Bound state solutions of the Schrödinger equation with energy-dependent molecular Kratzer potential via asymptotic iteration method

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ABSTRACT: In this paper, we obtained the exact bound state energy spectrum of the Schrödinger equation with energy dependent molecular Kratzer potential using asymptotic iteration method (AIM). The corresponding wave function expressed in terms of the confluent hypergeometric function was also obtained. As a special case, when the energy slope parameter in the energy-dependent molecular Kratzer potential is set to zero, then the well-known molecular Kratzer potential is recovered. Numerical results for the energy eigenvalues are also obtained for different quantum states, in the presence and absence of the energy slope parameter. These results are discussed extensively using graphical representation. Our results are seen to agree with the results in literature.

1. Introduction

The exact or approximate solutions of the Schrödinger equations play a vital role in many branches of modern physics and chemistry. The solution of this equation is used in the description of particle dynamics in the non-relativistic regime. Even though the Schrödinger equation was developed many decades ago, it is still very challenging to solve it analytically. The solution of the Schrödinger equation contains all the necessary information needed for the full description of a quantum state such as the probability density and entropy of the system. The Schrödinger equation with many physical potentials model have been investigated in recent times with different advance mathematical technique such as Nikiforov-Uvarov (NU) method, asymptotic iteration method (AIM), functional analysis approach, supersymmetric quantum mechanics (SUSYQM) among others. One of such potential models is the Kratzer potential

\[ V(r) = -2D \left( \frac{a^2}{r^2} - 1 \right) \] (1)

where \( D \) is the dissociation energy and \( a \) is the equilibrium internuclear length.

The Kratzer potential has been used as a potential model to describe internuclear vibration of diatomic molecules. Many authors have investigated the bound state solutions of the Kratzer potential within relativistic and non-relativistic quantum mechanics. Recently, Budaca studied an energy-dependent Coulomb-
like potential within the framework of Bohr Hamiltonian. Furthermore, Budaca\textsuperscript{27} had reported that the energy dependence on the coupling constant of the potential drastically changes the analytical properties of wave function and the corresponding eigenvalues of the system. The energy-dependent potentials have been studied in nuclear physics with applications to quark confinement\textsuperscript{28,29}. Several researchers have also given great attention to investigate the energy dependent potentials\textsuperscript{20,21}. Boumali and Labidi\textsuperscript{32} solved the Klein-Gordon equation with an energy-dependent potential, the Shannon and Fisher information theory was also considered. Also, Lombard \textit{et al.}\textsuperscript{33} studied the wave equation energy-dependent potential for confined systems. Therefore, the energy dependent potential in the Schrödinger equation or other wave equation in physics has many applications such as features in spectrum of confined systems and heavy quark systems in nuclear and molecular physics\textsuperscript{34}.

In this paper, we shall study the influence of the energy-dependent Kratzer potential on some diatomic molecules defined as:

\[ V(r, E) = -2D \left( \frac{a(1+\eta E)}{r} - \frac{1}{2} \frac{a^2(1+\eta E)}{r^2} \right) \quad (2) \]

where the energy slope parameter \( \eta \) must be positive definite in order to describe a physical system\textsuperscript{27}.

The shape of the energy dependent Kratzer molecular potential with different energy slope parameters, as it varies with equilibrium internuclear length are illustrated in Fig. 1A-1C, for four selected diatomic molecules (CO, NO, O\textsubscript{2} and I\textsubscript{2}).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{1A.png}
\caption{The shape of Energy-dependent Kratzer molecular potential for different diatomic molecules, with \( \eta=0 \).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{1B.png}
\caption{The shape of Energy-dependent Kratzer Molecular Potential for different diatomic molecules, with \( \eta=1 \).}
\end{figure}
Again by taking the \((k+1)th\) and \((k+2)th\) order derivative of Eq. 3 for \(k=1,2,3,...\), we obtain the following differential equations:

\[
y^{(k+1)}(x) = \lambda_{k-1}(x)y'(x) + s_{k-1}(x)y(x) \\
y^{(k+2)}(x) = \lambda_{k}(x)y'(x) + s_{k}(x)y(x)
\]

where,

\[
\lambda_{k-1}(x) = \lambda_{k-1}^0(x) + \lambda_{k-2}(x) + s_{k-2}(x) \\
s_{k-1}(x) = s_{k-1}(x) + s_{k}(x) + \lambda_{k-2}(x)
\]

\[
\lambda_{k}(x) = \lambda_{k}^0(x) + \lambda_{k-1}(x) + s_{k-1}(x) \\
s_{k}(x) = s_{k}(x) + s_{k-1}(x)
\]

