Methods of solving Coulombic three-body problems in hyperspherical coordinates

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A method for solving three-body problems in mass-weighted hyperspherical coordinates in the adiabatic approximation is presented. The adiabatic channel function is expanded in terms of analytical functions expressed in different sets of Jacobi coordinates to describe each dissociation limit naturally. Evaluation of matrix elements between functions in different Jacobi coordinates is achieved through the known transformation properties of hyperspherical harmonics in these coordinates. The method is applied to study the lowest channels for various Coulombic three-body systems such as H^-, $e^-e^-e^+$, $p^+p^+\mu^-$, $d^+d^+\mu^-$, $e^+p^+e^-$, $p^+d^+\mu^-$, and $d^+t^+\mu^-$ using only one or two analytical basis functions, and the results are compared with some known calculations. The behavior of the potential curves with respect to the variation of the masses of the three-body system is also examined.

I. INTRODUCTION

Hyperspherical coordinates have been applied extensively in recent years to study many new types of atomic, molecular, and nuclear three-body problems. In atomic physics, it has been shown[1,2] that electron correlations and the properties of doubly excited states of two-electron atoms are conveniently analyzed in hyperspherical coordinates. A new classification scheme of doubly excited states of atoms has emerged from such an analysis. In molecular physics, new hyperspherical normal modes[3] and novel features of reactive scatterings from collinear triatomic systems[4,5] have been identified using hyperspherical coordinates. In the last few years, progress had been made in the three-dimensional reactive scattering studies for molecular systems.[6-10] In nuclear physics, hyperspherical coordinates have also been used in a number of applications.[11]

From the quantum-mechanical three-body problem viewpoint, a two-electron atom is a special example where each pair of particles is governed by the Coulombic interaction. Another familiar Coulombic three-body system is H_2^+, i.e., the molecular hydrogenic ion. In the traditional approach, the theoretical methods for treating two-electron atoms and for H_2^+ are quite different: An independent electron approximation is used to describe the former and a Born-Oppenheimer approximation for the latter. A unification appears possible if these three-body problems are described in hyperspherical coordinates. From the mathematical viewpoint, the differences between two-electron atoms and one-electron diatomic molecular ions are only in the relative masses of the particles. How do the approximate quantum numbers used in the description of each type of problems emerge from the seemingly identical mathematical equations? The clues to this question again come from the recent analysis of electron correlations where the new quantum numbers are referred to the body frame of the atom[12] rather than to the quantum numbers of each individual electron as in the independent-particle approximation. Therefore, one of the interesting questions in the study of the three-body problem is how the quantum numbers used in the description of H^- (and He) evolve, as the mass of the two identical particles with respect to the mass of the third particle varies from the H^- limit to the H_2^+ limit. A general theoretical approach for Coulombic three-body problems would also allow us to study such intermediate systems as $e^-e^+e^-$, $p^+\mu^-p^+$, $d^+\mu^-d^+$, $e^-p^+e^+$, $p^+\mu^-d^+$, and $d^+\mu^-t^+$. The last muonic molecular ion $d^+\mu^-t^+$ is currently of great interest because of its im-

portance in the study of muon-catalyzed fusion.

There is one major complication in generalizing the hyperspherical coordinates used for two-electron atoms to arbitrary Coulombic three-body systems. While for the conventional atomic systems, one often neglects the motion of the nucleus, i.e., one assumes the mass of the nucleus to be infinite, this is not possible for the general three-body Coulombic systems.

In this article we address the methods of solving Coulombic three-body problems in hyperspherical coordinates. Within the hyperspherical method, there are different ways of choosing hyperspherical angles. In the early study, internal and external coordinates were used.[13] Such methods result in very complicated differential equations when the Schrödinger equation is expressed in internal coordinates. In our approach, we start with the Jacobi coordinates of the three particles. There is an important advantage in defining hyperspherical angles from the Jacobi coordinates since the wave functions are conveniently separable in the limit of two-body breakup.

A well-established procedure[1,14] for the study of the three-body system in hyperspherical coordinates is the adiabatic approximation. This is similar to the Born-Oppenheimer approximation in diatomic molecules. The Schrödinger equation in hyperspherical coordinates is solved at each fixed hyperradius to obtain a family of effective potential curves. These potential curves, similar to the molecular potential curves, contain essential informations about the structure of the three-body system.

The rest of this article is organized as follows. We first discuss in Sec. II A the hyperspherical coordinates in different sets of Jacobi coordiantes. The properties of the grand angular momentum operator and its eigenfunctions, the hyperspherical harmonics, and the transformation of hyperspherical harmonics from one set to another are discussed in Sec. II B. In Sec. II C we analyze the total Coulomb potential energy in different sets of hyperspherical coordinates. In Sec. II D we discuss the solution of the Schrödinger equation in the adiabatic approximation. We assume that the wave function varies slowly with respect to the hyperradius R so that the Schrödinger equation can be solved at each fixed R to obtain an effective potential $U(R)$ and a corresponding "channel function." At the end of this section we comment on the different hyperspherical angles chosen by other workers, particularly those used by quantum chemists. In Sec. III we discuss the various methods of solving the channel function and weigh the advantage as well as the disadvantages of the methods. We are interested in an efficient numerical method which can give reliable potentials $U(R)$ for the whole range of R and a wide range of masses of the three-body systems. This is achieved by analyzing the properties of the differential equations in the large- as well as the small-R limits. The adopted method is a generalization of the analytical channel functions[15] that was used in the study of two-electron atoms. In Sec. III D we discuss the symmetry consideration for cases where there are two identical particles. Some typical results for H^-, $e^-e^+e^-$, $p^+p^+\mu^-$, and $d^+d^+\mu^-$ are shown in Sec. IV, where the adiabatic potential curves

are calculated with a single basis function. We also consider three distinguishable particles such as $e^-p^+e^+$, $p^+\mu^-d^+$, and $d^+\mu^-t^+$, where the two lowest potential curves are calculated with two basis functions. The future directions and perspective of this general approach are discussed in Sec. V.

