Exact Polynomial Solutions of the Mie-Type Potential in the N–Dimensional Schrödinger Equation

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Abstract

The polynomial solution of the N-dimensional space Schrödinger equation for a special case of Mie potential is obtained for any arbitrary l-state. The exact bound-state energy eigenvalues and the corresponding eigenfunctions are calculated for diatomic molecular systems in the Mie-type potential. Keywords: Mie potential, Schrödinger equation, Eigenvalue, Eigenfunction, Diatomic molecules PACS number: 03.65.-w; 03.65.Fd; 03.65.Ge.

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1 Introduction

The solution of the Schrödinger equation for any spherically symmetric potential has attracted attention over the past years [1-16]. The motivation in this direction arises from considerable applications in the different fields of the material science and solid physics.

The Harmonic oscillator and H-atom (Coulombic) problems are two exactly solvable potentials which have been thoroughly studied in \( N \)-dimensional space quantum mechanics for any angular momentum \( \ell \). These two problems are related together and hence the resulting second-order differential equation has the normalized orthogonal polynomial function solution (cf. Ref.[17] and the references therein). On the other hand, the Pseudoharmonic and Mie type potentials are also two exactly solvable potentials other than Coulombic and Harmonic oscillator, their wavefunctions are vanishing at the origin.

The path integral solution for one-dimensional special case Mie-potential which is a perturbed Coulombic-type potential was obtained in [18]. Moreover, the Schrödinger equation for a system bound by a Mie-type potential was also solved by using the \( 1/N \) expansion method [19].

In this letter we will follow parallel solution to Refs.[17, 20] and give a complete normalized polynomial solution for the general \( N \)-dimensional Schrödinger equation for diatomic molecular systems interacting through Mie type potential, Coulombic-type potential with an additional centrifugal potential barrier, which reduces to the standard three dimensional case when the parameter \( N \) is set equal to 3. Our aim is to present a different approach to calculate the non-zero angular momentum solutions of the \( N \)-dimensional space of Schrödinger equation for the Mie-type potential.

The contents of this paper is as follows. In Section 2, we give the eigensolution of the \( N \) dimensional Schrödinger equation with Mie type potential for the analytical bound-state (real) and imaginary solutions. Finally, in Section 3 we give our results and conclusions.
2 The $N$-Dimensional Schrödinger Equation with Mie-Type Potential

We wish to solve the $N$-dimensional Schrödinger equation for a special case of the Mie-type potential [18] given by

$$ V(r) = D_0 \left[ \frac{k}{m-k} \left( \frac{r_0}{r} \right)^m - \frac{m}{m-k} \left( \frac{r_0}{r} \right)^k \right], $$  \hspace{1cm} (1)

where $D_0$ is the interaction energy between two atoms in a solid at $r = r_0$, and $m > k$ is always satisfied. By taking $m = 2k$ and choosing the special case $k = 1$, corresponding to a Coulombic-type potential with additional centrifugal potential barrier, Eq.(1) becomes

$$ V(r) = -\frac{a_1}{r} + \frac{a_2}{2r^2}, $$  \hspace{1cm} (2)

$$ r^2 = \sum_{i=1}^{N} x_i^2, $$  \hspace{1cm} (3)

where $a_1 = 2D_0r_0$ and $a_2 = 2D_0r_0^2$. For brevity, we write the radial part of the Schrödinger equation in $N$-dimensions as

$$ \left[ -\frac{\hbar^2}{2m} \nabla_N^2 + V(r) \right] \psi(r) = E_{nl} \psi(r), $$  \hspace{1cm} (4)

which reduces into the form

$$ \left\{ \frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} - \frac{l(l+N-2)}{r^2} + \frac{2m}{\hbar^2} \left[ E_{nl} + \frac{a_1}{r} - \frac{a_2}{2r^2} \right] \right\} R_{nl}(r) = 0. $$  \hspace{1cm} (5)

