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ARTICLE

Expectation Values and Energy Spectra of the Varshni Potential in Arbitrary Dimensions

Etido P. Inyang[a], **Joseph E. Ntibi**[b], **Effiong O. Obisung**[b], **Eddy S. William**[b], **Etebong E. Ibekwe**[c], **Ita O. Akpan**[b] and **Ephraim P. Inyang**[b]

[a] *Department of Physics, National Open University of Nigeria, Abuja, Nigeria.*
[b] *Theoretical Physics Group, Department of Physics, University of Calabar,P.M.B. 1115 Calabar Nigeria, Nigeria.*
[c] *Department of Physics, Akwa Ibom State University, Ikot Akpaden, P.M.B. 1167, Uyo, Nigeria.*

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Abstract: The Klein-Gordon equation with Varshni potential was solved through the Nikiforov-Uvarov method. The Greene and Aldrich approximation schemes were employed to overcome the centrifugal barrier. The energy eigenvalues were obtained in relativistic and non-relativistic regimes, as well as the corresponding normalized wave functions. Energy spectra and expectation values of the square of inverse of position $\langle r^{-2}\rangle$, kinetic energy $\langle T\rangle$ and the square of the momentum $\langle \hat{p}^2\rangle$ for five selected diatomic molecules: H_2, HCl, TiH, I_2 and CO, using their separate spectroscopic parameters were computed through Hellmann-Feynman Theorem. Bound-state energy eigenvalues were also computed for Varshni potential and the numerical results agree with the already existing literature.

Keywords: Expectation values, Varshni potential, Nikiforov-Uvarov method, Klein-Gordon equation.

1. Introduction

Relativistic equations, such as Klein-Gordon equation (KGE), are very essential in many aspects of modern physics and Klein-Gordon equation is the most suitably used wave equation for the treatment of spinless particles in relativistic quantum mechanics. Klein-Gordon equation has been studied with some exactly solvable potential [1-3]. The relativistic behavior of spin-zero particles needs understanding of the single-particle spectrum which contains a four-vector linear momentum operator and a rest mass and requires introducing the four-vector potential $V(r)$ and a space time scalar potential $S(r)$ with the configuration $S(r)=V(r)$ or $S(r)=-V(r)$ [2]. $S(r)=V(r)=2V(r)$ gives non-relativistic limits of the equation conforming exactly to that of the Schrödinger equation (SE) [4-7]. Different methods have been employed to obtain the solution of the relativistic and non-relativistic wave equations with interacting potential models. These include the factorization method [8], Nikiforov-Uvarov functional analysis(NUFA) method [9-13], supersymmetry quantum mechanics (SUSYQM) [14,15], asymptotic iteration method (AIM) [16,17], the WKB approximation [18-20], Nikiforov-Uvarov method (NU) [21-38], formula method [39], series expansion method [40-42], among

Corresponding Author: E. P.Inyang **Email**: etidophysics@gmail.com

others. With the above methods, many authors have solved both relativistic and non-relativistic wave equations with diverse potentials. For instance, Inyang *et al.* [43] obtained analytical solutions of the SE with the Kratzer–screened Coulomb potential model to study some diatomic molecules. Min-Cang [44] obtained relativistic and non-relativistic solutions of the inversely quadratic Yukawa potential. Arda and Sever [45] obtained the eigensolutions of the SE with the class of Yukawa potential *via* SUSYQM. Edet *et al*. [46] obtained bound-state solutions of the SE for the modified Kratzer potential plus screened Coulomb potential.

The Varshni potential is greatly important with applications cutting across nuclear physics, particle physics and molecular physics and takes the form [47]:

$$V(r) = \upsilon - \frac{\upsilon\chi e^{-\alpha r}}{r} \tag{1}$$

where υ and χ stand for the potential strength and α is the screening parameter which controls the shape of the potential-energy curve, as shown in Fig. 1, r stands for the inter-nuclear separation. The Varshni potential is a short-range repulsive potential energy function that plays an important role in both chemical and molecular physics [48-52]. This potential is generally used to describe bound states of the interaction of systems and has been applied in both classical and molecular physics. The Varshni potential was studied by Lim using the 2-body Kaxiras-Pandey parameters. The study observed that Kaxiras and Pandey used this potential to describe the 2-body energy portion of multi-body condensed matter [53]. The present study intends to investigate the relativistic Klein-Gordon equation with the Varshni-potential model in the framework of the NU method for bound-state problems and to employ Hellmann-Feynman theorem to compute expectation values for selected diatomic molecules. To the best of our knowledge, this is the first time Klein-Gordon equation is being studied with the Varshini-potential model to compute the expectation values of some diatomic molecules using the NU method.

It is noted that the exact solution of the Klein-Gordon equation with Varshni potential in Eq. (1) is not possible due to the presence of the inverse square term in Eq. (17). Therefore, to obtain approximate solutions, a suitable approximation scheme is employed. It is found that such approximation proposed by Greene and Aldrich [54]

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

is a good approximation to the centrifugal or inverse square term which is valid for $\alpha \ll 1$ for a short-range potential. The paper is organized as follows: In Section 2, the NU method is reviewed. In Section 3, the bound-state energy eigenvalues and the corresponding wave functions are calculated. In Section 4, the results are discussed. In Section 5, conclusion is presented.

2. Review of Nikiforov-Uvarov (NU) Method

The NU method was proposed by Nikiforov and Uvarov [55] as a suitable method to obtain the solution of the second-order differential equation *via* a coordinate transformation $s = s(r)$ of the form:

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

where $\tilde{\sigma}(s)$, and $\sigma(s)$ are polynomials, at most second-degree and $\tilde{\tau}(s)$ is a first-degree polynomial. The exact solution of Eq. (3) can be obtained by using the transformation:

$$\psi(s) = \phi(s)y(s) \ . \tag{4}$$

This transformation reduces Eq. (3) into a hypergeometric-type equation of the form:

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0. \tag{5}$$

The function $\phi(s)$ can be defined as the logarithm derivative.

