Hyperspherical Coulomb spheroidal representation in the Coulomb three-body problem

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Abstract
A new representation of the Coulomb three-body wavefunction via the well-known solutions of the separable Coulomb two-centre problem \( \phi_j(\xi, \eta) = X_j(\xi)Y_j(\eta) \) is obtained, where \( X_j(\xi) \) and \( Y_j(\eta) \) are the Coulomb spheroidal functions. Its distinguishing characteristic is the coordination with the asymptotic conditions of the scattering problem below the three-particle breakup. That is, the wavefunction of two colliding clusters in any open channel is the asymptotics of the single, corresponding to that channel, term of the suggested expansion. The effect is achieved due to a new relation between three internal coordinates of a three-body system and the parameters of \( \phi_j(\xi, \eta) \). It ensures the orthogonality of \( \phi_j(\xi, \eta) \) on a sphere of constant hyperradius, \( \rho = \text{const} \), in place of the surface \( R = |x_2 - x_1| = \text{const} \) appearing in the traditional Born–Oppenheimer approach. The independent variables \( \xi \) and \( \eta \) are the orthogonal coordinates on this sphere with three poles in the coalescence points. They are connected with the elliptic coordinates on the plane by means of a stereographic projection. For the total angular momentum \( J \geq 0 \) the products of \( \phi_j \) and the Wigner \( D \)-functions form a hyperspherical Coulomb spheroidal (HSCS) basis on a five-dimensional hypersphere, \( \rho \) being a parameter. The system of the differential equations and the boundary conditions for the radial functions \( f^J(\rho) \), the coefficients of the HSCS decomposition of the three-body wavefunction, are presented.

1. Introduction
The complete set of the solutions of a Coulomb two-centre problem has been widely used as a basis for the representation of a Coulomb three-body wavefunction for a long time ([1] and references therein). One of the most attractive features of that basis is its simplicity. First, due to the high symmetry of the Coulomb field, the Coulomb two-centre problem admits the separation of variables, and the basis elements are the completely factorized functions. Second, the cofactors composing the basis elements, the so-called Coulomb spheroidal functions (CSF), are well-investigated functions related to the Heun class. The principal results on CSF and further references are presented in [2–4].

The traditional way to use CSF for the analysis of the Coulomb three-body system with positive and negative charges \( (Z_1Z_2 > 0, Z_1Z_3 < 0) \) is an adiabatic representation [1], which is also known as the Born–Oppenheimer (BO) approach, the perturbed stationary states method, and the molecular orbitals method. In this approach, the distance \( R \) between the particles 1 and 2 is considered as an adiabatic parameter, and the basis functions are orthogonal at fixed \( R \). The numerous helpful properties of CSF allow us to construct the effective numerical algorithms for the calculation of bound states and cross sections of elastic and inelastic collisions for various Coulomb three-body systems. The method has been successfully used not only for the case of heavy particles 1, 2 and a light particle 3 [1, 5–9], but also for light particles 1, 2 (electrons) and a heavy particle 3 (nucleus) [10–13].

Nevertheless, the BO representation in the traditional form (i.e., with \( R \) as a parameter) has a well-known imperfection which decreases the efficiency of calculations of the scattering processes. The point is that the BO expansion is not coordinated with the physical asymptotic conditions of the scattering problem. It means that, at \( R \to \infty \), the
wavefunction of two colliding clusters in any open channel is formed as the sum of an infinite number of components, the selected terms of the BO series calculated at large $R$. This sum includes, in particular, the basis functions tending at large $R$ to the atomic wavefunctions of the closed channels. Thus, the terms of the BO expansion, generally speaking, are not divided into groups corresponding to open and closed channels. This peculiarity becomes apparent in the system of radial equations: the matrix elements coupling different basis states may remain nonzero at large $R$. This leads to the complication of the boundary conditions for the radial functions at $R \to \infty$ [8] and to the slow convergence of the expansion. The incoordination of the adiabatic representation with the physical asymptotic conditions of the three-body (not necessary Coulomb) scattering problem is peculiar to both the quantum approach and the semiclassical one. To overcome the difficulties in the frames of the semiclassical treatment the inclusion of ‘electron translation factors’ is used [14, 15]. The various methods in the improvement of the adiabatic representation for the scattering processes are also developed in the quantum approach ([16, 17] and references therein).

In contrast to the traditional BO representation, the adiabatic hyperspherical one [18–22] is coordinated with the asymptotic conditions of the three-body scattering problem. In this approach the hyperradius $\rho$ is used as an adiabatic parameter. The wavefunction of two colliding clusters in any open channel is the asymptotics of the single, corresponding to that channel, term of the expansion. The adiabatic hyperspherical approach is successfully applied to the calculations of the bound states, the cross sections of the elastic and inelastic collisions and the resonances in various Coulomb three-body systems [18, 20–28].

However, the adiabatic hyperspherical basis elements are, essentially, more complicated functions than the BO ones. In the general case, they are the non-factorized functions of five independent variables. In addition, for the Coulomb three-body systems the adiabatic hyperspherical terms as functions of $\rho$ have the numerous avoiding crossings which make difficulties for the numerical calculations [20, 22]. These avoiding crossings are closely connected with the exact crossings in the Coulomb two-centre problem [22]. Thus, in the adiabatic hyperspherical approach the high symmetry of the Coulomb field, instead of the simplification, paradoxically leads to additional difficulties. Efficient methods which overcome these difficulties are developed in papers [30, 31] (diabatization and truncation technique) and [32] (slow variable discretization). The avoiding crossings are removed in the original version of the hyperspherical approach developed in papers [33–37]. The basis suggested in these papers is completely factorized in the special four-pole elliptic coordinates on the hypersphere. The co-factors composing the basis elements in this approach are essentially more complicated functions as compared to CSF; they relate to the Heun class only at zero energy [36].

The goal of the present paper is to obtain the representation of the Coulomb three-body wavefunction which, on the one hand, contains only the well-known CSF and, on the other hand, is coordinated with the asymptotic conditions of the scattering problem at energies below the threshold of the three-particle breakup. In other words, our goal is to obtain the representation combining the advantages of the adiabatic hyperspherical approach (the coordination with the asymptotic conditions) and the advantages connected with the specific character of the Coulomb field (the complete factorization of the basis and the simplicity of its components, CSF). This task is interesting, firstly, for the development of efficient computing methods and, secondly, for the completeness of the theoretical description of CSF: it is desirable to present various ways to use these well-known functions in the Coulomb three-body problem.

The above goal is achieved in this paper with the help of a new relation between the parameters of CSF and the internal coordinates of the Coulomb three-body system. The suggested basis functions, just as the adiabatic hyperspherical basis functions, form the orthogonal set on the sphere $\rho = \text{const}$ in a three-dimensional space of the internal variables, in place of the surface $R = \text{const}$ appearing in the traditional BO approach.