Using the dimensionless abbreviations:

$$ x = r/r_0; \beta^2 = -\frac{2mr_0^2}{\hbar^2} E_{nl}; \gamma^2 = \frac{2mr_0^2}{\hbar^2} D_0, $$  \hspace{1cm} (6)

gives the following simple form

$$ \frac{d^2R_{nl}(x)}{dx^2} + \frac{N-1}{x} \frac{dR_{nl}(x)}{dx} + \left[ -\beta^2 + \frac{2\gamma^2}{x} - \frac{\gamma^2 + l(l+N-2)}{x^2} \right] R_{nl}(x) = 0, $$  \hspace{1cm} (7)
which restores its three-dimensional Schrödinger standard form once \( N = 3 \). Eq. (7) has an irregular singularity in the \( x \to \infty \) limit where its normalizable solutions in bound-states behave as [17, 20]

\[
\left( \frac{d^2}{dx^2} - \beta^2 \right) R_{nl}(x) = 0,
\]

so that \( R_{nl}(x) = A_{nl} \exp(-\beta x) + B_{nl} \exp(\beta x) \) In order that \( R_{nl}(x) \to 0 \) as \( x \to \infty \), we set \( B_{nl} = 0 \), so

\[
\lim_{x \to \infty} R_{nl}(x) = A_{nl} \exp(-\beta x),
\]

where \( A_{nl} \) is the normalization constant. Eq. (8) leads us to propose the trial solution

\[
R_{nl}(x) = N_{nl} \exp(-\beta x)g(x),
\]

where \( N_{nl} \) is another normalization constant. Putting this back into Eq. (7) yields an equation for \( g(x) \) of the form

\[
g''(x) + \left( \frac{N - 1}{x} - 2\beta \right) g'(x) + \left( \frac{2\gamma^2 - (N - 1)\beta}{x} - \frac{\gamma^2 + l(l + N - 2)}{x^2} \right) g(x) = 0,
\]

where the prime refers to the derivative with respect to \( x \). Because exponential behavior has already been taken out, one hopes that the solution for \( g(x) \) is a polynomial. Indeed, Eq. (7) has a singularity at \( x \to 0 \), the substitution of the trial solution \( g(x) = x^q \), provides the positive root solution:

\[
q = -\frac{(N - 2)}{2} + \sqrt{\left( l + \frac{N - 2}{2} \right)^2 + \gamma^2}.
\]

As \( q > 0 \), the wavefunction vanishes at \( x = 0 \), corresponding to the strong repulsion between the two atoms. It is reasonable to set

\[
R_{nl}(x) = N_{nl}x^q \exp(-\beta x)h(x),
\]

to Eq. (7), one gets

\[
h''(x) + \left( \frac{2q + N - 1}{x} - 2\beta \right) h'(x)
\]

\[
+ \left( \frac{2\gamma^2 - 2q\beta - (N - 1)\beta}{x} + q(q - 1) + \frac{(N - 1)q - \gamma^2 - l(l + N - 2)}{x^2} \right) h(x) = 0.
\]
Setting the numerator of $x^{-2}$ term equal to zero, in the last equation, and solving the resulting quadratic equation leads again to the solution given in Eq. (12) and thus gives the following differential equation

$$x h''(x) + [2q + N - 1 - 2\beta x] h'(x) + \left[2\gamma^2 - 2q\beta - (N - 1)\beta\right] h(x) = 0.$$  \hspace{1cm} (15)

The confluent series, for large values of $x$, is proportional to $\exp(2\beta x)$ so that $R_{nl}(x)$ diverges for $x \to \infty$ if the series $\text{I}_1 F_1$ does not break off. If it does, $\text{I}_1 F_1$ is a polynomial and $R_{nl}(x) \to 0$ for $x \to \infty$ becomes normalizable. After the substitution of series form [20]

$$h(x) = \sum_{i=0}^{i_{\text{max}}} C_i x^i,$$  \hspace{1cm} (16)

into Eq. (15), it provides

$$C_{i+1} = \frac{i + q + (N - 1)/2 - \gamma^2/\beta}{(i + 1)(i + 2q + N - 1)} C_i = \Gamma_i C_i, \quad \frac{C_{i+1}}{C_i} \to \frac{1}{i},$$  \hspace{1cm} (17)

which leads to a divergent wavefunction if not truncated to a maximum value for $i$. Nevertheless, the wavefunction is finite everywhere since $i$ and $l$ are finite, it follows

$$i_{\text{max}} + q + \frac{(N - 1)}{2} - \gamma^2/\beta = 0; \quad i_{\text{max}} = n; \quad (n = 0, 1, 2, ...).$$  \hspace{1cm} (18)

