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RESEARCH

Shifted Tietz–Wei oscillator for simulating the atomic interaction in diatomic molecules

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Abstract The shifted Tietz–Wei (sTW) oscillator is as good as traditional Morse potential in simulating the atomic interaction in diatomic molecules. By using the Pekeris-type approximation, to deal with the centrifugal term, we obtain the bound-state solutions of the radial Schrödinger equation with this typical molecular model via the exact quantization rule (EQR). The energy spectrum for a set of diatomic molecules ($\mathrm{NO}(a^4\Pi_i)$, $\mathrm{NO}(B^2\Pi_r)$, $\mathrm{NO}(L'^2\phi)$, $\mathrm{NO}(b^4\Sigma^-)$, $\mathrm{ICl}\left(X^1\Sigma_g^+\right)$, $\mathrm{ICl}(A^3\Pi_1)$ and $\mathrm{ICl}(A'^3\Pi_2)$ for arbitrary values of n and ℓ quantum numbers are obtained. For the sake of completeness, we study the corresponding wavefunctions using the formula method.

Keywords Exact quantization rule · Formula method · Shifted Tietz-Wei potential

Introduction

By employing the dissociation energy and the equilibrium bond length for a diatomic molecule as explicit parameters, Jia et al. [1] generated improved expressions for some well-known potentials including Rosen–Morse, Manning–Rosen, Tietz and Frost–Musulin potential energy functions. These authors found that the well-known Tietz potential function is conventionally defined in terms of five parameters but it actually has only four independent parameters. Furthermore, the Wei [2] and Tietz potential functions [3] are exactly same solvable empirical functions.

Wang et al. [4] also generated improved expressions for two versions of the Schiöberg potential energy function which are the Rosen–Morse and Manning–Rosen potential functions. By choosing the experimental values of the dissociation energy, equilibrium bond length and equilibrium harmonic vibrational frequency as inputs, the authors obtained the average deviations of the energies calculated with the potential model from the experimental data for five diatomic molecules, and find that no one of six three-parameter empirical potential energy functions is superior to the other potentials in fitting experimental data for all molecules examined.

All these efforts were made in an attempt to find a most suitable molecular potential in its description of diatomic molecules. Following Refs. [1, 4], we suggest sTW as a modification for the TW [2–8]. This potential can be written as

$$V(r) = V_\mathrm{e}\left[\frac{2(c_\mathrm{h}-1)e^{-b_h(r-r_\mathrm{e})}-(c_\mathrm{h}^2-1)e^{-2b_h(r-r_\mathrm{e})}}{\left(1-c_\mathrm{h}e^{-b_\mathrm{h}(r-r_\mathrm{e})}\right)^2}\right], \tag{1}$$

where $b_\mathrm{h} = \beta(1-c_\mathrm{h})$, r_e is the molecular bond length, β is the Morse constant, V_e is the potential well depth and c_h is an optimization parameter obtained from ab initio or

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Rydberg–Klein–Rees (RKR) intramolecular potentials. r is the internuclear distance. When the potential constant approaches zero, i.e. $c_h \rightarrow 0$, the sTW potential reduces to the Morse potential [9]. This potential is just the TW potential shifted by dissociation energy D_e. The shape of this potential is shown in Fig. 1a for different molecules.

Figure 1b compare between TW diatomic molecular potential, sTW diatomic molecular potential and the Morse potential using the parameters set for $H_2\left(X^1\Sigma_g^+\right)$ diatomic molecule. As it can be seen from this plot, the shifted Tietz–Wei and the Morse potentials are very close to each other for large values of r in the regions $r \approx r_e$ and $r > r_e$, but they are very different at $r \approx 0$. This implies that the shifted Tietz–Wei potential is as good as traditional Morse potential and better than the Tietz–Wei potential in stimulating the atomic interaction for diatomic molecules.

The scheme of our presentation is as follows. In the next section we give basic ingredient of exact quantization rule and all necessary formulas for our calculations. We solve the radial Schrödinger equation for the sTW and also obtain the rotational-vibrational energy spectrum for some diatomic molecules. Finally, results and conclusions are presented.

A brief review of the exact quantization rule

Here we give a brief review on the EQR. The details can be found in Refs. [10–24]. In 2005, Ma and Xu [12, 13] by carefully studying one-dimensional Schrödinger equation, have extended results to three-dimensional case by simply making the replacements $x \rightarrow r$ and $V(x) \rightarrow V_{\text{eff}}(r)$:

$$\int_{r_a}^{r_b} k(r)dr = N\pi + \int_{r_a}^{r_b} \phi(r)\left[\frac{\mathrm{d}k(r)}{\mathrm{d}r}\right]\left[\frac{\mathrm{d}\phi(r)}{\mathrm{d}r}\right]^{-1}\mathrm{d}r,$$
$$k(r) = \sqrt{\frac{2\mu}{\hbar^2}\left[E - V_{\text{eff}}(r)\right]}, \tag{2}$$

where r_A and r_B are two turning points determined by $E = V_{\text{eff}}(r)$. The $N = n+1$ is the number of the nodes of $\phi(r)$ in the region $E_{n\ell} = V_{\text{eff}}(r)$ and is larger by one than the number n of the nodes of wave function $\psi(r)$. The first term $N\pi$ is the contribution from the nodes of the logarithmic derivative of wave function, and the second is called the quantum correction.

