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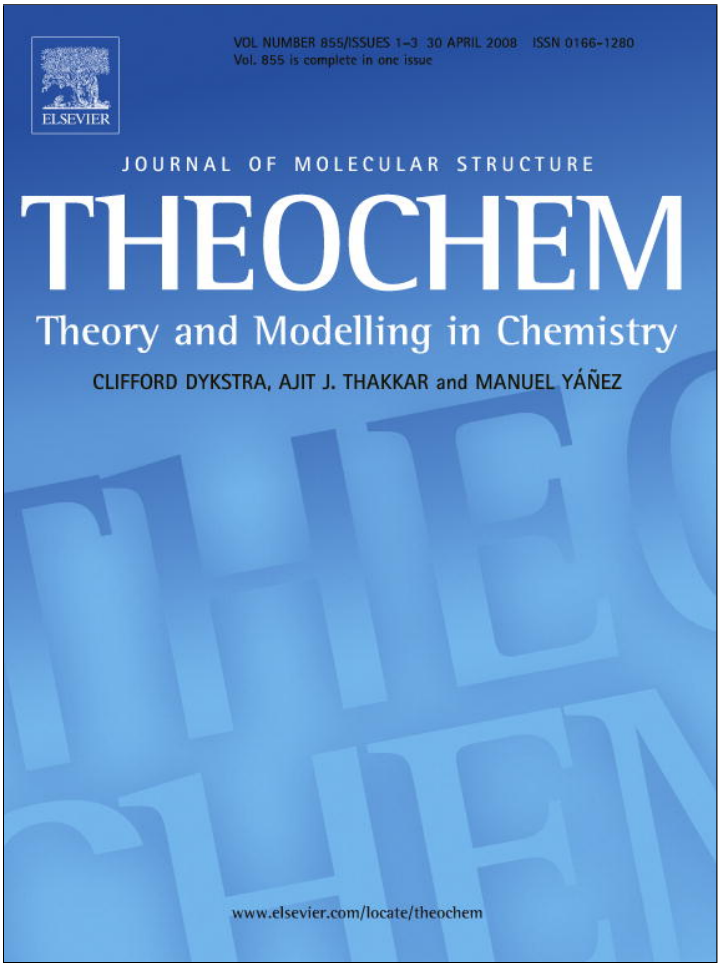

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Journal of Molecular Structure: THEOCHEM 855 (2008) 13–17

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Polynomial solutions of the Mie-type potential in the *D*-dimensional Schrödinger equation

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Received 13 November 2007; received in revised form 25 December 2007; accepted 25 December 2007
Available online 12 January 2008

Abstract

The polynomial solution of the *D*-dimensional Schrödinger equation for a special case of Mie potential is obtained with an arbitrary $l \neq 0$ states. The exact bound state energies and their corresponding wave functions are calculated. The bound state (real) and positive (imaginary) cases are also investigated. In addition, we have simply obtained the results from the solution of the Coulomb potential by an appropriate transformation.
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Keywords: Mie potential; Coulomb potential; Schrödinger equation; Bound states; Diatomic molecules

1. Introduction

The solution of the Schrödinger equation for any spherically symmetric (central) potential has attracted attention in the recent years [1–16]. The motivation in this direction arises from considerable applications in the different fields of the material science and solid state physics.

The anharmonic oscillator and H-atom (Coulombic) problems are exactly two solvable potentials studied in *D*-dimensional space for an arbitrary angular momentum $l \neq 0$ state. These two problems are related to each other 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 exactly solvable potentials other than Coulombic and anharmonic oscillator. Their wave functions vanish at origin.

The path integral solution of one-dimensional special case of Mie potential, i.e., Mie-type potential which is simply Coulomb potential with an additional centrifugal potential barrier was obtained before [18]. Further, the Schrödinger equation for Mie potential was also solved by using the $1/N$ expansion method [19].