The difference of our expansion from the traditional BO one can be outlined briefly for the simplest case of zero total angular momentum, $J = 0$, in the following way. Let $x_1$, $x_2$, and $x_3$ be the position vectors of the particles in the centre-of-mass frame:

$$m_1 x_1 + m_2 x_2 + m_3 x_3 = 0.$$  

(1)

In the case $J = 0$, the three-body wavefunction $\Psi$ depends on three independent internal variables, for example, $r_1$, $r_2$, $R$:

$$r_1 = |x_3 - x_1|, \quad r_2 = |x_3 - x_2|, \quad R = |x_2 - x_1|.$$  

(2)

In the traditional BO approach three independent variables are, in fact, $R$ and the prolate spheroidal coordinates $\xi \in [1, \infty)$ and $\eta \in [-1, 1]$ defined by the relations

$$\xi = (r_1 + r_2)/R, \quad \eta = (r_1 - r_2)/R.$$  

(3)

The variable $R$ is considered as a parameter of the basis, and the decomposition of the three-body wavefunction has the form

$$\Psi = \sum_j f_j(R) \phi_j(R|\xi, \eta),$$  

(4)

where the basis functions $\phi_j(R|\xi, \eta)$ are the factorized solutions of the Coulomb two-centre problem with the intercentre distance $R$. These solutions as the functions of $\xi$ and $\eta$ form the complete orthogonal system at fixed $R$.

In our approach, the independent variables are $\xi$, $\eta$ and the hyperradius

$$\rho = \sqrt{2(m_1 x_1^2 + m_2 x_2^2 + m_3 x_3^2)} = \sqrt{2(m_1 m_3 x_1^2 + m_2 m_3 x_2^2 + m_1 m_2 R^2)}/(m_1 + m_2 + m_3), \quad \rho \in [0, \infty).$$  

(5)

It is considered as the parameter of the basis. The decomposition of the three-body wavefunction has the form

$$\Psi = C(\rho, \xi, \eta) \sum_j f_j(\rho) \phi_j(\rho|\xi, \eta),$$  

(6)

where $C(\rho, \xi, \eta)$ is the special weight factor. Basis functions $\phi_j(\rho|\xi, \eta)$ are the factorized solutions of the Coulomb two-centre problem with the modified charges and the intercentre
distance proportional to the hyperradius \( \rho \). They form a complete orthogonal system at fixed \( \rho \), and coincide (up to a constant factor) with \( \Phi_j(\mathbf{R}|\xi, \eta) \) at large \( R \).

In the case \( J > 0 \), the suggested basis consists of the productions of CSF and the symmetrized Wigner functions. We call it ‘the hyperspherical Coulomb spheroidal (HSCS) basis’. The formulae are more complicated, but the principal idea is the same.

The principal notations and the starting equations are presented in section 2. Section 3 is devoted to the construction of the HSCS basis. In section 4 the definition of \( S \)-matrix in the appropriate representation is presented, and the asymptotical expressions for the radial functions in terms of the matrix elements of \( S \)-matrix are obtained. These formulae are deduced from the properties of the HSCS basis and the general relations defining \( S \)-matrix, without any analysis of the system of radial equations. This system and the statement of the scattering problem at energies below the three-particle breakup are presented in section 5.

2. Starting equations

We consider the system of three particles with charges \( Z_1 > 0, Z_2 > 0, Z_3 = -1 \) and masses \( m_1, m_2, m_3 \). The case of the identical particles 1 and 2 is not considered. The atomic units are used. The Jacobi coordinates \( R, r \) are expressed in terms of the position vectors of the particles \( x_1, x_2, x_3 \) (1) by the formulae

\[
R = x_2 - x_1, \quad r = x_3 - \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2},
\]

where \( M \) and \( \mu \) are the reduced masses:

\[
M = \frac{m_1 m_2}{m_1 + m_2}, \quad \mu = \frac{m_3(m_1 + m_2)}{m_1 + m_2 + m_3}.
\]

The Jacobi coordinates \( r_a, R_a \), which are suitable at large \( R \) for the clusterization \( \alpha (\alpha = 1 \) corresponds to the atom (1, 3) plus the distant particle 2; \( \alpha = 2 \) corresponds to (2, 3)+1), are defined by

\[
r_a = x_3 - x_a, \quad R_a = (-1)^{\alpha-1} \left[ x_{3-a} - \frac{m_a x_a + m_3 x_3}{m_a + m_3} \right],
\]

\[
\mu_a = \frac{m_a m_3}{m_a + m_3}, \quad M_a = \frac{m_3 - m_a (m_a + m_3)}{m_1 + m_2 + m_3}, \quad \alpha = 1, 2.
\]

The factor \((-1)^{\alpha-1}\) ensures the identical directions of \( R_a \) and \( R \) at large \( R \).

The Hamiltonian of the system in the coordinates \( R, r \) has the form

\[
H = T + V,
\]

\[
T = -\frac{1}{2M} \Delta_R - \frac{1}{2\mu} \Delta_r,
\]

\[
V = \frac{Z_1 Z_2}{R} - \frac{Z_1}{|r + RM/m_1|} - \frac{Z_2}{|r - RM/m_2|}.
\]

In the hyperspherical approach, six variables

\[
\Phi \in [0, 2\pi), \quad \Theta \in [0, \pi), \quad \varphi \in [0, 2\pi), \quad 
\rho \in [0, \infty), \quad \chi \in [0, \pi], \quad \vartheta \in [0, \pi]
\]

are generally used. Here \( \{\Phi, \Theta, 0\} \) are the Euler angles of a rotating frame with the third axis directed along \( R \). The variables \( \vartheta \) and \( \varphi \) are the spherical angles of \( r \) in the rotating frame. The hyperradius \( \rho \) and the hyperangle \( \chi \) are expressed in terms of \( R \) and \( r \) as

\[
\rho^2 = 2(MR^2 + \mu r^2), \quad \rho \in [0, \infty); \quad 

\tan \frac{\chi}{2} = (\mu/M)^{1/2}r/R, \quad \chi \in [0, \pi].
\]

The angles \( \Phi, \Theta, \varphi \) are the external coordinates defining the orientation of the triangle formed by three particles. The variables \( \rho, \chi, \vartheta \) are the internal coordinates of the system. In the hyperspherical coordinates the kinetic energy (12) takes the form [19, 22],

\[
T = -\frac{1}{\rho^2} \sin \vartheta \sin \beta \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{4}{\rho^2} \sin^2 \vartheta \left( \frac{\partial}{\partial \vartheta} \sin \beta \frac{\partial}{\partial \vartheta} \right) \sin^2 \varphi - \frac{\partial}{\partial \varphi} \frac{\partial}{\partial \varphi},
\]

\[
J^2 = -\frac{1}{\sin \Theta} \sin \Theta \frac{\partial}{\partial \Theta} \sin \Theta \frac{\partial}{\partial \Theta} \sin \Theta - \frac{1}{\sin^2 \Theta} \left( \frac{\partial}{\partial \Phi} \frac{\partial}{\partial \Phi} + \frac{\partial^2}{\partial \varphi^2} \sin^2 \Theta \frac{\partial}{\partial \Phi} \frac{\partial}{\partial \varphi} \right),
\]

\[
J \cdot l = \left[ \sin \varphi \left( \cos \Theta \frac{\partial}{\partial \Phi} - \sin \Phi \frac{\partial}{\partial \Phi} \right) - \cos \varphi \frac{\partial}{\partial \Theta} \sin \Phi \frac{\partial}{\partial \Phi} \right] \frac{\partial}{\partial \Theta} \sin \Phi \frac{\partial}{\partial \Phi} + \frac{\sin \varphi \frac{\partial^2}{\partial \Theta \partial \varphi} - \frac{\cos \varphi \frac{\partial^2}{\partial \Theta \varphi}}{\sin \Theta \sin \Phi \frac{\partial}{\partial \Phi} + \cos \varphi \cot \Theta \frac{\partial^2}{\partial \varphi^2}} \cot \varphi \right]
\]

\[
-\frac{\partial^2}{\partial \varphi^2}.
\]

