Schrödinger Equation

with the Potential $V(r) = ar^2 + br^{-4} + cr^{-6}$

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Abstract

By making use of an ansatz for the eigenfunction, we obtain the exact solutions to the Schrödinger equation with the anharmonic potential, $V(r) = ar^2 + br^{-4} + cr^{-6}$, both in three dimensions and in two dimensions, where the parameters $a$, $b$, and $c$ in the potential satisfy some constraints.

PACS numbers: 03.65.Ge.

Key words: Exact solution, Anharmonic potential, Schrödinger equation.

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1. Introduction

The exact solutions to the fundamental dynamical equations play crucial roles in physics. It is well-known that the exact solutions to the Schrödinger equation have been obtained only for a few potentials, and some approximate methods are frequently applied to arrive at the approximate solutions. In recent years, the higher order anharmonic potentials have drawn more attentions of physicists and mathematicians in order to partly understand a few newly discovered phenomena, such as the structural phase transitions [1], the polaron formation in solids [2], and the concept of false vacuo in field theory [3]. Interest in these anharmonic oscillator-like interactions comes from the fact that the study of the relevant Schrödinger equation, for example, in the atomic and molecular physics, provides us with insight into the physical problem in question.

For the Schrödinger equation ($\hbar = 2m = 1$ for convenience)

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

with the potential

$$V(r) = ar^2 + br^{-4} + cr^{-6}, \quad a > 0, \quad c > 0,$$

let

$$\psi(r, \theta, \varphi) = r^{-1} R_\ell(r) Y_{\ell m}(\theta, \varphi),$$

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

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

Znojil [4,5] converted Eq. (4) into a difference equation in terms of a Laurent-series ansatz for the radial function

$$R_\ell(r) = N_0 r^\alpha \exp\left[-(\sqrt{ar^2} + \sqrt{cr^{-2}})/2\right] \sum_{m=-M}^{N} h_m r^{2m}.$$  

He defined the continued fraction solutions to accelerate the convergence of the series, and obtained the solutions for the ground state and the first excited state.
Kaushal and Parashar highly simplified the ansatz for calculating those solutions

\[ R_0(r) = N_0 r^{\kappa_0} \exp[-(\sqrt{ar^2} + \sqrt{cr^2})/2], \quad \kappa_0 = (b + 3\sqrt{c})/(2\sqrt{c}), \] (6)

for the ground state [6], and

\[ R_0(r) = N_1 r^{\kappa_1} \left(1 + \beta r^2 + \gamma r^{-2}\right) \exp[-(\sqrt{ar^2} + \sqrt{cr^2})/2], \] (7)

for the first excited state [7]. By this ansatz, the parameters in the potential (2) have to satisfy two constraints:

\[ (2\sqrt{c} + b)^2 = c \left[(2\ell + 1)^2 + 8\sqrt{ac}\right], \] (8)

and

\[ \eta_\ell \left[(\eta_\ell - 4)^2 - 4(2\kappa_1 - 1)^2\right] = 64\sqrt{ac}(\eta_\ell - 4), \]

\[ \kappa_1 = (b + 7\sqrt{c})/(2\sqrt{c}), \quad \eta_\ell = \ell(\ell + 1) + 2\sqrt{ac} - \kappa_1^2 + \kappa_1. \] (9)

where there was a sign misprint in [7] (see Eq. (13) in [7]). They set the values of the parameters by

\[ \ell = 0, \quad a = 1.0, \quad c = 0.18, \quad b = 0.04082, \] (10)

and found that \( \beta = -0.1787 \) and \( \gamma = 0.8485 \), and the energies for the ground state and the first excited state were \( E_0 = 4.096214 \) and \( E_1 = 12.09621 \), respectively. Unfortunately, their parameters given in Eq. (10) do not satisfy the second constraint (9), such that the so-called solution of the first excited state in [7] does not satisfy Eq. (4). As a matter of fact, they assumed that the angular momentum \( \ell \) is same for both the ground state and the first excited state, and that the normalized factor \( N_1 \neq 0 \), so that they must obtain, as shown in Sec. 2 of the present letter, infinite solutions for \( \beta \) and \( \gamma \) if the parameters in the potential satisfy the constraints (8) and (9).