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{6}$$

with $\pi(s)$ being at most a first-degree polynomial. The second part of $\psi(s)$ being $y(s)$ in Eq. (5) is the hypergeometric function with its polynomial solution given by Rodrigues relation as:

$$y(s)=\frac{B_{nl}}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right] \tag{7}$$

where B_n is the normalization constant and $\rho(s)$ is the weight function which satisfies the condition below;

$$\left(\sigma(s)\rho(s)\right)'=\tau(s)\rho(s), \tag{8}$$

where also:

$$\tau(s)=\tilde{\tau}(s)+2\pi(s). \tag{9}$$

For bound solutions, it is required that:

$$\frac{d\tau(s)}{ds}<0. \tag{10}$$

The eigenfunctions and eigenvalues can be obtained using the definition of the following function $\pi(s)$ and parameter λ, respectively:

$$\left.\begin{aligned}\pi(s)&=\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\\ &\pm\sqrt{\left(\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\right)^2-\tilde{\sigma}(s)+k\sigma(s)}\end{aligned}\right\} \tag{11}$$

and

$$\lambda=k_-+\pi'_-(s)\ . \tag{12}$$

The value of k can be obtained by setting the discriminant in the square root in Eq. (11) equal to zero. As such, the new eigenvalues equation can be given as :

$$\lambda_n+n\tau'(s)+\frac{n(n-1)}{2}\sigma''(s)=0,(n=0,1,2,...). \tag{13}$$

3. Bound-state Solution of the Klein-Gordon Equation with Varshni Potential

The Klein-Gordon equation for a spinless particle for $\hbar=c=1$ in D-dimensions is given as [56, 57]:

$$\left.\begin{aligned}&\left[-\nabla^2+\left(M+S(r)\right)^2\right.\\ &\left.+\frac{(D+2l-1)(D+2l-3)}{4r^2}\right]\psi(r,\theta,\varphi)\\ &=\left[E-V(r)\right]^2\psi(r,\theta,\varphi)\end{aligned}\right\} \tag{14}$$

where ∇^2 is the Laplacian, M is the reduced mass, E is the energy spectrum and n and l are the radial and orbital angular momentum quantum numbers, respectively. It is a common practice that for the wave function to satisfy the boundary conditions, it can be rewritten as:

$$\psi(r,\theta,\varphi)=\frac{R_{nl}}{r}Y_{lm}(\theta,\varphi). \tag{15}$$

However, the spherical harmonic $Y_{lm}(\theta,\varphi)$ is known in literature [58].

The angular component of the wave function could be separated leaving only the radial part as shown below:

$$\left.\begin{aligned}\frac{d^2R(r)}{dr^2}+\left[\begin{aligned}&\left(E_{nl}{}^2-M^2\right)+V^2(r)-S^2(r)\\ &-2\left(E_{nl}V(r)+MS(r)\right)\\ &-\frac{(D+2l-1)(D+2l-3)}{4r^2}\end{aligned}\right]R(r)=0\end{aligned}\right\} \tag{16}$$

Thus, for equal vector and scalar potentials $V(r)=S(r)=2V(r)$, Eq. (16) becomes:

$$\left.\begin{aligned}\frac{d^2R(r)}{dr^2}+\left[\begin{aligned}&\left(E_{nl}{}^2-M^2\right)\\ &-V(r)\left(E_{nl}+M\right)\\ &-\frac{(D+2l-1)(D+2l-3)}{4r^2}\end{aligned}\right]R(r)=0\end{aligned}\right\}. \tag{17}$$

By substituting Eq. (1) into Eq. (17), the following equation is obtained:

$$\left.\begin{aligned}\frac{d^2R(r)}{dr^2}+\left[\begin{aligned}&\left(E_{nl}{}^2-M^2\right)\\ &-\left(\upsilon-\frac{\upsilon\chi e^{-\alpha r}}{r}\right)\left(E_{nl}+M\right)\\ &-\frac{(D+2l-1)(D+2l-3)}{4r^2}\end{aligned}\right]R(r)=0\end{aligned}\right\}. \tag{18}$$

The coordinate of Eq.(18) is transformed by setting

$$s = e^{-\alpha r}. \tag{19}$$

Differentiating Eq. (19) and simplifying it yield:

$$\frac{d^2R(r)}{dr^2} = \alpha^2 s^2 \frac{d^2R}{ds^2} + \alpha^2 s \frac{dR}{ds}. \tag{20}$$

Substituting Eqs. (2), (19) and (20) into Eq. (18), the result is:

$$\left.\begin{aligned} &\frac{d^2R(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dR(s)}{ds} \\ &+ \frac{1}{s^2(1-s)^2}\left[-\varepsilon(1-s)^2 + \beta\left(s-s^2\right) - \gamma\right]R(\mathrm{s}) \\ &= 0 \end{aligned}\right\} \tag{21}$$

where

$$\left.\begin{aligned} -\varepsilon &= \frac{E_{nl}^2 - M^2}{\alpha^2} \\ \beta &= \frac{\upsilon\chi(E_{nl}+M)}{\alpha} \\ \gamma &= \left(\frac{\upsilon(E_{nl}+M)}{\alpha^2} + \frac{(D+2l-1)(D+2l-3)}{4}\right) \end{aligned}\right\}. \tag{22}$$

Expanding the square bracket of Eq. (21), we get:

$$\left.\begin{aligned} &\frac{d^2R(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dR(s)}{ds} + \\ &\frac{1}{s^2(1-s)^2}\begin{bmatrix} -(\varepsilon+\beta)s^2 \\ +(2\varepsilon+\beta)s \\ -(\varepsilon+\gamma) \end{bmatrix}R(\mathrm{s}) = 0 \end{aligned}\right\}. \tag{23}$$

Comparing Eq. (23) with Eq. (3), the following parameters are obtained:

$$\left.\begin{aligned} \tilde{\tau}(s) &= 1-s \\ \sigma(\mathrm{s}) &= s(1-s) \\ \sigma'(s) &= 1-2s \\ \tilde{\sigma}(\mathrm{s}) &= -(\varepsilon+\beta)s^2 \\ &\quad +(2\varepsilon+\beta)s - (\varepsilon+\gamma) \end{aligned}\right\}. \tag{24}$$

By substituting Eq. (24) into Eq. (11), the result is:

$$\pi(s) = -\frac{s}{2} \pm \sqrt{(A-k)s^2 + (B+k)s + C} \tag{25}$$

where

$$\left.\begin{aligned} A &= \frac{1}{4} + \varepsilon + \beta \\ B &= -(2\varepsilon+\beta) \\ C &= \varepsilon + \gamma \end{aligned}\right\}. \tag{26}$$

To find the constant k, the discriminant of the expression under the square root of Eq. (25) must be equal to zero.

$$k = -(B+2C) - 2\sqrt{C}\sqrt{C+B+A} \tag{27}$$

Substituting Eq. (26) into Eq. (27), we get:

$$k_{\_} = \beta - 2\gamma - 2\sqrt{\varepsilon+\gamma}\sqrt{\frac{1}{4}+\gamma}. \tag{28}$$

Substituting Eq.(27) into Eq. (25), the result is:

$$\pi(s) = -\frac{s}{2} \pm \left[\left(\sqrt{C} + \sqrt{C+B+A}\right)S - \sqrt{C}\right]. \tag{29}$$

