Schrödinger Equation with the Potential $V(r) = Ar^{-4} + Br^{-3} + Cr^{-2} + Dr^{-1}$

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Abstract

Making use of an ansatz for the eigenfunction, we obtain exact closed form solutions to the Schrödinger equation with the inverse-power potential, $V(r) = Ar^{-4} + Br^{-3} + Cr^{-2} + Dr^{-1}$ both in three dimensions and in two dimensions, where the parameters of the potential $A, B, C, D$ satisfy some constraints.

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1. Introduction

The exact solutions to the fundamental dynamical equations play an important role in the different fields of physics. As far as the Schrödinger equation concerned, the exact solutions are possible only for the several potentials and some approximation methods are frequently used to arrive at the solutions. The problem of the inverse-power potential, $1/r^n$, has been widely carried out on the different fields of classic mechanics as well as on the quantum mechanics. For instance, the interatomic interaction potential in molecular physics [1-2], the inverse-power potentials $V(r) = -Z^2\alpha/r^4$ [3] (interaction between an ion and a neutral atom) and $V(r) = -d_1d_2/r^3$ [4] (interaction between a dipole $d_1$ and another dipole $d_2$) are often applied to explain the interaction between one matter and another one. The interaction in one-electron atoms, muonic and hadronic and Rydberg atoms also requires considering the inverse-power potentials [5]. Indeed, the interaction potentials mentioned above are only special cases of the inverse-power potential when some parameters of the potential vanishes.

The reason we write this paper is as follows. On the one hand, Özcelik and Simsek discussed this potential in the three-dimensional spaces [6]. They obtained the eigenvalues and eigenfunctions for the arbitrary node. Simultaneously, the corresponding constraints on the parameters of the potential were obtained. Unfortunately, they did not find that it is impossible to discuss the higher order excited state except for the ground state. In the later discussion, we will draw this conclusion and find some essential mistakes occurred in their calculations even for the ground state. We recalculate the solutions to the Schrödinger equation with this potential in three dimensions following their idea and correct their mistakes. On the other hand, with the advent of growth technique for the realization of the semiconductor quantum wells, the quantum mechanics of low-dimensional systems has become a major research field. Almost all of the computational techniques developed for the three-dimensional problems have already been extended to lower dimensions. Therefore, we generalize this method to the two-dimensional Schrödinger equation because of the wide interest in lower-dimensional fields theory. Besides, we has succeeded in dealing with the Schödinger equation with
the anharmonic potentials, such as singular potential both in two dimensions and in three dimensions[9, 10], the sextic potential [11], the octic potential [12] and the Mie-type potential [13] by this method. We now attempt to study the Schrödinger equation with the inverse-power potential by the same way both in three dimensions and in two dimensions.

This paper is organized as follows. In section 2, we study the three-dimensional Schrödinger equation with this potential using an ansatz for the eigenfunctions. The study of the two-dimensional Schrödinger equation with this potential will be discussed in section 3. The figures for the unnormalized radial functions are plotted in the last section.

2. Solutions in three dimensions

Throughout this paper the natural unit $\hbar = 1$ and $\mu = 1/2$ are employed. Consider the Schrödinger equation

$$-\nabla^2 \psi + V(r)\psi = E\psi, \quad (1)$$

where here and hereafter the potential

$$V(r) = Ar^{-4} + Br^{-3} + Cr^{-2} + Dr^{-1}, \quad A > 0, \quad D < 0. \quad (2)$$

Let

$$\psi(r, \theta, \phi) = r^{-\ell}R_{\ell}(r)Y_{\ell m}(\theta, \phi), \quad (3)$$

where $\ell$ and $E$ denote the angular momentum and the energy, respectively, and the radial wave function $R_{\ell}(r)$ satisfies

$$\frac{d^2 R_{\ell}(r)}{dr^2} + \left[ E - V(r) - \ell(\ell + 1)\frac{1}{r^2} \right] R_{\ell}(r) = 0. \quad (4)$$