In this approach, the energy spectrum equation is obtained by solving the two integrals involved in Eq. (2). This quantization rule has been used in many physical systems to obtain the exact solutions of many exactly solvable quantum systems [10–24]. EQR is a very important foundation to proper quantization rule (PQR) [10, 25–27].

The energy spectrum

To study any quantum physical model characterized by the diatomic molecular potential given by Eq. (1), we need to solve the following Schrödinger equation for spherically symmetric potential in any arbitrary dimensional space:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{D-1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\ell(\ell+D-2)}{r^2} + \frac{2\mu}{\hbar^2}\left(E_{n\ell} - V(r)\right)\right)$$
$$\psi_{n,\ell,m}(r,\Omega_D) = 0. \tag{3}$$

Now, by defining the wavefunction $\psi_{n,\ell,m}(r,\Omega_D)$ as $r^{(1-D)/2}R_{n\ell}(r)Y_{\ell m}(\theta,\phi)$ and taking $V(r)$ as the sTW

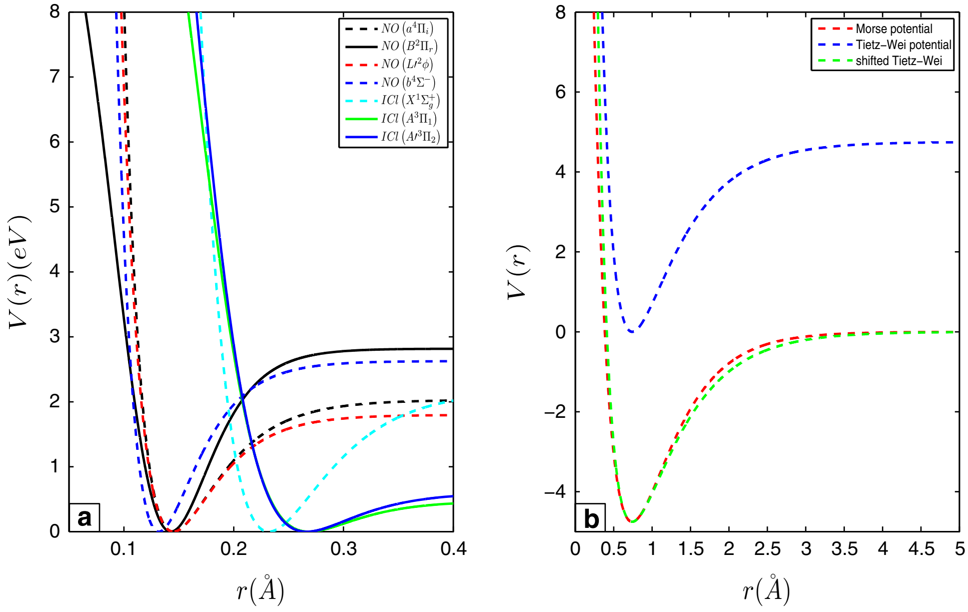

Fig. 1 **a** Shape of sTW diatomic molecular potential for different diatomic molecules. **b** Shape of the sTW, TW and Morse oscillator potentials for $H_2\left(X^1\Sigma_g^+\right)$ diatomic molecule with $c_h = 0.170066$, $b_h = 1.61890\,\text{Å}^{-1}$, $r_e = 0.7416\,\text{Å}$ and $V_e = 38318\,\text{cm}^{-1}$

diatomic molecular potential, the radial part of Eq. (3) can be found as

$$\frac{\mathrm{d}^2R_{n\ell}(r)}{\mathrm{d}r^2}+\frac{2\mu}{\hbar^2} \times\left[E_{n\ell}-V_{\mathrm{e}}\left[\frac{2(c_{\mathrm{h}}-1)e^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}-(c_{\mathrm{h}}^2-1)e^{-2b_h(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}e^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}\right]^2 -\frac{(\tilde{\eta}^2-\frac{1}{4})\hbar^2}{2\mu r^2}\right]R_{n\ell}(r)=0, \tag{4}$$

where n, ℓ and $E_{n\ell}$ denote the principal quantum number, orbital angular momentum number and the bound state energy eigenvalues of the system under consideration (i.e., $E_{n\ell}<0$), respectively. The parameter $\tilde{\eta}=\ell+\frac{1}{2}(D-2)$ which is a linear combination of the spatial dimensions D and the angular momentum quantum number ℓ. It is well known that for $\ell=0$, problem in the form (4) is exactly solvable. But for $\ell\neq 0$, it is not due to the centrifugal barrier. Therefore, in order to solve the above equation for $\ell\neq 0$ states, Hamzavi et al. [6] found that the following formula is a good approximation scheme to deal with the centrifugal barrier:

$$\frac{1}{r^2}\approx\frac{1}{r_{\mathrm{e}}^2}\left(D_0+D_1\frac{e^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}e^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+D_2\frac{e^{-2b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{(1-c_{\mathrm{h}}e^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})})^2}\right), \tag{5}$$