In what follows, we use instead of \( \chi \) the variable

\[
t = \tan \frac{\chi}{2}, \quad t \in [0, \infty).
\]

One can consider \( t \) and \( \vartheta \) as the polar coordinates on the half-plane presenting the stereographic projection of a hemisphere with radius \( \chi \), latitude \( \chi \) and longitude \( \vartheta \) on the equatorial plane (figure 1). Three independent variables \( t, \vartheta, \varphi \) are the spherical coordinates of the vector \( \mathbf{t} \) in the rotating frame. This vector differs from the relative vector \( r/R \) [38] by the mass factor:

\[
t = tr/r = (\mu/M)^{1/2}r/R.
\]

For the formulation of our approach it is suitable to write the three-body Hamiltonian (11), (12), (13) in terms of the variables \( \Phi, \Theta, \varphi, \rho, t, \vartheta \). Taking into account the expression for the six-dimensional elementary volume,
The coalescence points of the three-body system. The stereographic problem; Figure 1.

\[ \xi = \text{const}, \eta = \text{const} \] on the sphere \( \rho = \rho_0 = \text{const} \) in the three-dimensional space \( x = \rho \sin \chi \cos \theta, y = \rho \sin \chi \sin \theta, z = \rho \cos \chi; \gamma \neq 0 \) in our problem; \( \xi \) and \( \eta \) are given by (46), (47). The poles correspond to the coalescence points of the three-body system. The stereographic projection with the centre \( \chi = \pi, z = -\rho_0 \) onto the plane \( z = 0 \) gives the usual elliptic net on this plane. For \( \rho_0 = 1 \) the polar coordinates on the plane \( z = 0 \) coincide with the independent variables \( t \) and \( \theta \) of the Coulomb two-centre Hamiltonian (37).

\[ dR = (4M \mu)^{-3/2} g t^2 \sin \vartheta \sin \Theta d\vartheta d\varphi d\Theta d\Phi, \]
\[ g = \rho^5(1 + t^2)^{-3} \]

one can present the kinetic energy \( T \) as
\[ T = g^{-1/2} \tilde{T} g^{1/2}, \]
\[ \tilde{T} = -\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2} \left[ -(1 + t^2) \Delta_t (1 + t^2) + (1 + t^2)(J^2 - 2J \cdot l) + \frac{3}{4} \right], \]

where
\[ \Delta_t = \frac{1}{t^2} \frac{\partial}{\partial t} t^2 \frac{\partial}{\partial t} - \frac{1}{t^2}. \]

Using (22) and the notations
\[ t_a = (-1)^\alpha t_a R / R, \quad t_a = (\mu M)^{1/2} m_a^{-1}, \quad \alpha = 1, 2, \]

we obtain \( V \) (13) in the form
\[ V = \frac{(1 + t^2)^{1/2}}{\rho} \left( 2M(1 + t^2)^2 Z_1 Z_2 \right) \]
\[ - \left( 2 \mu_1 Z_1 \right) \left( 2 \mu_2 Z_2 \right) \frac{[t - t_1]}{[t - t_2]}, \]
\[ |t - t_a| = |t^2 + t_a^2 - 2(1 - \epsilon) t_a \cos \vartheta|^{1/2}, \quad \alpha = 1, 2. \]

The three-body wavefunction, \( \Psi = \Psi(\rho, t, \vartheta, \phi, \Theta, \varphi) \), satisfies the Schrödinger equation
\[ H \Psi = E \Psi. \]

Using the transformation (25) one can present it in the form
\[ \tilde{H} \tilde{\Psi} = E \tilde{\Psi}, \]

where the transformed wavefunction \( \tilde{\Psi} \) and the transformed three-body Hamiltonian \( \tilde{H} \) are given by the relations
\[ \tilde{\Psi} = g^{1/2} \Psi = \rho^{5/2}(1 + t^2)^{-3/2} \Psi, \]
\[ \tilde{H} = g^{1/2} \tilde{H} g^{-1/2} \]
\[ = -\frac{\partial^2}{\partial \rho^2} + \tilde{H}^{ad} + \frac{(1 + t^2)}{\rho^2} (J^2 - 2J \cdot l) + \frac{3}{4 \rho^2}, \]
\[ \tilde{H}^{ad} = -\rho^{-2}(1 + t^2) \Delta_t (1 + t^2) + V. \]

The transformed adiabatic hyperspherical Hamiltonian \( \tilde{H}^{ad} \) acts on functions of \( t, \vartheta, \phi, \) and depends on \( \rho \) parametrically. Its eigenfunctions are used as a basis for the representation of the three-body wavefunction in the reduced version of the adiabatic hyperspherical approach [22, 23]. (In the general version [19, 20], the adiabatic hyperspherical Hamiltonian \( \tilde{H}^{ad} \) includes the last two terms of (26) and acts on functions of five variables.)

3. The hyperspherical Coulomb spheroidal (HSCS) basis

3.1. The appropriate Coulomb two-centre Hamiltonian in \( t \)-space

It is seen that \( \tilde{H}^{ad} \) can be considered as the Hamiltonian of the particle with the variable mass \( \tilde{m}(t) \) moving in the field \( V \) in \( t \)-space:
\[ \tilde{H}^{ad} = -\frac{\partial^2}{\partial \rho^2} + \tilde{H}^{ad} + \frac{(1 + t^2)}{\rho^2} (J^2 - 2J \cdot l) + \frac{3}{4 \rho^2}, \]
\[ \tilde{H}^{ad} = -\rho^{-2}(1 + t^2) \Delta_t (1 + t^2) + V. \]

Here the form of kinetic energy ensures the self-conjugacy. The pure discrete character of the spectrum of \( \tilde{H}^{ad} \) is explained by the fast decrease of the mass \( \tilde{m}(t) \) at large \( t, \tilde{m}(t) \sim t^{-4} \).

Every eigenfunction of \( \tilde{H}^{ad} \) coincides, at large \( \rho \), with the wavefunction of certain bound state of the atom (1, 3) or (2, 3) [22].

For generating the basis functions in our approach we also use the Hamiltonian of the particle moving in \( t \)-space, but the mass of the particle is fixed. Namely, we use the traditional Coulomb two-centre Hamiltonian,
\[ \hbar = -\Delta_t - \frac{\tilde{Z}_1}{|t - t_1|} - \frac{\tilde{Z}_2}{|t - t_2|}. \]

It describes the motion of a particle with mass 1/2 and charge -1 in the field of two effective charges \( \tilde{Z}_1 \) and \( \tilde{Z}_2 \) located at the points \( t_1 \) and \( t_2 \) of \( t \)-space at the distance
\[ |t_2 - t_1| = |t_1 + t_2| = (\mu M)^{1/2} \]

from each other. In our approach, the effective charges \( \tilde{Z}_1 = \tilde{Z}_1(\rho) \) and \( \tilde{Z}_2 = \tilde{Z}_2(\rho) \) are chosen, so that every eigenfunction of the discrete spectrum of \( \hbar \) (37) at large \( \rho \) coincides, as well as in the case of \( \tilde{H}^{ad} \), with the wavefunction of some bound state of the atom (1, 3) or (2, 3). The simplest choice is the linear function \( \tilde{Z}_a(\rho) \) for which we easily obtain
\[ \tilde{Z}_a = \rho \tilde{Z}_a(2 \mu_1)^{1/2} (1 + t_a^2)^{-3/2} = \rho \tilde{Z}_a(2 \mu_1)^{1/2} (1 + t_a^2)^{-3/2} \]
\[ \alpha = 1, 2. \]

