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Approximate energy spectra of diatomic molecules (LiH, HCl, VH, I_2) case of the Hulthén plus screened Kratzer potential

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In this research, we used the Nikiforov Uvarov functional analysis method to solve the Schrödinger equation with the Hulthén plus screened Kratzer potential using the Greene Aldrich approximation to remove the centrifugal barrier. We determine the bound state energies and corresponding wave functions. We applied our results to several diatomic molecules (LiH, HCl, VH, and I_2) to analyze their energy spectra. Our technique produced accurate results, which were validated by comparing our eigenvalue data with numerical data obtained by other researchers. Given the precision of this analytical method, we recommend its application in solving problems in non-relativistic and relativistic systems, particularly those involving exponential potentials.

Keywords: Schrödinger equation; spectra of energy; screened Kratzer potential; Hulthén potential; Nikiforov Uvarov functional analysis approach.

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1. Introduction

Getting the precise analytical solution to the Schrödinger problem is crucial. One important aspect is a specific potential connected to certain physical systems that we find intriguing. The numerous obstacles that researchers face when studying quantum mechanics are some of the key challenges. This problem is encountered and observed frequently in almost every scientific field, including solid-state, nuclear, particle, atomic, and molecular research. Physics is just one of the many subfields within the discipline of study. Numerous fascinating and promising approximation methods have been devised since the theory was first introduced, showcasing their ability to produce accurate or nearly flawless results on occasion. [1-4].

Several methods and approaches, such as the Nikiforov-Uvarov method [5], the WKB approximation [6], the path integral approach [7], supersymmetry [8], the variational iteration method [9], and the semi-inverse variation principle [10], have demonstrated improvements and are frequently utilized in mathematical physics. Despite relying on the integration of second-order linear differential equations, this method can be considered an algebraic tool. The goal is to use this method to investigate relativistic problems such as the Schrödinger equation [11], the Klein-Gordon [12] equation, and the Dirac equation [13]. The methods may solve general second-order differential equations with linear solutions, such as extended orthogonal polynomial functions. The final option gives us an exact answer for the energy spectrum and wave functions. In addition to solving the Schrödinger equation with different potentials like modified Kratzer [14], Yukawa [15], Hylleraas [16], Morse [17], Woods Saxon [18], and Hellmann [19], we can employ one of the well-known methods. In this work, the NUFA method is applied to solve the Schrödinger equation. This technique is being utilized because of its accuracy, clarity, simplicity, and effectiveness. We have previously tested this technique on basic potentials like the Coulomb [20] and the screened Coulomb [21].

For instance, the screened Kratzer potential is used to investigate quark confinement. It also has two distinctive features: strong interaction-asymptotic freedom and confinement, and it has been used extensively in atomic and molecular physics and vibrational and rotational spectroscopy [22]. One of the significant short-range potentials in physics is the Hulthén potential. Researchers have recently become very interested in and concerned about its applicability to a variety of disciplines of physics, including nuclear and particle physics, atomic physics, molecular physics, condensed matter, and chemical physics [23].

This work aims to compute the energy spectrum of certain diatomic molecules (LiH, HCL, VH, I2) through the Schrödinger problem's solution following the NUFA approach while accounting for the modified Kratzer and Hulthén potentials. This potential is chosen because it is composed of attractive and repulsive components that act over long distances. Combining at least two potential processes and a wide variety of applications and using potentials with more suitable parameters often leads to improved results [24-30]. The scholarship on the energy spectrum of diatomic compounds is extensive and varied, illustrating the significant role that diatomic molecules perform in various fields of science and engineering [31-40].