II. HYPERSPHERICAL COORDINATES AND THE COULOMBIC THREE-BODY HAMILTONIAN

A. The coordinate systems

To be specific we confine ourselves to discuss three-body systems in the center-of-mass frame. Let $\mathbf{r}_i$ denote the coordinates of particle i in the laboratory frame, which has mass m_i. A possible set of Jacobi coordinates is given in Fig. 1(a). This is denoted as the α set. The vector from particle 1 to particle 2 is $\boldsymbol{\rho}_1$, with reduced mass $\mu_1 = m_1 m_2 /(m_1 + m_2)$. The second vector $\boldsymbol{\rho}_2$ is from the center of mass of particles 1 and 2 to particle 3, with reduced mass $\mu_2 = (m_1 + m_2)m_3 /(m_1 + m_2 + m_3)$. This choice of Jacobi coordinates is not unique. Two other possible sets are given in Figs. 1(b) and 1(c); they are designated as β and γ, respectively. This procedure can obviously be generalized to N-body systems.

Let $M = \sum m_i$ be the total mass of the system and $\mathbf{u}$ be the coordinates of the center of mass; there exist two important identities for the different sets of Jacobi coordinates for the N-body system,

$$\sum_{i=1}^{N} m_i \mathbf{r}_i^2 = \sum_{j=1}^{N-1} \mu_j \boldsymbol{\rho}_j^2 + M\mathbf{u}^2 , \tag{1}$$

$$\sum_{i=1}^{N} \frac{1}{m_i} \frac{\partial^2}{\partial^2 \mathbf{r}_i} = \sum_{j=1}^{N-1} \frac{1}{\mu_j} \frac{\partial^2}{\partial^2 \boldsymbol{\rho}_j} + \frac{1}{M} \frac{\partial^2}{\partial^2 \mathbf{u}} . \tag{2}$$

If we further introduce a set of mass-weighted vectors,

$$\boldsymbol{\xi}_i = (\mu_i /\mu)^{1/2} \boldsymbol{\rho}_i , \tag{3}$$

where μ is arbitrary, then Eqs. (1) and (2) become

$$\sum_{j=1}^{N-1} \boldsymbol{\xi}_j^{(\alpha)2} = \sum_{j=1}^{N-1} \boldsymbol{\xi}_j^{(\beta)2} = \sum_{j=1}^{N-1} \boldsymbol{\xi}_j^{(\gamma)2} , \tag{4}$$

$$\frac{1}{\mu} \sum_{j=1}^{N-1} \frac{\partial^2}{\partial^2 \boldsymbol{\xi}_j^{(\alpha)}} = \frac{1}{\mu} \sum_{j=1}^{N-1} \frac{\partial^2}{\partial^2 \boldsymbol{\xi}_j^{(\beta)}} = \frac{1}{\mu} \sum_{j=1}^{N-1} \frac{\partial^2}{\partial^2 \boldsymbol{\xi}_j^{(\gamma)}} , \tag{5}$$

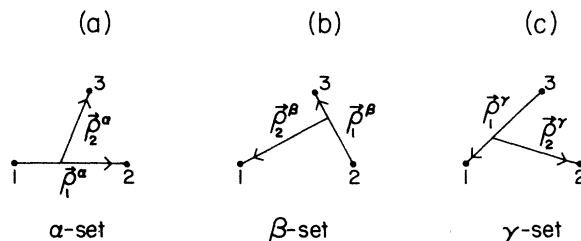where the ξ's are similar to Cartesian coordinates.

FIG. 1. Three different sets of Jacobi coordinates for three-body systems.

B. The grand angular momentum operator and hyperspherical harmonics

Kinetic-energy operator for the three-body system is

$$T = \frac{\hbar^2}{2}\sum_{i=1}^{3}\frac{1}{m_i}\nabla_{r_i}^2 = -\frac{\hbar^2}{2}\left[\sum_{j=1}^{2}\frac{1}{\mu_j}\frac{\partial^2}{\partial^2\rho_j} + \frac{1}{M}\frac{\partial^2}{\partial^2 u}\right].$$

(6)

By defining a hyperspherical radius R and a hyperangle ϕ,

$$R^2 = \xi_1^2 + \xi_2^2 ,$$

$$\tan\phi = \xi_2/\xi_1 ,$$

(7)

the kinetic-energy operator is rewritten as

$$T = -\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial^2 R} + \frac{5}{R}\frac{\partial}{\partial R} - \frac{\Lambda^2(\Omega)}{R^2}\right],$$

(8)

where Ω denotes the set of five angles, $\Omega = (\phi,\hat{\xi}_1,\hat{\xi}_2)$, and Λ^2 is the grand angular momentum operator

$$\Lambda^2(\Omega) = -\frac{1}{\sin^2\phi\cos^2\phi}\frac{d}{d\phi}\left[\sin^2\phi\cos^2\phi\frac{d}{d\phi}\right]$$

$$+ \frac{l_1^2(\hat{\xi}_1)}{\cos^2\phi} + \frac{l_2^2(\hat{\xi}_2)}{\sin^2\phi} .$$

(9)

The eigenvalues and the normalized eigenfunctions of $\Lambda^2(\Omega)$ are well known,

$$\Lambda^2(\Omega)Y_{[K]}(\Omega) = \lambda_{[K]}(\lambda_{[K]}+4)Y_{[K]}(\Omega) ,$$

(10)

where

$$\lambda_{[K]} = 2m + l_1 + l_2 ,$$

(11)

and the normalized eigenfunctions are

$$Y_{[K]}(\Omega) = Q_m^{l_2 l_1}(\phi)\mathscr{Y}_{l_1 l_2 LM}(\hat{\xi}_1,\hat{\xi}_2) ,$$

(12)

where $[K]$ denotes a set of quantum numbers m, l_1, l_2, L, and M, and

$$Q_m^{l_2 l_1}(\phi) = \theta_m^{l_2 l_1}\sin^{l_2}\phi\cos^{l_1}\phi\, P_m^{(l_2+1/2,l_1+1/2)} .$$

(13)

Here $\theta_m^{l_2 l_1}$ is a normalization constant and $P_m^{(\alpha,\beta)}$ is a

Jacobi polynomial. In (12), $\mathscr{Y}_{l_1 l_2 LM}(\hat{\xi}_1,\hat{\xi}_2)$ is the coupled total orbital angular momentum function. The eigenfunctions $Y_{[K]}(\Omega)$ form a complete and orthonormal set satisfying

$$\int d\Omega\, Y_{[K']}^*(\Omega)Y_{[K]}(\Omega) = \delta_{[K'][K]} ,$$

(14)

where the volume element $d\Omega = \cos^2\phi\sin^2\phi\,d\phi\,d\hat{\xi}_1 d\hat{\xi}_2$. The above equations, (6)–(14), can be written for each of the three sets of Jacobi coordinates.