Substituting Eq. (26) into Eq. (29) yields:

$$\pi_{\_}(\mathrm{s}) = -\frac{s}{2} - \begin{bmatrix} \left(\sqrt{\varepsilon+\gamma} + \sqrt{\frac{1}{4}+\gamma}\right)S \\ -\sqrt{\varepsilon+\gamma} \end{bmatrix}. \tag{30}$$

Differentiating Eq. (30), we obtain:

$$\pi'_{\_}(\mathrm{s}) = -\frac{1}{2} - \left(\sqrt{\varepsilon+\gamma} + \sqrt{\frac{1}{4}+\gamma}\right). \tag{31}$$

Substituting Eqs. (28) and (31) into Eq. (12), the result is:

$$\left.\begin{aligned}\lambda = \beta - 2\gamma - 2\sqrt{\varepsilon+\gamma}\sqrt{\frac{1}{4}+\gamma} \\ -\frac{1}{2}-\left(\sqrt{\varepsilon+\gamma}+\sqrt{\frac{1}{4}+\gamma}\right)\end{aligned}\right\}. \quad (32)$$

with $\tau(s)$ being obtained from Eq. (9) as:

$$\left.\begin{aligned}\tau(s) = 1 - 2s + 2\sqrt{\varepsilon+\gamma}\,s \\ -2\sqrt{\frac{1}{4}+\gamma}\,s + 2\sqrt{\varepsilon+\gamma}\end{aligned}\right\}. \quad (33)$$

Differentiating Eq. (33) yields:

$$\tau'(s) = -2 - 2\left(\sqrt{\varepsilon+\gamma}+\sqrt{\frac{1}{4}+\gamma}\right). \quad (34)$$

Taking the derivative of $\sigma'(s)$ with respect to s from Eq. (24) yields:

$$\sigma''(s) = -2\ . \quad (35)$$

Substituting Eqs. (34) and (35) into Eq. (13) and simplifying yield:

$$\lambda_n = n^2 + n + 2n\sqrt{\varepsilon+\gamma} + 2n\sqrt{\frac{1}{4}+\gamma}\ . \quad (36)$$

Equating Eqs. (32) and (36) and substituting Eq. (22) yield the energy eigenvalue equation of the Varshni potential in the relativistic limit as:

$$\begin{aligned}&M^2 - E_{nl}^2 = \\ &-\alpha^2\left(\frac{\upsilon\left(E_{nl}+M\right)}{\alpha^2}+\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4}\right) \\ &+\frac{\alpha^2}{4}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4}+\frac{\upsilon\left(E_{nl}+M\right)}{\alpha^2}}\right)^2-Q}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4}+\frac{\upsilon\left(E_{nl}+M\right)}{\alpha^2}}}\right]^2\end{aligned} \quad (37)$$

where

$$\left.\begin{aligned}Q = \frac{\upsilon\chi\left(E_{nl}+M\right)}{\alpha} \\ +\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4} \\ +\frac{\upsilon\left(E_{nl}+M\right)}{\alpha^2}\end{aligned}\right\}. \quad (37a)$$

3.1 Non-relativistic Limit

In this sub-section, the non-relativistic limit of Eq. (37) is studied. Considering a transformation of the form: $M + E_{nl} \to \frac{2\mu}{\hbar^2}$, $M - E_{nl} \to -E_{nl}$ and substituting it into Eq. (37), the non-relativistic energy eigenvalue equation reads:

$$\begin{aligned}E_{nl} = \upsilon + \frac{\alpha^2\hbar^2}{\mu}\left(\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{8}\right) \\ -\frac{\hbar^2\alpha^2}{8\mu}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4}+\frac{2\upsilon\mu}{\alpha^2\hbar^2}}\right)^2}{n+\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4}+\frac{2\upsilon\mu}{\alpha^2\hbar^2}}}\right]^2 \\ \frac{-\frac{2\upsilon\chi\mu}{\alpha\hbar^2}+\frac{\left(D+2l-1\right)\left(D+2l-3\right)}{4}+\frac{2\upsilon\mu}{\alpha^2\hbar^2}}{}\end{aligned}. \quad (38)$$

To obtain the corresponding wave function, Eq. (6) is considered and upon substituting Eqs. (24) and (33) and integrating, the result is:

$$\phi(\mathrm{s}) = s^{\sqrt{\varepsilon+\gamma}}\left(1-s\right)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\gamma}}\ . \quad (39)$$

To get the hypergeometric function considering Eq. (4), the weight function is determined first of Eq. (8) upon differentiating the left-hand side to get:

$$\frac{\rho'(\mathrm{s})}{\rho} = \frac{\tau(\mathrm{s})-\sigma'(\mathrm{s})}{\sigma(\mathrm{s})}\ . \quad (40)$$

Substituting Eqs. (24) and (33) into Eq. (40), then integrating and simplify, we obtain:

$$\rho(\mathrm{s}) = s^{2\sqrt{\varepsilon+\gamma}}\left(1-s\right)^{2\sqrt{\frac{1}{4}+\gamma}}\ . \quad (41)$$

By substituting Eqs. (24) and (41) into Eq. (7), the Rodrigue's equation is obtained as:

$$\begin{aligned}&y_n(s) = \\ &B_n s^{-2\sqrt{\varepsilon+\gamma}}\left(1-s\right)^{-2\sqrt{\frac{1}{4}+\gamma}}\frac{d^n}{ds^n}\left[s^{n+2\sqrt{\varepsilon+\gamma}}\left(1-s\right)^{n+2\sqrt{\frac{1}{4}+\gamma}}\right]\end{aligned} \quad (42)$$

where B_n is the normalization constant.

Eq. (42) is an equivalent to

$$P_n^{\left(2\sqrt{\varepsilon+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}(1-2s), \tag{43}$$

where $p_n^{(\alpha,\beta)}$ is Jacobi polynomial.

