	1	-0.6899105635741887	-0.6899105635	-0.6896035396138025	-2.9950021250000005	-2.995002125	-2.9940045000000000
1	1	-0.5722309407225661	-0.5722309407	-0.5718076188414074	-1.4980010000000001	-1.498001000	-1.4970045000000000
2	1	-0.537583483535231	-0.5375834835	-0.5371277912043335	-1.220779125	-1.220779125	-1.2197845000000000
3	1	-0.5228774304841995	-0.5228774305	-0.5224100938146438	-1.123752125	-1.123752125	-1.1227601250000000
0	2	-0.563225533945468	-0.5632255334	-0.5630508543825075	-1.3025877142229958	-1.302587714	-1.302201872184403
1	2	-0.5340428340959917	-0.5340428341	-0.5337240097533026	-1.1560413139290355	-1.156041314	-1.155363939225181
2	2	-0.5211298050006393	-0.5211298050	-0.5207493205425896	-1.0947354815483925	-1.094735482	-1.093938232041968
3	2	-0.5143067798181733	-0.5143067798	-0.5138959792881225	-1.0634048059092762	-1.063404806	-1.062548531648839
0	3	-0.5327236750416858	-0.5327236750	-0.5326018749170197	-1.1439479771348375	-1.143947977	-1.143685816860237
1	3	-0.5204455614642278	-0.5204455615	-0.5201906956637058	-1.0888465729587917	-1.088846573	-1.088310737089324
2	3	-0.5139022861640776	-0.5139022862	-0.5135787736130005	-1.060095327212972	-1.060095327	-1.059418943879603
3	3	-0.5100083296014261	-0.5100083296	-0.5096463318898519	-1.0432245157920812	-1.043224516	-1.042468019323530
0	4	-0.5199924479677669	-0.5199924480	-0.5199025668480347	-1.0858620535674184	-1.085862054	-1.085664968464422
1	4	-0.5136230845573435	-0.5136230846	-0.5134143288870058	-1.0583723432870422	-1.058372343	-1.057929861731356
2	4	-0.5098212016802128	-0.5098212017	-0.5095438530724833	-1.0421338120069923	-1.042133812	-1.041548732718895
3	4	-0.5073721220797552	-0.5073721221	-0.5070530264169021	-1.0317502207342404	-1.031750221	-1.031076397206152

Note: NU and PQR denote the comparison methods reported by Edet, *et al* (2019) and Oluwadare and Oyewumi (2017) respectively. The original energy values are preserved.

Table 2: Energy spectra of the Inverse quadratic Yukawa potential model in 3D, $D_e = r_e = 0$, $a = -1$, $b = 1$, $D = 3$, $\theta=0.01$, $\hbar = \mu = 1$

$\backslash(n)$	$\backslash(l)$	Present $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	NU	PQR	Present $\backslash(E_{nl})$, $\backslash(V_0=1)$	NU	PQR
0	1	-0.6803042120574261	-0.6803042120	-0.6774133455125515	-2.9502125000000006	-2.950212500	-2.9404500000000000
1	1	-0.565837636172278	-0.5658376361	-0.5619400365376546	-1.4801000000000002	-1.480100000	-1.4704500000000000
2	1	-0.5321979244508102	-0.5321979244	-0.5281909972598103	-1.2079125	-1.207912500	-1.1984500000000000
3	1	-0.5179887920767261	-0.5179887921	-0.5141450483150030	-1.1127125	-1.112712500	-1.1035125000000000
0	2	-0.5547330505827409	-0.5547330506	-0.5533867400061118	-1.28271760423246	-1.282717604	-1.279268338661399
1	2	-0.5274476689996761	-0.5274476690	-0.5249118232916035	-1.1414855760980793	-1.141485576	-1.135367365171019
2	2	-0.5154443910714022	-0.5154443911	-0.5125947736790960	-1.0824717934967991	-1.082471793	-1.075445608618366
3	2	-0.5091769501318238	-0.5091769501	-0.5063882922242523	-1.0523864093101456	-1.052386409	-1.045120125270810