The Hulthén plus screened Kratzer potential is given by :

$$V(r) = -\frac{V_0 e^{-\alpha r}}{1-e^{-\alpha r}} - 2De\left(\frac{r_e}{e} - \frac{R_e^2}{2r^2}\right)e^{-\alpha r}, \quad (1)$$

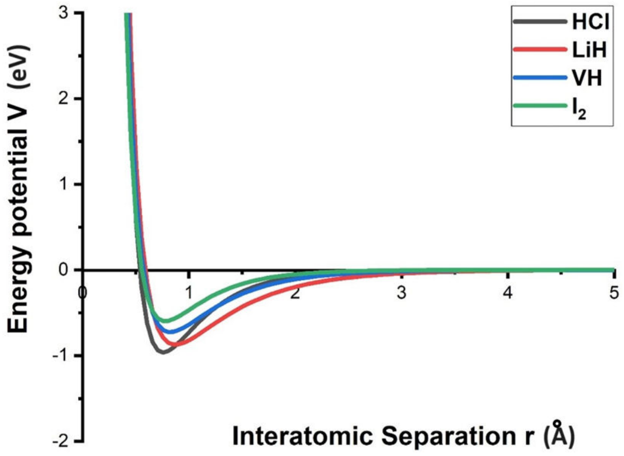

FIGURE 1. Plotting the Hulthén plus screened Kratzer potential for selected diatomic molecules.

where De represents the dissociation energy, re defined as the molecular bond length, V_0 strength of potential, α is the screening parameter, r the inter-atomic separation, α is the screening parameter. The plot of the potential $V(r)$ against the inter-nuclear distance is displayed in Fig. 1.

2. Review of the Nikiforov-Uvarov-Functional Analysis (NUFA) method

NUFA is an elegant and straightforward technique for resolving a second-order differential equation. The probabilistic NUFA methodology is a more basic and straightforward method. For the NUFA to compute wave and composition, accurate translation of waveform formulas and discontinuity recognition are required. Because of the essential particular choices of the required parameters in this technique, the application of this method is very powerful to the Schrödinger and Klein Gordon and Dirac equations with sophisticated potential profiles. Also, the NUFA method cannot be utilized effectively to solve more realistic physical systems. Ignoring the complexity of the NU technique, which involves, among other things, finding the square roots of polynomial functions, can lead to ineffective solutions [41].

$$\varphi''(s) + \frac{\tilde{\tau}(z)}{\sigma(z)}\varphi'(s) + \frac{\tilde{\sigma}(z)}{\sigma^2(z)}\varphi(z) = 0, \tag{2}$$

where $\tilde{\sigma}(z)$ polynomial typically from the 2nd degree also $\sigma(z)$, $\tilde{\tau}(z)$ 1st degree polynomial. Then

$$\begin{aligned}\varphi''(z) + \frac{c_1 - c_2 z}{s(1-c_3 z)}\varphi'(s) + \frac{1}{s^2(1-c_3 s)^2} \\ \times [-\gamma_1 z^2 + \gamma_2 z - \gamma_3]\varphi(z) = 0,\end{aligned} \tag{3}$$

with c_i and γ_i are constants with $i = 1, 2 \ldots$

Then

$$\varphi(z) = z^{\lambda}(1-z)^{v} f(z). \tag{4}$$

Equation (3) plus Eq. (4) yields the subsequent expression:

$$\begin{aligned}(1-c_3 z)f''(z) + (c_1 + 2\lambda - [2\lambda c_3 + 2vc_3 + c_2]s)f'(z) - c_3\left(\lambda + v + \left[\frac{c_2}{2c_3} - \frac{1}{2}\right] + \sqrt{\frac{c_2}{2c_3} - \frac{\gamma_1}{c_3^2}}\right) \\ \times \left(\lambda + v + \left[\frac{c_2}{2c_3} - \frac{1}{2}\right] + \sqrt{\left[\frac{c_2}{2c_3} - \frac{1}{2}\right]^2 + \frac{\gamma_1}{c_3^2}}\right) \\ + \left(\frac{\lambda(\lambda-1) + c_1\lambda - \gamma_3}{s} + \frac{v(v-1)c_3 + c_2 v - c_1 c_3 v - \frac{\gamma_1}{c_3} + \gamma_2 - \gamma_3 c_3}{1 - c_3 s}\right) f(z) = 0.\end{aligned} \tag{5}$$