Solving Eq. 8, we obtain the following relation:

\[
\frac{y^{(k+2)}(x)}{y^{(k+1)}(x)} = \frac{\lambda_{k}(x)}{\lambda_{k-1}(x)} \left[ \frac{y'(x) + \frac{s_{k-1}(x)}{\lambda_{k-1}(x)}y(x)}{y'(x) + \frac{s_{k}(x)}{\lambda_{k}(x)}y(x)} \right]
\]

For sufficiently large values of \(k\), the \(\alpha(x)\) values are obtained as

\[
\frac{s_{k}(x)}{\lambda_{k}(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x)
\]

This method consists of converting the Schrödinger-like equation into the form of Eq. 3 for a given potential model. The corresponding energy eigenvalues are calculated by means of the quantization condition\(^{12-16}\).

\[
\delta_{k}(x) = s_{k}(x)\lambda_{k-1}(x) - \lambda_{k}(x)s_{k-1}(x), k=1,2,3,...
\]

The general solutions of Eq. 3 is obtain from Eq. 10 as:

\[
y(x) = \exp\left(-\int^{x} \alpha(x)dx\right)\left[ C_{2} + C_{1} \int^{x} \exp\left(\int^{x} [\lambda_{0}(x_{2}) + 2\alpha(x_{2})]dx_{2}\right)dx_{1}\right]
\]

where \(C_{1}\) and \(C_{2}\) are integration constant.

### 2 Asymptotic Iteration Method

The AIM has been proposed and used to solve the homogenous linear second-order differential equation of the form\(^{12-16}\):

\[
y''(x) = \lambda_{0}(x)y'(x) + s_{0}(x)y(x)
\]

where \(\lambda_{0} \neq 0\) and the prime denote the derivative with respect to \(x\).

The functions, \(s_{0}(x)\) and \(\lambda_{0}(x)\) must be sufficiently differentiable. Differentiating Eq. 3 with respect to \(x\), we get

\[
y'''(x) = \lambda_{1}(x)y'(x) + s_{1}(x)y(x)
\]

where,

\[
\lambda_{1}(x) = \lambda_{1}^{0}(x) + \lambda_{0}^{2}(x) + s_{0}(x) \\
s_{1}(x) = s_{0}'(x) + s_{0}(x)\lambda_{0}(x)
\]

Taking the second derivative of Eq. 3 yields

\[
y''''(x) = \lambda_{2}(x)y'(x) + s_{2}(x)y(x)
\]

where,

\[
y(x) = \exp\left(-\int^{x} \alpha(x)dx\right)\left[ C_{2} + C_{1} \int^{x} \exp\left(\int^{x} [\lambda_{0}(x_{2}) + 2\alpha(x_{2})]dx_{2}\right)dx_{1}\right]
\]

with \(\lambda_{2}(x) = \lambda_{1}'(x) + \lambda_{0}(x)\lambda_{1}(x) + s_{1}(x)\)

\[
s_{2}(x) = s_{1}'(x) + s_{0}(x)\lambda_{0}(x)
\]

\[
(7)
\]

\[
\delta_{k}(x) = s_{k}(x)\lambda_{k-1}(x) - \lambda_{k}(x)s_{k-1}(x), k=1,2,3,...
\]

\[
(12)
\]

where \(C_{1}\) and \(C_{2}\) are integration constant.
Also, the eigenfunction can be obtained by transforming the Schrödinger-like equation of the form:

\[ y''(x) = 2\left( \frac{ax^n}{1-bx^{n+2}x} - \frac{t+1}{x} \right) y'(x) - \frac{Wx^n}{1-bx^{n+2}} y(x) \] (14)