0	3	-0.5243377329215011	-0.5243377329	-0.5238335921350012	-1.12585102584645	-1.125851026	-1.123949057454857
1	3	-0.5135708752784635	-0.5135708753	-0.5120761646075057	-1.0742821975792922	-1.074282198	-1.069983262515873
2	3	-0.5079081522284276	-0.5079081522	-0.5061129917794308	-1.0474487326313557	-1.047448733	-1.042124745183449
3	3	-0.5046167138658402	-0.5046167139	-0.5028802557635820	-1.0317812426794297	-1.031781243	-1.026091932802665
0	4	-0.5115902203637018	-0.5115902204	-0.5118093030597658	-1.0682664897003769	-1.068266490	-1.067417988764047
1	4	-0.5065129323597443	-0.5065129324	-0.5059709010589428	-1.0435758179062147	-1.043575818	-1.040702385388879
2	4	-0.5035609347346595	-0.5035609347	-0.5028023247194076	-1.0290689464829375	-1.029068946	-1.025236123010328
3	4	-0.5017404815344207	-0.5017404815	-0.5010876689076859	-1.0198734498128765	-1.019873450	-1.015671686891542

Note: NU and PQR denote the comparison methods reported by Edet, *et al* (2019) and Oluwadare and Oyewumi (2017) respectively

Table 3: Energy spectra of H₂ for Kratzer - Inverse quadratic Yukawa potential model for $a = -1, b = 1$

$\backslash(n \backslash l)$	$\backslash(l \backslash)$	2D $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	3D $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	4D $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	2D $\backslash(E_{nl})$, $\backslash(V_0=1)$	3D $\backslash(E_{nl})$, $\backslash(V_0=1)$	4D $\backslash(E_{nl})$, $\backslash(V_0=1)$
0	1	-1.659057252319493	-1.659025159721949	-1.658980230084302	-1.676183593418949	-1.676151535402831	-1.676106654178635
1	1	-1.843418424318692	-1.843386809498955	-1.843342548748066	-1.838221146070405	-1.838189634994944	-1.838145519484411
2	1	-2.035605829280594	-2.035574692238664	-2.035531100374533	-2.008084931684564	-2.008053967549761	-2.00801061775289
3	1	-2.235619467205198	-2.235588807941075	-2.235545884963702	-2.185774950261426	-2.185744533067281	-2.185701948984070
0	2	-1.658980230084302	-1.658922463405464	-1.658851859684041	-1.676106654178635	-1.676048949744734	-1.675978422099032
1	2	-1.843342548748066	-1.843285642062764	-1.843216089438861	-1.838145519484411	-1.838088799533917	-1.838019475137177
2	2	-2.035531100374533	-2.035475053682766	-2.035406552156385	-2.00801061775289	-2.007954882285803	-2.007886761138025
3	2	-2.235545884963702	-2.235490698265470	-2.235423247836611	-2.185701948984070	-2.185647198000392	-2.185580280101577
0	3	-1.658851859684041	-1.658768418918324	-1.658672141106299	-1.675978422099032	-1.675895071238967	-1.675798897161517
1	3	-1.843216089438861	-1.843133890871238	-1.843039046353843	-1.838019475137177	-1.837937546286510	-1.837843012972841
2	3	-2.035406552156385	-2.035325595786854	-2.03523218456409	-2.007886761138025	-2.007806254296756	-2.007713361746868
3	3	-2.235423247836611	-2.235343533665173	-2.235251555737040	-2.185580280101577	-2.185501195269706	-2.185409943483599
0	4	-1.658672141106299	-1.658563026245635	-1.658441074333697	-1.675798897161517	-1.675689899863187	-1.675568079340023
1	4	-1.843039046353843	-1.842931555879694	-1.842811419440878	-1.837843012972841	-1.837735875185694	-1.837616132913202
2	4	-2.03523218456409	-2.035126318476456	-2.035007997510764	-2.007713361746868	-2.007608083470904	-2.007490419449083
3	4	-2.235251555737040	-2.235147314035919	-2.235030808543351	-2.185409943483599	-2.185306524718817	-2.1851909389

Table 4. Energy spectra of LiH under the Kratzer-inverse quadratic Yukawa potential model for different spatial dimensions