Özcelik and Simsek [6] make an ansatz for the ground state

$$R_{\ell}^0(r) = \exp[g(r)], \quad (5)$$

where

$$g(r) = \frac{a}{r} + br + c \ln r, \quad a < 0, \quad b < 0. \quad (6)$$
After calculating, one can obtain the following equation
\[
\frac{d^2 R_0^\ell(r)}{dr^2} - \left[\frac{d^2 g(r)}{dr^2} + \left(\frac{dg(r)}{dr}\right)^2\right] R_0^\ell(r) = 0. \tag{7}
\]

Compare Eq. (7) with Eq. (4) and obtain the following sets of equations
\[
a^2 = A, \quad b^2 = -E, \tag{8a}
\]
\[
2bc = D, \quad 2a(1 - c) = B, \tag{8b}
\]
\[
C + \ell(\ell + 1) - \frac{1}{4} = c^2 - 2ba - c. \tag{8c}
\]

It is not difficult to obtain the value of the parameter \(a\) from Eq. (8a) written as \(a = \pm \sqrt{A}\). In order to retain the well-behaved solution at \(r \to 0\) and at \(r \to \infty\), they choose negative sign in \(a\), i. e. \(a = -\sqrt{A}\). According to this choice, they arrive at a constraint on the parameters of the potential from Eq. (8c) written as
\[
C = \frac{B^2}{4A} + \frac{B}{2\sqrt{A}} + \frac{2AD}{B + 2\sqrt{A}} - \ell(\ell + 1). \tag{9}
\]

Then the energy is read as
\[
E_0^+ = -\frac{1}{16A} \left\{C + \ell(\ell + 1) \pm \sqrt{[C + \ell(\ell + 1)]^2 - 2BD}\right\}^2. \tag{10}
\]

It is readily to find that Eq. (10) is a wrong result. From Eqs. (6) and (8b), as we know, since the parameter \(b\) is negative, when we calculate the energy \(E\) from Eq. (8a), we only take the \(b\) as a negative value, so that Eq. (10) only takes the negative sign. Actually, it is not difficult to obtain the corresponding values of the parameters for the \(g(r)\) from Eq. (8), i. e.
\[
c = \frac{B + 2\sqrt{A}}{2\sqrt{A}}, \quad b = \frac{D\sqrt{A}}{B + 2\sqrt{A}}. \tag{11}
\]

The eigenvalue \(E\), however, will be simply expressed as from Eq. (8a)
\[
E = -\frac{AD^2}{B^2 + 4A + 4B\sqrt{A}}. \tag{12}
\]

The corresponding eigenfunction Eq. (5) can now be read as
\[
R_0^\ell = N_0 r^c \exp\left[\frac{1}{r}a + br\right], \tag{13}
\]
where \( N_0 \) is the normalized constant and here and hereafter the parameters \( a, b \) and \( c \) are given above.

After their discussing the ground state, Özcelik and Simsek continue to study the first excited state. They make the \textit{ansatz} for the first excited state,

\[
R_1^\ell (r) = f(r) \exp[g(r)],
\]

where \( g(r) \) is the same as Eq. (6) and \( f(r) = r - \alpha_1 \), where \( \alpha_1 \) is a constant. For short, it is readily to find from Eq. (14) that the radial wave function \( R_1^\ell (r) \) satisfies the following equation

\[
R_1^\ell (r)'' - \left[ g(r)'' + (g(r)')^2 + \frac{f(r)'' + 2g(r)'f(r)'}{f(r)} \right] R_1^\ell (r) = 0,
\]

where the prime denotes the derivative of the radial wave function with respect to the variable \( r \).

Compare Eq. (15) with Eq. (4) and obtain the following sets of equations

\[
\begin{align*}
-2b - 2bc + D + b^2\alpha_1 + e\alpha_1 &= 0, \\
-b^2 - E &= 0, \\
\alpha_1 &= A, \\
-a^2 + A + 2\alpha_1 - B\alpha_1 - 2ac\alpha_1 &= 0, \\
2ab - c - c^2 + C + \ell(\ell + 1) + 2bc\alpha_1 - D\alpha_1 &= 0, \\
B + 2ac - 2ab\alpha_1 - c\alpha_1 + c^2\alpha_1 - C\alpha_1 - \ell\alpha_1 - \ell^2\alpha_1 &= 0,
\end{align*}
\]