From Eqs. (4) and (5), it is clear that the grand angular momentum operator is independent of the chosen Jacobi coordinates,

$$\Lambda^2(\Omega^\alpha) = \Lambda^2(\Omega^\beta) = \Lambda^2(\Omega^\gamma) .$$

(15)

Therefore, it is possible to expand the eigenfunction of one set in terms of the eigenfunctions of another set within the given subset with $\lambda_{[K]} = \lambda_{[K']}$,

$$Y_{[K]}(\Omega^\alpha) = \sum_{[K']} A\begin{bmatrix}K\\K'\end{bmatrix}^{\alpha\to\alpha'}(\eta)Y_{[K']}(\Omega^{\alpha'}) .$$

(16)

Here α' denotes either the β or γ set and η is related to the mass ratio of the particles. The expansion coefficients

$$A\begin{bmatrix}K\\K'\end{bmatrix}^{\alpha\to\alpha'}(\eta) = \int d\Omega^{\alpha'}Y_{[K']}^*(\Omega^{\alpha'})Y_{[K]}(\Omega^\alpha)$$

(17)

are called the transformation brackets[16] of the hyperspherical harmonic functions. A program for their evaluations has been written and is given in Ref. 16.

C. Coulomb particles in different sets of Jacobi coordinates

If the charges of the three particles are given by $Z_1 e$, $Z_2 e$, and $Z_3 e$, respectively, the total Coulomb potential is

$$V = \frac{Z_1 Z_2 e^2}{r_{12}} + \frac{Z_2 Z_3 e^2}{r_{23}} + \frac{Z_3 Z_1 e^2}{r_{31}}$$

$$= \frac{Z_1 Z_2 e^2}{\rho_1^{(\alpha)}} + \frac{Z_2 Z_3 e^2}{\rho_1^{(\beta)}} + \frac{Z_3 Z_1 e^2}{\rho_1^{(\gamma)}} ,$$

(18)

where r_{ij} is the distance between particles i and j. The second equation above expresses that the total Coulomb potential is most simply given in terms of combinations of different sets of Jacobi coordinates. In practice, it is desirable to express the potential in one set of Jacobi coordinates only. From the simple geometric construction, the following relations can be derived:

$$\rho_1^{(\alpha)} = -\rho_2^{(\beta)} - \frac{m_3}{m_2+m_3}\rho_1^{(\beta)} = -\left[\left(\frac{\mu}{\mu_2^{(\beta)}}\right)^{1/2}\xi_2^{(\beta)} + \frac{m_3}{m_2+m_3}\left(\frac{\mu}{\mu_1^{(\beta)}}\right)^{1/2}\xi_1^{(\beta)}\right]$$

$$= \rho_2^{(\gamma)} - \frac{m_3}{m_1+m_3}\rho_1^{(\gamma)} = \left[\left(\frac{\mu}{\mu_2^{(\gamma)}}\right)^{1/2}\xi_2^{(\gamma)} - \frac{m_3}{m_1+m_3}\left(\frac{\mu}{\mu_1^{(\gamma)}}\right)^{1/2}\xi_1^{(\gamma)}\right] ,$$

(19a)

$$\rho_1^{(\beta)} = \rho_2^{(\alpha)} - \frac{m_1}{m_1+m_2}\rho_1^{(\alpha)} = \left[\left[\frac{\mu}{\mu_2^{(\alpha)}}\right]^{1/2}\xi_2^{(\alpha)} - \frac{m_1}{m_1+m_2}\left[\frac{\mu}{\mu_1^{(\alpha)}}\right]^{1/2}\xi_1^{(\alpha)} \right]$$

$$= -\rho_2^{(\gamma)} - \frac{m_1}{m_1+m_3}\rho_1^{(\gamma)} = -\left[\left[\frac{\mu}{\mu_2^{(\gamma)}}\right]^{1/2}\xi_2^{(\gamma)} + \frac{m_1}{m_1+m_3}\left[\frac{\mu}{\mu_1^{(\gamma)}}\right]^{1/2}\xi_1^{(\gamma)} \right] , \qquad (19b)$$

$$\rho_1^{(\gamma)} = -\rho_2^{(\alpha)} - \frac{m_2}{m_1+m_2}\rho_1^{(\alpha)} = -\left[\left[\frac{\mu}{\mu_2^{(\alpha)}}\right]^{1/2}\xi_2^{(\alpha)} + \frac{m_2}{m_1+m_2}\left[\frac{\mu}{\mu_1^{(\alpha)}}\right]^{1/2}\xi_1^{(\alpha)} \right]$$

$$= \rho_2^{(\beta)} - \frac{m_2}{m_2+m_3}\rho_1^{(\beta)} = \left[\left[\frac{\mu}{\mu_2^{(\beta)}}\right]^{1/2}\xi_2^{(\beta)} - \frac{m_2}{m_2+m_3}\left[\frac{\mu}{\mu_1^{(\beta)}}\right]^{1/2}\xi_1^{(\beta)} \right] . \qquad (19c)$$