The wave function is given by:

$$\psi_{nl}(s) = B_{nl}s^{\sqrt{\varepsilon+\gamma}}(1-s)^{\frac{1}{2}+\sqrt{\frac{1}{4}+\gamma}}P_n^{\left(2\sqrt{\varepsilon+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}(1-2s) \tag{44}$$

Using the normalization condition, the normalization constant can be obtained as follows:

$$\int_0^\infty |\psi_{nl}(r)|^2\, dr = 1\ . \tag{45}$$

Using the coordinate transformation of Eq. (19), we get:

$$-\frac{1}{\alpha s}\int_1^0 |\psi_{nl}(\mathrm{s})|^2\, ds = 1\ . \tag{46}$$

By letting $y = 1-2s$, the result is:

$$\frac{B_{nl}^2}{\alpha}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{2\sqrt{\varepsilon+\gamma}}\left(\frac{1+y}{2}\right)^{1+2\sqrt{\frac{1}{4}+\gamma}}\left[P_n^{\left(2\sqrt{\varepsilon+\gamma},2\sqrt{\frac{1}{4}+\gamma}\right)}y\right]^2 dy\Bigg\}. = 1 \tag{47}$$

Let

$$\left.\begin{aligned}\mu &= 1+2\sqrt{\frac{1}{4}+\gamma}\\ \mu-1 &= 2\sqrt{\frac{1}{4}+\gamma}\\ u &= 2\sqrt{\varepsilon+\gamma}\end{aligned}\right\}. \tag{48}$$

Substituting Eq. (48) into Eq. (47) yields:

$$\frac{B_{nl}^2}{\alpha}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{u}\left(\frac{1+y}{2}\right)^{\mu}\left[P_n^{(2\,\mathrm{u},\mu-1)}y\right]^2 dy = 1\,. \tag{49}$$

According to Onate et al. [59], the integral of the form in Eq. (49) can be expressed as:

$$\left.\begin{aligned}&\int_{-1}^{1}\left(\frac{1-p}{2}\right)^{x}\left(\frac{1+p}{2}\right)^{y}\left[P_n^{(2\mathrm{x},2y-1)}p\right]^2 dp\\ &= \frac{2\Gamma(x+n+1)\Gamma(y+n+1)}{n!\,x\Gamma(x+y+n+1)}\end{aligned}\right\}. \tag{50}$$

Hence, comparing Eq. (49) with the standard integral of Eq. (50), the normalization constant is obtained as:

$$B_{nl} = \sqrt{\frac{n!u\alpha\Gamma(\mathrm{u}+\mu+\mathrm{n}+1)}{2\Gamma(u+n+1)\Gamma(\mu+n+1)}}\ . \tag{51}$$

3.2 Application of Hellmann-Feynman Theorem to the Varshni Potential

Hellmann-Feynman Theorem (HFT) is one of the useful means of obtaining expectation values of some quantum mechanical observables for any arbitrary values of n and l quantum numbers. Assume that the Hamiltonian $\hat{H}$ for a particular quantum mechanical system is a function of some parameter q. Let $E(\mathrm{q})$ and $\Psi(q)$ be the eigenvalues and the eigenfunctions of the Hamiltonian $\hat{H}(q)$. Then, the Hellmann-Feynman Theorem (HFT) states that:

$$\frac{\partial E_{nl}(q)}{\partial q} = \langle\psi_{nl}(q)\left|\frac{\partial\hat{H}(q)}{\partial q}\right|\psi_{nl}(q)\rangle\ , \tag{52}$$

provided that the associated normalized eigenfunction $\psi_{nl}(q)$ is continuous with respect to the parameter q [60-62].

The effective Hamiltonian is given as:

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu r^2}l(l+1) + \upsilon - \frac{\upsilon\chi e^{-\alpha r}}{r}. \tag{53}$$

3.2.1 Expectation Value of $\langle r^{-2}\rangle$

Substituting $q = l$ into Eq. (53) gives:

$$\frac{\partial E_{nl}(l)}{\partial l} = \langle\psi_{nl}(l)\left|\frac{\partial\hat{H}(l)}{\partial l}\right|\psi_{nl}(l)\rangle\,. \tag{54}$$

Taking the partial derivative of Eq. (53) with respect to l gives:

$$\langle\psi(l)\left|\frac{\partial H(l)}{\partial l}\right|\psi(l)\rangle = \frac{\hbar^2}{2\mu}(2l+1)\langle r^{-2}\rangle\,. \tag{55}$$

Taking the partial derivative of Eq. (38) with respect to l gives:

$$\frac{\partial E_{nl}(l)}{\partial l}=\frac{4\alpha^2\hbar^2}{8\mu}\left\{-2BV\left[\frac{1}{2\sqrt{U}}-\frac{\left(n+\frac{1}{2}+\sqrt{U}\right)+\left(\frac{4\upsilon\chi\mu}{\hbar^2\alpha}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2}\right)\frac{1}{2\sqrt{U}}}{\left(n+\frac{1}{2}+\sqrt{U}\right)^2}\right]\right\} \quad (56)$$

where

$$B=\frac{\hbar^2\alpha^2}{8\mu} \quad (57)$$

$$U=\frac{1}{4}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2} \quad (58)$$

$$V=\left(n+\frac{1}{2}+\sqrt{U}\right)-\frac{\left(\frac{4\upsilon\chi\mu}{\hbar^2\alpha}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2}\right)}{\left(n+\frac{1}{2}+\sqrt{U}\right)}. \quad (59)$$

Equating Eqs. (55) and (56) yields the expectation values of $\langle r^{-2}\rangle$ for different orbital quantum numbers. Hence,

$$\langle r^{-2}\rangle=\frac{\alpha^2}{(2l+1)}-\frac{4\mu BV}{\hbar^2(2l+1)}\left\{\frac{1}{2\sqrt{U}}-\frac{\left(n+\frac{1}{2}+\sqrt{U}\right)+\left(\frac{4\upsilon\chi\mu}{\hbar^2\alpha}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2}\right)\frac{1}{2\sqrt{U}}}{\left(n+\frac{1}{2}+\sqrt{U}\right)^2}\right\}. \quad (60)$$

3.2.2 Expectation Values for $\langle T\rangle$ and $\langle\hat{P}^2\rangle$

Substituting $q=\mu$ into Eq. (52), we get:

$$\frac{\partial E_{nl}(\mu)}{\partial\mu}=\langle\psi_{nl}(\mu)\left|\frac{\partial\hat{H}(\mu)}{\partial\mu}\right|\psi_{nl}(\mu)\rangle. \quad (61)$$

Taking the partial derivative of Eq. (61) with respect to μ gives:

$$\frac{\partial H(\mu)}{\partial\mu}=\frac{\hbar^2}{2\mu^2}\frac{d^2}{dr^2}+\frac{\hbar^2}{2\mu^2r^2}l(l+1), \quad (62)$$

which implies:

$$\frac{\partial H(\mu)}{\partial\mu}=-\frac{1}{\mu}\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{\hbar^2}{2\mu r^2}l(l+1)\right). \quad (63)$$

Eq. (63) implies:

$$-\frac{1}{\mu}\langle T\rangle=-\frac{1}{\mu}(H-V). \quad (64)$$

Hence,

$$\langle\psi_{nl}(\mu)\left|\frac{\partial\hat{H}(\mu)}{\partial\mu}\right|\psi_{nl}(\mu)\rangle=-\frac{1}{\mu}\langle T\rangle. \quad (65)$$

From the relation $T=\frac{p^2}{2\mu}$, substituting for T in Eq. (64), we obtain:

$$-\frac{1}{\mu}\langle T\rangle=-\frac{1}{2\mu^2}\langle\hat{P}^2\rangle. \quad (66)$$