In our viewpoint, Kaushal and Parashar presented a good idea for studying the Schrödinger equation (1) with the higher order anharmonic potential (2), but their calculation was wrong. In the present letter, we recalculate the solutions following their idea, and then, generalize this method to the two-dimensional Schrödinger equation because of the wide interest in lower-dimensional field theories recently. Besides, 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 two dimensions.

This letter is organized as follows. In Sec. 2, we recalculate the ground state and the first excited state of the Schrödinger equation with this potential using an ansatz for the eigenfunctions. This method is applied to two dimensions in Sec. 3. The figures for the unnormalized radial functions of the solutions are plotted in the due sections.

\section{Ansatz}

Assume that the radial function in Eq. (3) is

\[ R_\ell(r) = r^\kappa \left( \alpha + \beta r^2 + \gamma r^{-2} \right) \exp\left[ -\left( \sqrt{a}r^2 + \sqrt{c}r^{-2} \right)/2 \right] \]  

(11)

where \( \beta = \gamma = 0 \) and \( \kappa = \kappa_0 \) for the ground state, and \( \beta \neq 0, \gamma \neq 0 \) and \( \kappa = \kappa_1 \) for the first excited state. Substituting Eq. (11) into Eq. (4), we have

\[
\frac{d^2 R_\ell(r)}{dr^2} = \{r^4 a \beta + r^2[\alpha a - \beta E] + [-\alpha E + \beta \ell(\ell + 1) + \gamma a] \\
+ r^{-2}[\alpha \ell(\ell + 1) + \beta b - \gamma E] + r^{-4}[\alpha b + \beta c + \gamma \ell(\ell + 1)] \\
+ r^{-6}[\alpha c + \gamma b] + r^{-8}\gamma c\} r^\kappa \exp\left[ -\left( \sqrt{a}r^2 + \sqrt{c}r^{-2} \right)/2 \right].
\]  

(12a)

On the other hand, the derivative of the radial function can be calculated directly from Eq. (11),

\[
\frac{d^2 R_\ell(r)}{dr^2} = \{r^4 a \beta + r^2[\alpha a - \beta \sqrt{a}(2\kappa + 5)] \\
+ [-\alpha \sqrt{a}(2\kappa + 1) + \beta(2 + 3\kappa + \kappa^2 - 2\sqrt{ac}) + \gamma a] \\
+ r^{-2}[\alpha(\kappa^2 - \kappa - 2\sqrt{ac}) + \beta \sqrt{c}(2\kappa + 1) - \gamma \sqrt{a}(2\kappa - 3)] \\
+ r^{-4}[\alpha \sqrt{c}(2\kappa - 3) + \beta c + \gamma(6 - 5\kappa - 2\sqrt{ac} + \kappa^2)] \\
+ r^{-6}[\alpha c + \gamma \sqrt{c}(2\kappa - 7) + r^{-8}\gamma c] r^\kappa \exp\left[ -\left( \sqrt{a}r^2 + \sqrt{c}r^{-2} \right)/2 \right].
\]  

(12b)

Comparing the coefficients in the same power of \( r \), we obtain

\[
\beta[E - \sqrt{a}(2\kappa + 5)] = 0, \quad \text{(13a)}
\]

\[
\alpha[E - \sqrt{a}(2\kappa + 1)] = \beta[\ell(\ell + 1) + 2\sqrt{ac} - \kappa^2 - 3\kappa - 2], \quad \text{(13b)}
\]
\[\alpha[\ell(\ell + 1) + 2\sqrt{ac} - \kappa^2 + \kappa] = \beta[-b + \sqrt{c}(2\kappa + 1)] + \gamma[E - \sqrt{a}(2\kappa - 3)], \tag{13c}\]
\[\alpha[b - \sqrt{c}(2\kappa - 3)] = -\gamma[\ell(\ell + 1) + 2\sqrt{ac} - \kappa^2 + 5\kappa - 6], \tag{13d}\]
\[\gamma[b - \sqrt{c}(2\kappa - 7)] = 0. \tag{13e}\]