In this letter we follow the method given in Refs. [17,20,21] to get a complete normalized polynomial eigensolutions to the general *D*-dimensional Schrödinger equation for diatomic molecular systems interacting via Mie-type potential. These eigensolutions can be reduced to a three-dimensional case. We obtain the analytic solution of the *D*-dimensional Schrödinger with Mie-type potential for the $l \neq 0$ states by using a standard method. It is not difficult to verify that our results can be also obtained from the solution of the Coulomb potential by employing an appropriate transformation.

This paper is organized as follows. In Section 2, we present the analytic eigensolutions for both bound state (real) and imaginary cases. We can also obtain the eigensolutions of the Mie-type potential from the Coulombic solutions by utilizing an appropriate transformation. Finally, some concluding remarks are given in Section 3.

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0166-1280/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.theochem.2007.12.044

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2. The *D*-dimensional Schrödinger equation for the Mie-type potential

The Mie-type potential [18] is

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

where the parameter D_0 determines the interaction energy between two atoms in a solid at $r=r_0$, and $j>k$ is always satisfied. Taking $j=2k$ and further setting $k=1$, the potential reduces to the Coulombic-type form:

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

$$r^2=\sum_{i=1}^{D}x_i^2, \tag{3}$$

where $a_1=2D_0r_0$ and $a_2=2D_0r_0^2$ are two constants. The D-dimensional Schrödinger equation for the central potential (2) is given by [22–25]

$$\begin{aligned}
&\left\{\nabla_D^2+\frac{2\mu}{\hbar^2}[E-V(r)]\right\}\psi_{l_1\cdots l_{D-2}}^{(l_{D-1}=l)}(\mathbf{x})=0,\\
&\quad\nabla_D^2=\sum_{j=1}^{D}\frac{\partial^2}{\partial x_j^2},\\
&\nabla_D^2=\frac{\partial^2}{\partial r^2}+\frac{(D-1)}{r}\frac{\partial}{\partial r}\\
&\qquad+\frac{1}{r^2}\left[\frac{1}{\sin^{D-2}\theta_{D-1}}\frac{\partial}{\partial\theta_{D-1}}\left(\sin^{D-2}\theta_{D-1}\frac{\partial}{\partial\theta_{D-1}}\right)\right.\\
&\qquad\left.-\frac{L_{D-2}^2}{\sin^2\theta_{D-1}}\right],\ \psi_{l_1\cdots l_{D-2}}^{(l_{D-1}=l)}(\mathbf{x})=R_l(r)Y_{l_1\cdots l_{D-2}}^{(l_{D-1}=l)}(\widehat{\mathbf{x}}),\\
&-L_{D-1}^2=\frac{1}{\sin^{D-2}\theta_{D-1}}\frac{\partial}{\partial\theta_{D-1}}\left(\sin^{D-2}\theta_{D-1}\frac{\partial}{\partial\theta_{D-1}}\right)-\frac{L_{D-2}^2}{\sin^2\theta_{D-1}},\\
&L_j^2Y_{l_1\cdots l_{D-2}}^{(l_{D-1}=l)}(\widehat{\mathbf{x}})=l_j(l_j+j-1)Y_{l_1\cdots l_{D-2}}^{(l_{D-1}=l)}(\widehat{\mathbf{x}}),\\
&\quad j\in[1,D-1],
\end{aligned}\tag{4}$$

where μ and E denote the reduced mass and energy of two interacting particles, respectively. $\mathbf{x}$ is a D-dimensional position vector with the hyperspherical Cartesian components $x_1,x_2,\cdots,x_D$.[1] This allows us to obtain the following radial wave equation [22–25]:

$$\begin{aligned}&\left\{\frac{d^2}{dr^2}+\frac{D-1}{r}\frac{d}{dr}-\frac{l(l+D-2)}{r^2}\right.\\&\qquad\left.+\frac{2\mu}{\hbar^2}\left[E_{nl}+\frac{a_1}{r}-\frac{a_2}{2r^2}\right]\right\}R_{nl}(r)=0.\end{aligned}\tag{5}$$