Equation (5) may be made simpler by applying the subsequent the Gaussian hypergeometric process:

$$\lambda(\lambda-1) + c_1\lambda - \gamma_3 = 0. \tag{6}$$

Then

$$v(v-1) + c_2 v - c_1 c_3 v - \frac{\gamma_1}{c_3} + \gamma_2 - \gamma_3 c_3 = 0. \tag{7}$$

Equation (3) turns into:

$$\begin{aligned}s(1-c_3 s)f''(z)(c_1 + 2\lambda - [2\lambda c_3 + 2vc_3 + c_2]s)f'(z) - \left(\lambda + v + \left[\frac{c_2}{2c_3} - \frac{1}{2}\right] + \sqrt{\left[\frac{c_2}{2c_3} - \frac{1}{2}\right]^2 - \frac{\gamma_1}{c_3^2}}\right) \\ + \left(\lambda + v + \frac{1}{2}\left[\frac{c_2}{2c_3} - \frac{1}{2}\right] + \sqrt{\left[\frac{c_2}{2c_3} - \frac{1}{2}\right]^2 + \frac{\gamma_1}{c_3^2}}\right) c_3 f(z) = 0.\end{aligned} \tag{8}$$

As a result of Eqs. (6) and (7),

$$\lambda = \frac{1}{2}(1-c_1) \pm \frac{1}{2}\sqrt{(1-c_1)^2+4\gamma_3}, \tag{9}$$

and

$$v = \frac{1}{2c_3}\left([c_3+c_1c_3-c_2] \pm \sqrt{[c_3+c_1c_3-c_2]^2+4\left[\frac{\gamma_1}{c_3}+c_3\gamma_3-\gamma_2\right]}\right), \tag{10}$$

and

$$y(1-y)f''(z)+(c+[a+b+1]s)f'(z)-(ab)f(z)=0, \tag{11}$$

and a, b and c are:

$$a = \sqrt{c_3}\left(v+\lambda+\frac{1}{2}\left[\frac{c_2}{c_3}-1\right]+\sqrt{\frac{1}{4}\left[\frac{c_2}{c_3}-1\right]^2+\frac{\gamma_1}{c_3^2}}\right), \tag{12}$$

$$a = \sqrt{k_3}\left(v+\lambda+\frac{1}{2}\left[\frac{k_2}{k_3}-1\right]-\sqrt{\frac{1}{4}\left[\frac{k_2}{k_3}-1\right]^2+\frac{\gamma_1}{k_3^2}}\right), \tag{13}$$

$$c = c_1+2\lambda. \tag{14}$$

Using the fundamental standards listed below:

$$\sqrt{c_3}\left(\lambda+v+\left[\frac{c_2}{2c_3}-\frac{1}{2}\right)+\sqrt{\left[\frac{c_2}{2c_3}-\frac{1}{2}\right]^2+\frac{\gamma}{c_3^2}}\right)=-n, \tag{15}$$

$$v+\lambda+\left[\frac{c_2}{2c_3}-\frac{1}{2}\right]+\frac{n}{\sqrt{c_3}}=-\sqrt{\left[\frac{c_2}{2c_3}-\frac{1}{2}\right]^2+\frac{c_1}{c_3^2}}. \tag{16}$$

After squaring and flipping each component of Eq. (26), we obtain:

$$\lambda^2+2\lambda\left(v+\left[\frac{c_2}{2c_3}-\frac{1}{2}\right]+\frac{n}{\sqrt{c_3}}\right)+\left(v+\left[\frac{c_2}{2c_3}-\frac{1}{2}\right]+\frac{n}{\sqrt{c_3}}\right)^2-\left[\frac{c_2}{2c_3}-\frac{1}{2}\right]-\frac{\gamma_1}{c_3^2}=0. \tag{17}$$

For this NUFA, the waveform Equation might turn into:

$$\begin{aligned} R_{nl} = {} & N_z\frac{(1-c_1)+\sqrt{(c_1-1)^2+4\gamma_3}}{2}(1-c_3s) \\ & \times \frac{(c_3+c_1c_3-c_2)+\sqrt{(c_3+c_1c_3-c_2)^2+4\left(\frac{\gamma_1}{c_3^2}+c_3\gamma_3-\gamma_2\right)}}{2c_3} 2F_1(a,b,c;z), \end{aligned} \tag{18}$$

where N is the normalization parameter.