The exact solutions for Eq. 14 are given by

\[ y(x) = (-1)^n C(N+2)|\sigma|^{2} F_{l} (\sigma, \rho+n; x; bx^{n+2}) \] (15)

where,

\[ \sigma_n = \frac{\Gamma(\sigma+n)}{\sigma}, \sigma = \frac{2t+N+3}{N+2}, \rho = \frac{(2t+1)b+2a}{(N+2)b} \] (16)

\[ \frac{d^2\psi_{nl}}{dx^2} + \frac{2\mu}{\hbar^2} \left( E_{nl} + 2D \left( \frac{a(1+\eta E)}{r} - \frac{a^2(1+\eta E)}{2} \right) \right) - \frac{l(l+1)\hbar^2}{2\mu r^2} \psi_{nl}(r) = 0 \] (17)

Substituting Eq. 1 into Eq. 17 yields,

\[ \frac{d^2\psi_{nl}}{dy^2} + \left( -\frac{\epsilon_n}{y} + \frac{\beta}{y^2} \right) \psi_{nl}(y) = 0 \] (18)

with the following definitions for the used parameters:

\[ \epsilon_n = -\frac{2\mu E_{nl}}{\hbar^2 a^2}, \beta = \frac{4\mu D(1+\eta E)}{\hbar^2}, \gamma(y+1) = \frac{2\mu Da^2(1+\eta E)}{\hbar^2} + l(l+1) \] (19)

In order to transform Eq. 19 into form suitable for the AIM, we write the wave function in the form:

\[ \psi_{nl}(y) = y^{\gamma+1} e^{\epsilon_n y} f(y) \] (20)

Substituting Eq. 21 into Eq. 19, we obtain:

\[ f''(y) = \left[ \frac{2\epsilon_y - 2(\gamma+1)}{y} \right] f'(y) + \left[ \frac{2\epsilon_y (\gamma+1) - \beta}{y} \right] f(y) \] (21)

3. Bound state solution of the Schrödinger equation with energy-dependent Kratzer potential

The radial part of the Schrödinger equation with energy dependent potential \( V(r, E_{nl}) \) reads:

\[ \frac{d^2\psi_{nl}}{dr^2} + \frac{2\mu}{\hbar^2} \left( E_{nl} - V(r, E_{nl}) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right) \psi_{nl}(r) = 0 \] (22)

By applying the AIM quantization of Eq. 12 by substituting Eq. 23, we obtain the following iterations:

\[ \frac{s_0}{\alpha_0} \Rightarrow \epsilon_0 = \frac{\beta}{2(\gamma_0+1)}, n = 0, \]

\[ \frac{s_1}{\alpha_1} \Rightarrow \epsilon_1 = \frac{\beta}{2(\gamma_1+2)}, n = 1, \] (24)

\[ \frac{s_2}{\alpha_2} \Rightarrow \epsilon_2 = \frac{\beta}{2(\gamma_2+3)}, n = 2 \]

Generally, for arbitrary \( n \), we have

\[ \epsilon_n = \frac{\beta}{2(\gamma_n+n+1)} \] (25)

Using Eq. 20 with Eq. 25, the energy eigenvalues of the Schrödinger equation with energy-dependent Kratzer potential is obtained as:
\[ E_{nl} = -\frac{1}{8\mu} \left( n + \frac{1}{2} \right)^2 - \frac{\beta^2 \hbar^2 a^2}{1 + \frac{1}{2} \left( 1 + \frac{1}{2} \right)^2} \]  
\[(26)\]

This is a very complicated transcendental energy equation. As a special case, when the energy slope parameter \( \eta = 0 \), Eq. 26 reduces to the result of the standard Kratzer potential given as:

\[ E_{nl} = -\frac{2\mu D^2 a^2}{\hbar^2} \left( n + \frac{1}{2} \right)^2 \]  
\[(27)\]

This result is consistent with those reported by Bayrak, Boztosun and Ciftci.\(^\text{29}\)

### 4. Results and Discussion

We compute the energy eigenvalues (in eV) of energy dependent Kratzer molecular potential for CO, NO, O\(_2\) and I\(_2\) diatomic molecules. This was done using the spectroscopic parameters given in Table 1, and the conversion \( \hbar c = 1973.29 \text{ eV} \AA^{-1} \).\(^{26}\)