with

$$D_0=1-\frac{1}{\alpha}(1-c_{\mathrm{h}})(3+c_{\mathrm{h}})+\frac{3}{\alpha^2}(1-c_{\mathrm{h}})^2, \quad \lim_{c_{\mathrm{h}}\to 0}D_0=1-\frac{3}{\alpha}+\frac{3}{\alpha^2} \tag{6a}$$

$$D_1=\frac{2}{\alpha}(1-c_{\mathrm{h}})^2(2+c_{\mathrm{h}})-\frac{6}{\alpha^2}(1-c_{\mathrm{h}})^3, \quad \lim_{c_{\mathrm{h}}\to 0}D_1=\frac{4}{\alpha}-\frac{6}{\alpha^2} \tag{6b}$$

$$D_2=-\frac{1}{\alpha}(1-c_{\mathrm{h}})^3(1+c_{\mathrm{h}})+\frac{3}{\alpha^2}(1-c_{\mathrm{h}})^4, \quad \lim_{c_{\mathrm{h}}\to 0}D_2=-\frac{1}{\alpha}+\frac{3}{\alpha^2}, \tag{6c}$$

Constant $\alpha=b_{\mathrm{h}}r_{\mathrm{e}}$ has been introduced for mathematical simplicity. Now, by inserting this approximation into Eq. (4) and then introducing a new transformation of the form $r\to\zeta=\frac{r-r_{\mathrm{e}}}{r_{\mathrm{e}}}$ through the mapping function $\zeta=f(r)$ with r in the domain $[0,\infty)$ or ζ in the domain $[-1,\infty]$, we obtain the following second order differential equation:

$$\frac{1}{r_{\mathrm{e}}^2}\frac{\mathrm{d}^2R_{n\ell}(\zeta)}{\mathrm{d}\zeta^2}+\frac{2\mu}{\hbar^2}[E_{n\ell}-V_{\mathrm{eff}}(\zeta)]R_{n\ell}(\zeta)=0, \quad \text{with}$$

$$V_{\mathrm{eff}}(\zeta)=\left[\mathcal{A}+\frac{\mathcal{B}}{e^{\alpha\zeta}-c_{\mathrm{h}}}+\frac{\frac{\ell(\ell+1)D_2}{r_{\mathrm{e}}^2}+\frac{2\mu V_{\mathrm{e}}}{\hbar^2}(c_{\mathrm{h}}-1)^2}{(e^{\alpha\zeta}-c_{\mathrm{h}})}+\mathcal{F}\left(e^{\alpha\zeta}-c_{\mathrm{h}}\right)^2\right],$$

$$\mathcal{A}=\left(\frac{\tilde{\eta}^2-\frac{1}{4}}{r_{\mathrm{e}}^2}\right)\frac{D_0\hbar^2}{2\mu},\ \mathcal{B}=\left(\frac{\tilde{\eta}^2-\frac{1}{4}}{r_{\mathrm{e}}^2}\right)\frac{D_1\hbar^2}{2\mu}+2V_{\mathrm{e}}(c_{\mathrm{h}}-1),$$

$$\mathcal{F}=\left(\frac{\tilde{\eta}^2-\frac{1}{4}}{r_{\mathrm{e}}^2}\right)\frac{D_2\hbar^2}{2\mu}+V_{\mathrm{e}}(c_{\mathrm{h}}-1)^2. \tag{7}$$

If we define $\tilde{\varsigma}=\frac{1}{e^{\alpha\zeta}-c_{\mathrm{h}}}$, then we can obtain the two turning points $\tilde{\varsigma}_a$ and $\tilde{\varsigma}_b$ as well as their sum and product properties by solving $V_{\mathrm{eff}}(\zeta)-E_{n\ell}=0$ or $V_{\mathrm{eff}}(\tilde{\varsigma})-E_{n\ell}=0$ as:

$$\tilde{\varsigma}_a=-\frac{\mathcal{B}}{2\mathcal{F}}-\frac{1}{2\mathcal{F}}\sqrt{\mathcal{B}^2-4\mathcal{F}(\mathcal{A}-E_{n\ell})}, \quad \text{and}$$
$$\tilde{\varsigma}_b=\frac{\mathcal{B}}{2\mathcal{F}}+\frac{1}{2\mathcal{F}}\sqrt{\mathcal{B}^2-4\mathcal{F}(\mathcal{A}-E_{n\ell})}$$
$$\tilde{\varsigma}_a+\tilde{\varsigma}_b=-\frac{\mathcal{B}}{\mathcal{F}}, \quad \tilde{\varsigma}_a\tilde{\varsigma}_b=\frac{\mathcal{A}-E_{n\ell}}{\mathcal{F}} \quad \text{and} \tag{8}$$
$$k(y)=\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}}[-(\tilde{\varsigma}-\tilde{\varsigma}_a)(\tilde{\varsigma}-\tilde{\varsigma}_b)]^{1/2}.$$