Owing to the symmetry of the potential, the present problem is reduced to a one-dimensional radial eigenvalue problem which in turn can be solved by a standard way. We first study the solution of the bound states, i.e., $E_{nl}<0$, in the region $r\in(0,\infty)$. Defining the following dimensionless quantities:

$$x=r/r_0;\quad \gamma^2=\frac{2\mu r_0^2}{\hbar^2}D_0,\quad \beta=r_0\varepsilon_{nl},\quad \varepsilon_{nl}=\sqrt{-\frac{2\mu}{\hbar^2}E_{nl}}, \tag{6}$$

allows one to obtain the following one-dimensional Schrödinger equation:

$$\begin{aligned}&\frac{d^2R_{nl}(x)}{dx^2}+\frac{D-1}{x}\frac{dR_{nl}(x)}{dx}\\&\qquad+\left[-\beta^2+\frac{2\gamma^2}{x}-\frac{\gamma^2+l(l+D-2)}{x^2}\right]R_{nl}(x)=0.\end{aligned}\tag{7}$$

We now proceed to solve Eq. (7) which has an irregular singularity in the $x\to\infty$ limit where its normalizable solutions for bound states behave as [17,20]

$$\left(\frac{d^2}{dx^2}-\beta^2\right)R_{nl}(x)=0, \tag{8}$$

which suggests the general solution be expressed by $R_{nl}(x)=A_{nl}\exp(-\beta x)+C_{nl}\exp(\beta x)$. Considering the fact that the function $R_{nl}(x)$ must be bounded everywhere, including at infinity and since $\beta>0(\varepsilon_{nl}>0)$ from Eq. (6), we should set $C_{nl}=0$. Therefore, we must have the following exponentially decreasing solution:

$$\lim_{x\to\infty}R_{nl}(x)=A_{nl}\exp(-\beta x), \tag{9}$$

where A_{nl} is the normalization constant. This result suggests that we look for a trial solution for Eq. (7) having the general form

$$R_{nl}(x)=N_{nl}\exp(-\beta x)g(x), \tag{10}$$

where N_{nl} is another normalization constant. Inserting this back into Eq. (7), we find that the function $g(x)$ satisfies the following differential equation:

$$\begin{aligned}&g''(x)+\left(\frac{D-1}{x}-2\beta\right)g'(x)\\&\qquad+\left(\frac{2\gamma^2-(D-1)\beta}{x}-\frac{\gamma^2+l(l+D-2)}{x^2}\right)g(x)=0,\end{aligned}\tag{11}$$

where the prime refers to the derivative with respect to x. Because exponential behavior has already been taken out, one expects 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:

$$q=-\frac{(D-2)}{2}+\sqrt{\left(l+\frac{D-2}{2}\right)^2+\gamma^2}. \tag{12}$$

As $q>0$, the wave function vanishes at $x=0$, corresponding to the strong repulsion between the two atoms. It is reasonable to substitute

$$R_{nl}(x)=N_{nl}x^q\exp(-\beta x)h(x), \tag{13}$$

[1] It should be mentioned that such a definition was introduced by Erdélyi early in 1950s (cf. [26], pp. 232–235, Chapter 11) even though the notation used by him is quite different from that by Louck and Chatterjee [27,28].

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into Eq. (7), in order to obtain

$$h''(x)+\left(\frac{2q+D-1}{x}-2\beta\right)h'(x)+\left(\frac{2\gamma^2-2q\beta-(D-1)\beta}{x}+\frac{q(q-1)+(D-1)q-\gamma^2-l(l+D-2)}{x^2}\right)h(x)=0. \tag{14}$$

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). Hence, one obtains the following wave function $h(x)$ satisfying

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

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 ${}_1F_1$ does not break off. If it does, ${}_1F_1$ is a polynomial and $R_{nl}(x)\to 0$ for $x\to\infty$ becomes normalizable. Substitution of the following series form [20]

$$h(x)=\sum_{i=0}^{i_{\max}}C_i x^i, \tag{16}$$

into Eq. (15) gives

$$C_{i+1}=\frac{i+q+(D-1)/2-\gamma^2/\beta}{(i+1)(i+2q+D-1)}C_i=\Gamma_{il}C_i,\ \frac{C_{i+1}}{C_i}\to\frac{1}{i}, \tag{17}$$

which leads to a divergent wave function if not truncated to a maximum value for i. Nevertheless, the wave functions should be convergent everywhere since i and l are finite and consequently it follows

$$i_{\max}+q+\frac{(D-1)}{2}-\frac{\gamma^2}{\beta}=0;\quad i_{\max}=n;\quad n=0,1,2,\ldots. \tag{18}$$