From (18) and (19), for example, we can write the Coulomb potential in terms of the β-set coordinates,

$$V^{(\beta)} = e^2 \left\{ \frac{Z_1 Z_2}{\left| \left[\frac{\mu}{\mu_2^{(\beta)}}\right]^{1/2}\xi_2^{(\beta)} + \frac{m_3}{m_2+m_3}\left[\frac{\mu}{\mu_1^{(\beta)}}\right]^{1/2}\xi_1^{(\beta)} \right|} + \frac{Z_2 Z_3}{\left| \left[\frac{\mu}{\mu_1^{(\beta)}}\right]^{1/2}\xi_1^{(\beta)} \right|} \right.$$

$$\left. + \frac{Z_3 Z_1}{\left| \left[\frac{\mu}{\mu_2^{(\beta)}}\right]^{1/2}\xi_2^{(\beta)} - \frac{m_2}{m_2+m_3}\left[\frac{\mu}{\mu_1^{(\beta)}}\right]^{1/2}\xi_1^{(\beta)} \right|} \right\} . \qquad (20)$$

An expression like (20) is used in the evaluation of matrix elements when the wave functions are given in β coordinates.

D. Adiabatic treatment in hyperspherical coordinates

Using the mass-weighted Jacobi coordinates, the Schrödinger equation in the center-of-mass coordinate system is

$$\left[-\frac{\hbar^2}{2\mu}(\nabla_{\xi_1}^2 + \nabla_{\xi_2}^2) + V \right]\overline{\Psi} = E\overline{\Psi} . \qquad (21)$$

Equation (21) resembles the Schrödinger equation for the two-electron atoms except that the potential has complicated mass-weighted factors. In terms of hyperspherical coordinates, letting $\overline{\Psi} = \psi R^{-5/2}$, (21) becomes

$$\left[-\left[\frac{\partial^2}{\partial^2 R} - \frac{15}{4R^2} - \frac{\Lambda^2(\Omega)}{R^2}\right] + U - \varepsilon \right](\overline{\Psi}R^{5/2}) = 0 , \qquad (22)$$

where $U = 2\mu/\hbar^2 V$, $\varepsilon = 2\mu/\hbar^2 E$, and Λ^2 is the grand angular momentum operator defined in (9). Following the success of applying the quasiseparable approximation in hyperspherical coordinates in the study of doubly excited states of atoms, we expand

$$\psi(R,\Omega) = \sum_\mu F_\mu(R)\Phi_\mu(R;\Omega) , \qquad (23)$$

where the channel function Φ_μ satisfies the equation

$$\left[\frac{\Lambda^2(\Omega)}{R^2} + U \right]\Phi_\mu(R;\Omega) = U_\mu(R)\Phi_\mu(R;\Omega) \qquad (24)$$

and the hyperradial wave function satisfies

$$\left[\frac{d^2}{dR^2} - \frac{15}{4R^2} - U_\mu + \varepsilon + W_{\mu\mu}(R) \right]F_\mu(R)$$

$$+ \sum_\nu W_{\mu\nu}(R)F_\nu(R) = 0 , \qquad (25a)$$

where

$$W_{\mu\nu} = 2\langle \Phi_\mu | d/dR | \Phi_\nu\rangle d/dR + \langle \Phi_\mu | d^2/dR^2 | \Phi_\nu\rangle . \qquad (25b)$$

By dropping the interchannel coupling, the hyperradial wave function satisfies the one-dimensional equation

$$\left[\frac{d^2}{dR^2} - \frac{15}{4R^2} - U_\mu + \varepsilon + W_{\mu\mu}(R) \right]F_\mu(R) = 0 . \qquad (26)$$

The validity of (26) has been demonstrated for two-electron atoms.[1] Its validity will be assumed here.

The quasiseparability approximation allows us to examine the correlation, or equivalently, the geometric structure of the three particles if the particles are confined to a sharp-density distribution in configuration space. One of our goals in the study of Coulombic three-body problems is to examine how the shape varies with respect to the masses of the three particles.

It is appropriate to comment on the specific hyper-

spherical angles chosen in our approach. We retain the spherical angles $\hat{\xi}_1, \hat{\xi}_2$ of the two Jacobi radius vectors in each set of Jacobi coordinates. This has the advantage that the wave function for each adiabatic channel reduces to the independent particle wave function directly in the limit of two-body breakup, i.e., in the limit of large hyperradius. This choice is in contrast with the hyperspherical coordinates being used by quantum chemists[6-10] where three of the hyperspherical angles were chosen to be the Euler angles of the three-body system. The latter methods reduce the six-dimensional Schrödinger equation to a set of coupled three-dimensional partial differential equations in the two internal angles and the hyperradius.[13] Upon applying the quasiseparable approximation, the three-dimensional equations are reduced to eigenvalue problems in the two remaining hyperangles at each R which are then solved using finite-element methods.[6-8] The latter approach has the disadvantage that the structure of the differential equation becomes more complicated for nonzero total angular momentum states and that the solution of the adiabatic potential curves appears to be more complicated. In the present approach, we take advantage of the known solutions of Eq. (24) in the asymptotic region $(R \to \infty)$ and generalize them to the smaller-R region, to be described in Sec. III.

III. METHODS OF THE SOLUTION OF HYPERSPHERICAL CHANNEL FUNCTIONS

The major task in the hyperspherical approach is the numerical solution of the channel equation (24). For Coulombic three-body systems, the potential energy scales like $1/R$, while the kinetic-energy term in (24) scales like $1/R^2$. Thus the solution of (24) can be expanded in terms of hyperspherical harmonics at small R. At large R, if we only consider two-body breakup channels, then in the asymptotic limit the system reduces to a pair of charged particles which are described by hydrogenic wave functions (as functions of ξ_1) and a particle at a large distance. To find the most convenient method for solving the channel equation (24), we need to examine the properties of channel functions in the limit of $R \to 0$ and of $R \to \infty$.

The Coulombic three-body systems consist either of three distinguishable charged particles ABC or of two identical charged particles and a third different particle AAC. For bound states to exist, the sign of the charge in two of the particles has to be different. We adopt the convention that the two particles which have the same sign in charge are A and B if they are distinguishable and that they are also labeled as particles 1 and 2, respectively. For AAC systems, C is always designated as the third particle. According to this convention, the two-body breakup combinations are $A + (BC)$ or $B + (AC)$, and they are described most conveniently by the β-set Jacobi coordinates and γ-set Jacobi coordinates, respectively. For AAC systems, the two-body breakup is $A + (AC)$. In this case, proper symmetrization of the wave function is required.