Now, we can write the non-linear Riccati equation for the ground state is as

$$-\alpha\frac{\tilde{\varsigma}(1+\tilde{\varsigma})}{r_{\mathrm{e}}}\phi_0'(\tilde{\varsigma})+\phi_0^2(\tilde{\varsigma})+\frac{2\mu}{\hbar^2}\left[E_{0\ell}-V_{eff}(\tilde{\varsigma})\right]=0\,. \tag{9}$$

Since the logarithmic derivative $\phi_0(\tilde{\varsigma})$ for the ground state has one zero and no pole, it has to take the linear form in $\tilde{\varsigma}$. Thus, we assume the following solution for the ground states

$$\phi_0(\tilde{\varsigma})=A+B\tilde{\varsigma}\,. \tag{10}$$

By putting Eqs. (10) into (9), we can solve the non-linear Riccati equation. After proper comparison, it is straightforward to obtain the ground state energy and values of A and B as

$$E_{0\ell}=\mathcal{A}-\frac{\hbar^2A^2}{2\mu} \quad \text{with} \quad A=\frac{\mu}{\hbar^2}\frac{\mathcal{B}-\mathcal{F}/c_{\mathrm{h}}^2}{B}+\frac{B}{2} \quad \text{and}$$
$$B=\frac{\alpha c_{\mathrm{h}}}{2r_{\mathrm{e}}}+\frac{\alpha c_{\mathrm{h}}}{2r_{\mathrm{e}}}\sqrt{1+\frac{8\mu\mathcal{F}r_{\mathrm{e}}^2}{\alpha^2\hbar^2c_{\mathrm{h}}^2}}. \tag{11}$$

Since we now have all basic ingredient required to perform our calculations, thus, we proceed to calculating integrals (2)

$$
\begin{aligned}
\int_{r_a}^{r_b} k(r)\mathrm{d}r &= -\frac{r_\mathrm{e}}{\alpha}\int_{\tilde{\varsigma}_a}^{\tilde{\varsigma}_b}\frac{k(\tilde{\varsigma})}{a\tilde{\varsigma}(1+\tilde{\varsigma})}d\tilde{\varsigma} = -\frac{r_\mathrm{e}}{\alpha}\int_{\tilde{\varsigma}_{0a}}^{\tilde{\varsigma}_{0b}} \\
&\quad\times\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}\frac{\left[-(\tilde{\varsigma}-\tilde{\varsigma}_a)(\tilde{\varsigma}-\tilde{\varsigma}_b)\right]^{1/2}}{\tilde{\varsigma}(1+\tilde{\varsigma}c_\mathrm{h})}}\mathrm{d}\tilde{\varsigma} \\
&= -\frac{\pi r_\mathrm{e}}{\alpha}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}} \\
&\quad\times\left[\frac{\sqrt{(1+\tilde{\varsigma}_a c_\mathrm{h})(1+\tilde{\varsigma}_b c_\mathrm{h})}}{c_\mathrm{h}}-\frac{1}{c_\mathrm{h}}-\sqrt{\tilde{\varsigma}_a\tilde{\varsigma}_b}\right] \\
&= -\frac{\pi r_\mathrm{e}}{\alpha}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}} \\
&\quad\times\left[\frac{\sqrt{(\mathcal{A}-E_{n\ell})c_\mathrm{h}^2-\mathcal{B}c_\mathrm{h}+\mathcal{F}}}{\mathcal{F}c_\mathrm{h}}-\frac{1}{c_\mathrm{h}}-\sqrt{\frac{\mathcal{A}-E_{n\ell}}{\mathcal{F}}}\right],
\end{aligned}
\tag{12}
$$

where we have used the following standard integral

$$
\begin{aligned}
&\int_{x_a}^{x_b}\frac{\sqrt{(x_a-x)(x-x_b)}}{x(1+Qx)}dx \\
&= \pi\left[\frac{\sqrt{(Qx_a+1)(Qx_b+1)}}{Q}-\frac{1}{Q}-\sqrt{x_a x_b}\right].
\end{aligned}
\tag{13}
$$