$\backslash(n \backslash l)$	$\backslash(l \backslash)$	2D $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	3D $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	4D $\backslash(E_{nl})$, $\backslash(V_0=0.5)$	2D $\backslash(E_{nl})$, $\backslash(V_0=1)$	3D $\backslash(E_{nl})$, $\backslash(V_0=1)$	4D $\backslash(E_{nl})$, $\backslash(V_0=1)$
0	1	-0.806867486111934	-0.806848509749156	-0.806821942841085	-1.146189300517335	-1.146170327033465	-1.146143764155841
1	1	-0.883711491183900	-0.883692642105009	-0.883666253394018	-1.21977300896926	-1.219754168527094	-1.219727791907442



2	1	-0.962066321568483	-0.962047599773479	-0.962021389259568	-1.294867542733802	-1.294848835333339	-1.294822644971659
3	1	-1.041931977265683	-1.041913382754565	-1.041887350437733	-1.371472901810960	-1.371454327452200	-1.371428323348493
0	2	-0.806821942841085	-0.806787785387543	-0.806746037388294	-1.146143764155841	-1.146109611884257	-1.146067870218446
1	2	-0.883666253394018	-0.883632325050387	-0.883590857073418	-1.219727791907442	-1.219693879109686	-1.21965243013303
2	2	-0.962021389259568	-0.961987690025848	-0.961946502071157	-1.294822644971659	-1.294788971647732	-1.294747815360230
3	2	-1.041887350437733	-1.041853880313926	-1.041812972381515	-1.371428323348493	-1.371394889498394	-1.371354025900047
0	3	-0.806746037388294	-0.806696698843058	-0.806639769751497	-1.146067870218446	-1.146018539158086	-1.145961618702792
1	3	-0.883590857073418	-0.883541849462260	-0.883485302215906	-1.21965243013303	-1.219603444976501	-1.219546923638951
2	3	-0.961946502071157	-0.961897825394079	-0.961841659992933	-1.294747815360230	-1.294699176107533	-1.294643053887726
3	3	-1.041812972381515	-1.041764626638515	-1.041708843082577	-1.371354025900047	-1.371305732551182	-1.371250009449118
0	4	-0.806639769751497	-0.806575250113224	-0.806503139927802	-1.145961618702792	-1.145897108852124	-1.145825009605580
1	4	-0.883485302215906	-0.883421215333197	-0.883349588812814	-1.219546923638951	-1.219482866119053	-1.219411272415305
2	4	-0.961841659992933	-0.961778005865786	-0.961706863010443	-1.294643053887726	-1.294579448698598	-1.294508360537646
3	4	-1.041708843082577	-1.041645621710992	-1.041574962520688	-1.371250009449118	-1.371186856590761	-1.371116273972604

Note: n and l denote the quantum numbers, while 2D, 3D, and 4D represent two-, three-, and four-dimensional spaces, respectively. V_0 is the potential-depth parameter. All numerical values are retained as supplied.

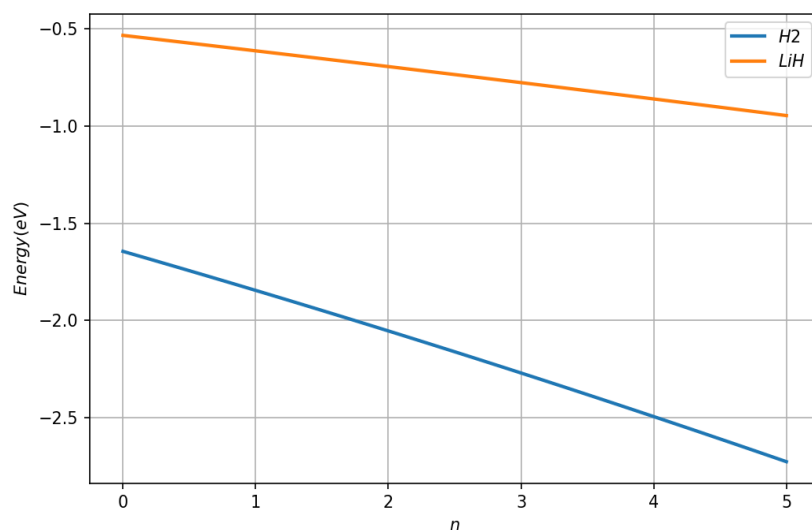


Fig. 1: A graph of ro-vibrational energy spectrum for varying vibrational quantum number