**Table 1. Spectroscopic parameters of the various diatomic molecules\(^{20}\)**

| Molecule | \( D \) (eV) | \( a \) (\( \AA \)) | \( \mu \) (amu) |
|----------|--------------|-----------------|--------------|
| CO       | 10.84514471  | 1.1282          | 6.860586000  |
| NO       | 8.043782568  | 1.1508          | 7.468441000  |
| O\(_2\)  | 5.156658828  | 1.2080          | 7.997457504  |
| I\(_2\)  | 1.581791863  | 2.6620          | 63.45223502  |

The energy eigenvalues of energy dependent molecular Kratzer potential for the ground state diatomic molecules selected are shown in Tables 2 and 3, in the absence of the energy slope parameter \( \eta \).

**Table 2. Energy eigenvalues (in eV) of energy dependent Kratzer molecular potential for different values of \( n \) and \( \ell \) for ground states CO and NO diatomic molecules, with \( \eta = 0 \).**

| \( n \) | \( \ell \) | CO          | CO\(^{29}\)   | NO          | NO\(^{29}\)   |
|--------|--------|-------------|---------------|-------------|---------------|
| 0      | 0      | -10.79431511 | -10.79431532  | -8.002659248 | -8.002659417  |
| 1      | 0      | -10.69383928 | -10.69383992  | -7.921456326 | -7.921456839  |
|        | 1      | -10.69337058 | -10.69337123  | -7.92104332  | -7.921043834  |
| 2      | 0      | -10.59475984 | -10.59476089  | -7.841483114 | -7.841483956  |
|        | 1      | -10.59429764 | -10.59429869  | -7.841076336 | -7.841077188  |
| 3      | 0      | -10.49705101 | -10.49705246  | -7.762714900 | -7.762716066  |
|        | 1      | -10.49659519 | -10.49659664  | -7.762314236 | -7.762315413  |
|        | 2      | -10.49568366 | -10.49568512  | -7.761513040 | -7.761514218  |
| 4      | 0      | -10.40068763 | -10.40068947  | -7.685127602 | -7.685129079  |
|        | 1      | -10.40023807 | -10.40023992  | -7.684732928 | -7.684734417  |
|        | 2      | -10.39933907 | -10.39934092  | -7.683943714 | -7.683945203  |
|        | 3      | -10.39799086 | -10.39799272  | -7.682760192 | -7.682761696  |
|        | 4      | -10.39619379 | -10.39619567  | -7.681182728 | -7.681184246  |
Table 3. Energy eigenvalues (in eV) of energy dependent Kratzer molecular potential for different values of \( n \) and \( \ell \) for ground states \( O_2 \) and \( I_2 \) diatomic molecules, with \( \eta = 0 \).

Our results are very consistent with the results obtained by Bayrak, Boztosun and Ciftci. Also, it is observed that the energy eigenvalues become more bounded as the quantum states of these molecules increases. Moreover, with the introduction of the energy slope parameter, the energy eigenvalues for the different diatomic molecules tends to increase drastically (See Tables 4-6), as compared to the absence of energy slope parameter in Tables 2 and 3.
Table 4. Energy eigenvalues (in eV) of energy dependent Kratzer molecular potential for different values of \( n \) and \( \ell \) for ground states CO, NO, \( O_2 \) and \( I_2 \) diatomic molecules, with \( \eta = 0.5 \).