3. Analytical solutions of SE with Hulthén-Screened Kratzer potential using NUFA method

The Schrödinger equation for the Hulthén plus screened Kratzer potential is presented by [42]:

$$\left(\frac{d^2}{dr}-\frac{2\mu}{\hbar^2}\left[E+\frac{V_0e^{-\alpha r}}{1-e^{-\alpha r}}+2D_e\left\{\frac{r_e}{r}-\frac{r_e^2}{2r^2}\right\}e^{-\alpha r}-\frac{\hbar^2 l(l+1)}{2\mu r^2}\right]\right)R_{nl}(r)=0. \tag{19}$$

We apply the Greene -Aldrich approximation [43]. Applying the approximation solves the centrifugal issue. This strategy is good for $\alpha \ll 1$ and operates effectively for the centrifugal problem:

$$\frac{1}{r^2}=\left(\frac{\alpha^2}{[1-e^{-\alpha r}]^2}\right), \qquad \frac{1}{r}=\left(\frac{\alpha}{[1-e^{-\alpha r}]^2}\right). \tag{20}$$

The Eq. (19) becomes

$$\left(\frac{d^2}{dr^2}-\frac{2\mu}{\hbar^2}\left[E+\frac{V_0e^{-\alpha r}}{1-e^{-\alpha r}}+2D_e\left\{\frac{\alpha r_e}{1-e^{-\alpha r}}-\frac{(\alpha^2/2)r_e^2}{(1-e^{-\alpha r})^2}\right\}e^{-\alpha r}-\frac{\alpha^2\hbar^2 l(l+1)}{2\mu(1-e^{-\alpha r})^2}\right]\right)R_{nl}(r)=0. \tag{21}$$

Applying the transformation $y=e^{-\alpha r}$ we obtain

$$\begin{aligned}&\left(\frac{d^2}{dy^2}+\frac{1-y}{y(1-y)}\frac{d}{dy}+\left[\frac{1}{y(1-y)^2}\right]\left[\left\{\frac{2\mu E}{\alpha^2\hbar^2}(1-y)^2\right.\right.\right.\\&\left.\left.\left.+\frac{2\mu V_0}{\hbar^2}y(1-y)+\frac{4\mu D_e r_e}{\alpha\hbar^2}y(1-y)-\frac{2\mu D_e r_e^2}{\hbar^2}y-l(l+1)\right\}\right]\right)R_{nl}(r)=0.\end{aligned} \tag{22}$$

To be able to use the NUFA method, modify Eq. (22) as follows:

$$\left(\left[\frac{d^2}{dy^2}+\frac{1-y}{y(1-y)}\frac{d}{dy}+\left[\frac{1}{y(1-y)^2}\right](-\gamma_1y^2+\gamma_2y-\gamma_3)\right]\right)R_{nl}(y)=0, \tag{23}$$

with

$$-\gamma_1=\frac{2\mu E}{\alpha^2\hbar^2}-\frac{2\mu V_0}{\alpha^2\hbar^2}-\frac{4\mu D_e r_e}{\alpha\hbar^2}, \tag{24}$$

$$\gamma_2=-\frac{4\mu E}{\alpha^2\hbar^2}+\frac{2\mu V_0}{\alpha^2\hbar^2}+\frac{4\mu D_e r_e}{\alpha\hbar^2}-\frac{2\mu D_e r_e^2}{\hbar^2}, \tag{25}$$

$$-\gamma_3=\frac{2\mu E}{\alpha^2\hbar^2}-l(l+1). \tag{26}$$

Equations (24), (25), and (26) are compared to the NUFA preceding Eqs. (3), (9), and (23) to obtain

$$c_1=c_2=c_3=1, \tag{27}$$

$$\lambda=\sqrt{-\frac{2\mu E}{\alpha^2\hbar^2}+l(l+1)}, \tag{28}$$

$$v=\frac{1}{2}+\frac{1}{2}\sqrt{\frac{8\mu D_e r_e^2}{\hbar^2}+(2l+1)^2}. \tag{29}$$