The wave functions considered here include only the

spatial part. For AAC systems, the spatial wave functions have to be combined properly with the spin functions to obtain correct overall symmetries for the total wave functions. This combination depends on whether particle A is a Fermi particle or a Bose particle.

This section is organized into a few subsections. In Sec. III A we discuss the symmetry of hyperspherical harmonic functions in α set coordinates. In Sec. III B we examine the potential surface for a number of systems in α- and in β-set coordinates. This is followed by Sec. III C, where we describe how the channel equation (24) can be solved by expanding in terms of a complete set of hyperspherical harmonic functions. This method, although quite straightforward, is not very useful in practice because of its slow convergence. This slow convergence is attributed to the fact that the asymptotic solutions are not easily expanded in terms of hyperspherical harmonics. In Sec. III D the asymptotic behavior of the channel equation $(R \to \infty)$ is examined. Following Lin,[15] we propose a new set of analytical channel functions as the basis functions for the solution of (24). In Sec. III E we discuss the "mixed" basis functions where analytical channel functions in different Jacobi coordinates are used to solve Eq. (24). Practical problems in the evaluation of matrix elements in this approach are addressed in Sec. III F. Some preliminary results are given in Sec. IV.

A. Symmetries in hyperspherical harmonic functions

The symmetry of the wave functions for AAC systems is most conveniently examined if the wave functions are expressed in the α-set coordinates. Since there are no spin interactions, the spatial wave function has well-defined quantum numbers L, M, and parity. At small R, it is convenient to expand the channel function in hyperspherical harmonics,

$$\Phi_\mu(R;\Omega) = \sum_{[K]} g_{[K]}(R) Y_{[K]}(\Omega^\alpha) , \qquad (27)$$

where $[K] = [l_1, l_2, m]$ and where the explicit dependence of these quantum numbers on α has been dropped for simplicity. The interchange of particles 1 and 2 is equivalent to changing ρ_1 to $-\rho_1$, while ρ_2 remains unchanged. From (12), the hyperspherical harmonics acquires a phase $(-1)^{l_1}$ under such an operation. If the spatial wave function is symmetric under interchange of particles 1 and 2, then only even l_1 values are allowed in the expansion. If the spatial wave function is antisymmetric, then only odd l_1 is allowed. There are no other restrictions on the values of l_1 and l_2 except that they have to satisfy the triangular relation with L and that the sum $l_1 + l_2$ is even (odd) for even (odd) parity states. There is no restriction on the values of m.

The symmetry conditions for wave functions expressed in β- and γ-set coordinates are more complicated. They are discussed in Sec. III E below.

B. Potential surfaces in hyperspherical coordinates

The total Coulomb potential energy between three charged particles can be written in hyperspherical coordinates in the form
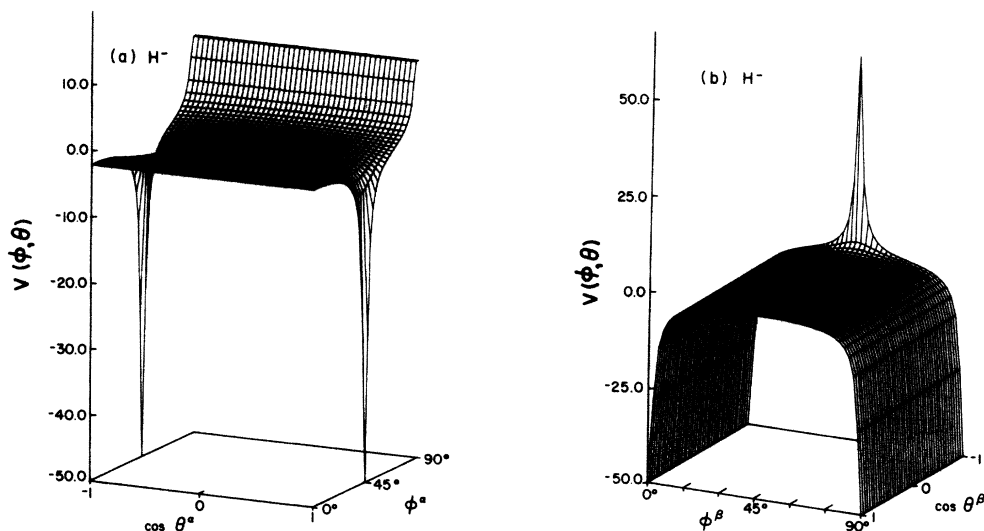
FIG. 2. Potential surfaces of H^- at constant hyperradius in (a) α-set and (b) β-set Jacobi coordinates. The repulsive "wall" at $\phi = 90°$ in (a) has been "chopped" off. Potential energies are given in arbitrary units.

$$V(R,\Omega) = C(\phi,\theta)/R , \tag{28}$$

where θ is the angle between the two Jacobi coordinates ξ_1 and ξ_2 and the effective charge C depends on the angles used. Contour plots of the effective charges C in α- and in β-set coordinates are shown in Figs. 2, 3, and 4 for H^-, $e^-e^-e^+$ and $d^+d^+\mu^-$, respectively, and in Fig. 5 for the $e^+p^+e^-$ system.