| \( n \) | \( \ell \) | \( CO \)    | \( NO \)    | \( O_2 \)    | \( I_2 \)    |
|-------|-------|-----------|-----------|-----------|-----------|
| 0     | 0     | -1.685470983 | -1.598084322 | -1.436597363 | -0.8821098304 |
| 1     | 0     | -1.679305517 | -1.590871796 | -1.427770406 | -0.8798579292 |
|       | 1     | -1.679233740 | -1.590790708 | -1.427673989 | -0.8798527834 |
| 2     | 0     | -1.673229781 | -1.583767938 | -1.419089433 | -0.8776117488 |
|       | 1     | -1.673159611 | -1.583530439 | -1.418806171 | -0.8776015171 |
| 3     | 0     | -1.667239060 | -1.576767407 | -1.410544994 | -0.8753865376 |
|       | 1     | -1.667170554 | -1.57689982  | -1.410453001 | -0.8753814511 |
|       | 2     | -1.667033643 | -1.57653242  | -1.410269138 | -0.8753712785 |
|       | 3     | -1.666828530 | -1.576303400 | -1.409993648 | -0.8753560203 |
| 4     | 0     | -1.661329077 | -1.569865334 | -1.402133902 | -0.8731668498 |
|       | 1     | -1.661262070 | -1.569789595 | -1.402043954 | -0.8731617926 |
|       | 2     | -1.661128150 | -1.569638220 | -1.401864174 | -0.8731516783 |
|       | 3     | -1.660927510 | -1.569411413 | -1.401594794 | -0.8731365078 |
|       | 4     | -1.660660434 | -1.569109476 | -1.401236158 | -0.8731162818 |
| 5     | 0     | -1.655495943 | -1.563057265 | -1.393849636 | -0.8709577054 |
|       | 1     | -1.655430353 | -1.562983126 | -1.393761633 | -0.8709526770 |
|       | 2     | -1.655299265 | -1.562834945 | -1.393585738 | -0.8709426205 |
|       | 3     | -1.655102858 | -1.562612914 | -1.393322171 | -0.8709275367 |
|       | 4     | -1.654841404 | -1.562317323 | -1.392971259 | -0.8709074262 |
|       | 5     | -1.654515258 | -1.561948551 | -1.392533439 | -0.8708822905 |
Table 5. Energy eigenvalues (in eV) of energy dependent Kratzer molecular potential for different values of $n$ and $\ell$ for ground states CO, NO, O$_2$ and I$_2$ diatomic molecules, with $\eta = 1$.

| $n$ | $\ell$ | CO       | NO       | O$_2$      | I$_2$     |
|-----|--------|----------|----------|-----------|----------|
| 0   | 0      | -0.9143283175 | -0.8879121698 | -0.8355872569 | -0.6120188036 |
| 0   | 1      | -0.9118740953 | -0.8849352196 | -0.8316829851 | -0.6107178506 |
| 1   | 0      | -0.9118356154 | -0.8848906520 | -0.8316274353 | -0.6107142849 |
| 1   | 1      | -0.9094616292 | -0.8820091632 | -0.827942378 | -0.6094196340 |
| 2   | 0      | -0.9070878461 | -0.8791305048 | -0.8240785907 | -0.6081347096 |
| 2   | 1      | -0.9070515614 | -0.879084168 | -0.8240260842 | -0.6081311896 |
| 3   | 0      | -0.9047500576 | -0.8762961642 | -0.8203702568 | -0.6068523785 |
| 3   | 1      | -0.9047147491 | -0.8762551852 | -0.8203191212 | -0.6068488809 |
| 3   | 2      | -0.9046442191 | -0.8761733203 | -0.8202169568 | -0.6068418862 |
| 4   | 0      | -0.9045386403 | -0.8760507547 | -0.8200639757 | -0.6068313948 |
| 5   | 0      | -0.9024458954 | -0.8735034094 | -0.8167197533 | -0.6055761139 |
| 5   | 1      | -0.9024114949 | -0.8734634655 | -0.816669025 | -0.6055726385 |
| 5   | 2      | -0.9023427747 | -0.8733836647 | -0.8165703009 | -0.6055656880 |
| 5   | 3      | -0.9022398959 | -0.8732641797 | -0.8164211473 | -0.6055552630 |
| 5   | 4      | -0.9021030976 | -0.8731052679 | -0.8162227378 | -0.6055413644 |
| 5   | 5      | -0.9019326946 | -0.8729072681 | -0.8159754631 | -0.6055239934 |
Table 6. Energy eigenvalues (in eV) of energy dependent Kratzer molecular potential for different values of $n$ and $\ell$ for ground states CO, NO, O$_2$ and I$_2$ diatomic molecules, with $\eta=2$.