Indeed, under this condition each eigenfunction of the discrete spectrum of \( \hbar \) (37) at \( \rho \to \infty \) is localized (with the exception
of the case $\tilde{Z}_1 = \tilde{Z}_2$, see below) in the neighbourhood of one of the centres and coincides with the eigenfunction of the one-centre Hamiltonian [3]. For example, in the asymptotic region
\[ R \to \infty, \quad |x_3 - x_1| = r_1 = O(1), \]
(40)
or, in the hyperspherical variables,
\[ \rho \to \infty, \quad |t - t_1| = (\mu/M)^{1/2} r_1/R = r_1(2/\mu_1)^{1/2} \mu + O(\rho^{-2}), \]
(41)
the corresponding one-centre Hamiltonian is given by
\[ -\Delta + \frac{\tilde{Z}_1}{|t - t_1|} \approx \frac{\rho^2 \mu_1^2}{\mu^2} \left( -\frac{1}{2} \Delta_1 - \frac{Z_1}{r_1} \right). \]
(42)
The expression in the parenthesis coincides with the Hamiltonian of the atom (1, 3). Hence, the eigenfunction of $h$ (37) localized at $\rho \to \infty$ in the domain (40), (41) coincides up to a constant factor with the wavefunction of some bound state of the atom (1, 3). The indices of the state are unimportant here.

As is seen from equation (39) in the case
\[ Z_1/Z_2 = (\mu_2/\mu_1)^{3/2}, \]
(43)
the effective charges are equal, $\tilde{Z}_1 = \tilde{Z}_2$. In this case the Hamiltonian (37) has an additional symmetry, and its eigenfunctions are divided into symmetric and antisymmetric ones. Thus, every eigenfunction is localized at $\rho \to \infty$ near both centres. For the construction of the basis in this case it is suitable to use the corresponding linear combinations of symmetric and antisymmetric eigenfunctions, which are localized at large $\rho$ in the vicinity of one of the centres. That transformation does not present any difficulties. Taking into account the abstract character of the condition (43) for the non-identical particles 1 and 2 we do not consider this case and suppose hereinafter
\[ \tilde{Z}_1 \neq \tilde{Z}_2. \]
(44)

3.2. Coulomb spheroidal functions on the sphere $\rho = \text{const}$

The equation defining the spectrum of the Hamiltonian $h(\rho|t)$ (37),
\[ (h - \varepsilon) \psi = 0, \]
(45)
is investigated in details [2, 3]. The problem admits the separation of variables in the prolate spheroidal coordinates $\xi \in [1, \infty)$ and $\eta \in [-1, 1]$,
\[ \xi = |t_1 - t_2|^{-1}(|t - t_1| + |t - t_2|) = R^{-1}(r_1 + r_2), \]
\[ \eta = |t_1 - t_2|^{-1}(|t - t_1| - |t - t_2|) = R^{-1}(r_1 - r_2). \]
(46)
(47)
The eigenfunction $\psi_{jm}^{\pm}(\rho|t)$, which corresponds to the eigenvalue $\varepsilon \in \varepsilon_{jm} < 0$ in the discrete spectrum and to $\varepsilon > 0$ in the continuous spectrum, is presented as the product
\[ \psi_{jm}^{\pm}(\rho|t) = \phi_{jm}(\rho|\xi, \eta) e^{\pm \im \mathbf{p} \cdot \mathbf{r}/\sqrt{2m}}, \]
\[ \phi_{jm}(\rho|\xi, \eta) = X_{jm}(\xi)Y_{jm}(\eta). \]
(48)
(49)
Here $m = 0, 1, 2, \ldots$ is the absolute value of the projection of the total momentum on the rotating axis. The multi-index $j$ is defined for the discrete spectrum ($\varepsilon < 0$) and for the continuous one ($\varepsilon > 0$) by the equation
\[ j = \begin{cases} (n_z, n_y), & \varepsilon < 0, \\ (n_z, n_y), & \varepsilon > 0, \end{cases} \]
(50)
where $n_z$ and $n_y$ are the number of nodes of radial $X(\xi)$ and angle $Y(\eta)$ functions, respectively. These functions, the so-called Coulomb spheroidal functions, satisfy the system of equations
\[ \left[ \frac{d}{d\varepsilon} (\xi^2 - 1) \right] - \lambda - \rho^2 (\xi^2 - 1) + a\xi X(\xi) = 0, \]
(51)
\[ \left[ \frac{d}{d\eta} (1 - \eta^2) \right] + \lambda - \rho^2 (1 - \eta^2)^2 + b\eta Y(\eta) = 0, \]
(52)
and the corresponding boundary conditions [3]. Here $\lambda$ is the separation constant. The parameters $a, b$ and $\rho$ are connected with the parameters of the Hamiltonian $h$ (37) by the relations
\[ a = \frac{1}{2}(\tilde{Z}_1 + \tilde{Z}_2)(t_1 + t_2) = \frac{\rho}{\sqrt{2\mu M}} (Z_1\mu_1^{3/2} + Z_2^{3/2}), \]
\[ b = \frac{1}{2}(\tilde{Z}_2 - \tilde{Z}_1)(t_1 + t_2) = \frac{\rho}{\sqrt{2\mu M}} (Z_2^{3/2} - Z_1\mu_1^{3/2}), \]
(53)
(54)
(55)
CSF defined by (51)–(55) differ from traditional CSF [1, 3] by a new connection of the parameters $a$ and $b$ with the coordinates and the masses of three particles (53), (54). The most important point is that our $a$ and $b$ are proportional to $\rho$ instead of $R$ in the traditional approach.

The functions $\phi_{jm}(\rho|\xi, \eta)$ at fixed $m$ and all possible $j$ form the complete set in the space of functions of two internal coordinates ($|\chi, \theta|$, $|t, \theta|$ or $|\xi, \eta|$) at fixed third internal coordinate, $\rho = \text{const}$. The normalization accepted in the paper is defined by the equation
\[ \langle f|g \rangle = 1/2 \int_0^\pi \sin^2 \chi/2 \int_0^\pi \int_0^\pi \sin \theta \sin \phi f^* g^* \]
\[ = \int_0^{t_1 + t_2} d\varepsilon \int_0^\pi \sin \theta \sin \phi f^* g^*, \]
(56)
\[ = \int_0^{t_1 + t_2} d\varepsilon \int_1^\infty d\eta (\xi^2 - \eta^2)^2 f^* g. \]
(57)
The completeness condition takes the form
\[ \sum_j \phi_{jm}(\rho|\xi, \eta) \phi_{jm}(\rho|\xi', \eta') = \sum_{n_z=0}^{\infty} \sum_{n_y=0}^{\infty} \phi_{n_z,n_y}(\rho|\xi, \eta) \phi_{n_z,n_y}(\rho|\xi', \eta') \]
\[ + \int_0^\infty \phi_{n_z,n_y}(\rho|\xi, \eta) \phi_{n_z,n_y}(\rho|\xi', \eta') d\varepsilon = 8(t_1 + t_2)^{-3}(\xi^2 - \eta^2)^{-3} \delta(\xi - \xi') \delta(\eta - \eta'). \]
(58)
3.3. HSCS basis on a five-dimensional hypersphere

