WAVE FUNCTIONS AND ENERGY TERMS OF
THE SCHRÖDINGER EQUATION
WITH TWO-CENTER COULOMB PLUS
HARMONIC OSCILLATOR POTENTIAL

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Abstract

Schrödinger equation for two center Coulomb plus harmonic oscillator potential is solved by the method of ethalon equation at large intercenter separations. Asymptotical expansions for energy term and wave function are obtained in the analytical form.

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The Schrödinger equation with two-center potentials is of considerable interest in various problems related with few body systems treating in Born-Oppenheimer approximation. It describes the bound states of light particle in the field of two heavy particles. Usually such type of systems arise in molecular physics. However last years there is a considerable interest to another systems modelling by two-center Schrödinger equations, namely baryons containing two heavy quarks (QQq- baryons) and heavy flavoured hybryd mesons (QQg-mesons) are becoming subject of extensive investigation now. The motion of light quark (gluon) in the field of two heavy quarks (quark-antiquark pair) can be described in the nonrelativistic approach by the Schrödinger equation with two-center Coulomb plus confinement potential. In this paper we concerned with the Schrödinger equation with two-center Coulomb plus harmonic oscillator potential which
is, to our knowledge, the only Coulomb plus confinement potential allowing separation of variables in the Schrödinger equation. Using the method of ethalon equation, widely applying for the solution of two-center Coulomb Schrödinger equation in molecular physics, we obtain wave functions and eigenvalues of the Schrödinger equation with two-center Coulomb plus harmonic oscillator potential in the form of asymptotical expansion in terms of inverse powers of the intercenter distance.

So we want to find energy eigenvalues and wave functions of the following Schrödinger equation

\[
\left[ -\frac{1}{2}\Delta - \frac{Z}{r_1} - \frac{Z}{r_2} + \omega^2(r_1^2 + r_2^2) \right] \psi = E \psi \tag{1}
\]

In the prolate spheroidal coordinates, which are defined as follows:

\[
\xi = \frac{r_1 + r_2}{R} \quad (1 < \xi < \infty), \quad \eta = \frac{r_1 - r_2}{R} \quad (-1 < \eta < 1)
\]

this potential can be written in the form

\[
V(r_1, r_2) = -\frac{2}{R^2} \frac{a(\xi) + b(\eta)}{\xi^2 - \eta^2} + \frac{\omega^2 R^2}{2} \tag{2}
\]

where

\[
a(\xi) = 2ZR - \frac{\omega^2 R^4}{4} \xi^2(\xi^2 - 1), \quad b(\eta) = 2ZR - \frac{\omega^2 R^4}{4} \eta^2(\eta^2 - 1)
\]

As is well known [1], the Schrödinger equation with potential in the form (2) is separable in the prolate spheroidal coordinates. After separation we have three ordinary differential equations connected by separation constants \(\lambda\) and \(m\):

\[
\left[ \frac{\partial}{\partial \xi}(\xi^2 - 1)\frac{\partial}{\partial \xi} + a\xi + (p^2 - \gamma'\xi^2)(\xi^2 - 1) - \frac{m^2}{(\xi^2 - 1)} - \lambda \right] X(\xi) = 0
\]

\[
\left[ \frac{\partial}{\partial \eta}(\eta^2 - 1)\frac{\partial}{\partial \eta} + (p^2 - \gamma'\eta^2)(\eta^2 - 1) - \frac{m^2}{(\eta^2 - 1)} - \lambda \right] Y(\eta) = 0
\]

\[
(\frac{\partial^2}{\partial \phi^2} + m^2) Z(\phi)
\]

where

\[
p = \frac{R}{2}\sqrt{2E'}
\]
\[ E' = E - \frac{\omega^2 R^2}{2}, \quad \gamma' = \frac{\omega^2 R^4}{4}, \quad a = 2ZR. \]

Boundary conditions for \( U \) and \( V \) are

\[ U(\xi) \mid_{\xi=1} = 0, \quad U(\xi) \mid_{\xi \to \infty} \to 0, \quad (3) \]

\[ V(\eta) \mid_{\eta=\pm 1} = 0. \quad (4) \]

After substitutions

\[ U(\xi) = \frac{1}{\sqrt{\xi^2 - 1}} X(\xi), \]

\[ V(\eta) = \frac{1}{\sqrt{1 - \eta^2}} Y(\eta), \]

these equs. can be reduced to the following canonical form:

\[ U''(\xi) + \left[ \frac{h^2}{4} + \frac{h(\alpha \xi - \lambda)}{\xi^2 - 1} - h^4 \gamma \xi^2 + \frac{1 - m^2}{(\xi^2 - 1)^2} \right] U(\xi) = 0 \quad (5) \]

\[ V''(\eta) + \left[ \frac{h^2}{4} + \frac{h\lambda}{1 - \eta^2} - h^4 \gamma \eta^2 + \frac{1 - m^2}{(1 - \eta^2)^2} \right] V(\eta) = 0 \quad (6) \]

where \( \alpha = 2Z/\sqrt{2E'} \), \( \gamma = \omega^2/8E'^2 \),

\[ h = 2p \quad (7) \]