We first compare the potential surfaces of H^- in different sets of Jacobi angles. In Fig. 2(b) we note that the potential surface in β-set coordinates is similar to the one examined in previous studies for H^- (see Fig. 2 of Ref. 1). This is not surprising since in this case the Jacobi

coordinates $\rho_1^{(\beta)} \approx -r_2$, $\rho_2^{(\beta)} \approx r_1$, where r_1 and r_2 are the vectors from the nucleus to the two electrons. The two potential valleys are due to the strong electron-nucleus attraction and the spike is due to the Coulomb repulsion between the two electrons when they are nearly on top of each other. The same potential takes on quite a different look when expressed in the α-set coordinates. As shown in Fig. 2(a), the special features of this surface are the two sharp attractive singular potential "holes" and the infinite repulsion wall (chopped off in the figure) at $\phi = 90°$. The two holes correspond to the two potential valleys and the repulsive wall corresponds to the spike in Fig. 2(b), respectively.
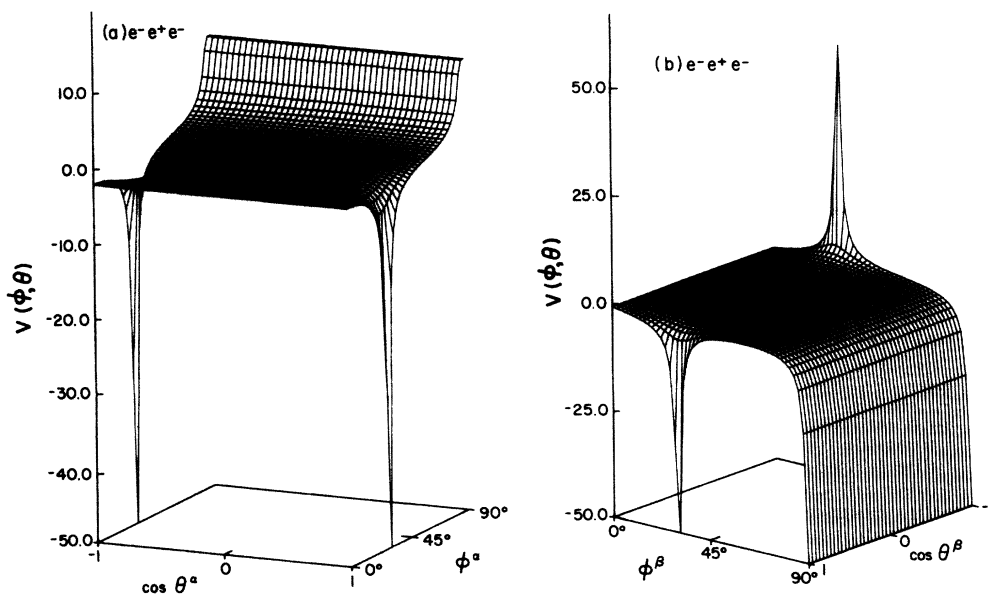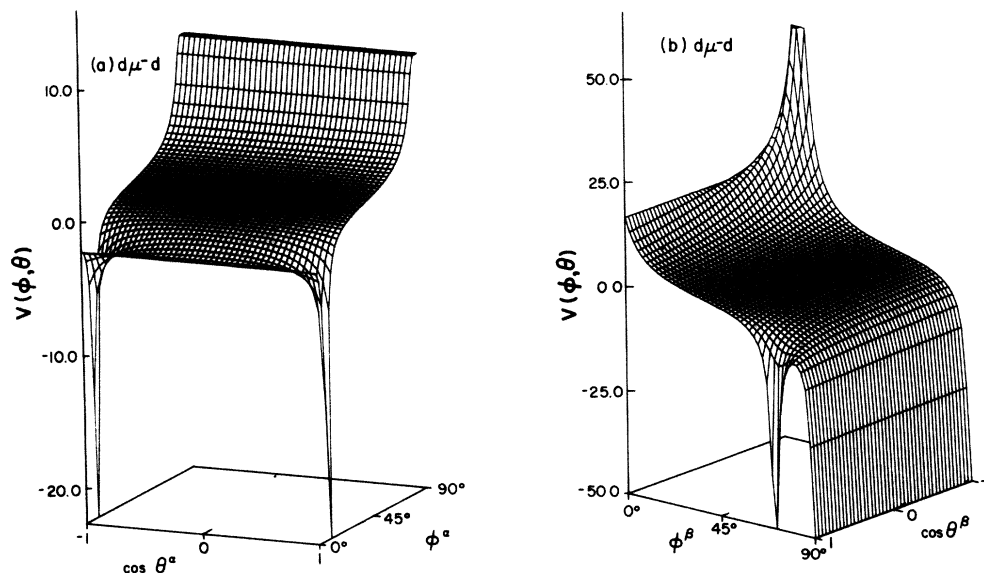

FIG. 3. Same as Fig. 2 but for $e^-e^+e^-$.

FIG. 4. Same as Fig. 2 but for $d^+\mu^-d^+$.

The location of singularities in the potential surface in a given set of Jacobi angles can be easily found by examining the expression of the Coulomb potential expressed in that coordinate system. In α-set coordinates, the repulsive singularity occurs when $\cos\phi=0$ or $\phi=90°$. Two attractive singularities occur at $(\theta,\phi)=(0°,\phi_0^\alpha)$ and $(180°,\phi_0^\alpha)$, where

FIG. 5. Potential surface for $e^+p^+e^-$ in the β-set Jacobi coordinates. The repulsive wall at $\phi=0$ has been "chopped" off.

$$\tan\phi_0^\alpha = \frac{m_1}{m_1+m_2} \left[\frac{\mu_2^{(\alpha)}}{\mu_1^{(\alpha)}} \right]^{1/2}. \qquad (29)$$

This angle is 44.98° for H^-. If the mass of the proton is assumed to be infinite, this angle would be 45°.

We now look at the potential surfaces in α-set coordinates for other systems. From Figs. 2(a), 3(a), and 4(a), we note that the potential surfaces for all three systems are very similar. The repulsive wall is always located at $\phi=90°$, and the two attractive holes are always located symmetrically at $(\theta,\phi)=(0°,\phi_0^\alpha)$ and $(180°,\phi_0^\alpha)$, with $\phi_0^\alpha=44.98°$, 30°, and 9.40° for H^-, $e^-e^+e^-$, and $d^+\mu^-d^+$, respectively. In fact, this angle is 0.945° for H_2^+. The similarity of these potential surfaces, as seen in α-set coordinates, provides a first hint of possible similar physical behaviors of these Coulombic three-body systems. We comment that this coordinate system is the "natural" one used in the Born-Oppenheimer treatment of the H_2^+ molecular ion. However, this is also the coordinate system where the potential surface is symmetric with respect to $\theta=90°$, or with respect to the interchange of the two identical particles. We further stress that the axis between the two identical particles, i.e., the symmetry axis, has been shown recently to be an approximate internal axis of rotation for the doubly excited states[12,17] as well as for double-escape states[18] of atomic systems such as H^- and He. The physical basis of this internal axis of rotation may be attributed to the fact that this axis is the symmetry axis for any three-body system with two identical particles.