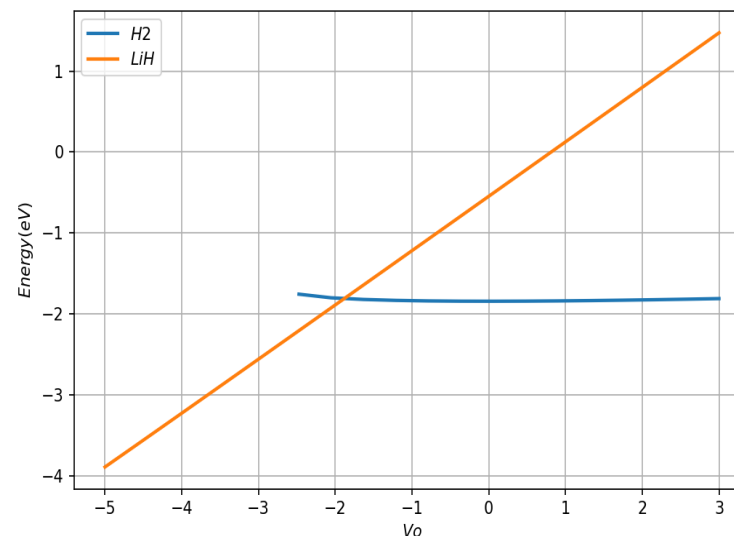


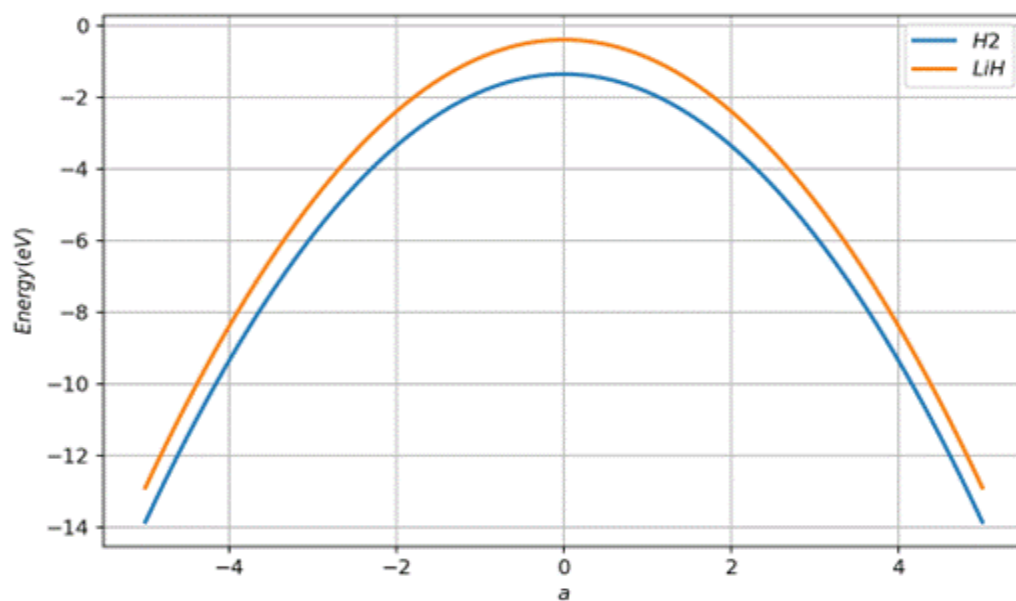
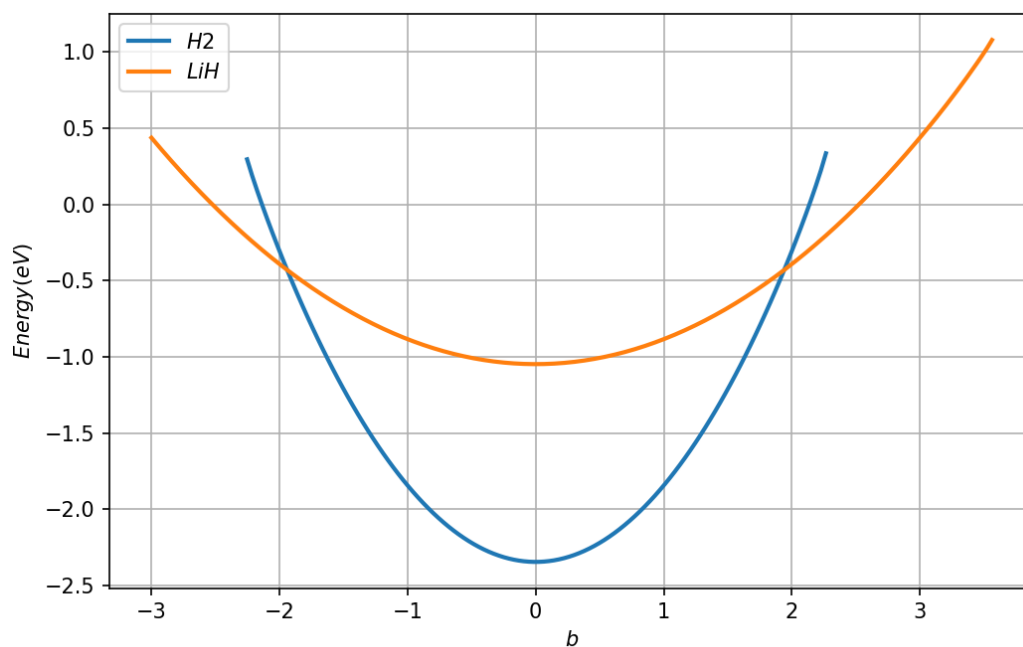
Fig. 2: A graph of ro-vibrational energy spectrum for varying potential depth



