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КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

SYMBOLIC COMPUTATIONS FOR THE TWO COULOMB CENTRES PROBLEM IN THE SPACE OF ARBITRARY DIMENSION

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The case of small intercentre distances in the D-dimensional two Coulomb centres problem $(Z_1eZ_2)_D$ $(D \geqslant 2)$ is studied by solving separated wave equations. The usage of Maple symbolic computation system (Maple Waterloo Software, Inc., see http://www.maplesoft.com) for solving the problem is under discussion. The obtained results are compared with the previous asymptotic and numerical treatments. The correspondence between energy terms of the systems $(Z_1eZ_2)_3$ and $(Z_1eZ_2)_D$ is found.

Случай малых расстояний между центрами в D-мерной задаче двух кулоновских центров $(Z_1eZ_2)_D$ $(D \geqslant 2)$ исследуется путем решения разделенных волновых уравнений. Обсуждается использование программы символьных вычислений Maple. Полученные результаты сравниваются с предыдущими асимптотическими и численными расчетами. Обнаружено соответствие энергетических членов систем $(Z_1eZ_2)_3$ и $(Z_1eZ_2)_D$.

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INTRODUCTION

This work is devoted to the generalization of results of the asymptotic theory for the quantum mechanics two Coulomb centres problem Z_1eZ_2 [1] by inflating the number of spacial dimension (briefly $(Z_1eZ_2)_D$ problem). Separating the problem in hyperspheroidal coordinates [2] leads to two coupled confluent Heun equations [3], the singularities of which are located at ± 1 and at infinity. To calculate the energy levels of the two Coulomb centres system is a two-parameter boundary-eigenvalue problem. We solve this problem in the case of small intercentre separations by means of asymptotic methods that have been proposed in [1] and developed in [3]. The two-dimensional two centres problem $(Z_1eZ_2)_2$ at small intercentre separations was studied in work [4].

The solution of the Schrödinger equation with two-centre potential is of considerable interest in various problems of few-body systems. They describe the bound states of light particles in the field of two heavy particles. Usually such a type of systems arises in molecular physics. However, during the last years interest has been shown in other systems modelled by the two-centre Schrödinger equation; namely, baryons containing heavy quarks (QQq baryons) [5] and heavy flavoured hybrid mesons (QQg mesons) are now becoming the subject of extensive investigation. There is a close connection between the $(Z_1eZ_2)_D$ problem and $SU(2)$ monopole [6]. The five-dimensional bound system of «charge-dion» with $SU(2)$ Yang monopole is described by equations which we obtain at the separation of variables of (1) (see below) in hyperspheroidal coordinates. Besides, equation (1) is connected with the well-known Teukolsky equation [7].

1. FORMULATION OF THE PROBLEM

The Schrödinger equation for the $(Z_1eZ_2)_D$ problem in atomic units ($m = e = \hbar = 1$) reads

$$\left(-\frac{1}{2}\Delta - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}\right)\Psi(\mathbf{r}; R) = E\Psi(\mathbf{r}; R), \tag{1}$$

where r_1 and r_2 are distances from the electron to charges Z_1 and Z_2; R is the intercentre distance. Here the vectors $\mathbf{r}$, $\mathbf{r}_1$, $\mathbf{r}_2$ belong to the D-dimensional vector space $\mathbb{R}^D$ and $\Delta = \sum\limits_{i=1}^{D} \dfrac{\partial^2}{\partial x_i^2}$. We only consider bound states with $E < 0$.

In the case of $D \geqslant 3$ the variables in equation (1) are separated in a hyperspheroidal coordinate system [2]. And we come to necessity of solving the following boundary problems:

$$\left[\frac{1}{(\xi^2-1)^{\frac{D-3}{2}}}\frac{d}{d\xi}(\xi^2-1)^{\frac{D-1}{2}}\frac{d}{d\xi} - \lambda^{(\xi)} - p^2(\xi^2-1) + \right.$$
$$\left. + 2p\alpha\xi - \frac{m(m+D-3)}{\xi^2-1}\right]\Pi^{(D)}(\xi) = 0, \tag{2}$$

$$|\Pi^{(D)}(1)| < \infty, \qquad |\Pi^{(D)}(\xi)| \stackrel{\xi\to\infty}{\longrightarrow} 0, \tag{3}$$

$$\left[\frac{1}{(1-\eta^2)^{\frac{D-3}{2}}}\frac{d}{d\eta}(1-\eta^2)^{\frac{D-1}{2}}\frac{d}{d\eta} + \lambda^{(\eta)} - p^2(1-\eta^2) + \right.$$
$$\left. + 2p\beta\eta - \frac{m(m+D-3)}{1-\eta^2}\right]\Xi^{(D)}(\eta) = 0, \tag{4}$$

$$|\Xi^{(D)}(\pm 1)| < \infty, \tag{5}$$

where

$$p = (R/2)(-2E)^{1/2}, \quad \alpha = (Z_2 + Z_1)(-2E)^{-1/2}, \quad \beta = (Z_2 - Z_1)(-2E)^{-1/2},$$