Inserting Eqs. (24), (27), (28) and (29) into Eq. (17), we obtain

$$E=\frac{\alpha^2\hbar^2 l(l+1)}{2\mu}-\frac{\alpha^2\hbar^2}{2\mu}\left(\frac{(n+v)^2+\left[\frac{2\mu V_0}{\alpha^2\hbar^2}+\frac{4\mu D_e r_e}{\alpha\hbar^2}+l(l+1)\right]}{n+v}\right)^2. \tag{30}$$

Equation (18) may also be used to get the radial wave function. It is expressed in the form:

$$R_{nl}(y)=Ny^{\sqrt{(2\mu E/\alpha^2\hbar^2)-l(l+1)}}(1-y)^{(1/2)+(1/2)\sqrt{(8\mu D_e r_e^2/\hbar^2)+(2l+1)^2}}{}_2F_1(a,b,c;z), \tag{31}$$

with N is the parameter normalization.

The spectroscopic parameter in Table I is adopted to obtain energy spectrum of the selected diatomic molecules. These specifications come from references [44,45]. We utilize the conversions $1\text{amu}=931.494028$ Mev/c and $c=1973.29$ eV [46] to carry out the remaining computations.

TABLE I. Parameters of selected diatomic molecules.

Molecule	D_e (eV)	α (Å^{-1})	r_e (Å)	μ (amu)
HCl	4.619061175	1.8677	1.2746	0.9801045
LiH	2.5152672118	1.1280	1.5956	0.8801221
VH	2.33	1.4437	1.719	0.09203207571
I2	1.5556	1.8643	2.6986	63.45224

TABLE II. Spectra of energy of the Hulthén plus screened modified Kratzer potential of LiH, HCl, VH and I_2.

n	l	HCl	LiH	VH	I_2
0	0	-21.3940468	-8.06537323	-10.9179947	-18.2056622
0	1	-21.3922026	-8.06536029	-10.9161572	-18.2054235
0	2	-21.3885755	-8.06533488	-10.9125488	-18.2049462
0	3	-21.3832831	-8.06529788	-10.9072968	-18.2042304
0	4	-21.3764897	-8.06525053	-10.9005777	-18.2032764
0	5	-21.3683936	-8.06519428	-10.8926032	-18.2020847
1	0	-22.2248882	-8.24339054	-11.4633412	-18.3944526
1	1	-22.2224964	-8.24343586	-11.4611451	-18.3942134
1	2	-2.,217779	-8.24352506	-11.4568195	-18.3937353
1	3	-22.2108637	-8.24365542	-11.4504922	-18.3930183
1	4	-22.2019302	-8.24382312	-11.4423425	-18.3920627
1	5	-22.1911981	-8.24402356	-11.4325876	-18.3908689
2	0	-23.4018013	-8.59408422	-12.194766	-18.5866915
2	1	-23.399682	-8.59442709	-12.1927844	-18.5864522
2	2	-23.3954957	-8.59510288	-12.1888749	-18.5859736
2	3	-23.389344	-8.59609249	-12.1831403	-18.5852561
2	4	-23.3813701	-8.59736921	-12.1757259	-18.5842997
2	5	-23.3717507	-8.59890068	-12.166809	-18.5831049
3	0	-24.8667539	-9.08066827	-13.0830175	-18.782336
3	1	-24.8655961	-9.0815646	-13.0817074	-18.7820967
3	2	-24.8633067	-9.083333	-13.0791196	-18.7816182
3	3	-24.8599367	-9.08592683	-13.0753165	-18.7809006
3	4	-24.8555586	-9.08928062	-13.0703865	-18.7799443
3	5	-24.8502618	-9.09331468	-13.064438	-18.7787495
4	0	-26.5826633	-9.68080744	-14.1096736	-18.9813453
4	1	-26.5830307	-9.68248777	-14.1093956	-18.9811062
4	2	-26.5837577	-9.68580562	-14.108846	-18.9806281
4	3	-26.5848293	-9.69067854	-14.1080372	-18.9799112
4	4	-26.5862239	-9.6969905	-14.1069866	-18.9789557
4	5	-26.5879147	-9.7045997	-14.1057158	-18.9777619

In this study, we calculated the bound energies of several diatomic molecules, considering the Hulthén plus screened Kratzer potential. Equation (30) served as the basis for all the computations. The findings were computed using the parameters given in Table I.