The three-body Hamiltonian (11) has three commuting integrals of motion [1]: the square of the total angular momentum \( J^2 \); its projection on the third axis of the laboratory frame \( J_3 \) and the inversion of all Jacobi coordinates \( P \). It is therefore suitable to use for the construction of the basis of the symmetrized Wigner \( D \)-functions \( D_{Km}^J(\Phi, \Theta, \varphi) \) which are the eigenfunctions of these operators. The functions \( D_{Km}^J(\Phi, \Theta, \varphi) \) are, in addition, the eigenfunctions of the operator \( J_3^2 \) where \( J_3 \) is the projection of the total angular momentum on the third axis of the rotating frame:

\[
J_3^2 D_{Km}^J = J(J+1) D_{Km}^J, \quad J_3 D_{Km}^J = K D_{Km}^J, \quad J_3^2 D_{Km}^J = K D_{Km}^J, \quad J_3 D_{Km}^J = \pm K D_{Km}^J.
\]

The normalized symmetrized \( D \)-functions, \( D_{Km}^J(\Phi, \Theta, \varphi) \), are given by the expression [22]

\[
D_{Km}^J = A_{Km}^J \left[ D_{K+m}^J + \lambda(-1)^{J+1} D_{K-m}^J \right],
\]

where

\[
A_{Km}^J = (-1)^K [2J+1] / (2\omega_0(J+\lambda)).
\]

The standard Wigner functions \( D_{Km}^J(\Phi, \Theta, \varphi) \) are defined via functions \( d\Phi^J(\Phi, \Theta, \varphi) \) [41]:

\[
d\Phi^J(\Phi, \Theta, \varphi) = \exp \left( -iK \Phi \right) d\Phi^J(\Theta, \varphi) \exp \left( -i\mu \varphi \right),
\]

\[
\int_0^{2\pi} d\Phi \int_0^\pi \sin \Theta d\Theta \int_0^{2\pi} d\varphi D_{Km}^{J\varphi} \Phi D_{Km}^{J\varphi'} = \delta_{JJ'} \delta_{KK'} \delta_{mm'} \delta_{\varphi\varphi'}.
\]

We define the hyperspherical Coulomb spheroidal (HSCS) basis on the five-dimensional hypersphere

\[
\Omega = [t, \vartheta, \Phi, \Theta, \varphi] = [\xi, \eta, \Phi, \Theta, \varphi],
\]

\[
d\Omega = t^2 \sin \vartheta dt d\vartheta \sin \Theta d\Phi d\Theta d\varphi
\]

\[
= \left[ (1 + t^2)^{3/2}(\xi^2 - t^2)^2 \right] \sin \Theta d\vartheta d\Theta d\Phi d\Theta d\varphi,
\]

as the system of the common eigenfunctions of the operators \( J^2, J_3, J_3^2, P \) and the Coulomb two-centre Hamiltonian \( h \) depending on the parameter \( \rho \):

\[
\Phi_{jm}^{JK}(\rho|\Omega) = D_{Km}^J(\Phi, \Theta, \varphi) \phi_{jm}(\rho|\xi, \eta).
\]

Due to the completeness and the orthonormality of the system \( \{ \Phi_{jm}^{JK} \} \) (67) the three-body wavefunction \( \Psi \) (33) with fixed \( J, K, \lambda \) is presented in the form of the HSCS decomposition:

\[
\Psi_{jm}^{JK}(\rho|\Omega) = \rho^{3/2}(1 + t^2)^{-3/2} \Phi_{jm}^{JK}(\rho|\Omega),
\]

\[
\sum_{jm} J_{jm}^{JK}(\rho) \Phi_{jm}^{JK}(\rho|\Omega),
\]

where the sum by \( j \) includes both the discrete spectrum and the continuum (see (58)). The coefficients of the decomposition (68), the radial functions \( f_{jm}^{JK}(\rho|\Omega) \) are given by the integral

\[
f_{jm}^{JK}(\rho) = \int \Phi_{jm}^{JK}(\rho|\Omega) \Phi_{jm}^{JK}(\rho|\Omega) d\Omega.
\]

4. S-matrix and radial functions

4.1. Basis functions of the discrete spectrum at large \( \rho \)

Every eigenfunction of the discrete spectrum of \( h \) (37) at large \( \rho \) tends to the wavefunction of the bound state of the atom (1, 3) or the atom (2, 3). Detailed analysis [3] shows that the limiting atomic states are the states with definite parabolic quantum numbers in the rotating frame. Thus, the basis functions (49) can be enumerated by the indices \( \alpha \) (the number of the nucleus forming the atom), \( n \) (the principal quantum number), \( s \) (the first parabolic quantum number) and \( m \) (the absolute value of the projection of the atomic orbital momentum on the axis \( R \)):

\[
\phi_{\alpha n sm}(\rho|\xi, \eta) = \phi_{\alpha n sm}(\rho|\xi, \eta).
\]

The formulae determining the one-to-one correspondence,

\[
[n, n, m] \leftrightarrow [\alpha, n, s, m],
\]

for different cases are presented in [3].

To obtain the factor connecting the asymptotics of \( \phi_{\alpha n sm}(\rho|\xi, \eta) \) and the normalized atomic function in the region \( \rho \to \infty \),

\[
r_{\alpha} = O(1),
\]

(71) one has to use the asymptotic formula

\[
[t - t_1] = r_{\alpha} / r_{\alpha} \ln(\rho)/\rho + O(\rho^{-2})
\]

(73) and relations (56), (57) defining the normalization of basis functions. The result is

\[
\phi_{\alpha n sm}(\rho|\xi, \eta)_{\rho \to \infty} = (\mu_\alpha \rho^2 / 2\mu^2)^{3/4} \phi_{\alpha n sm}(r_{\alpha}, \vartheta_{\alpha}).
\]

Here \( \phi_{\alpha n sm}(r_{\alpha}, \vartheta_{\alpha}) \) is the normalized atomic function of the atom \( \alpha \) without the factor \exp(\pm im\varphi) \sqrt{2\pi}

\[
\int_0^{2\pi} d\varphi \phi_{\alpha n sm}(r_{\alpha}, \vartheta_{\alpha}) = 1,
\]

(75) where \( \vartheta_{\alpha} \) is the angle between \( r_{\alpha} \) and \( R \). The atomic function is factorized in the parabolic coordinates, but we conserve the notation \( \phi_{\alpha n sm}(r_{\alpha}, \vartheta_{\alpha}) \) for convenience.