The potential surfaces in β-set coordinates also show singularities. There are two attractive singularities, one is a line along $\phi^\beta=90°$, the other is at the point $\theta=0°$ and $\phi=\phi_0^\beta$, where

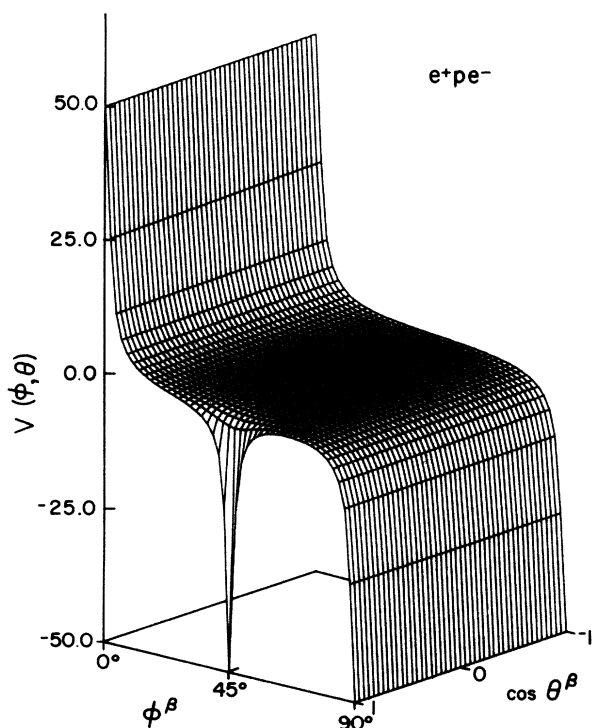$$\tan\phi_0^\beta = \frac{m_2}{m_2+m_3} \left[\frac{\mu_2^{(\beta)}}{\mu_1^{(\beta)}} \right]^{1/2}. \qquad (30)$$

Thus there is a potential valley along $\phi^\beta = 90°$ and an attractive potential hole at $(\theta,\phi) = (0°, \phi_0^\beta)$. The angle ϕ_0^β is 0.0312°, 30°, 71.20°, 88.11° for H^-, $e^- e^- e^+$, $d^+ d^+ \mu^-$, and H_2^+, respectively. The repulsive singularity occurs at $\theta = 180°$ and

$$\tan\phi_1^\beta = \frac{m_3}{m_2 + m_3} \left[\frac{\mu_2^{(\beta)}}{\mu_1^{(\beta)}} \right]^{1/2} , \qquad (31)$$

where $\phi_1^\beta = 44.984°$, 30°, 9.4°, and 0.945° for H^-, $e^- e^- e^+$, $d^+ d^+ \mu^-$, and H_2^+, respectively. The potential surfaces do *not* exhibit any symmetries in β-set coordinates. For AAC systems, the potential surface in the γ set would look like the corresponding one in the β set.

It may be noted that the potential hole for H^- at $(\theta,\phi) = (0°, 0.0312°)$ does not show up as a hole in Fig. 2(b) but rather as a potential valley. The graphic resolution was unable to pick up such details in a small angular range. We note that the potential surface in Fig. 2(b) displays symmetry only if the mass of the proton can be approximated as infinite, or correspondingly, when the mass polarization effect is neglected. The singularities in the potential surfaces are summarized for a number of three-body Coulombic systems in Table I.

C. Expansions in hyperspherical harmonics

Equation (24) can in principle be solved by expanding the channel function in terms of hyperspherical harmonics. For ABC systems, one can choose hyperspherical harmonics among the α-, β-, or γ-set coordinates. For a converged calculation, the result would not depend on the coordinate set chosen. For the AAC system, it is more convenient to use the α set since the exchange symmetry between the two identical particles can then be conveniently carried out (see Sec. III A). In terms of hyperspherical harmonics in the α set, the repulsive potential between particles 1 and 2 [to be abbreviated as the (12) interaction] is diagonal in (l_1, l_2). Mixture of (l_1, l_2) pairs is due to the attractive interactions between 1 and 3, and between 2 and 3. This is very different from the conventional independent-particle approximation in atoms where the interelectronic repulsion is responsible for the breakdown of l_1 and l_2 quantum numbers. Of course, the l_1 and l_2 used here are not the angular momenta of any two particles; rather, they are those due to the composite reduced particles in the α set.

The expansion in hyperspherical harmonics is known to converge very slowly. In the limit of large hyperradii,

TABLE I. Singular points in the potential surfaces in different Jacobi coordinates for Coulombic three-body systems.

	H^-	$e^- e^- e^+$	$d^+ d^+ \mu^-$	H_2^+	$e^+ p^+ e^-$	$d^+ t^+ \mu^-$
			α set			
Repulsive line						
$\phi =$	90°	90°	90°	90°	90°	90°
Attractive point						
$\theta =$	0°	0°	0°	0°	0°	0°
$\phi =$	44.98°	30°	9.40°	0.945°	0.0312°	6.912°
Attractive point						
$\theta =$	180°	180°	180°	180°	180°	180°
$\phi =$	44.98°	30°	9.40°	0.945°	44.98°	10.307°
			β set			
Repulsive point						
$\theta =$	180°	180°	180°	180°	180°	180°
$\phi =$	44.984°	30°	9.40°	0.945°	0.0312°	6.91°
Attractive line						
$\phi =$	90°	90°	90°	90°	90°	90°
Attractive point						
$\theta =$	0°	0°	0°	0°	0°	0°
$\phi =$	0.0312°	30°	71.20°	88.11°	44.98°	72.78°
			γ set			
Repulsive point						
$\theta =$	0°	0°	0°	0°	0°	0°
$\phi =$	44.984°	30°	9.40°	0.945°	44.98°	10.307°
Attractive line						
$\phi =$	90°	90°	90°	90°	90°	90°
Attractive point						
$\theta =$	180°	180°	180°	180°	180°	180°
$\phi =$	0.0312°	30°	71.20°	88.11°	44.98°	72.78°