Table II shows the bound energies of LiH, HCl, VH, and I_2 for quanta states n and l. It shows that the energy eigenvalues drop for each of the specific diatomic compounds when the quantum states are different from n to l. The energy increases by increasing the vibration number n and the rotation number l.

Specific cases

1.- By Putting $V_0 = 0$ we obtain energy spectra of screened Kratzer potential on the form:

$$E = \frac{\alpha^2\hbar^2}{2\mu}l(l+1) - \frac{\alpha^2\hbar^2}{8\mu}\left(\frac{(n+v)^2 + \left[\frac{4\mu D_e r_e}{\alpha\hbar^2} +\right]}{n+v}\right)^2 . \tag{32}$$

The findings are displayed in Table III.

TABLE III. Spectra of energy of screened Kratzer potential of LiH and HCl.

n	l	Our results LiH	Ref [47] LiH	Our results HCl	Ref [47] HCl
0	0	-9.0709681363	-9.070968135	-22.1932905150	-22.19329052
1	0	-9.0594461198	-9.059446120	-22.2695372170	-22.26953722
	1	-9.0470561241	-9.047056120	-22.2426601076	-22.24266011
2	0	-9.05443111855	-9.054431115	-22.3566328803	-22.35663288
	1	-9.04227809368	-9.042278085	-22.3301252097	-22.33012521
	2	-9.017997941977	-9.017997940	-22.2771478258	-22.27714784
3	0	-9.0555658678	-9.055565865	-22.4541271909	-22.27714784
	1	-9.04363707225	-9.043637070	-22.4279726546	-22.42797265
	2	-9.0198039856	-9.019803985	-22.3756997899	-22.42797265
	3	-8.9841153576	-8.984115355	-22.2973807185	-22.29738072
4	0	-9.0625244751	-9.062524470	-22.5616048355	-22.56160484
	1	-9.0508081726	-9.050808170	-22.5357882509	-22.53578825
	2	-9.0273987751	-9.027398770	-22.4841896449	-22.48418965
	3	-8.9923424559	-8.992342455	-22.4068778664	-22.40687787
	4	-8.9457078747	-8.945707875	-22.3039554976	-22.30395550
5	0	-9.0750091716	-9.075009170	-22.6786822859	-22.67868230
	1	-9.0634945347	-9.063494530	-22.6531894991	-22.65318950
	2	-9.0404872599	-9.040487255	-22.6022369402	-22.60223694
	3	-9.0060311194	-9.006031120	-22.5258903759	-22.52589037
	4	-8.9601912095	-8.960191210	-22.4242478046	-22.42424781
	5	-8.9030532894	-8.903053285	-22.2974386839	-22.29743871

In this specific scenario, the screened Kratzer potential is utilized. Table III provides the energy spectrum of LiH and HCl for various quanta states of n and l. Although there is some disagreement between the calculated findings and Ref. [47], overall, the results indicate high consistency. This implies that the energy level of such molecules may be reliably estimated using the energy-based SK molecular potential. The bounded energies often tend to increase as the quantum number n grows. One possible explanation for the increase in energy might be the addition of nodes to the framework wave solution. The presence of these inclusion nodes augments the probability of finding the electron close to the atomic nucleus.