it is not hard to obtain the following sets of equations from Eqs. (16a-16c)

\[
\begin{align*}
E &= -b^2, \\
a^2 &= A, \\
c &= \frac{B + 2\sqrt{A}}{2\sqrt{A}},
\end{align*}
\]

\[
b = \frac{D\sqrt{A}}{B + 4\sqrt{A}},
\]

where the constant \( \alpha_1 \neq 0 \) and it is determined by Eqs. (16d) and (16e). Furthermore, it is evident to find that Eq. (17b) does not coincide with Eq. (11) with respect to the same parameter \( b \), which will lead to the their wrong calculation for the first excited state. In fact, they obtained two different relations during their calculation through
the compared equation, i.e. $D = 2bc$ (see Eq. (9) in [6]) and $D = 2b(c + 1)$ (see Eq. (16) in [6]). The parameter $D$ does not exist if the parameter $b$ is not equal to zero. It is another main mistaken that arises their wrong result, that’s to say, it is impossible to discuss the first excited state for the Schrödinger equation by this method. We only discuss the ground state by this simpler ansatz method as mentioned above.

As a matter of fact, the normalized constants $N_0$ can be calculated in principle from the normalized relation

$$\int_0^\infty |R_0^0|^2 dr = 1.$$  \hspace{1cm} (18)

In the course of calculation, making use of the standard integral [14]($\text{Re}\lambda_1 > 0$, $\text{Re}\lambda_2 > 0$ and $\text{Re}\nu > 0$)

$$\int_0^\infty r^{\nu-1} \exp[-(\lambda_1 r + \lambda_2 r^{-1})] dr = 2 \left(\frac{\lambda_2}{\lambda_1}\right)^{\nu/2} K_\nu(2\sqrt{\lambda_1\lambda_2}),$$  \hspace{1cm} (19)

which implies

$$N_0 = \left[\frac{1}{2(a^2+b^2+1/4)\sqrt{ab}}\right],$$  \hspace{1cm} (20)

where the values of the parameters $b, c$ and $a$ are given by Eq. (11) and $-\sqrt{A}$, respectively. The figure 1 for the unnormalized radial eigenfunction in three dimensions is plotted in the last section.

3. Solutions in tow dimensions

We now generalize this method to the two-dimensional Schrödinger equation. Consider Schrödinger equation with a potential $V(r)$ that depends only on the distance $r$ from the origin

$$H\psi = \left(\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2}\right) \psi + V(r)\psi = E\psi.$$  \hspace{1cm} (21)

Let

$$\psi(r, \varphi) = r^{-1/2} R_m(r) e^{\pm im\varphi}, \quad m = 0, 1, 2, \ldots,$$  \hspace{1cm} (22)

where the radial wave function $R_m(r)$ satisfies the following radial equation

$$\frac{d^2 R_m(r)}{dr^2} + \left[ E - V(r) - \frac{m^2 - 1/4}{r^2}\right] R_m(r) = 0,$$  \hspace{1cm} (23)
where $m$ and $E$ denote the angular momentum and energy, respectively. For the solution of Eq. (23), we make an *ansatz* [6-13] for the ground state

$$R_0^m(r) = \exp[g_m(r)], \quad (24)$$

where

$$g_m(r) = \frac{a_1}{r} + b_1 r + c_1 \ln r. \quad (25)$$

After calculating, we arrive at the following equation

$$\frac{d^2 R_0^m(r)}{dr^2} - \left[ \frac{d^2 g_m(r)}{dr^2} + \left( \frac{dg_m(r)}{dr} \right)^2 \right] R_0^m(r) = 0. \quad (26)$$