$\lambda^{(\xi)}$ and $\lambda^{(\eta)}$ are eigenvalues and m is an azimuthal quantum number ($m = 0, 1, 2, \ldots$).

Both equations (2) and (4) are singly confluent Heun equations [3]. It is convenient to consider boundary problems with functions $\Pi^{(D)}(\xi)$ and $\Xi^{(D)}(\eta)$ that satisfy boundedness conditions at the ends of the corresponding intervals. The eigenfunctions of the problems

(2), (3) and (4), (5) are respectively called the radial and angular Coulomb hyperspheroidal functions (RCHFs and ACHFs).

In the case of $D = 2$ the variables are separated in an elliptic coordinate system [4] and we obtain the two following boundary-eigenvalue problems:

$$\left[\frac{d^2}{du^2} + 2p\alpha\cosh u - p^2\left(\cosh^2 u - 1\right) - \lambda^{(u)}\right]\Pi^{(2)}(u) = 0, \tag{6}$$

$$\Pi^{(2)}(u + 2\pi i) = \Pi^{(2)}(u), \qquad |\Pi^{(2)}(0)| < \infty, \qquad |\Pi^{(2)}(u)| \overset{u\to\infty}{\longrightarrow} 0, \tag{7}$$

$$\left[\frac{d^2}{dv^2} + 2p\beta\cos v - p^2\left(1 - \cos^2 v\right) + \lambda^{(v)}\right]\Xi^{(2)}(v) = 0, \tag{8}$$

$$\Xi^{(2)}(v + 2\pi) = \Xi^{(2)}(v). \tag{9}$$

Here $\lambda^{(u)}$ and $\lambda^{(v)}$ are eigenvalues. Equations (6) and (8) belong to the class of ODEs with periodic coefficients. The equations can be transformed to the Ince equation [8] by means of changing the dependent and independent variables. The eigenfunctions of the problems (6), (7) and (8), (9) are respectively called the radial and angular Coulomb elliptic functions (RCEFs and ACEFs).

In spite of the fact that equations (6) and (8) have forms that are radically different from the forms of equations (2) and (4), the former ones can be solved by methods slightly different from the methods which are used in this paper for solving equations (2) and (4). As far as equations (6) and (8) are concerned, they are investigated in papers [4] in detail and we do not include this matter in the current letter.

2. CONSTRUCTING ACHFs

It is useful for further deductions to introduce the B-function by the following formula:

$$\mathbf{B}_n^{(D),\,m}(z) = \frac{\Gamma(n+m+D-2)}{\Gamma(n-m+1)}(z^2-1)^{\frac{3-D}{4}} P_{n+\frac{D-3}{2}}^{-m-\frac{D-3}{2}}(z), \tag{10}$$

where n and z are unrestricted, $P_n^m(z)$ are Legendre functions [9]. We will restrict ourselves to $D = 3, 4, 5, \ldots$ and $m = 0, 1, 2, \ldots$ in further deductions. In addition, we also introduce the modified B-function

$$\mathbb{B}_n^{(D),\,m}(x) = \frac{\Gamma(n+m+D-2)}{\Gamma(n-m+1)}(1-x^2)^{\frac{3-D}{4}} \mathbb{P}_{n+\frac{D-3}{2}}^{-m-\frac{D-3}{2}}(x), \tag{11}$$

where $-1 \leqslant x \leqslant 1$, $\mathbb{P}_n^m(x)$ are Legendre functions on the cut [9].