Moreover, inserting the following abbreviations

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

in Eq. (15), then it reduces to the general type of Kummer's (Confluent Hypergeometric) differential equation of the form

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

Essentially, the solution of Eq. (20) is given by

$$h(x)={}_1F_1(a,c;z)={}_1F_1\left(-n;2\frac{\gamma^2}{\beta}-2n;2\beta x\right)=L_n^{\left(2\frac{\gamma^2}{\beta}-2n-1\right)}(2\beta x), \tag{21}$$

where ${}_1F_1(-n,\nu+1;z)=L_n^{(\nu)}(z)$ denotes the Kummer's function. In addition, we may also rewrite Eq. (15) in the following general form

$$zh''(z)+[\nu+1-z]h'(z)+nh(x)=0, \tag{22}$$

where $\nu=2q+D-2$ and $n_{\max}=\frac{\gamma^2}{\beta}-q-\frac{(D-1)}{2}=0,1,2,\ldots$. If n is a non-negative integer, then a finite polynomial solution is allowed. This part of wave function combined with the rest of $R_{nl}(x)$ yields a normalizable (physical) solution. In particular, the solution of Eq. (22) is proportional to the generalized Laguerre polynomial $L_n^{(\nu)}(2\beta x)$. Combining everything we finally arrive at the ansatz for the wave functions with the following form:

$$R_{nl}(r)=N_{nl}\left(\frac{r}{r_0}\right)^{\frac{\gamma^2}{\beta}-n-\frac{(D-1)}{2}}\exp\left(-\frac{\beta r}{r_0}\right)L_n^{(2\frac{\gamma^2}{\beta}-2n-1)}\left(\frac{2\beta r}{r_0}\right), \tag{23}$$

where $\frac{\gamma^2}{\beta}=n+\frac{1}{2}+\sqrt{(l+\frac{D-2}{2})^2+\gamma^2}$. Since the radial volume element in a D-dimensional space is $r^{D-1}\mathrm{d}r$, one obtains [17]

$$N_{nl}=\left[\int_0^\infty \mathrm{d}r r^{D-1}\mathrm{e}^{-2\beta x}x^{2q}(L_n^{(2q+D-2)}(2\beta x))^2\right]^{-1/2},$$
$$N_{nl}=\frac{(2\beta)^{q+N/2}}{r_0^{N/2}}[J_{n,\nu}^{(1)}(2\beta x)]^{-1/2};J_{n,\nu}^{(1)}=\frac{(\nu+n)!}{n!}(2n+\nu+1), \tag{24}$$

or equivalently

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

On the other hand, following Ref. [21], we obtain the solutions of the Mie-type potential from the solution of the Coulomb potential by employing the transformation, $L(L+D-2)=l(l+D-2)+\frac{2\mu D_0 r_0^2}{\hbar^2}$. Thus, Eq. (5) can be reduced to the following Schrödinger-like equation:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{D-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{L(L+D-2)}{r^2}+\frac{2\mu}{\hbar^2}\left(E_{nL}+\frac{A}{r}\right)\right]R_{nL}(r)=0, \tag{26}$$

where

$$A=a_1\quad\text{and}\quad L=-\frac{(D-2)}{2}+\sqrt{\left(l+\frac{D-2}{2}\right)^2+\frac{2\mu D_0 r_0^2}{\hbar^2}}. \tag{27}$$

It should be mentioned that the last equation is the usual case of the Schrödinger equation with a Coulombic potential, $V(r)=-\frac{A}{r}$. The bound state energy levels of Eq. (26) are [29,30]

$$E_{nL}=-\frac{\mu A^2}{2\hbar^2\left(n+\frac{D-1}{2}+L\right)^2},\quad n=0,1,2,\cdots, \tag{28}$$