| $n$ | $\ell$ | CO       | NO       | O$_2$    | I$_2$    |
|-----|--------|----------|----------|----------|----------|
| 0   | 0      | -0.4774929881 | -0.4701556293 | -0.4550063750 | -0.3795921052 |
|     | 1      | -0.476518304  | -0.4690143732  | -0.4534445388  | -0.3789570351  |
| 1   | 0      | -0.476520739  | -0.4689911448  | -0.4534147167  | -0.3789548282  |
|     | 1      | -0.475699234  | -0.4678965624  | -0.4519148304  | -0.3783251918  |
| 2   | 0      | -0.474753199  | -0.4667999700  | -0.4504144000  | -0.3776965243  |
|     | 1      | -0.4747669984 | -0.466783719   | -0.4503865989  | -0.3776943507  |
|     | 2      | -0.4756130152 | -0.4678295473  | -0.4518286336  | -0.3783186218  |
| 3   | 0      | -0.4739163936 | -0.4657227183  | -0.4489409312  | -0.3770709835  |
|     | 1      | -0.4738986862 | -0.4657018233  | -0.4489140099  | -0.3770688262  |
|     | 2      | -0.4738633478 | -0.4656601156  | -0.4488602625  | -0.3770645119  |
|     | 3      | -0.4738105292 | -0.4655977580  | -0.4487798774  | -0.3770580413  |
|     | 4      | -0.4737404532 | -0.4655149913  | -0.4486731336  | -0.3770494152  |
| 4   | 0      | -0.4730617690 | -0.4646632066  | -0.4474923542  | -0.376485216   |
|     | 1      | -0.4730446207 | -0.4646429544  | -0.447462416   | -0.376463803   |
|     | 2      | -0.4730103939 | -0.4646025252  | -0.4474141038  | -0.3764420979  |
|     | 3      | -0.4729592263 | -0.4645420684  | -0.4473361143  | -0.3764356752  |
|     | 4      | -0.4728913214 | -0.4644618046  | -0.4472325300  | -0.3764271130  |
| 5   | 0      | -0.4728069445 | -0.4643620221  | -0.4471036873  | -0.3764164124  |
|     | 1      | -0.4728069445 | -0.4643620221  | -0.4471036873  | -0.3764164124  |

But, the variation of the quantum state with the energy eigenvalues in the presence of the energy slope parameter is in the reverse direction. As the quantum number increases, the energy eigenvalues of energy dependent molecular Kratzer potential becomes more bounded.

Figures 2 and 3 shows the energy eigenvalues variation with the energy slope parameter for different quantum numbers. Both graphs show a similar close trend of increase in energy eigenvalues as the energy slope parameter increases, for different quantum numbers.
Figure 2. Energy eigenvalues of energy-dependent Kratzer molecular potential vs $\eta$ for different values of $n$.

Figure 3. Energy eigenvalues of energy-dependent Kratzer Molecular Potential Vs $\eta$ for different values of $\ell$.

In Fig. 4, there is a diverse behavior of the energy eigenvalues with the potential strength, for different values of the energy slope parameter. Here, there is a direct decrease in energy eigenvalue as the potential strength increase in the absence of the energy slope parameter ($\eta = 0$). With the presence of the energy slope parameter ($\eta = -1$), the energy eigenvalue becomes very bounded with a maximum potential strength of about 1 eV. Similarly, there is a stunted decrease in energy eigenvalue (not more than 1 eV), as the potential strength increase ($\eta = 1$).

Figure 4. Energy eigenvalues of energy-dependent Kratzer molecular potential vs $D$ for different values of $\eta$.

5. Conclusions

We applied the asymptotic iteration method (AIM) to solve the Schrödinger equation with energy dependent molecular Kratzer potential. Its energy eigenvalues and corresponding wave functions in terms of confluent hypergeometric function have been obtained. The numerical results of the energy eigenvalues have been presented in the presence and absence of the energy slope parameter, respectively, for four different diatomic molecules (CO, NO, O$_2$ and I$_2$). Our results agree with the results in available literature, especially when the energy slope parameter is set to zero. We have also shown graphically the variation of the energy eigenvalues with some of the potential parameters like energy slope parameter and the potential strength. The behavior of the energy eigenvalues with these parameters is similar in all the diatomic molecules studied. The result obtained in this study finds application in quantum chemistry, molecular physics amongst others.

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