1 Asymptotics of quasi-angular equation.

We will solve eqs.\((3)\) and\((6)\) for large \( R \) approximately by the method of ethalon equation. This method is sucessfully applied to the solution of nonrelativistic two center Coulomb problem \([1, 2, 4]\) and in the theory of diffracion of waves. Details of the method of ethalon equation are given in \([1, 2, 3, 4]\). Let’s start from the angular eq.\((6)\). As an ethalon equation for eq.\((6)\) we choose the Whittaker equation \([7]\):

\[ W'' + \left[ -\frac{h^4}{4} + \frac{h^2 k}{z} + \frac{1 - m^2}{4z^2} \right] W \quad (8) \]

and seek solution in the form

\[ V = [z'(\eta)]^{-\frac{1}{2}} M_{\frac{3}{2}, \frac{m}{2}}(h^2 z), \quad (9) \]
where $M_k \varphi_k (h^2 z)$ is the solution (regular at zero) of eq. (8). After substitution (3) into (5) we get following equation for $z$:

$$
\frac{z'^2}{4} - \gamma (x - 1)^2 - \frac{1}{h^2} \left( \frac{1}{4} + \frac{k z'^2}{z} - \frac{\lambda}{2x(1 - x/2)} \right) + \frac{\tau}{h^2} \left( \frac{1}{x^2(1 - x^2)} - \frac{z'^2}{z^2} \right) - \frac{1}{2h^2} [z, x] = 0
$$

(10)

where $\tau = \frac{1 - m^2}{4}$, $x = 1 + \eta$. Requirement coincidence of transition points

$$z(x) \big|_{x=0} = 0$$

leads to the following "quantum condition"

$$\lambda = 2kz'(0) + \frac{2\tau}{h^2} \left( \frac{z''(0)}{z'(0)} - 1 \right)
$$

(11)

We will seek the solution of eq. (10) and eigenvalues $\lambda$ in the form of following asymptotical expansion:

$$z = \sum_{k=0}^{\infty} \frac{z_k}{h^k}, \quad \lambda = \sum_{k=0}^{\infty} \frac{\lambda_k}{h^k}
$$

Substitution these expansions into (10) gives us the recurrence system of differential equations for $z$:

$$
\begin{align*}
z_0' &= 2\gamma^\frac{1}{2}(x - 1) \\
z_1' &= 0 \\
z_2' &= \frac{1}{2z_0'} + \frac{2kz_0'}{z_0} - \frac{(z_1')^2}{2z_0'} - \frac{2\lambda_0}{z_0x(1 - x/2)} - \frac{z_2'}{2}
\end{align*}
$$

and for $\lambda$:

$$
\begin{align*}
\lambda_0 &= 2kz_0'(0) \\
\lambda_1 &= 2kz_1'(0) \\
\lambda_2 &= 2kz_2'(0) + 2\tau \left( \frac{z_0''(0)}{z_1'(0)} - 1 \right)
\end{align*}
$$

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Solving these recurrence equations we have for $\lambda$:

$$\lambda^{(n)} = 4k\gamma^\frac{1}{2} + \frac{2k\beta - 4\tau}{h^2} + O\left(\frac{1}{h^4}\right)$$ \hspace{1cm} (12)

and for $z$:

$$z = \gamma^\frac{1}{2}x(2 - x) + \frac{1}{h^2}\beta\ln(1 - x) + O\left(\frac{1}{h^4}\right)$$ \hspace{1cm} (13)

From boundary conditions one can obtain for quantum number $k$ [3, 4]:

$$k = q + \frac{m + 1}{2},$$

where $q = 0, 1, 2, \ldots$.

## 2 Asymptotics of quasi-radial equation

For equation (5) as an ethalon equation we take equation:

$$W'' + \left[h^2s - h^4y^2 - \frac{4\tau + 3}{4y^2}\right]W = 0$$ \hspace{1cm} (14)

solution of which expressed by the confluent hypergeometric functions[?, ?]

$$W = ye^{-\frac{h^4y^2}{2}}F\left(\frac{s - 2c - 1}{4}, c + \frac{1}{2}, h^4y^2\right)$$

where $c = \frac{1 + \sqrt{m^2 + 3}}{2}$.