Substituting Eq. (66) into Eq. (65) yields:

$$\langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle = -\frac{1}{2\mu^2} \langle \hat{P}^2 \rangle \,. \quad (67)$$

Taking the partial derivative of Eq. (38) with respect to μ gives:

$$\frac{\partial E_{nl}(\mu)}{\partial \mu} = -\frac{\alpha^2\hbar^2}{\mu^2}\left(\frac{(D+2l-1)(D+2l-3)}{8}\right) + 2BV\left[\frac{2\upsilon}{\hbar^2\alpha^2\sqrt{U}} - \frac{\left(n+\frac{1}{2}+\sqrt{U}\right)\left(\frac{4\upsilon\chi}{\hbar^2\alpha}+\frac{4\upsilon}{\alpha^2\hbar^2}\right)+\left(\frac{4\upsilon\chi\mu}{\hbar^2\alpha}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2}\right)\frac{2\upsilon}{\hbar^2\alpha^2\sqrt{U}}}{\left(n+\frac{1}{2}+\sqrt{U}\right)^2}\right]. \quad (68)$$

Equating Eqs. (65) and (68) yields the expectation values of $\langle T \rangle$ for different orbital quantum numbers. Hence,

$$\langle T \rangle = \frac{\alpha^2\hbar^2}{\mu}\left(\frac{(D+2l-1)(D+2l-3)}{8}\right) - 2\mu BV\left[\frac{2\upsilon}{\hbar^2\alpha^2\sqrt{U}} - \frac{\left(n+\frac{1}{2}+\sqrt{U}\right)\left(\frac{4\upsilon\chi}{\hbar^2\alpha}+\frac{4\upsilon}{\alpha^2\hbar^2}\right)+\left(\frac{4\upsilon\chi\mu}{\hbar^2\alpha}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2}\right)\frac{2\upsilon}{\hbar^2\alpha^2\sqrt{U}}}{\left(n+\frac{1}{2}+\sqrt{U}\right)^2}\right]. \quad (69)$$

Equating Eqs. (67) and (68) yields the expectation values of $\langle \hat{P}^2 \rangle$ for different orbital quantum numbers. Hence,

$$\langle \hat{P}^2 \rangle = 2\alpha^2\hbar^2\left(\frac{(D+2l-1)(D+2l-3)}{8}\right) - 4\mu^2 BV\left[\frac{2\upsilon}{\hbar^2\alpha^2\sqrt{U}} - \frac{\left(n+\frac{1}{2}+\sqrt{U}\right)\left(\frac{4\upsilon\chi}{\hbar^2\alpha}+\frac{4\upsilon}{\alpha^2\hbar^2}\right)+\left(\frac{4\upsilon\chi\mu}{\hbar^2\alpha}+\frac{(D+2l-1)(D+2l-3)}{4}+\frac{4\upsilon\mu}{\hbar^2\alpha^2}\right)\frac{2\upsilon}{\hbar^2\alpha^2\sqrt{U}}}{\left(n+\frac{1}{2}+\sqrt{U}\right)^2}\right]. \quad (70)$$

4. Results and Discussion

TABLE 1. Molecular parameters for selected diatomic molecules [52].

Molecule	$\overset{0}{\alpha}(A)$	$\mu(amu)$
H_2	1.9426	0.50391
CO	2.2994	6.8606719
I_2	1.8643	63.45223502
HCl	1.8677	0.9801045
TiH	1.32408	0.987371

TABLE 2. Energy spectra $E_{nl}(eV)$ and expectation values for $\left\langle r^{-2}\right\rangle_{nl}$, $\langle T\rangle_{nl}$ and $\left\langle P^2\right\rangle_{nl}$ of the Varshni potential for $D=3$ with various n and l quantum numbers for H_2 diatomic molecules.

n	l	$E_{nl}(eV)$	$\left\langle r^{-2}\right\rangle_{nl}\left(\mathring{A}\right)^{-2}$	$\langle T\rangle_{nl}(\mathrm{eV})$	$\left\langle P^2\right\rangle_{nl}(\mathrm{eV}/c)^2$
0	0	-1.284911706	0.03579269260	-9.162774801	-3.737481180
0	1	-0.1054081970	0.36962978560	-9.130996387	-3.727330813
0	2	-0.07608090100	0.05920818721	-9.067311521	-3.707110307
0	3	-0.03243091400	0.00123608902	-8.971470241	-3.676977983
1	0	-0.3670952040	0.10200937101	-8.513336108	-3.336311615
1	1	-0.3529862820	0.03668385200	-8.480836963	-3.327012768
1	2	-0.3248963660	0.02520795230	-8.480836963	-3.308484628
1	3	-0.2830783740	0.02139776540	-8.415734312	-3.280864490
2	0	-0.6248777810	0.5426331240	-7.873022427	-2.973831503
2	1	-0.6113588380	0.1832125510	-7.839974593	-2.965273962
2	2	-0.5844399920	0.1127128246	-7.773793971	-2.948219351
2	3	-0.5443566640	0.08346423870	-7.674314879	-2.922787033
3	0	-0.8931843390	0.9361674190	-7.246074828	-2.645561145
3	1	-0.8802253930	0.3140913608	-7.212613314	-2.637650798
3	2	-0.8544184310	0.1908832726	-7.145621284	-2.621882798
3	3	-0.8159828870	0.1389220179	-7.044964233	-2.598361166

TABLE 3. Energy spectra $E_{nl}(eV)$ and expectation values for $\left\langle r^{-2}\right\rangle_{nl}$, $\langle T\rangle_{nl}$ and $\left\langle P^2\right\rangle_{nl}$ of the Varshni potential for $D=3$ with various n and l quantum numbers for CO diatomic molecules.

n	l	$E_{nl}(\mathrm{eV})$	$\left\langle r^{-2}\right\rangle_{nl}\left(\mathring{A}\right)^{-2}$	$\langle T\rangle_{nl}(\mathrm{eV})$	$\left\langle P^2\right\rangle_{nl}(\mathrm{eV}/c)^2$
0	0	-0.1170808900	2.489514420	-22.31946683	-159.1662412
0	1	-0.1166026000	0.8298635421	-22.31624311	-159.1581250
0	2	-0.1156461300	0.4979486091	-22.30979559	-159.1418921
0	3	-0.1142114900	0.3557102344	-22.30012416	-159.1175444
1	0	-0.3517501900	2.540359848	-22.05602493	-156.4563020
1	1	-0.3512725000	0.8468115465	-22.05279699	-156.4482544
1	2	-0.3503172600	0.5081168442	-22.04634099	-156.4321590
1	3	-0.3488847200	0.3629726517	-22.03665686	-156.4080174
2	0	-0.5873492500	2.590492590	-21.79265536	-153.7806669
2	1	-0.5868722700	0.8635219961	-21.78942332	-153.7726868
2	2	-0.5859183600	0.5181425575	-21.78295914	-153.7567266
2	3	-0.5844877300	0.3701332794	-21.77326272	-153.7327874
3	0	-0.8238764800	2.540359848	-21.52940447	-151.1388219
3	1	-0.8234001700	0.8468115465	-21.52616847	-151.1309081
3	2	-0.8224476800	0.5081168442	-21.51969637	-151.1150804
3	3	-0.8210190800	0.3629726517	-21.50998802	-151.0913399