Further, using the following abbreviations in Eq. (15):

$$z = 2\beta x; \quad c = \left(q + \frac{N - 1}{2}\right); \quad -n = \left(c/2 - \gamma^2/\beta\right),$$  \hspace{1cm} (19)

gives the general type of Kummer’s (Confluent Hypergeometric) differential equation of the form

$$z h''(z) + [c - z] h'(z) + n h(x) = 0; \quad (n = 0, 1, 2, ...),$$  \hspace{1cm} (20)

having the solution

$$h(x) = _1 F_1(a, c; z) = _1 F_1(-n; 2\gamma^2/\beta - 2n; 2\beta x) = L_n^{(2\gamma^2/\beta - 2n - 1)}(2\beta x),$$  \hspace{1cm} (21)

where $ _1 F_1(-n, m + 1; z) = L_n^{(m)}(z)$ denotes the Kummer’s function. On the other hand, we may also write Eq. (15) in the following general form
\[ zh''(z) + [m + 1 - z] h'(z) + nh(x) = 0, \tag{22} \]

where \( m = 2q + N - 2 \) and \( n_{\text{max}} = \frac{x^2}{\beta} - q - \frac{(N-1)}{2} = 0, 1, 2, \ldots \). If \( n \) is a non-negative integer, then a finite polynomial solution is allowed. (This when combined with the rest of \( R_{nl}(x) \) yields a normalizable solution.) In particular, this solution to Eq. (22) is the generalized Laguerre polynomial \( L_n^{(m)}(2\beta x) \). Combining everything one finally has

\[ R_{nl}(r) = N_{nl} \left( \frac{r}{r_0} \right)^{\frac{x^2}{\beta} - n - \frac{(N-1)}{2}} \exp \left( -\frac{\beta r}{r_0} \right) L_n^{(2\beta^2 - 2n - 1)} \left( \frac{2\beta r}{r_0} \right). \tag{23} \]

Since the radial volume element in \( N \)-dimensional space is \( r^{N-1} dr \), one can obtain [17]

\[ N_{nl} = \left[ \int_0^\infty dr r^{N-1} e^{-2\beta x} x^{2q} \left( L_n^{(2q+N-2)}(2\beta x) \right)^2 \right]^{-1/2}, \]

\[ N_{nl} = \frac{(2\beta)^{q+N/2}}{r_0^{N/2}} \left[ J_{n,m}^{(1)}(2\beta x) \right]^{-1/2}; J_{n,m}^{(1)} = \frac{(m+n)!}{n!} \left( 2n + m + 1 \right), \tag{24} \]

or equivalently as

\[ N_{nl} = \left( \frac{2\beta}{r_0} \right)^{N/2} (2\beta)^{\frac{x^2}{\beta} - n - \frac{(N-1)}{2}} \left[ \frac{n!}{\frac{2\beta^2}{\beta} - n} \right]^{1/2}. \tag{25} \]

### 2.1 Negative Energy

For bound-states, \( \beta > 0 \), the solution becomes in arbitrary normalization constant is given by means of Eq. (23) in which \( R_{nl}(x) \to 0 \) for \( x \to \infty \) becomes normalizable. On the other hand, from Eq. (6) with the aid of Eqs. (12) and (18), the eigenvalue becomes [21]

\[ E_{nl} = -\frac{\hbar^2 \gamma^4}{2mr_0^2} \left[ n + \frac{1}{2} + \sqrt{\left( l + \frac{N-2}{2} \right)^2 + \gamma^2} \right]^{-2}. \tag{26} \]

Since the parameter \( \gamma \gg 1 \) for most diatomic molecules, we may expand into powers of \( 1/\gamma \). This leads to

\[ E_{nl} = D_0 \left[ -1 + \frac{2 \left( n + \frac{1}{2} \right)}{\gamma} + \frac{\left( l + \frac{N-2}{2} \right)^2}{\gamma^2} - \frac{3 \left( n + \frac{1}{2} \right)^2}{\gamma^2} - \frac{3 \left( n + \frac{1}{2} \right) \left( l + \frac{N-2}{2} \right)^2}{\gamma^3} + \ldots \right]. \tag{27} \]
The Mie-type potential, Eq.(2), can be expanded about its minimum at \( r = r_0 \) as

\[
V(r) = D_0 \frac{(r - r_0)^2}{r_0^2} - D_0. \tag{28}
\]