Boundary condition (3) and properties of functions $F$ [7, 8] give rise to the following expression for $s$:

$$s = 4n + \sqrt{m^2 + 3} + 2.$$

Substituting

$$U = [y(\xi)]^{-\frac{1}{2}}W(y(\xi))$$

into eq.(3) we have

$$\frac{y^2y'^2}{4} - \gamma\xi^2 + \frac{1}{h^2}\left(\frac{1}{4} - sy^2 - \frac{\lambda}{\xi^2 - 1}\right) + \frac{1}{h^3}\frac{\alpha\xi}{\xi^2 - 1} +$$

$$\frac{4\tau}{h^4(\xi^2 - 1)^2} - \frac{3 - 4\tau y'^2}{4h^4 y^2} - \frac{1}{2h^4}[y, \xi] = 0.$$ \hspace{1cm} (15)
After substitution

\[ \phi = \frac{y^2(t)}{4} \]

this eq. can be reduced to the form

\[
\phi'' - \gamma(t + 1) + \frac{1}{h^2} \left( \frac{1}{4} - \left( n + \frac{1}{2} \right) \frac{\phi'^2}{\phi} - \frac{\lambda}{t(t + 2)} \right) + \frac{1}{h^3} \frac{\alpha(t + 1)}{t(t + 2)} + \frac{\tau}{h^4} \left( \frac{\phi'^2}{\phi^2} - \frac{4}{t^2(t + 2)^2} \right) - [\phi, t] = 0. \tag{16}
\]

where \( t = \xi - 1 \) Quantization condition which follows from \( \phi(x) = 0 \) is written in the form

\[
\lambda = -2s\phi'(0) + \frac{\alpha}{h} - \frac{1}{h^2} \left[ \frac{\phi''}{\phi'} + 1 \right] \bigg|_{t=0} \tag{17}
\]

Inserting into eq.(16) asymptotical expansions

\[
\phi = \sum_{k=0}^{\infty} \frac{\phi_k}{h^k}, \quad \lambda = \sum_{k=0}^{\infty} \frac{\lambda_k}{h^k}
\]

and solving obtained equations we have for \( y \):

\[
y = 2\gamma^\frac{1}{2}(t^2 + 2t)^\frac{1}{2} + \frac{1}{h^2} \delta \gamma^{-\frac{1}{2}}(t^2 + 2t)^{-\frac{1}{2}} \ln(t + 1) + \frac{1}{h^3} \alpha \gamma^{-\frac{3}{4}}(t^2 + 2t)^{-\frac{1}{4}} \ln \frac{2(t + 1)}{t + 1} + O(\frac{1}{h^4}) \tag{18}
\]

and for \( \lambda \)

\[
\lambda(\xi) = -2s\gamma^\frac{1}{2} - \frac{\alpha}{h} + \frac{4\tau - s\delta}{h^2} - \frac{s\alpha \gamma^{-\frac{3}{4}}}{2h^3} + O(\frac{1}{h^4}) \tag{19}
\]

3 Asymptotical expansion for energy and wave functions.

Asymptotical expansions (12) and (19) give us expression for energy in the form of multipole expansion. In order to obtain this expansion one should insert

\[ E' = E_0 + \frac{E_1}{R} + \frac{E_2}{R^2} + \ldots \]

into (12) and (19). Equating \( \lambda^\eta \) and \( \lambda^\xi \) and taking into account (7) we get following equations for coefficients \( E_1, E_2, \ldots \):
\[ E_1 = \frac{1}{6Z}[(s\omega - 2k\omega^{-1})(2E_0)^{\frac{3}{2}} + (4s^2 - 16k^2 - 16\tau)(2E_0)^{\frac{1}{2}}], \]
\[ E_2 = \frac{5}{2}E_1^2 + 2s\omega^{-1}E_0 + E_1(2E_0)^{\frac{1}{2}}Z^{-1}(16\tau^2 + 16k^2 - 4s^2), \]

\[ \cdots \cdots \cdot \]

Now we need to find \( E_0 \). In order to find this one we note that for \( R \to \infty \) \( E' = E_0 \) or
\[ E = E_0 + \frac{\omega^2 R^2}{2}. \]  \hspace{1cm} (20)

On the other hand for large \( R \)
\[ V(r_1, r_2) = \frac{2Z}{R} \sum_{l=0}^{\infty} \left( \frac{r}{R} \right)^l p_l(\cos\theta) + \omega^2 [r^2 + 2rR\cos\theta + \frac{R^2}{4}] + (r^2 - 2rR\cos\theta + \frac{R^2}{4}) \approx \omega^2 (2r^2 + \frac{R^2}{2}). \]  \hspace{1cm} (21)

Hence for the energy term with this potential we have
\[ E = 2\omega(N + \frac{3}{2}) + \frac{\omega^2 R^2}{2}, \]  \hspace{1cm} (22)

where \( N = 2n + q + m \) is the principal quantum number. Comparing (20) and (22) we have
\[ E_0 = 2\omega(N + \frac{3}{2}). \]

Thus we have obtained an asymptotical expansion for wave functions and energy eigenvalues of the Schrödinger equation with two-center Coulomb plus harmonic oscillator potential. Derived formulas have to be useful for farther numerical calculations in nonasymptotical region and can be also used for estimation QQq baryon energy spectra.

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