TABLE 4. Energy spectra $E_{nl}(eV)$ and expectation values for $\left\langle r^{-2}\right\rangle_{nl}$, $\langle T\rangle_{nl}$ and $\left\langle P^2\right\rangle_{nl}$ of the Varshni potential for $D=3$ with various n and l quantum numbers for I_2 diatomic molecules.

n	l	$E_{nl}(eV)$	$\left\langle r^{-2}\right\rangle_{nl}\left(\mathring{A}\right)^{-2}$	$\langle T\rangle_{nl}(\mathrm{eV})$	$\left\langle P^2\right\rangle_{nl}(\mathrm{eV}/c)^2$
0	0	-0.01508951000	2.638248562	-3.099862014	-291.4735778
0	1	-0.01508020000	0.8794171616	-3.099633021	-291.4698897
0	2	-0.01506158000	0.5276514661	-3.099175029	-291.4625149
0	3	-0.01503373000	0.3768951573	-3.098488021	-291.4514518
1	0	-0.04534811000	2.646393504	-3.077186434	-288.7271469
1	1	-0.04533873000	0.8821321334	-3.076957406	-288.7234675
1	2	-0.04532011000	0.5292804395	-3.076499321	-288.7161083

n	l	$E_{nl}(eV)$	$\left\langle r^{-2}\right\rangle_{nl}\left(\text{Å}\right)^{-2}$	$\langle T\rangle_{nl}(\text{eV})$	$\left\langle P^2\right\rangle_{nl}(\text{eV}/c)^2$
1	3	−0.04529214000	0.3780586989	−3.075812191	−288.7050692
2	0	−0.07572465000	2.654493607	−3.054512093	−285.9946808
2	1	−0.07571527000	0.8848321597	−3.054283017	−285.9910092
2	2	−0.07569657000	0.5309004451	−3.053824839	−285.9836658
2	3	−0.07566856000	0.3792158351	−3.053137580	−285.9726510
3	0	−0.1062188700	2.662549139	−3.031839794	−283.2760989
3	1	−0.1062095400	0.8875173285	−3.031610673	−283.2724353
3	2	−0.1061907500	0.5325115362	−3.031152415	−283.2651083
3	3	−0.1061626700	0.3803666034	−3.030465013	−283.2541175

TABLE 5. Energy spectra $E_{nl}(eV)$ and expectation values for $\left\langle r^{-2}\right\rangle_{nl}$, $\langle T\rangle_{nl}$ and $\left\langle P^2\right\rangle_{nl}$ of the Varshni potential for $D=3$ with various n and l quantum numbers for HCl diatomic molecules

n	l	$E_{nl}(eV)$	$\left\langle r^{-2}\right\rangle_{nl}\left(\text{Å}\right)^{-2}$	$\langle T\rangle_{nl}(\text{eV})$	$\left\langle P^2\right\rangle_{nl}(\text{eV}/c)^2$
0	0	−0.1529847700	1.473532445	−9.051930929	−8.807283121
0	1	−0.1503699400	0.4914243720	−9.037010945	−8.801602065
0	2	−0.1451447400	0.2951505825	−9.007166779	−8.790245776
0	3	−0.1373179400	0.2111383936	−8.962389926	−8.773225855
1	0	−0.4610450100	1.600333990	−8.680100390	−8.289787149
1	1	−0.4584503900	0.5336755706	−8.665105589	−8.284282842
1	2	−0.4532654700	0.3204821440	−8.635112115	−8.273279650
1	3	−0.4454988800	0.2292118785	−8.590112330	−8.256788452
2	0	−0.7730904500	1.600333990	−8.309501194	−7.795407708
2	1	−0.7705168300	0.5336755706	−8.294439840	−7.790069215
2	2	−0.7653738100	0.3204821440	−8.264313630	−7.779397292
2	3	−0.7576697900	0.2292118785	−8.219115671	−7.763402108
3	0	−1.089108990	1.835403060	−7.940841730	−7.322926754
3	1	−1.086557120	0.6120030134	−7.925721251	−7.317743878
3	2	−1.081457530	0.3674439523	−7.895477132	−7.307382871
3	3	−1.073818390	0.2627189638	−7.850103134	−7.291853231

TABLE 6. Energy spectra $E_{nl}(eV)$ and expectation values for $\left\langle r^{-2}\right\rangle_{nl}$, $\langle T\rangle_{nl}$ and $\left\langle P^2\right\rangle_{nl}$ of the Varshni potential for $D=3$ with various n and l quantum numbers for TiH diatomic molecules.

n	l	$E_{nl}(eV)$	$\left\langle r^{-2}\right\rangle_{nl}\left(\text{Å}\right)^{-2}$	$\langle T\rangle_{nl}(\text{eV})$	$\left\langle P^2\right\rangle_{nl}(\text{eV}/c)^2$
0	0	−0.07152099500	0.7302912690	−4.012170649	−3.913689181
0	1	−0.07019219700	0.2435742016	−4.004725407	−3.910814081
0	2	−0.06753717000	0.1463168492	−3.989832450	−3.905067256
0	3	−0.06356104800	0.1046963051	−3.967486874	−3.896455495
1	0	−0.2155946040	0.7988103264	−3.836743540	−3.669035737
1	1	−0.2116448370	0.2664039745	−3.829258062	−3.666256471
1	2	−0.2116448370	0.1600028318	−3.814284905	−3.660701110
1	3	−0.2077025790	0.1144593050	−3.791819641	−3.652375937
2	0	−0.3616429120	0.8637003948	−3.661975352	−3.436039830
2	1	−0.3603372950	0.2880247719	−3.654454412	−3.433350099
2	2	−0.3577285070	0.1729642548	−3.639410531	−3.427973564
2	3	−0.3538214230	0.1237056446	−3.616839747	−3.419916089
3	0	−0.5096601390	0.9251749007	−3.488241204	−3.214046403
3	1	−0.5083667450	0.3085076864	−3.480689005	−3.211440334
3	2	−0.5057823400	0.1852437113	−3.465582832	−3.206230934
3	3	−0.5019116790	0.1324656811	−3.442919112	−3.198423645

TABLE 7. Bound-state energy eigenvalues of the Varshni potential as a function of the screening parameter with $2\mu = \hbar = 1, \upsilon = \chi = -1$, $D = 3$.