For the ground state, \(\beta = \gamma = 0\) and \(\alpha \neq 0\), we obtain a constraint (8) and
\[\kappa_0 = (3\sqrt{c} + b)/(2\sqrt{c}), \quad E_0 = \sqrt{a/c} (b + 4\sqrt{c}). \tag{14}\]

For the first excited state, \(\beta \neq 0\) and \(\gamma \neq 0\). From Eqs. (13a) and (13e) we have
\[\kappa_1 = (7\sqrt{c} + b)/(2\sqrt{c}), \quad E_1 = \sqrt{a/c} (b + 12\sqrt{c}). \tag{15}\]

It is easy to see from Eqs. (8) and (15) that the right hand side of Eq. (13d) becomes zero, namely, \(\alpha = 0\). Since Kaushal and Parashar [7] assumed \(\alpha \neq 0\), they must obtain the infinite \(\gamma\) if the parameters in the potential satisfy two constraints (8) and (9).

Now, we obtain from Eq. (13)
\[\alpha = 0, \quad \gamma = -\sqrt{c/a} \beta, \tag{16}\]
and another constraint
\[b = -6\sqrt{c}. \tag{17}\]

It is easy to check that the constraints (8) and (17) coincide with the constraints (8) and (9).

Setting \(\ell = 0\) and \(a = 1.0\) for comparison with Znojil [4] and Kaushal-Parashar [7], we obtain
\[b = -11.25, \quad \sqrt{c} = 1.875, \quad \gamma = -1.875\beta, \quad \kappa_0 = -1.5, \quad \kappa_1 = 0.5, \quad E_0 = -2, \quad E_1 = 6. \tag{18}\]

Thus, the radial functions \(R_0^{(0)}(r)\) for the ground state and \(R_0^{(1)}(r)\) for the first excited state are
\[R_0^{(0)}(r) = N_0 r^{-1.5} \exp\{-r^2 + 1.875r^{-2}/2\}, \tag{19}\]
\[R_0^{(1)}(r) = N_1 r^{-0.5}(r^2 - 1.875r^{-2}) \exp\{-r^2 + 1.875r^{-2}/2\}, \]
where the normalized factors are calculated by the normalized condition:

$$\int_0^\infty |R_i^i(r)|^2 dr = 1, \quad i = 0 \text{ and } 1. \quad (20)$$

Without loss of any main property, we show the unnormalized radial functions in Fig. 1 and Fig. 2.

Furthermore, if the angular momentum $\ell'$ for the first excited state is different from the angular momentum $\ell$ for the ground state, equation (16) and the constraint (17) become

$$\begin{align*}
\beta &= 4\alpha \sqrt{a}/[\ell'(\ell' + 1) - \ell(\ell + 1) - 4(b + 6\sqrt{c})/\sqrt{c}], \\
\gamma &= 4\alpha \sqrt{c}/[\ell'(\ell' + 1) - \ell(\ell + 1)], \\
[\ell'(\ell' + 1) - \ell(\ell + 1) - 2(b + \sqrt{c})/\sqrt{c}] / (32\sqrt{ac}) \\
&= [\ell'(\ell' + 1) - \ell(\ell + 1) - 4(b + 6\sqrt{c})/\sqrt{c}]^{-1} + [\ell'(\ell' + 1) - \ell(\ell + 1)]^{-1}. \\
\end{align*} \quad (21)$$

Setting $a = 1.0$, $\ell = 0$ and $\ell' = 1$, we obtain

$$\begin{align*}
b &= -4.2011, \quad c = 0.75878, \quad \kappa_0 = -0.91144, \quad \kappa_1 = 1.08856, \\
\beta &= -1.47683 \, \alpha, \quad \gamma = 1.74216 \, \alpha, \quad E_0 = -0.82288, \quad E_1 = 7.17713. \quad (22)
\end{align*}$$