Using equation (74) we obtain the asymptotics of the HSCS basis function \( \Phi_{jm}^{JK} \) (49) in the form

\[
\Phi_{jm}^{JK}(\rho|\xi, \eta)_{\rho \to \infty} = (\mu_\alpha \rho^2 / 2\mu^2)^{3/4} F_{jm}^{JK}(\Phi, \Theta, \varphi, r_{\alpha}, \vartheta_{\alpha}).
\]

(76)
where

\[ F^{JK}_{\alpha\nu\sigma}(\Phi, \Theta, \varphi, \rho, \theta_a) = D^{J}_{K}(\Phi, \Theta, \varphi) \phi_{\alpha\nu\sigma}(r_a, \theta_a) \]

\[ = A^{\alpha}_{\nu, \sigma}(d^{J}_{K}(\Theta) \exp(-im\varphi) + \lambda(-1)^{J+m} d^{J}_{K,-\nu}(\Theta) \exp(im\varphi)) \]

\[ \times \exp(iK\Phi) \phi_{\alpha\nu\sigma}(r_a, \theta_a). \]  

(77)

It is seen that \( F^{JK}_{\alpha\nu\sigma} \) is the combination of two atomic functions with opposite projections of the orbital momentum on the rotating axis \( R \) with coefficients depending on \( \Phi \) and \( \Theta \). Functions \( F^{JK}_{\alpha\nu\sigma} \) corresponding to the same atom (\( \alpha = \alpha' \)) satisfy the orthogonality condition

\[ \int_{0}^{2\pi} \int_{0}^{\pi} \sin \Theta \, d\Theta \int_{0}^{2\pi} \int_{0}^{\infty} r_a^2 \, dr_a \]

\[ \times \int_{0}^{2\pi} \sin \varphi \, d\varphi \int_{0}^{\pi} \sin \theta \, d\theta \int_{0}^{\infty} r_m^2 \, dr_m \]

\[ \delta_{J\lambda} \delta_{K\lambda} \delta_{n\alpha} \delta_{\nu\sigma} \delta_{\beta\lambda}(r_{a}) \delta_{\beta\lambda}(r_{m}). \]  

(78)

4.2. S-matrix in the \((\alpha\nu\sigma)\) representation

The product of \( F^{JK}_{\alpha\nu\sigma} \) and the ingoing (outgoing) wave,

\[ F^{JK}_{\alpha\nu\sigma}(\Phi, \Theta, \varphi, \rho, \theta_a) \cdot R_{\nu\sigma}^{-1} \exp(\pm i(k_a R_a - \gamma_{an})), \]

(79)

presents the state of the colliding atom and the remaining particle \((1, 3) + 2 \) for \( \alpha = 1 \) or \((2, 3) + 1 \) for \( \alpha = 2 \) at large distance \( R_a \) between them. Here \( k_{an} \) is the relativistic momentum

\[ k_{an} = \sqrt{2M_{a}(E - E_{an})} = M_{a}v_{an}, \]

where \( E_{an} \) is the energy of the isolated atom \( \alpha \); the logarithmic phase \( \gamma_{an} \) is given by

\[ \gamma_{an} = \gamma_{an}(R_a) = (Z_{a} - 1)Z_{3-a}M_{a}k_{an}^{-1} \log 2k_{an}R_{a}. \]  

(81)

The asymptotics of any three-body wavefunction at energy below the threshold of the three-particle breakup is presented as the combination of the products (79).

Consider a three-body system with fixed \( J, K, \lambda \). These indices are omitted hereinafter. According to the general theory [40] for the definition of S-matrix we have to consider the three-body wavefunction which contains a single ingoing wave in the input channel \([\alpha, n, s, m]\) and the outgoing waves in all open channels \([\alpha' n', s', m']\).

\[ \Psi_{an\sigma} \]

\[ = \frac{F_{an\sigma}}{R_{\nu\sigma} \sqrt{\gamma_{an}}} \exp(-i(k_{a} R_{a} - \gamma_{an})) \]

\[ - \sum_{\alpha' n' s' m'} \hat{S}_{an\sigma} \hat{F}_{\alpha' n' s' m'} \exp[i(k_{a} R_{a} - \gamma_{an})]. \]  

(82)

Here the coefficients \( \hat{S}_{an\sigma} \) are the matrix elements of the operator

\[ \hat{S} = \hat{S} Y, \]

(83)

where \( \hat{S} \) is the S-matrix, and \( \hat{Y} \) is the inversion operator which changes the sign of the relative coordinate \( R_a \) at fixed \( r_a \). It acts on any function of \( \Phi, \Theta, \varphi, \theta_a \) as follows:

\[ \hat{Y} \Phi(\Phi, \Theta, \varphi, \theta_a) = \Phi(\Phi + \pi, \Theta - \pi, \varphi - \pi, \theta_a). \]  

(84)

The matrix elements of S-matrix in any representation can be obtained from \( \hat{S}_{an\sigma} \) in a regular way with the use of relations (83), (84) and the transformation matrix connecting the set \( \{F^{JK}_{\alpha\nu\sigma}\} \) with the corresponding new set.

4.3. The asymptotics of radial functions in terms of \( \hat{S}_{an\sigma} \)

According to (68), (69) the wavefunction \( \Psi_{an\sigma} \) defined by the asymptotical condition (82) can be presented in the form of the HSCS decomposition:

\[ \Psi_{an\sigma} = \rho^{-5/2}(1 + \rho^2)^{-3/2} \sum_{jm' \nu' \sigma'} f_{an\sigma}(\rho) \Phi_{jm'(\rho)}^{\nu'} \]  

(85)

where the radial functions are given by

\[ f_{jm'(\rho)}^{\nu'}(\rho) = \int \Phi_{jm'}^{\nu'}(\rho, \Omega) \rho^{5/2}(1 + \rho^2)^{-3/2} \Psi_{an\sigma}(\rho | \Omega) \, d\Omega. \]  

(86)

Using this relation and the asymptotical formula (82) for \( \Psi_{an\sigma} \) we can express the asymptotics of \( f_{an\sigma}(\rho) \) in terms of the matrix elements \( \hat{S}_{an\sigma} \). To this end we have to rewrite expression (82) in the hyperspherical coordinates using the relation

\[ R_a = (2M_a)^{-1/2} \rho + O(\rho^{-1}), \]

(87)

which is valid in the asymptotical region (72). As a result, we have

\[ \Psi_{an\sigma}(\rho | \Omega) \]

\[ \rho \rightarrow \infty \]

\[ = F_{an\sigma} 2^{1/4} M_{a}^{1/4} \exp[-i(q_{an} \rho - \gamma_{an})] \]

\[ \frac{q_{an}^{1/2}}{q_{an}^{1/2}} \]

\[ - \sum_{\alpha' n' s' m'} \hat{S}_{an\sigma} F_{an\sigma} 2^{1/4} M_{a}^{1/4} \exp[i(q_{an} \rho - \gamma_{an})] \]

\[ \frac{q_{an}^{1/2}}{q_{an}^{1/2}}. \]  

(88)

where

\[ q_{an} = \sqrt{E - E_{an}}, \]

(89)

\[ \gamma_{an} = \gamma_{an}(\rho) = (Z_{a} - 1)Z_{3-a}M_{a}k_{an}^{-1} \log 2q_{an} \rho. \]  

(90)

The substitution of \( \Psi_{an\sigma}(\rho | \Omega) \) by the asymptotic expression (88) in equation (86) and the integration taking into consideration (76) and (78) lead to the asymptotical formulae for radial functions \( f_{an\sigma}(\rho) \), where \( \{an\sigma\} \) is the index of the input channel. For indices \( \{jm'\} = \{\alpha' n' s' m'\} \) corresponding to open channels, we obtain

\[ f_{an\sigma}(\rho) \]

\[ \rho \rightarrow \infty \]

\[ = 2(\pi \mu)^{1/4} q_{an}^{-1/2} \delta_{an} \delta_{\nu' \sigma'} \delta_{s' s} \delta_{m' m} \exp[-i(q_{an} \rho - \gamma_{an})] \]

\[ - (q_{an}/q_{\alpha' n'})^{1/2} \hat{S}_{an\sigma} \exp[i(q_{an} \rho - \gamma_{an})]. \]  

(91)

For \( \{jm', \sigma'\} \) corresponding to the closed channels and continuous spectrum of the Hamiltonian \( h \) the result is

\[ f_{an\sigma}(\rho) \]

\[ \rho \rightarrow \infty \]

\[ = 0. \]  

(92)

4.4. The coordination with the asymptotic conditions of the scattering problem

The relations (91) and (92) show that the radial function \( f_{an\sigma}(\rho) \) does not vanish at \( \rho \rightarrow \infty \) only if its indices \( \alpha' n' s' m' \) correspond to one of the open channels. In this case, its asymptotics contains the single matrix element \( \hat{S}_{an\sigma} \). In other words, the function describing the motion of two colliding clusters in the definite open channel (the definite term of expression (82)) is the asymptotics of the single term
of the decomposition (85). Other terms of (85) do not make a contribution to this function. Thus, the HSCS expansion (85) is coordinated with the asymptotic conditions of the scattering problem.