An expansion for the eigenfunction $\Xi^{(D)}(\eta)$ of the boundary problem (8), (9) can be presented in the form

$$\Xi^{(D)}(\eta) = \sum_{n=m-l}^{\infty} g_n \mathbb{B}_{l+n}^{(D),\,m}(\eta). \tag{12}$$

The coefficients g_n satisfy the system of recurrent equations

$$\begin{aligned} & p^2\Omega_n\Omega_{n+1}g_{n+2} + 2p\beta\Omega_n g_{n+1} + \\ & \quad + \Big[\lambda^{(\eta)} - (l+n)(l+n+D-2) - p^2 + p^2\left(\Omega_{n-1}\Gamma_n + \Omega_n\Gamma_{n+1}\right)\Big] g_n + \\ & \quad\quad + 2p\beta\Gamma_n g_{n-1} + p^2\Gamma_n\Gamma_{n-1}g_{n-2} = 0, \quad g_{m-l-1} = 0, \quad g_{m-l-2} = 0, \quad (13) \end{aligned}$$

$$\Omega_n = \frac{l+n+m+D-2}{2l+2n+D}, \qquad \Gamma_n = \frac{l+n-m}{2n+2l+D-4}.$$

The asymptotic procedure of getting the succeeding coefficients g_n in expansion (12) and separation constant $\lambda^{(\eta)}$ is based on the formal series

$$g_n = p^{|n|}\sum_{j=0}^{\infty}[g_n]_{2j}p^{2j}, \qquad g_0 \equiv 1, \qquad \lambda^{(\eta)} = \sum_{j=0}^{\infty}[\lambda]_{2j}p^{2j}. \qquad (14)$$

Expansions (14) are inserted into the recurrent equations (13). Then we equate coefficients of alike powers of p. On the first step of the recursive procedure, $[\lambda]_0$ is obtained. On the next step the coefficients $[g_{\pm 1}]_0$ are obtained, then $[\lambda]_2$ and so on.

Now we will consider the realization of the recurrent procedure in Maple. Firstly, we have to enter formal series (14) for the coefficient g_n:

```
> g:=proc (n) local Res; if n=0 then Res:=1 else
  Res:=p^abs(n)*sum(G(n,2*j)*p^(2*j), j=0..2); fi; Res; end proc;
```

Secondly, we enter the recurrent equation (13):

```
> Eq:=(n)-> p^2*Omega(n)*Omega(n+1)*g(n+2) + 2*p*beta*Omega(n)*g(n+1) +
  (L-(n+l)*(n+l+D-2)-p^2+p^2*(Omega(n-1)*Gamma(n)+Omega(n)*Gamma(n+1)))
  *g(n) + 2*p*beta*Gamma(n)*g(n-1) + p^2*Gamma(n)*Gamma(n-1)*g(n-2);
```

Thirdly, formal series (14) for $\lambda^{(\eta)}$ is entered:

```
> L:= L0 + L2*p^2 + L4*p^4;
```

It is useful to introduce an additional procedure which collects the terms of alike powers of p:

```
> COEF:=(N,M)->coeff( expand(Eq(N)), p, M);
```

Finally, we have all necessary procedures to realize the recurrent scheme

```
> L0:=solve(COEF(0,0)=0, L0);
> G(1,0):=solve(COEF(1,1)=0, G(1,0));
> G(-1,0):=solve(COEF(-1,1)=0, G(-1,0));
> L2:=combine(solve(COEF(0,2)=0, L2));
> G(2,0):=solve(COEF(2,2)=0,G(2,0));
> G(1,2):=solve(COEF(1,3)=0,G(1,2));
> G(-2,0):=solve(COEF(-2,2)=0, G(-2,0));
> G(-1,2):=solve(COEF(-1,3)=0, G(-1,2));
> L4 := solve(COEF(0,4)=0, L4);
```

3. CONSTRUCTING RCHFs

The expansion of the solution $\Pi_<^{(D)}(\xi)$ of equation (2), which is finite at $\xi = 1$, has the following form:

$$\Pi_<^{(D)}(\xi) = \mathrm{e}^{-p\xi} \sum_{n=-\infty}^{\infty} d_n(\nu) \mathbf{B}_{\nu+n}^{(D),\, m}(\xi), \quad d_0(\nu) \equiv 1, \quad d_n(\nu) = p^{|n|} \sum_{j=0}^{\infty} [d_n(\nu)]_{2j} p^{2j}. \tag{15}$$

The coefficients $d_n(\nu)$ satisfy three-term recurrent equations which can be easily obtained by substituting series (15) into equation (2). The coefficients $d_n(\nu)$ can be calculated by means of the recurrent procedure which was described in Sec. 2.