Compare Eq. (26) with Eq. (23) and obtain the following sets of equations

$$a_1^2 = A, \quad b_1^2 = -E, \quad (27a)$$

$$2b_1 c_1 = D, \quad 2a_1 (1 - c_1) = B, \quad (27b)$$

$$C + m^2 - \frac{1}{4} = c_1^2 - 2b_1 a_1 - c_1. \quad (27c)$$

It is not difficult to obtain the values of the parameters $a_1$ from Eq. (27a) written as $a_1 = \pm \sqrt{A}$. Likely, in order to retain the well-behaved solution at $r \to 0$ and at $r \to \infty$, we choose negative sign in $a_1$, i. e. $a_1 = -\sqrt{A}$. According to this choice, Eq. (27b) will give the other parameter values as

$$c_1 = \frac{B + 2\sqrt{A}}{2\sqrt{A}}, \quad b_1 = \frac{D\sqrt{A}}{B + 2\sqrt{A}}. \quad (28)$$

Besides, it is readily to obtain from Eq. (27c) that

$$C = \frac{B^2}{4A} + \frac{B}{2\sqrt{A}} + \frac{2AD}{B + 2\sqrt{A}} - (m^2 - 1/4), \quad (29)$$

which is the constraint on the parameters for the two-dimensional Schrödinger equation with the inverse-power potential.

The eigenvalue $E$, however, will be given by Eq. (27a) as

$$E = -\frac{AD^2}{B^2 + 4A + 4B\sqrt{A}}. \quad (30)$$
The corresponding eigenfunction Eq. (24) can now be read as

\[ R_m^0 = N r^{c_1} \exp \left[ \frac{1}{r} a_1 + b_1 r \right], \quad (31) \]

Similarly, the normalized constants \( N \) can be calculated in principle from the normalized relation

\[ \int_0^\infty |R_m^0|^2 dr = 1. \quad (32) \]

According to Eq. (19), we can obtain

\[ N = \left[ \frac{1}{2^{(a_1+b_1)^2} \sqrt{a_1 b_1} K_{2c_1+1}(4\sqrt{a_1 b_1})} \right], \quad (33) \]

where the values of the parameters \( a_1, b_1 \) and \( c_1 \) are given above. The figure 2 for the unnormalized radial eigenfunction in two dimensions is plotted in the last section.

Considering the values of the parameters of the potential, we fix them as follows. The values of parameters \( A, C, D \) are first fixed, for example \( A = 4.0, C = 2.0 \) and \( D = -2.0 \), the value of the parameter \( B \) is given by Eq. (10) and Eq. (29) for the cases both in three dimensions and two dimensions for \( \ell = 0 \) and \( m = 0 \), respectively. By this way, the parameter \( B \) turns out to \( B = 5.87 \) in three dimensions and \( B = 5.65 \) in two dimensions, respectively. The ground state energy corresponding to these values are obtained as \( E = -0.164 \) for the case in three dimensions and \( E = -0.172 \) for the case in two dimensions. Actually, when we study the properties of the ground state, as we know, the unnormalized radial wave functions do not affect the main features of the wave functions. We have plotted the unnormalized radial wave functions in figures 1 and 2 for the cases both in three dimensions and in two dimensions, respectively. With respect to figures 1 and 2, it is easy to find that they are similar to each other, which stems from the same values of the angular momentum \( \ell = 0 \) and \( m = 0 \). They will be different if we take the different values of the angular momentum in the course of calculations.

In conclusion, we obtain the exact analytic solutions to the Schrödinger equation with the inverse-power potential \( V(r) = Ar^{-4} + Br^{-3} + Cr^{-2} + Dr^{-1} \) using a simpler ansatz for the eigenfunction both in three dimensions and in two dimensions, and
simultaneously the constrains on the parameters of the potential are arrived at from the compared equations. Finally, we remark that this simple and intuitive method can be generalized to other potential. The study of the Schrödinger equation with the asymmetric potential is in progress.

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Figure 1: The ground state wave functions in three dimensions as a function of $r$ for the potential (2) with the values $A = 4.0$, $B = 5.87$, $C = 2.0$ and $D = -2.0$. The $y$-axis denotes the values of wave functions and the $x$-axis denotes the variable $r$.

Figure 2: The ground state wave functions in two dimensions as a function of $r$ for the potential (2) with the values $A = 4.0$, $B = 5.65$, $C = 2.0$ and $D = -2.0$. The $y$-axis denotes the values of wave functions and the $x$-axis denotes the variable $r$. 