That is not right for the traditional BO approach where \( R \) is an adiabatic parameter. The reason is that the BO basis functions form an orthogonal system on the surface \( R = \text{const} \), so that the surface appears in the integral for the radial function which replaces (86) in the BO case. For the calculation of this integral one has to use for \( R \) the expansion in powers of \( R^{-1} \). But this expansion, in contrast to the expansion in powers of \( \rho^{-1} \) (87), contains a non-vanishing term depending on the atomic coordinate \( r \).

\[
R_a \big|_{R \to \infty} = R + (-1)^d m_s (m_a + m_3)^{-1} R^{-1} r_a \cdot R + O(R^{-1}).
\]  

Consequently, the asymptotic formula for the ingoing (outgoing) wave \( \exp(\pm i k_a R_a) \) contains the factor

\[
\exp[\pm i k_a m_s (m_a + m_3)^{-1} R^{-1} r_a \cdot R].
\]

(94)

The matrix elements of that factor differ from zero for all states of the atom \( \alpha \) including the excited states corresponding to the closed channels. So the radial function does not vanish at \( R \to \infty \) for all states with \( \alpha' = \alpha \). It means that all terms of the traditional BO decomposition with given \( \alpha \) make a contribution to the wavefunctions of all open channels with that \( \alpha \).  

4.5. The real radial functions

In the numerical calculations it is used instead of the complex functions \( \Psi_{anm} \) (85), (82) their real linear combinations \( G_{anm} \) which contain \( \sin(k_a R_a - \gamma_{an} - \pi J/2) \) in the input channel and \( \cos(k_{\alpha'} R_{\alpha'} - \gamma_{\alpha' \alpha'} - \pi J/2) \) in all open channels. The HSCS representation for \( G_{anm} \) has the form

\[
G_{anm} = \rho^{-5/2} (1 + i t^2)^{3/2} \sum_{jm'} g_{jm'}^{anm}(\rho) \Phi_{jm'}(\rho|\Omega).
\]

(95)

where the asymptotics of the radial function \( g_{jm'}^{anm}(\rho) \) with indices \( \{jm'\} = \{\alpha' \text{'s} m' \} \) corresponding to the open channel is given by

\[
g^{anm}_{\alpha' \text{'s} m'}(\rho) \big|_{\rho \to \infty} = \delta_{\alpha \alpha'} \delta_{\gamma_{an} \gamma_{an'}} \delta_{\text{angm}} \sin(\eta_{an} \rho - \gamma_{an} - \pi J/2) - (\eta_{an}/\eta_{a' \alpha'})^{1/2} K_{\alpha\text{'s} m}^{anm} \cos(\eta_{a' \alpha'} \rho - \gamma_{a' \alpha'} - \pi J/2).
\]

(96)

For \( \{j, m'\} \) corresponding to the closed channels and the continuum spectrum we have

\[
g_{jm}^{anm}(\rho) \big|_{\rho \to \infty} = 0.
\]

(97)

The relation between \( K_{anm}^{\alpha' \text{'s} m'} \) (96) and \( S_{anm}^{\alpha' \text{'s} m'} \) (91) can be written as follows:

\[
K = i(1 - (-1)^d) \mathcal{S}[1 + (-1)^d]^{-1},
\]

\[
\mathcal{S} = (-1)^d [1 - i\mathbf{k}]^{-1} [1 + i\mathbf{k}],
\]

(98)

where \( \mathcal{S} \) and \( K \) are matrices with matrix elements \( \mathcal{S}_{ji} = \delta_j^i, \quad K_{ji} = K_j^i, \quad f = \{\alpha' \text{'s} m' \}, \quad i = \{anm\}. \)

The relation between the functions \( \Psi_{anm} \) and \( G_{anm} \) is given by

\[
G_i = 2^{-1}(M \mu)^{-3/4} q_i^{1/2} \times \exp[i(\mathbf{J} + 1)/2 \sum_j \Psi_j [1 + (-1)^d \mathcal{S}]_{ji}].
\]

(101)

5. The scattering problem for the radial system

For the calculation of the \( K \)-matrix it is necessary to solve the system of equations for the radial functions which follows from the Schrödinger equation. To obtain this system in the simplest form it is suitable to present the adiabatic hyperspherical Hamiltonian \( \tilde{H} \) (35) as the sum

\[
\tilde{H} = \rho^{-2}(1 + i t^2) h(1 + i t^2) + W,
\]

(102)

where the additional potential \( W(\rho, t) \) has no singularities in the coalescence points. It is given by the formulae

\[
W = V + \frac{(1 + i t^2)}{\rho^2} \left( \frac{Z_1}{|t - t_1|} + \frac{Z_2}{|t - t_2|} \right)
\]

\[
\rho \to \infty = \frac{1}{\rho} \left[ u^{(12)} + u^{(13)} + u^{(23)} \right],
\]

(103)

\[
w^{(12)} = \frac{Z_1 Z_2 (2M)^{1/2} (1 + i t^2)^{1/2}}{|t - t_1|} \left( \left[ 1 + \frac{1 + i t^2}{1 + t_1^2} \right]^{3/2} - 1 \right)
\]

\[
\rho \to \infty = \frac{Z_1 Z_2 (2M)^{1/2} (1 + i t^2)^{1/2}}{|t - t_1|} \left( \left[ 1 + \frac{1 + i t^2}{1 + t_1^2} \right]^{3/2} - 1 \right)
\]

\[
\rho \to \infty = \frac{Z_1 Z_2 (2M)^{1/2} (1 + i t^2)^{1/2}}{|t - t_2|} \left( \left[ 1 + \frac{1 + i t^2}{1 + t_2^2} \right]^{3/2} - 1 \right)
\]

(104)

The three-body Hamiltonian \( \tilde{H} \) (34) takes the form

\[
\tilde{H} = -\frac{\partial^2}{\partial \rho^2} + \frac{3}{4 \rho^2} - E \]

\[
+ (1 + i t^2)(J^2 - 2J \cdot L) \frac{3}{4} + W.
\]

(105)

The substitution of \( \Psi_{\text{'J'K'\lambda}} \) by the decomposition (68) in the Schrödinger equation (32), (105) and projecting onto the state \( \Phi_{\text{'J'K'\lambda}}(\rho|\Omega) \) lead to the system of the differential equations for radial functions

\[
\left( -\frac{d^2}{d \rho^2} + \frac{3}{4 \rho^2} - E \right) f_{jm}(\rho) + \sum_j \left[ \left[ 2 Q_{ij}^m \frac{d}{d \rho} + \sum_j d P_{ij}^m + \sum_j U_{ij}^m + W_{ij}^m + R_{ij}^m \right] f_{jm}(\rho) + \frac{1}{\rho^2} \right]
\]

\[
\times \left( T_{jm} f_{jm-1}(\rho) + T_{jm+1} f_{jm+1}(\rho) \right) = 0,
\]

(106)

where the sum over \( j \) includes both the discrete spectrum and the continuum (see (58)). The indices \( J, K, \lambda \) corresponding to the integrals of motion are omitted.