3. Solutions in two dimensions

For the Schrödinger equation in two dimensions with the potential,

$$V(\rho) = a\rho^2 + b\rho^{-4} + c\rho^{-6}, \quad a > 0, \quad c > 0, \quad (23)$$

let

$$\psi(\rho, \varphi) = \rho^{-1/2} R_m(\rho) e^{\pm im\varphi}, \quad m = 0, 1, 2, \cdots, \quad (24)$$

where the radial function $R_m(\rho)$ satisfies the radial equation

$$\frac{d^2 R_m(\rho)}{d \rho^2} + \left[ E - V(r) - \frac{m^2 - 1/4}{r^2} \right] R_m(\rho) = 0. \quad (25)$$

Making the ansatz for the radial functions of the ground state and the first excited state:

$$\begin{align*}
R_m^{(0)}(\rho) &= N_0 \rho^{\kappa_0} \exp[-(\sqrt{a}\rho^2 + \sqrt{c}\rho^{-2})/2], \\
R_m^{(1)}(\rho) &= N_1 \rho^{\kappa_1} (\alpha + \rho^2 + \gamma \rho^{-2}) \exp[-(\sqrt{a}\rho^2 + \sqrt{c}\rho^{-2})/2]. \\
\end{align*} \quad (26)$$
where $\gamma \neq 0$, and substituting Eq. (26) into Eq. (25), we have

$$\beta [E - \sqrt{a}(2\kappa + 5)] = 0,$$

$$\alpha [E - \sqrt{a}(2\kappa + 1)] = \beta [m^2 - 1/4 + 2\sqrt{ac} - \kappa^2 - 3\kappa - 2],$$

$$\alpha [m^2 - 1/4 + 2\sqrt{ac} - \kappa^2 + \kappa] = \beta [-b + \sqrt{c}(2\kappa + 1)] + \gamma [E - \sqrt{a}(2\kappa - 3)],$$

$$\alpha [b - \sqrt{c}(2\kappa - 3)] = -\gamma [m^2 - 1/4 + 2\sqrt{ac} - \kappa^2 + 5\kappa - 6],$$

$$\gamma [b - \sqrt{c}(2\kappa - 7)] = 0.$$

Hence, if the angular momentum $m$ of the ground state is the same as that of the first excited state, we obtain from Eq. (27)

$$\frac{2\sqrt{c} + b}{2} = 4c [m^2 + 2\sqrt{ac}], \quad b = -6\sqrt{c},$$

$$\kappa_0 = \frac{3\sqrt{c} + b}{2\sqrt{c}}, \quad E_0 = \sqrt{a/c} \left( b + 4\sqrt{c} \right),$$

$$\kappa_1 = \frac{7\sqrt{c} + b}{2\sqrt{c}}, \quad E_1 = \sqrt{a/c} \left( b + 12\sqrt{c} \right),$$

$$\alpha = 0, \quad \gamma = -\sqrt{c}.$$  

(28)

If $m = 0$ and $a = 1.0$, the values of the corresponding parameters are

$$b = -12, \quad c = 4, \quad \gamma = -2,$$

$$\kappa_0 = -1.5, \quad \kappa_1 = 0.5, \quad E_0 = -2, \quad E_1 = 6.$$  

(29)

The unnormalized radial functions are shown in Fig. 3 and Fig. 4.

To summarize, we discuss the ground state and the first excited state for the Schrödinger equation with the potential $V(r) = ar^2 + br^{-4} + cr^{-6}$ using a simple ansatz for the eigenfunctions. Two constraints on the parameters in the potential are arrived at from the compared equations. This simple and intuitive method can be generalized to the other potentials, such as the sextic potential, the octic potential, and the inverse potential.

**Acknowledgments.** This work was supported by the National Natural Science Foundation of China and Grant No. LWTZ-1298 from the Chinese Academy of Sciences.
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