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and the wave functions are

$$\psi^{(l)}_{l_1\cdots l_{D-2}}(\mathbf{x}) = A_{nL} r^L \exp(-\varepsilon_{nl} r) L_n^{(2L+D-2)}(2\varepsilon_{nl} r) Y^{(L)}_{L_1\cdots L_{D-2}}(\widehat{\mathbf{x}}), \tag{29}$$

where A_{nL} is a normalization constant and $Y^{(L)}_{L_1\cdots L_{D-2}}(\widehat{\mathbf{x}})$ is the angular part of the wave functions. With the aid of Eq. (27), we may rewrite Eq. (28) in a more explicit form as

$$E_{nl} = -\frac{2\mu D_0^2 r_0^2}{\hbar^2\left(n+\frac{1}{2}+\sqrt{\left(l+\frac{D-2}{2}\right)^2+\frac{2\mu D_0 r_0^2}{\hbar^2}}\right)^2}, \quad n = 0,1,2,\cdots. \tag{30}$$

2.1. Negative energy

For bound state case, i.e., $\beta > 0$, the solution given by means of Eq. (23), in which $R_{nl}(x) \to 0$ for $x \to \infty$, becomes convergent and normalized. Further, Eq. (30) with the aid of Eq. (6) can be rewritten as [31]

$$E_{nl} = -\frac{\hbar^2\gamma^4}{2\mu r_0^2}\left[n+\frac{1}{2}+\sqrt{\left(l+\frac{D-2}{2}\right)^2+\gamma^2}\right]^{-2}. \tag{31}$$

Since the parameter $\gamma \gg 1$ for most diatomic molecules, we may expand Eq. (31) into powers of $1/\gamma$ as

$$E_{nl} = D_0\left[-1+\frac{2\left(n+\frac{1}{2}\right)}{\gamma}+\frac{\left(l+\frac{D-2}{2}\right)^2}{\gamma^2}-\frac{3\left(n+\frac{1}{2}\right)^2}{\gamma^2} - \frac{3\left(n+\frac{1}{2}\right)\left(l+\frac{D-2}{2}\right)^2}{\gamma^3}+\ldots\right]. \tag{32}$$

Moreover, the Mie-type potential given by Eq. (2) can be expanded about its minimum at $r = r_0$ as

$$V(r) = D_0\frac{(r-r_0)^2}{r_0^2} - D_0. \tag{33}$$

Hence, with classical frequency for small harmonic vibrations,

$$\omega = \sqrt{\frac{2D_0}{\mu r_0^2}}, \tag{34}$$

and the moment of inertia

$$I = \mu r_0^2, \tag{35}$$

we finally arrive at

$$E_{nl} = -\frac{1}{2}I\omega^2 + \hbar\omega\left(n+\frac{1}{2}\right)+\frac{\hbar^2}{2I}\left(l+\frac{D-2}{2}\right)^2 - \frac{3\hbar^2}{2I}\left(n+\frac{1}{2}\right)^2 - \frac{3\hbar^3}{2I^2\omega}\left(n+\frac{1}{2}\right)\left(l+\frac{D-2}{2}\right)^2+\ldots. \tag{36}$$

2.2. Positive energy

For $\beta < 0$, i.e., $E_{nl} > 0$, it is now no longer real but purely complex, $\beta x = -\mathrm{i}\kappa r$ with $\kappa = \sqrt{\frac{2\mu E_{nl}}{\hbar^3}}$. Hence, the wave functions become [31]

$$R_{nl}(r) = A_{nl}(r/r_0)^q \exp(\mathrm{i}\kappa r)\,{}_1F_1\left(q+\frac{D}{2}-\frac{1}{2}-\frac{\mathrm{i}\gamma^2}{\kappa r_0}, 2q+D-1; -2\mathrm{i}\kappa r\right), \tag{37}$$

which vanishes at $r = 0$. Its asymptotic may be found from the formula [31]