Furthermore, we can find the integral on the right hand side as

$$
\begin{aligned}
&\int_{r_{0a}}^{r_{0a}}\phi(r)\left[\frac{\mathrm{d}k_0(r)}{\mathrm{d}r}\right]\left[\frac{\mathrm{d}\phi(r)}{\mathrm{d}r}\right]^{-1}\mathrm{d}r \\
&= -\frac{r_\mathrm{e}}{\alpha}\int_{\tilde{\varsigma}_{0a}}^{\tilde{\varsigma}_{0b}}\left[\frac{\mathrm{d}k(r)}{\mathrm{d}r}\right]\left[\frac{\mathrm{d}\phi(\tilde{\varsigma})}{\mathrm{d}\tilde{\varsigma}}\right]^{-1}\left(\frac{A}{B}+\tilde{\varsigma}\right)\mathrm{d}\tilde{\varsigma} \\
&= \frac{r_\mathrm{e}}{2\alpha}\int_{\tilde{\varsigma}_{0a}}^{\tilde{\varsigma}_{0b}}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}}\frac{\left[2\tilde{\varsigma}-(\tilde{\varsigma}_a+\tilde{\varsigma}_b)\right]\left[\frac{A}{B}+\tilde{\varsigma}\right]}{\tilde{\varsigma}(1+\tilde{\varsigma}c_\mathrm{h})\sqrt{-(\tilde{\varsigma}-\tilde{\varsigma}_a)(\tilde{\varsigma}-\tilde{\varsigma}_b)}}\mathrm{d}\tilde{\varsigma} \\
&= \frac{r_\mathrm{e}}{2\alpha}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}}\int_{\tilde{\varsigma}_{0a}}^{\tilde{\varsigma}_{0b}}\left[\left(\frac{A}{B}-\frac{1}{c_\mathrm{h}}\right)\left(1+\frac{\tilde{\varsigma}_{0a}+\tilde{\varsigma}_{0b}}{2}c_\mathrm{h}\right)\frac{1}{1+\tilde{\varsigma}c_\mathrm{h}}\right. \\
&\quad\left.+\frac{1}{c_\mathrm{h}}.-\frac{A}{B}\left(\frac{\tilde{\varsigma}_{0a}+\tilde{\varsigma}_{0b}}{2}\right)\frac{1}{\tilde{\varsigma}}\right]\times\frac{\mathrm{d}\tilde{\varsigma}}{\sqrt{-(\tilde{\varsigma}-\tilde{\varsigma}_a)(\tilde{\varsigma}-\tilde{\varsigma}_b)}} \\
&= \left[\left(\frac{A}{B}-\frac{1}{c_\mathrm{h}}\right)\left(1-\frac{\mathcal{B}c_\mathrm{h}}{2\mathcal{F}}\right)\frac{1}{\sqrt{1-\frac{\mathcal{B}c_\mathrm{h}}{\mathcal{F}}+\frac{\mathcal{A}-E_{0\ell}}{\mathcal{F}}c_\mathrm{h}^2}}\right. \\
&\quad\left.+\frac{A}{B}\left(\frac{\mathcal{B}}{2\mathcal{F}}\right)\frac{\sqrt{\mathcal{F}}}{\sqrt{\mathcal{A}-E_{0\ell}\mathcal{F}}}\right]\frac{\pi r_\mathrm{e}}{\alpha}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}} \\
&= \frac{\pi r_\mathrm{e}}{\alpha}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}}\left[\frac{1}{Bc_\mathrm{h}}\sqrt{\frac{2\mu\mathcal{F}}{\hbar^2}}+\frac{1}{c_\mathrm{h}}\right].
\end{aligned}
\tag{14}
$$

Using the results in Eqs. (12) and (14) together with Eq. (1), we can find the energy eigenvalues equation for the sTW diatomic molecular potential as

$$
\begin{aligned}
E_{n\ell}^D &= \frac{\hbar^2\left(\tilde{\eta}^2-\frac{1}{4}\right)D_0}{2\mu r_\mathrm{e}^2}-\frac{\alpha^2\hbar^2}{2\mu r_\mathrm{e}^2} \\
&\quad\times\left[\frac{(\delta+n)^2+\frac{\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2c_\mathrm{h}^2}(D_1c_\mathrm{h}-D_2)+\frac{2\mu V_\mathrm{e}r_\mathrm{e}^2}{\alpha^2\hbar^2}\left(1-\frac{1}{c_\mathrm{h}^2}\right)}{2(\delta+n)}\right]^2 \\
&\quad\text{with }\ \delta=\frac{1}{2}+\frac{1}{2}\sqrt{1+\frac{4}{c_\mathrm{h}^2}\left(\frac{D_2\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2}+\frac{2\mu V_\mathrm{e}r_\mathrm{e}^2}{\alpha^2\hbar^2}(1-c_\mathrm{h})^2\right)}.
\end{aligned}
\tag{15}
$$

In three-dimensional $(D=3)$ space, it can be reduced to the form

$$
\begin{aligned}
E_{n\ell} &= \frac{\hbar^2\ell(\ell+1)D_0}{2\mu r_\mathrm{e}^2}-\frac{\alpha^2\hbar^2}{2\mu r_\mathrm{e}^2} \\
&\quad\times\left[\frac{(\delta+n)^2+\frac{\ell(\ell+1)}{\alpha^2c_\mathrm{h}^2}(D_1c_\mathrm{h}-D_2)+\frac{2\mu V_e r_e^2}{\alpha^2\hbar^2}\left(1-\frac{1}{c_h^2}\right)}{2(\delta+n)}\right]^2 \\
&\quad\text{with }\ \delta=\frac{1}{2}+\frac{1}{2}\sqrt{1+\frac{4}{c_h^2}\left(\frac{D_2\ell(\ell+1)}{\alpha^2}+\frac{2\mu V_e r_e^2}{\alpha^2\hbar^2}(1-c_h)^2\right)}.
\end{aligned}
\tag{16}
$$