State	Screening parameter (α)	Present work E_{nl}	[39]
2P	0.001	-1.061750235	-1.0617502
	0.050	-1.025625010	-1.0256250
	0.100	-0.991000001	-0.9900000
3P	0.001	-1.027168072	-1.0271680
	0.050	-1.000645080	-1.0006250
	0.100	-0.980278864	-0.9802778
4P	0.001	-1.015065656	-1.0150656
	0.050	-0.995156336	-0.9951563
	0.100	-0.992000008	-0.9900000
4d	0.001	-1.014939102	-1.0149391
	0.050	-0.985156474	-0.9851563
	0.100	-0.962500063	-0.9625000
4f	0.001	-1.014750243	-1.0147502
	0.050	-0.972500081	-0.9725000
	0.100	-0.930625006	-0.9306250

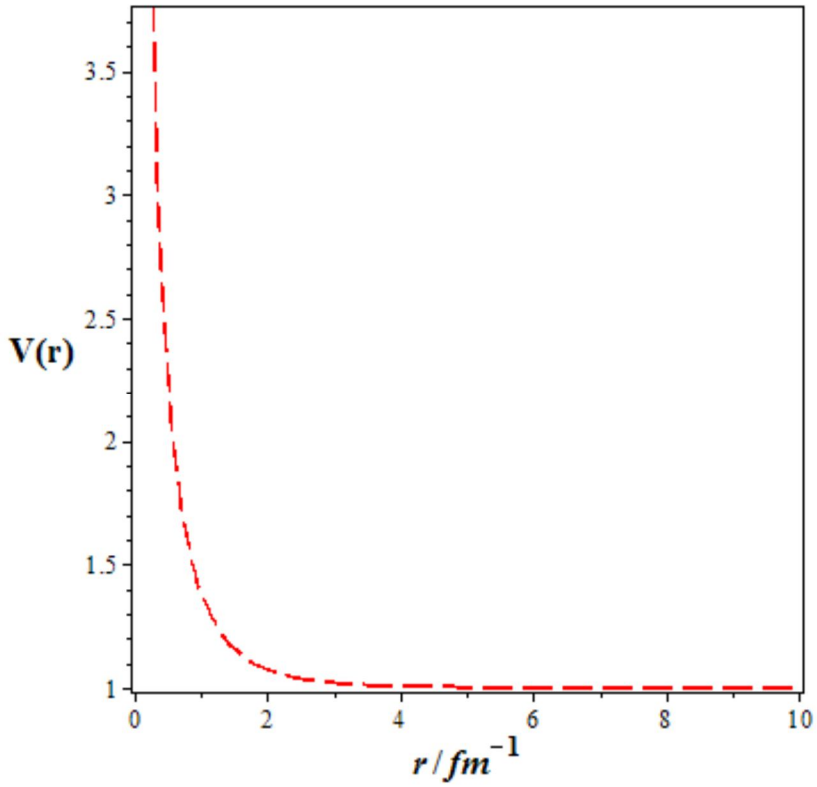

FIG. 1. Plots of Varshni potential with inter-nuclear distance r in (fm^{-1}).

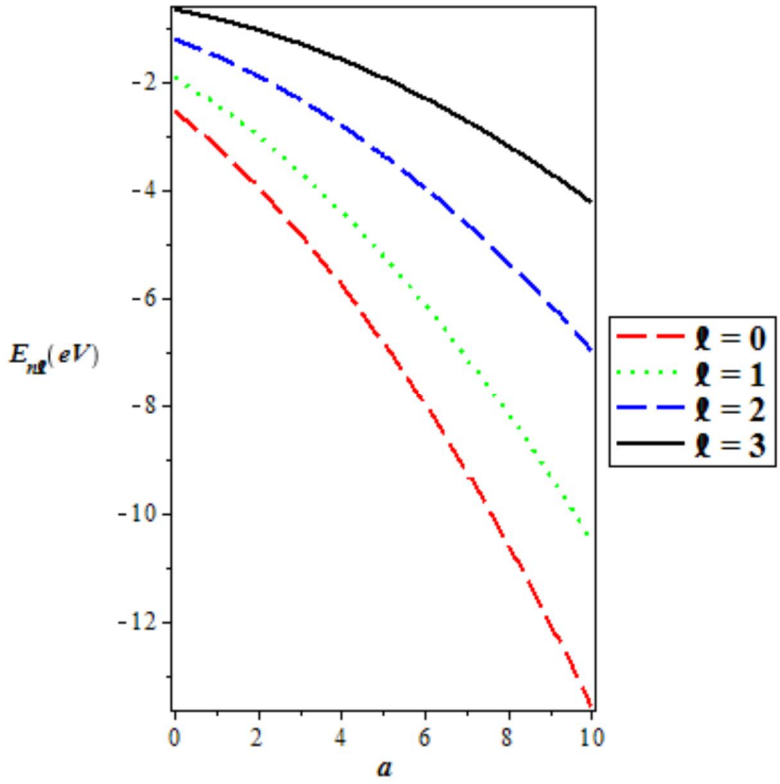

FIG. 2. Energy eigenvalues' variation with parameter a for various vibrational quantum numbers.

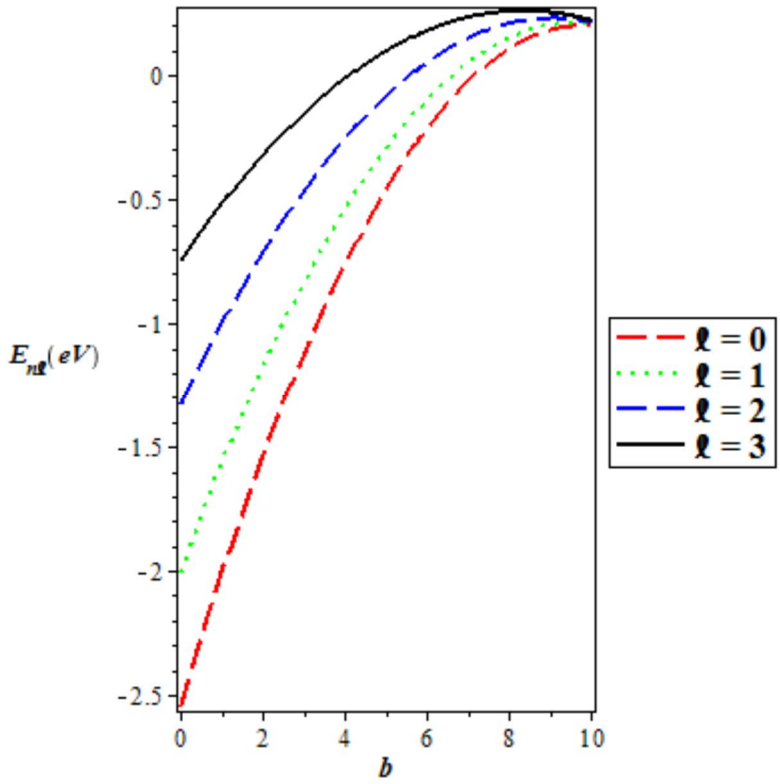

FIG. 3. Energy eigenvalues' variation with potential parameter b for various quantum numbers.