According to a symmetry property we have to construct the function $\Pi_>^{(D)}(\xi)$ that is the continuation of the function $\Pi_<^{(D)}(\xi)$ to large ξ in the form

$$\begin{gathered}
\Pi_>^{(D)}(\xi) = g(\nu) y_\nu^{(1)}(\xi) + (-1)^{D-3} g(-\nu - D + 2) y_{-\nu-D+2}^{(1)}(\xi), \\
y_\nu^{(1)}(\xi) = \frac{(\xi - 1)^{\frac{m}{2}}}{(\xi + 1)^{\frac{m+D-3}{2}}} \sum_{n=-\infty}^{\infty} h_n(\nu) R_{\nu + \frac{D-3}{2} + n}\Big(p(\xi + 1)\Big), \\
h_n(\nu) = p^{|n|} \sum_{j=0}^{\infty} [h_n(\nu)]_{2j} p^{2j}, \\
h_0(\nu) \equiv 1, \quad R_\tau(x) = x^\tau \, \mathrm{e}^{-x} {}_1F_1\Big(-\alpha + \tau + 1; 2\tau + 2; 2x\Big).
\end{gathered} \tag{16}$$

Here $g(\nu)$ and $g(-\nu - D + 2)$ are matching constants, ${}_1F_1(a; c; x)$ is the regular in the origin solution of confluent hypergeometric equation [9].

In order to match solutions (15) and (16) we have to present function (15) as a linear combination of further solutions of equation (2)

$$\Pi_<^{(D)}(\xi) = y_\nu^{(2)}(\xi) + (-1)^{D-3} y_{-\nu-D+2}^{(2)}(\xi). \tag{17}$$

The form of $y_\nu^{(2)}(\xi)$ is rather cumbersome and we do not present it here. It is important that the function $y_\nu^{(2)}(\xi)$ is a series of the hypergeometric function ${}_2F_1(a, b; c; x)$ [9].

According to some transformation property of the functions $y_\nu^{(1)}(\xi)$ and $y_\nu^{(2)}(\xi)$, the condition of matching solutions (15) and (16) has the following form:

$$y_\nu^{(2)}(\xi) = g(\nu) y_\nu^{(1)}(\xi).$$

The matching constant $g(\nu)$ can be obtained by expanding a hypergeometric series representation $y_\nu^{(2)}(\xi)$ and the confluent hypergeometric representation for $y_\nu^{(1)}(\xi)$ and comparing alike terms.

When α and ν have arbitrary values, the solution $\Pi_>^{(D)}(\xi)$ in the limit $\xi \to \infty$ has the form of a linear combination of the two exponents, one decreasing and the other increasing. Declaring the coefficient in front of the increasing exponent to be zero, we get the dispersive equation that connects the values of the parameters α, ν and p

$$\tan(\pi\alpha) = \tan \pi \left(\nu + \frac{D-3}{2} \right) \frac{1 - \varepsilon}{1 + \varepsilon}, \qquad \varepsilon = O\left(p^{2\nu + D - 2}\right). \tag{18}$$

CONCLUSIONS

We can calculate the energy of the system $(Z_1eZ_2)_D$ from the dispersive equation (18). The first step in deriving asymptotic expansions for the energy is to obtain the expansion of the parameter ν in powers of p. The asymptotic expansion for ν can be derived by equating $\lambda^{(\eta)}$ and $\lambda^{(\xi)}$. Inserting the expression for ν into the dispersion equation (18) and solving this equation by successive approximations, we obtain the asymptotic expressions for the energy terms of the system $(Z_1eZ_2)_D$.

We have checked our approximate results with numerical solutions. The comparison of our results for the values ν (in the case of $D = 3$) with those of the previous asymptotic and numerical treatments [10] shows that, as should be expected, evaluation of additional terms in the asymptotic expansions for ν improves agreement between asymptotic and numerical results. We have compared high energy levels of the two-dimensional (2D) H_2^+ with high energy levels of the three-dimensional (3D) H_2^+. We have seen that high energy levels of the 2D H_2^+ approximate to the corresponding energy levels of the 3D H_2^+. This result confirms a well-known fact: the motion of an electron in the Rydberg state becomes approximately planar. The energy terms $E_{nlm}^{(D)}$ of the system $(Z_1eZ_2)_D$ are connected with the energy terms $E_{nlm}^{(3)}$ of Z_1eZ_2 by the following relation:

$$E_{nlm}^{(D)} = E_{nlm}^{(3)}\Bigg|_{\substack{n \to n + \frac{D-3}{2} \\ l \to l + \frac{D-3}{2}, \\ m \to m + \frac{D-3}{2}}} \tag{19}$$

where n, l, m are spherical quantum numbers. The $1/D$-expansion of energy for the $(Z_1eZ_2)_D$ problem was calculated in work [11] for the first time. But this expansion gives poor results in the case of small separations. We have obtained expansion for the energy which is convergent not only for the small intercentre separations but also for a large number of spatial dimension.

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