The Eigenfunctions

For the sake of completeness, we study the corresponding wavefunctions for this potential. For this purpose we introduce a new transformation of the form $t=e^{-b_\mathrm{h}(r-r_\mathrm{e})}\in(e^{\alpha},0)$ in Eq. (7), which maintained the finiteness of the transformed wave functions on the boundary conditions. Thus, we can find

$$
\begin{aligned}
&\frac{\mathrm{d}^2U_{n\ell}(t)}{\mathrm{d}t^2}+\frac{1}{t}\frac{\mathrm{d}U_{n\ell}(t)}{\mathrm{d}t}+\frac{1}{t^2(1-c_\mathrm{h}t)^2} \\
&\times\left\{\left[\frac{2\mu r_\mathrm{e}^2E_{n\ell}}{\hbar^2\alpha^2}-\frac{\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2}D_0\right]\right. \\
&+\left[-2c_\mathrm{h}\left(\frac{2\mu r_\mathrm{e}^2(E_{n\ell}+V_\mathrm{e})}{\alpha^2\hbar^2}-\frac{\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2}D_0\right)\right. \\
&\left.+\frac{4\mu r_\mathrm{e}^2V_\mathrm{e}}{\hbar^2\alpha^2}-\frac{\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2}D_1\right]t \\
&+\left[c_\mathrm{h}^2\left(\frac{2\mu r_\mathrm{e}^2(E_{n\ell}+V_\mathrm{e})}{\alpha^2\hbar^2}-\frac{\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2}D_0\right)\right. \\
&\left.\left.+\frac{\left(\tilde{\eta}^2-\frac{1}{4}\right)}{\alpha^2}(D_1c_\mathrm{h}-D_2)-\frac{2\mu r_\mathrm{e}^2V_\mathrm{e}}{\hbar^2\alpha^2}\right]t^2\right\}U_{n\ell}(t)=0.
\end{aligned}
\tag{17}
$$

Following the procedure described in Ref. [28], we can write the solution $U_{n\ell}(t)$ in terms of hypergeometric polynomials and thus the wave function takes the form

Table 1 Model parameters of the diatomic molecules studied in the present work

Molecules (states)	c_h	$\mu/10^{-23}$ (g)	b_h (Å^{-1})	r_e (Å)	$D\,(\mathrm{cm}^{-1})$
NO $(a^4\Pi_i)$	0.0082003	1.249	2.408413	1.451	16,361
NO $(B^2\Pi_r)$	−0.482743	1.249	3.42650	1.428	22,722
NO $(L'^2\phi)$	−0.073021	1.249	2.73796	1.451	14,501
NO $(b^4\Sigma^-)$	−0.085078	1.249	3.01538	1.318	21,183
ICl $\left(X^1\Sigma_g^+\right)$	−0.086212	4.55237	2.008578	2.3209	17,557
ICl $(A^3\Pi_1)$	−0.167208	4.55237	2.542557	2.6850	3814.7
ICl $(A'^3\Pi_2)$	−0.157361	4.55237	2.373450	2.6650	4875

Table 2 The bound states energy eigenvalues ($D = 2$ and 3) for set of diatomic molecules for various n and rotational ℓ quantum numbers in sDF diatomic molecular potential