Therefore, with classical frequency for small harmonic vibrations,

\[
\omega = \sqrt{\frac{2D_0}{mr_0^2}}, \tag{29}
\]

and the moment of inertia

\[
I = mr_0^2, \tag{30}
\]

we arrive at

\[
E_{nl} = -\frac{1}{2} I \omega^2 + \hbar \omega \left( n + \frac{1}{2} \right) + \frac{\hbar^2}{2I} \left( l + \frac{N - 2}{2} \right)^2 - \frac{3\hbar^2}{2I} \left( n + \frac{1}{2} \right)^2
\]

\[
- \frac{3\hbar^3}{2I^2 \omega} \left( n + \frac{1}{2} \right) \left( l + \frac{N - 2}{2} \right)^2 + .... \tag{31}
\]

### 2.2 Positive Energy

For \( \beta < 0 \) or \( E_{nl} > 0 \), it is no longer real but purely complex, \( \beta x = -i\kappa r \) with \( \kappa = \sqrt{\frac{2mE}{\hbar^2}} \) which gives the wavefunction [21]

\[
R_{nl}(r) = A_{nl} \frac{r^q}{r_0^q} \exp(i\kappa r) \frac{1}{\Gamma(2q+N-1)} \Gamma(q + \frac{N-1}{2}) \exp\left(-\frac{i\gamma^2}{2\kappa r_0} + \frac{N-1}{2}ight).
\]

which vanishes at \( r = 0 \). Its asymptotic may be found from the well-known formula [21]

\[
\frac{1}{\Gamma(2q+N-1)} \Gamma(q + \frac{N-1}{2}) \exp\left(-\frac{i\gamma^2}{2\kappa r_0} + \frac{N-1}{2}ight) = 0,
\]

holding for the whole complex \( z \)-plane cut along the positive imaginary axis.

\[
R_{nl}(r) = C_{nl} r^q \exp(i\kappa r) \left[ e^{-i\pi \left(q - \frac{\kappa^2 r_0^2}{2} + \frac{N-1}{2} \right)} \frac{\Gamma(2q+N-1)}{\Gamma(q + \frac{N-1}{2})} \left(-2i\kappa r\right)^{-q + \frac{\kappa^2 r_0^2}{2} - \eta} \right]
\]

\[
+ \frac{\Gamma(2q+N-1)}{\Gamma(q + \frac{N-1}{2})} e^{-2i\kappa r} \left(-2i\kappa r\right)^{-q - \frac{\kappa^2 r_0^2}{2} + \frac{N-1}{2} - \eta}, \tag{34}
\]
with $\frac{\gamma^2}{\kappa r_0} = \sqrt{\frac{2m}{\kappa^2 E^2} r_0}$. Therefore, the eigenenergy reads as

$$E_{nl} = \frac{\hbar^2 \gamma^4}{2m r_0^2} \left[ n + \frac{1}{2} + \sqrt{\left( l + \frac{N - 2}{2} \right)^2 + \gamma^2} \right]^{-2}. \quad (35)$$

### 3 Results and Conclusions

We have studied the solution for a Mie-type potential. Considering the special case of the Mie potential with $m = 2k$ and for $k = 1$, the problem was reduced to a Coulombic potential with the additional centrifugal potential barrier of order $1/r^2$. The exact solutions for this particular case have been obtained, which are similar to the Hydrogenic solutions [17]. We have calculated the eigenvalue and the corresponding wave function considering the negative (bound-states) and positive (imaginary) cases for any quantum-mechanical system bound by a special case of the Mie potential.

The present results for the potential parameters $a_1 = 1$ and $a_2 = 0$ in Eq. (2) correspond to the Coulombic potential case. They are the same with the previous calculations in [17-19]. Thus, for this particular case the energy terms in the expansion, Eq. (27), take the form

$$E_n = -\frac{1}{n^2}. \quad (36)$$

This value is the exact nonrelativistic H-atom energy expression. Further, setting $N = 3$, $D_0 = V_0/2$, $r_0 = \sigma$, $A = \frac{1}{2} \sigma^2 V_0$ and $B = \sigma^2 V_0$, Eq.(27) becomes

$$E_n = -\frac{2m}{\hbar^2} B^2 \left[ 2n' + 1 + \left( (2l + 1)^2 + \frac{8mA}{\hbar^2} \right)^{1/2} \right]^{-2}, \quad n' = n - s - 1 = 1, 2, 3... \quad (37)$$

which consequently recovers the formula (28) in Ref. [18] and also Eq. (19) in Ref. [19]. For the H-atom case this energy expression also gives $-0.5$ a.u. exactly. Thus, the present result reproduces exactly the path integral, $1/N$-expansion, and the non-relativistic Schrödinger equation solutions.

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