By Putting $\alpha \rightarrow 0$ and $V_0 = 0$ we conclude the bound energies of the Kratzer potential.

$$E = \frac{\alpha^2\hbar^2}{2\mu}\left(\frac{\frac{4\mu D_e r_e^2}{\hbar^2}}{\left[2n+1+\sqrt{\frac{8\mu D_e r_e^2}{\hbar^2}+(2l+1)^2}\right]}\right)^2 . \tag{33}$$

Table IV shows the Kratzer potential energy spectrum of LiH and HCl for different quanta states of n and l. The results show high consistency despite occasional discrepancies between the computed findings and references [48]. This suggests that the energy-based Kratzer molecular potential can be a useful tool for accurately estimating the energy level of such molecules. As the quantum number n increases, the bound energies frequently show an increasing trend. Including nodes in the framework and solutions could be one reason for the increase in energy. These inclusion nodes increase the likelihood of discovering the electron near the atomic nucleus.

TABLE IV. Energy spectrum of Kratzer potential for specified diatomic molecules LiH and HCl.

Quantum numbers		LiH	LiH [26]	HCl	HCl [26]
n	l				
0	0	-2.4673101	-2.467310304097	-4.54184788	-4.541848211101
1	0	-2.37581864	-2.375819214406	-4.39372703	-4.393727956046
	1	-2.37410739	-2.374107972668	-4.3912929	-4.391293850595
2	0	-2.28932336	-2.289324266253	-4.25273564	-4.252737112329
	1	-2.28770469	-2.287705602815	-4.25041772	-4.250419208735
	2	-2.28447428	-2.284475215373	-4.24578952	-4.245791052967
3	0	-2.20746701	-2.207468200275	-4.11842341	-4.118425371585
	1	-2.20593435	-2.205935555783	-4.11621441	-4.116216389518
	2	-2.20287552	-2.202876749755	-4.11180361	-4.111805631214
	3	-2.19830341	-2.198304679122	-4.10520538	-4.105207449232
4	0	-2.12992367	-2.129925128672	-3.99037501	-3.990377425087
	1	-2.12847105	-2.128472514560	-3.98826822	-3.988270645562
	2	-2.12557186	-2.125573350591	-3.98406142	-3.984063879462
	3	-2.12123818	-2.121239701434	-3.97776815	-3.977770657506
	4	-2.11548794	-2.115489505754	-3.96940857	-3.969411138650
5	0	-2.0563956	-2.056397286593	-3.86820694	-3.868209749404
	1	-2.05501753	-2.055019226505	-3.86619614	-3.866198963636
	2	-2.05226707	-2.052268785922	-3.86218095	-3.862183802008
	3	-2.04815552	-2.048157264859	-3.85617413	-3.856177032746
	4	-2.04269968	-2.042701466576	-3.84819472	-3.848197679994
	5	-2.03592169	-2.035923524667	-3.83826784	-3.838270872139

4. Conclusion

In this study, the centrifugal barrier was eliminated by solving the Schrödinger equation with the Hulthén plus screened Kratzer potential using the Greene Aldrich approximation and the Nikiforov Uvarov functional analysis approach. We ascertain the associated wave functions and bound state energy. The bound energies of the Hulthén plus SK potential of diatomic molecules (VH, I2, LiH, HCl) are computed computationally. We could also reduce the bound energy expression for the HPSK potential to those of the conventional SK and Kratzer and Hulthén potential by altering the Hulthén plus screened Kratzer potential parameters. Our numerical results for the SK and Kratzer potentials likely standards agree with those reported in the literature. It is crucial to emphasize that our research cannot be compared to any of Kratzer's possible calculations in published works. The results were used to derive the energy spectrum of well-known diatomic chemicals in this specific Kratzer potential example and (HCl, LiH) for the SK likely instance. The current method has the advantage of allowing for quick identification of bound energies. When diatomic molecules are considered, the method presented in this work may be used to find determined energies and matching wave functions for the Schrödinger equation within a given potential. The results are highly valuable in determining properties of diatomic molecules, such as the thermodynamic one, and in concluding the mass spectra of certain heavy quarkoniums. Our works in the future is to apply the validate method to determine spectrum of energy for non-relativistic case by applying the approach on the Klein-Gordon and Dirac equations.

Data availability statements

No data associated in the manuscript.

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