D	n	ℓ	NO $(a^4\Pi_i)$	NO $(B^2\Pi_r)$	NO $(L'^2\phi)$	NO $(b^4\Sigma^-)$	ICl $\left(X^1\Sigma_g^+\right)$	ICl $(A^3\Pi_1)$	ICl $(A'^3\Pi_2)$
	0	0	−1.971298585	−2.88233770	−1.855428285	−2.695026855	−2.200695845	−0.4861418795	−0.618432865
	1	0	−1.859308585	−3.01386965	−1.972859085	−2.834614855	−2.248819245	−0.5129225795	−0.646829015
		1	−1.859148585	−3.01373250	−1.972723585	−2.834451355	−2.248804845	−0.5129118495	−0.646818105
	2	0	−1.750608585	−3.14759050	−2.093631485	−2.977436555	−2.297420945	−0.5403157895	−0.675774025
		1	−1.750468585	−3.14745280	−2.093493685	−2.977270755	−2.297406745	−0.5403049695	−0.675763045
		2	−1.750098585	−3.14703970	−2.093081285	−2.976773655	−2.297363645	−0.5402725095	−0.675730195
2	3	0	−1.645178585	−3.28347662	−2.217724085	−3.123472855	−2.346500045	−0.5683148895	−0.705263165
		1	−1.645068585	−3.28333841	−2.217584185	−3.123304955	−2.346485745	−0.5683039695	−0.705252125
		2	−1.644678585	−3.28292375	−2.217165185	−3.122801255	−2.346442645	−0.5682712195	−0.705219005
		3	−1.644058585	−3.28223274	−2.216466785	−3.121961855	−2.346370345	−0.5682166495	−0.705163785
	4	0	−1.543078585	−3.42150558	−2.345115985	−3.272704955	−2.396055245	−0.5969133695	−0.735291785
		1	−1.542938585	−3.42136686	−2.344973985	−3.272534755	−2.396040945	−0.5969023495	−0.735280655
		2	−1.542598585	−3.42095075	−2.344548485	−3.272024355	−2.395997445	−0.5968693195	−0.735247275
		3	−1.541978585	−3.42025729	−2.343839285	−3.271173455	−2.395924945	−0.5968142695	−0.735191635
		4	−1.541118585	−3.41928647	−2.342846285	−3.269982555	−2.395823745	−0.5967371995	−0.735113745
	0	0	−1.971278585	−2.88230356	−1.855395085	−2.694986655	−2.200692145	−0.4861392095	−0.618430175
	1	0	−1.859278585	−3.01383536	−1.972825385	−2.834574055	−2.248815545	−0.5129198795	−0.646826285
		1	−1.859008585	−3.01356106	−1.972554585	−2.834247155	−2.248787045	−0.5128984495	−0.646804535
	2	0	−1.750568585	−3.14755607	−2.093596885	−2.977395155	−2.297417445	−0.5403130995	−0.675771295
		1	−1.750288585	−3.14728068	−2.093321985	−2.977063955	−2.297388745	−0.5402914395	−0.675749345
		2	−1.749808585	−3.14672991	−2.092771985	−2.976400855	−2.297331445	−0.5402481695	−0.675705525
3	3	0	−1.645158585	−3.28344206	−2.217689085	−3.123430855	−2.346496645	−0.5683121595	−0.705260395
		1	−1.644908585	−3.28316563	−2.217409585	−3.123095155	−2.346467645	−0.5682903295	−0.705238345
		2	−1.644418585	−3.28261279	−2.216850885	−3.122423255	−2.346410245	−0.5682466595	−0.705194145
		3	−1.643678585	−3.28178358	−2.216012785	−3.121415755	−2.346323545	−0.5681811695	−0.705127915
	4	0	−1.543028585	−3.42147091	−2.345080285	−3.272662455	−2.396051945	−0.5969106095	−0.735288995
		1	−1.542798585	−3.42119348	−2.344796885	−3.272322355	−2.396022645	−0.5968885995	−0.735266735
		2	−1.542328585	−3.42063869	−2.344229385	−3.271641355	−2.395964745	−0.5968445495	−0.735222225
		3	−1.541588585	−3.41980654	−2.343378185	−3.270620455	−2.395877945	−0.5967784695	−0.735155455
		4	−1.540608585	−3.41869709	−2.342243285	−3.269259655	−2.395761945	−0.5966903895	−0.735066435

$$U_{n\ell}(\zeta) = N_{n\ell} e^{-p\alpha\zeta} (1 - c_{\mathrm{h}} e^{-\alpha\zeta})^{q} \; {}_2F_1(-n, n + 2(p+q); \\ 2p + 1, c_{\mathrm{h}} e^{-\alpha\zeta}), \tag{18}$$

with

$$p = \sqrt{\left[\left(\frac{\tilde{\eta}^2 - \frac{1}{4}}{\alpha^2}\right) D_0 - \frac{2\mu r_{\mathrm{e}}^2}{\hbar^2 \alpha^2} E_{n\ell}\right]} \quad \text{and}$$

$$q = \frac{1}{2}\left\{1 + \sqrt{1 + \frac{4}{c_{\mathrm{h}}^2}\left[\left(\frac{\tilde{\eta}^2 - \frac{1}{4}}{\alpha^2}\right) D_2 + \frac{2\mu r_{\mathrm{e}}^2 V_{\mathrm{e}}}{\hbar^2 \alpha^2}(1 - c_{\mathrm{h}})^2\right]}\right\}, \tag{19}$$

where $N_{n\ell}$ is the normalization constant. For a further detail on the calculation of similar potential models solved using formula method, one is advised to refer to other work [28]

Results and conclusions

In this study, in an attempt to find a more suitable potential that simulate the atomic interaction in diatomic molecules, we suggested sTW diatomic molecular potential as a modification for the TW diatomic molecular potential. The bound state solution of this potential has been found in an arbitrary D-dimension via the improved exact quantization rule.

Further, using the spectroscopic parameters presented in Table 1 which are taken from Ref. [8], we computed rotational-vibrational energy spectrum of some diatomic molecules in 2,3,4,5-dimensions. The results are presented in Tables 2 and 3. In our numerical computations, we have used the following conversions: 1 amu = 931.494028

Table 3 The bound states energy eigenvalues (D = 4 and 5) for set of diatomic molecules for various n and rotational ℓ quantum numbers in sDF diatomic molecular potential