Table 5: Spectroscopic constants of the diatomic molecules in this study

Molecules	$D_e(\text{eV})$	$r_e(\text{\AA})$	$\alpha (\text{\AA}^{-1})$	$\mu(\text{amu})$
H_2	4.7446	0.7416	1.9426	0.50391

LiH	2.5152672118	1.5956	1.1280	0.8801221
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Fig. 3: A graph of ro-vibrational energy spectrum for varying potential fitting parameter a Fig. 4: A graph of ro-vibrational energy spectrum for varying potential fitting parameter b 

These phenomena are further presented in plots for visualization purposes, as seen in Figures 1 – 4, where we investigate the dependency of the ro-vibration energy spectrum on the potential parameters and the ro-vibrational quantum numbers in 3D.

Figure 1 shows a linear decrease in the ro-vibrational spectra for both molecules as the vibrational quantum number increases. But LiH spectrum is about 1.2eV higher than that of H₂ as observed.

Figure 2 is the investigation of the nature of the spectra of both molecules for varying potential depth. It is observed that, the LiH spectrum increases linearly as the potential depth increases. While the H₂ spectrum remains roughly constant from -3.4 eV, beyond which ro-vibrational energy eigenvalues are not possible.

In figure 3 and 4, we present the ro-vibrational spectra for varying potential parameters a and b , where it is observed that, the spectra are centered on 0 (Gaussian or normal distribution). There is monotonic increase in the spectra up to 0, followed by a mirror monotonic decrease for increasing a . While for increasing b , the spectra decreases exponentially up to 0, followed by a mirror exponential decrease.

5.0 Conclusion

We have obtained explicitly the non-relativistic energy and normalized wave function of the Kratzer – inverse quadratic Yukawa potential using the EQR and found our results to be in excellent agreement with literature. We then investigated the dependence of the ro-vibrational energy spectra on the potential parameters as shown in tables and figures. However, the energy of the LiH molecules is higher than that of the H₂.

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Declarations

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Conflict of Interest

The author declared no conflict of interest

Data Availability

Data shall be made available upon request

Ethical Considerations

Not applicable

Author Contributions

Peter Obeten Okoi conceptualized the study and developed the methodology. Joseph Abebe Obu contributed to theoretical formulation and interpretation of the energy spectra. Etido Patrick Inyang performed analytical derivations and validated the computational results. William Egbe Azogor contributed to the literature review and manuscript editing. All authors reviewed and approved the final manuscript.