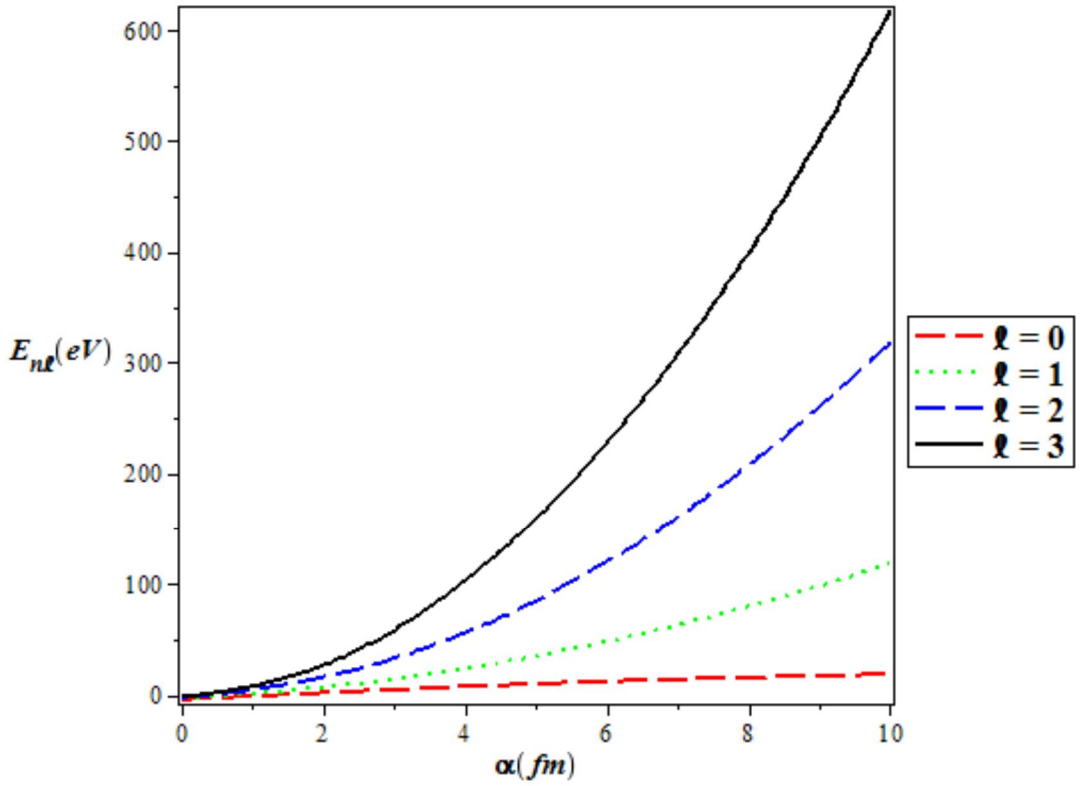

FIG. 4. Energy eigenvalues' variation with screening parameter for various vibrational quantum numbers.

4.1 Discussion of Results

The numerical values of five diatomic molecules were computed with spectroscopic parameters adopted from Oluwadare and Oyewumi (2017) [52] for energy spectra and expectation values of $\langle r^{-2}\rangle, \langle T\rangle$ and $\langle \hat{p}^2\rangle$, respectively. Equation (38) was used for energy spectra, while Eqs. (60), (69) and (70) were used for expectation values. The diatomic molecules considered in this work are H_2, HCl, TiH, I_2 and CO as presented in Tables 2-6.The constants, 1 amu = $931.494028\ \mathrm{MeV}/c^2$ and $\hbar c = 1973.29$ eVA are adopted from Ituen *et al*. [62] for the computation. Equation (38), was also used to compute for bound state of Varshni potential as presented in Table 7.

Table 1 is the spectroscopic constant used in the numerical computation of the energy spectra and expectation values. Tables 2-6 show numerical energy spectra and expectation values of $\langle r^{-2}\rangle$, $\langle T\rangle$ *and* $\langle \hat{P}^2\rangle$, respectively for the five selected diatomic molecules. The results show that the energy spectra $E_{nl}(eV)$ of these diatomic molecules increase as the principal quantum number n and orbital angular momentum quantum number l increase. The tables also show that some of the expectation values increase with an increase in quantum state, while some decrease with an increase in quantum state. For instance, it is observed that as n and l increase, the expectation values of $\langle r^{-2}\rangle$ decrease. Also, it is observed that the expectation values of $\langle T\rangle$ and $\langle \hat{P}^2\rangle$ increase as n and l increase. The bound-state energy for Varshni potential is generated with $\upsilon = \chi = -1$ and $D = 3$ for different states with three different values of the potential range. It is observed that as the potential range increases, the energy of the system increases, as shown in Table 7, which agrees with the work of Ebomwonyi *et al*. [39]. We plotted the energy eigenvalues with the potential-strength parameters and screening parameter of Varshni potential, as shown in Figs. 2-4, for various values of quantum numbers. In Fig. 2, a decrease in energy eigenvalues is noticed as n and l increase. In Fig. 3, energy eigenvalues increase as n and l increase and converge at zero. Finally, in Fig.4, the increase in energy tends to spread out from zero for different vibrational quantum numbers.

5. Conclusion

In this work, analytical solutions have been obtained of the Klein-Gordon equation for the Varshni potential with an approximation to the centrifugal term using the Nikiforov-Uvarov method. The energy eigenvalues are obtained both in relativistic and non-relativistic regimes and the corresponding normalized eigenfunctions. Energy spectra and expectation values of the square of inverse position $\langle r^{-2} \rangle$, kinetic energy $\langle T \rangle$ and square of momentum $\langle \hat{P}^2 \rangle$ for five selected diatomic molecules are computed using Hellmann-Feynman Theorem, as presented in Tables 2-6. Bound-state energy is obtained for Varshni potential, which agrees with Ebomwonyi *et al*. [39], proving the success of the formalism. The variation in the energy eigenvalues with potential parameters was also plotted and discussed.

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