D	n	ℓ	NO $(a^4\Pi_i)$	NO $(B^2\Pi_r)$	NO $(L'^2\phi)$	NO $(b^4\Sigma^-)$	ICl $\left(X^1\Sigma_g^+\right)$	ICl $(A^3\Pi_1)$	ICl $(A'^3\Pi_2)$
	0	0	−1.971158585	−2.88220112	−1.855295085	−2.694865755	−2.200681645	−0.4861312495	−0.618422105
	1	0	−1.859148585	−3.01373250	−1.972723585	−2.834451355	−2.248804845	−0.5129118495	−0.646818105
		1	−1.858778585	−3.01332103	−1.972317885	−2.833961155	−2.248762245	−0.5128796695	−0.646785525
	2	0	−1.750468585	−3.14745280	−2.093493685	−2.977270755	−2.297406745	−0.5403049695	−0.675763045
		1	−1.750098585	−3.14703970	−2.093081285	−2.976773655	−2.297363645	−0.5402725095	−0.675730195
		2	−1.749438585	−3.14635128	−2.092393885	−2.975945655	−2.297292045	−0.5402183995	−0.675675405
3	3	0	−1.645068585	−3.28333841	−2.217584185	−3.123304955	−2.346485745	−0.5683039695	−0.705252125
		1	−1.644678585	−3.28292375	−2.217165185	−3.122801255	−2.346442645	−0.5682712195	−0.705219005
		2	−1.644058585	−3.28223274	−2.216466785	−3.121961855	−2.346370345	−0.5682166495	−0.705163785
		3	−1.643188585	−3.28126535	−2.215488785	−3.120786155	−2.346269545	−0.5681402395	−0.705086495
	4	0	−1.542938585	−3.42136686	−2.344973985	−3.272534755	−2.396040945	−0.5969023495	−0.735280655
		1	−1.542598585	−3.42095075	−2.344548485	−3.272024355	−2.395997445	−0.5968693195	−0.735247275
		2	−1.541978585	−3.42025729	−2.343839285	−3.271173455	−2.395924945	−0.5968142695	−0.735191635
		3	−1.541118585	−3.41928647	−2.342846285	−3.269982555	−2.395823745	−0.5967371995	−0.735113745
		4	−1.540048585	−3.41803836	−2.341569785	−3.268451355	−2.395693345	−0.5966380895	−0.735013565
	0	0	−1.970998585	−2.88203041	−1.855128785	−2.694664455	−2.200663845	−0.4861179795	−0.618408615
	1	0	−1.859008585	−3.01356106	−1.972554585	−2.834247155	−2.248787045	−0.5128984495	−0.646804535
		1	−1.858508585	−3.01301246	−1.972013385	−2.833593555	−2.248729945	−0.5128555495	−0.646761065
	2	0	−1.750288585	−3.14728068	−2.093321985	−2.977063955	−2.297388745	−0.5402914395	−0.675749345
		1	−1.749808585	−3.14672991	−2.092771985	−2.976400855	−2.297331445	−0.5402481695	−0.675705525
		2	−1.749048585	−3.14590380	−2.091946885	−2.975407055	−2.297245545	−0.5401832395	−0.675639815
4	3	0	−1.644908585	−3.28316563	−2.217409585	−3.123095155	−2.346467645	−0.5682903295	−0.705238345
		1	−1.644418585	−3.28261279	−2.216850885	−3.122423255	−2.346410245	−0.5682466595	−0.705194145
		2	−1.643678585	−3.28178358	−2.216012785	−3.121415755	−2.346323545	−0.5681811695	−0.705127915
		3	−1.642668585	−3.28067802	−2.214895385	−3.120072855	−2.346208245	−0.5680938395	−0.705039565
	4	0	−1.542798585	−3.42119348	−2.344796885	−3.272322355	−2.396022645	−0.5968885995	−0.735266735
		1	−1.542328585	−3.42063869	−2.344229385	−3.271641355	−2.395964745	−0.5968445495	−0.735222225
		2	−1.541588585	−3.41980654	−2.343378185	−3.270620455	−2.395877945	−0.5967784695	−0.735155455
		3	−1.540608585	−3.41869709	−2.342243285	−3.269259655	−2.395761945	−0.5966903895	−0.735066435
		4	−1.539388585	−3.41731030	−2.340824985	−3.267557955	−2.395617345	−0.5965802895	−0.734955135

MeV/c^2, $1\ \mathrm{cm}^{-1} = 1.239841875 \times 10^{-4}$ eV, and $\hbar c = 1973.29 eV$Å.

From Eq. (15), it can be seen that two interdimensional states are degenerate whenever $(n, \ell, D) \rightarrow (n, \ell \pm 1, D \mp 2) \Rightarrow E^{D}_{n,\ell} = E^{(D\mp 2)}_{n,\ell\pm 1}$. Thus, a knowledge of $E^{D}_{n,\ell}$ for D = 2 to 5 provides the information necessary to find $E^{D}_{n,\ell}$ for other higher dimensions. For example, $E^{(2)}_{0,4} = E^{(4)}_{0,3} = E^{(6)}_{0,2} = E^{(8)}_{0,1}$. This is the same transformational invariance described for bound states of free atoms and molecules [29–31] and demonstrates the existence of interdimensional degeneracies among states of the confined Hulthén potential.

The advantage of the approach employed in this study is that it gives the eigenvalues through the calculation of two integral given by Eq. (2) and solving the resulting algebraic equation. Firstly, we can easily obtain the quantum correction by only considering the solution of the ground state of the quantum system since it is independent of the number of nodes of the wave function for exactly solvable quantum system. The general expressions obtained for the energy eigenvalues and wave functions can be easily reduced to the 3D space (D = 3) and for s-wave (i.e. $\ell = 0$ state). The EQR produce as good results as the PQR, however the procedure followed using PQR is more shorter and quick.

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