The matrix elements \( P_{ij}^m, Q_{ij}^m, R_{ij}^m, T_{jm}, U_{ij}^m, W_{ij}^m \) in (106) are the two-dimensional integrals containing the
factorized solutions of the Coulomb two-centre problem \( \phi_{jm}(\rho|\xi, \eta) \) (49):

\[
P_{ij}^{\alpha}(\rho) = P_{ji}^{\alpha}(\rho) = \left( \frac{\partial}{\partial \rho} \phi_{im} \right) \left( \frac{\partial}{\partial \rho} \phi_{jm} \right),
\]

\[
Q_{ij}^{\alpha}(\rho) = -Q_{ji}^{\alpha}(\rho) = \left( \frac{\partial}{\partial \rho} \phi_{im} \right),
\]

\[
R_{ij}^{\alpha}(\rho) = R_{ji}^{\alpha}(\rho) = [J(J+1) - 2m^2][\phi_{im}](1+i^2)\phi_{jm},
\]

\[
T_{jm,lm}(\rho) = 1[J(J+1) - m(m+1)]^{1/2}(1+\delta_{lm})^{1/2}
\times \langle \phi_{im}(1+i^2)(-\partial/\partial \theta + m\cot \theta)\phi_{jm} \rangle,
\]

\[
U_{ij}^{\alpha}(\rho) = \frac{1}{\rho^2} \langle \phi_{im}(1+i^2)h_{lm}(1+i^2)\phi_{jm} \rangle,
\]

\[
W_{ij}^{\alpha}(\rho) = \langle \phi_{im}|W|\phi_{jm} \rangle = \frac{1}{\rho^2} \langle \phi_{im}|w^{(12)} + w^{(13)} + w^{(23)}\phi_{jm} \rangle,
\]

(107)

the operator \( h_{lm} \) is given by the expression

\[
h_{lm} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{-im\varphi} h e^{in\varphi} d\varphi
\]

\[
= \frac{1}{i^2} \left[ \frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} \right] - \frac{1}{\sin \theta} \left[ \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{m^2}{\sin \theta} \right]
\]

\[
= \frac{1}{|t - t_1|} - \frac{Z_2}{|t - t_2|}.
\]

(108)

It is evident that the real radial functions \( g_{jm}^{\alpha}(\rho) \) (95) also satisfy the system (106) as well as the coefficients of the HSCS decomposition of any solution of the Schrödinger equation (32).

We did not study the asymptotics of the matrix elements at large \( \rho \) in detail as it is not necessary for the statement of the scattering problem. However, the principal term of the asymptotics of the diagonal matrix element \( U_{ii}^{\alpha}(\rho) \) is obtained without any complicated calculations:

\[
U_{ii}^{\alpha}(\rho)|_{\rho \to \infty} = E_{an}, \quad i = \{\alpha ns \}.
\]

(109)

Other matrix elements in (106) vanish at \( \rho \to \infty \).

To find the matrix \( K_{\alpha ns}^{\alpha'ns'} \) (96) one has to solve the system (106) for the real radial functions \( g_{jm}^{\alpha}(\rho) \) for all sets [\( \alpha ns m \)] (the input channel) corresponding to open channels. The solutions have to satisfy the boundary conditions at \( \rho = 0 \):

\[
g_{jm}^{\alpha}(0) = 0,
\]

(110)

which follow from the finiteness of the Coulomb three-body wavefunction \( G(\rho) \), and the asymptotical conditions (96), (97) at \( \rho \to \infty \). The matrix elements \( S_{\alpha ns}^{\alpha'ns'} \) are expressed in terms of \( K_{\alpha ns}^{\alpha'ns'} \) in accordance with (99). The matrix elements of \( S \)-matrix can be expressed in terms of \( S_{\alpha ns}^{\alpha'ns'} \) with the help of relation (83).

### 6. Concluding remarks

The suggested hyperspherical Coulomb spheroidal (HSCS) representation is a novel way to use the solutions of the Coulomb two-centre problem for the expansion of the Coulomb three-body wavefunction which differs considerably from the Born–Oppenheimer one. It combines two important qualities. On the one hand it is coordinated with the asymptotic conditions of the scattering problem for energies below the three-particle breakup threshold (section 4); on the other hand the HSCS basis consists of relatively simple and well-known functions, the Coulomb spheroidal functions and the Wigner D-functions (section 3). The combination of these properties is achieved at the cost of the deviation from the adiabatic idea and the corresponding complication of the radial equations. Indeed, the Coulomb two-centre Hamiltonian \( h \) (37) generating our basis functions differs from the adiabatic hyperspherical Hamiltonian \( \tilde{h}_{ad} \) (36) by both the potential energy and the kinetic one. Therefore, the radial system (106) contains the non-diagonal matrices \( U_{ij}^{\alpha}(\rho) \) and \( W_{ij}^{\alpha}(\rho) \) (107) instead of the diagonal matrix of \( \tilde{h}_{ad} \) in the adiabatic hyperspherical approach. This complication, however, looks insignificant as compared with the advantages resulting from the properties of the HSCS expansion. First, the avoided crossings of the adiabatic hyperspherical terms are changed by the exact crossings of the Coulomb two-centre terms. Second, the use of the well-known and relatively simple CSF allows us to perform the precise calculations in a wide range of \( \rho \) including extremely large values which are essential for the calculation of \( S \)-matrix. Therefore, the HSCS approach can be greatly helpful for the construction and modernization of numerical methods in the investigations of scattering processes in the Coulomb three-body systems at energies below the three-particle breakup threshold.

It is interesting also to apply the HSCS expansion to the calculation of the bound states of these systems. This problem is simpler than the scattering one as all radial functions vanish at \( \rho \to \infty \).

The applied three-pole coordinate system on the sphere \( \rho = \text{const} \), which is connected with the elliptic coordinate system on the plane by means of the stereographic projection, may be interesting in different versions of the hyperspherical approach to the three-body problem as it presents a natural way to take into consideration three coalescent points.

The essential difference between HSCS and adiabatic hyperspherical expansions is that the first one includes both discrete and continuous spectra while the second one has a pure discrete spectrum. In the adiabatic hyperspherical approach (as well as in the approach of papers [33–37]) every basis function at large \( \rho \) is localized in the vicinity of the coalescent point where it coincides with the wavefunction of the bound state of the corresponding atom. Thus, this basis is not suitable for the representation of the Coulomb three-body wavefunction at energies above the threshold of the three-particle breakup. In contrast to the adiabatic hyperspherical basis, the HSCS one includes the basis functions of the continuous spectrum which are not localized in the vicinities of the coalescent points at any \( \rho \). This allows us to hope that in certain problems the HSCS basis can be used for the suitable representation of the Coulomb three-body wavefunction at energies above the threshold mentioned.

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