$${}_1F_1(a,c;z) \to \exp(-\mathrm{i}\pi a)\frac{\Gamma(c)}{\Gamma(c-a)}z^{-a} + \frac{\Gamma(c)}{\Gamma(a)}\exp(z)z^{a-\eta_l} = 0, \tag{38}$$

which is true for the whole complex z-plane cut along the positive imaginary axis. The total wave functions become

$$R_{nl}(r) = C_{nl} r^q \exp(\mathrm{i}\kappa r)\left[\mathrm{e}^{-\mathrm{i}\pi\left(q-\frac{\mathrm{i}\gamma^2}{\kappa r_0}+\frac{D}{2}-\frac{1}{2}\right)}\frac{\Gamma(2q+D-1)}{\Gamma\left(q+\frac{\mathrm{i}\gamma^2}{\kappa r_0}+\frac{D-1}{2}\right)} \times(-2\mathrm{i}\kappa r)^{-q+\frac{\mathrm{i}\gamma^2}{\kappa r_0}-\frac{(D-1)}{2}} + \frac{\Gamma(2q+D-1)}{\Gamma\left(q-\frac{\mathrm{i}\gamma^2}{\kappa r_0}+\frac{D-1}{2}\right)}\mathrm{e}^{-2\mathrm{i}\kappa r} \times(-2\mathrm{i}\kappa r)^{q-\frac{\mathrm{i}\gamma^2}{\kappa r_0}+\frac{D-1}{2}-\eta_l}\right], \frac{\gamma^2}{\kappa r_0} = \sqrt{\frac{2\mu}{\hbar^3}\frac{D_0^2}{E_{nl}}}r_0. \tag{39}$$

Finally, for this system, the energy states become

$$E_{nl} = \frac{\hbar^2\gamma^4}{2\mu r_0^2}\left[n+\frac{1}{2}+\sqrt{\left(l+\frac{D-2}{2}\right)^2+\gamma^2}\right]^{-2}. \tag{40}$$

3. Conclusions

We have obtained the solutions of the D-dimensional Schrö dinger equation for the Mie-type potential. Considering the special case of the Mie potential with $j = 2k$ where $k = 1$, the problem has been reduced into Coulomb potential with the additional centrifugal potential barrier of order $1/r^2$. The exact solutions for this particular case have been obtained from the known Hydrogenic solution by using a convenient transformation [17]. In addition, we have calculated the eigenvalues and the corresponding wave functions for any quantum-mechanical system bounded by such special case of the Mie potential. We have also studied the negative (bound state) and positive (imaginary) cases.

Taking the potential parameters $a_1 = 1$ and $a_2 = 0$ in Eq. (2), this reduces the present analysis to the Coulombic results. Our calculations are similar to the previous calculations given in Refs. [17–19]. On the other hand, for this particular case, the energy terms in the expansion (28) take the following form

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$$E_n = -\frac{1}{n^2}, \tag{41}$$

which is the exact non-relativistic H-atom energy expression. Putting $D = 3$, $D_0 = V_0/2$, $r_0 = \sigma$, $A = \frac{1}{2}\sigma^2 V_0$ and $B = \sigma V_0$ in Eq. (31), gives

$$E_{nl} = -\frac{2\mu}{\hbar^2}B^2\left[2n' + 1 + \left[(2l+1)^2 + \frac{8\mu A}{\hbar^2}\right]^{1/2}\right]^{-2},$$
$$n' = n - s - 1 = 1, 2, 3 \ldots \tag{42}$$

which consequently recovers the formula (28) in Ref. [18] and also formula (19) in Ref. [19]. It should be pointed out that Eq. (42), in the H-atom case, gives -0.5 a.u. exactly. Finally, we emphasize that the present results reproduce exactly the path integral, $1/N$-expansion, and the non-relativistic Schrödinger equation solutions.

Acknowledgements

The authors wish to thank the kind referee for the positive and invaluable suggestions which have improved the manuscript greatly. This research was partially supported by the Scientific and Technological Research Council of Turkey.

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