the channel function reduces to hydrogenic solutions near the deep potential wells at $(\phi, \theta) = (\phi_0^\alpha, 0°)$ and $(\phi_0^\alpha, 180°)$ (see Table I). We expect that the physical solutions to concentrate near these two singularities. Such localized solutions cannot be conveniently expanded in hyperspherical harmonics which are polynomial functions in ϕ and θ. In other words, it would take a very large set of hyperspherical harmonic functions including large values of (l_1, l_2) and m quantum numbers to obtain reasonable accuracy for the channel functions at large R. Although this can be done by selective prediagonalization of a subset of hyperspherical harmonics,[19,20] the need of a large basis set makes such a method less appealing.

D. Asymptotic solutions in the large-R limit

To describe physical solutions in the large-R limit where particles 2 and 3 form a bound state, it is convenient to use β-set Jacobi coordinates. In this limit, the angular momentum l_1 is the orbital angular momentum of the two-body system (23) which is limited to small values if only low-lying states are considered. Since l_1 and l_2 have to form a triangular relation with L, the con-

vergence in terms of the expansion in (l_1, l_2) pairs is quite fast. (Note: All the quantities in this subsection refer to the β set.) Furthermore, the approximate channel solutions in the large-R limits are known—they are hydrogenic solutions of the (23) system. By taking advantage of these known solutions, we follow Lin[15] in developing a set of analytic channel functions for each pair of (l_1, l_2). Define

$$\Phi_\mu = X_\mu(R;\Omega)/(\sin\phi \, \cos\phi) . \tag{32}$$

Equation (24) becomes

$$\left[\frac{1}{R^2} \left[-\frac{\partial^2}{\partial^2 \phi} - 4 + \frac{l_1^2(\hat{\xi}_1)}{\cos^2\phi} + \frac{l_2^2(\hat{\xi}_2)}{\sin^2\phi} \right] + V \right] X_\mu = U_\mu X_\mu . \tag{33}$$

In the large-R limit, particle 1 is far away from the (23) pair, and we have

$$\xi_1 = R \cos\phi, \quad \xi_2 = R \sin\phi \simeq R \quad \text{as } \phi \to \pi/2 , \tag{34}$$

and (33) reduces to

$$\left[\left[-\frac{\partial^2}{\partial^2 \xi_1} + \frac{l_1^2}{\xi_1^2} + \frac{2\mu e^2}{\hbar^2} \frac{Z_2 Z_3}{\left[\frac{\mu}{\mu_1} \right]^{1/2} \xi_1} \right] \right.$$

$$+ \frac{2\mu e^2}{\hbar^2} \left[\frac{Z_1 Z_2}{\left| \left[\frac{\mu}{\mu_2} \right]^{1/2} \xi_2 + \frac{m_3}{m_2 + m_3} \left[\frac{\mu}{\mu_1} \right]^{1/2} \xi_1 \right|} + \frac{Z_3 Z_1}{\left| \left[\frac{\mu}{\mu_2} \right]^{1/2} \xi_2 - \frac{m_2}{m_2 + m_3} \left[\frac{\mu}{\mu_1} \right]^{1/2} \xi_1 \right|} \right]$$

$$\left. + \frac{1}{R^2} \left[\xi_1^2 \frac{\partial^2}{\partial^2 \xi_1} + \xi_1 \frac{\partial}{\partial \xi_1} + l_2^2 - 4 \right] + \theta \left[\frac{1}{R^4} \right] \right] X_\mu = U_\mu X_\mu . \tag{35}$$

The first terms in the large parentheses are the hydrogenic Hamiltonian with effective charge $Z = (\mu_1/\mu)^{1/2} Z_2 Z_3$ and mass μ. Its eigenvalue is $-\mu_1 Z_2^2 Z_3^2 / n^2$ Ry $(e = \hbar = 1)$, where n is the principal quantum number. This is identical to the energy of the hydrogenic system (23) with charges Z_2 and Z_3 and reduced mass μ_1. By expanding the terms in the second large parentheses to order $1/\rho_2^2$, we obtain

$$V \to \frac{Z_1 Z_2}{\rho_2} \left[1 - \frac{m_2}{m_2 + m_3} \frac{\rho_1}{\rho_2} \cos\theta \right]$$

$$+ \frac{Z_3 Z_1}{\rho_2} \left[1 + \frac{m_2}{m_2 + m_3} \frac{\rho_1}{\rho_2} \cos\theta \right] , \tag{36}$$

where ρ_1 is the radius of the hydrogenic system (23). It can be shown[14] that the terms in the last large parentheses excluding l_2^2 in (35) are canceled by the diagonal nonadiabatic coupling term $\langle X_\mu | d^2/dR^2 | X_\mu \rangle$. By specializing to $Z_1 = Z_2 = -1$, $Z_3 = +1$ or $Z_1 = Z_2 = +1$,

$Z_3 = -1$, the asymptotic potential to order $1/R^2$ can be obtained by diagonalizing the operator

$$U_\mu(R) = -\mu_1 \frac{1}{n^2} + \frac{1}{R^2} (-2\mu_2 \rho_1 \cos\theta + l_2^2) . \tag{37}$$

Note that the dipole term in the $1/R^2$ coefficient has the correct reduced mass. For states which lie below the $N \geq 2$ hydrogenic limit, this dipole term contributes to the long-range coupling. In this case, the channel function in the asymptotic region is a linear combination of hydrogenic wave functions.[15] These channel functions are said to be in the dipole representation.

In the asymptotic limit, the function X_μ for each (l_1, l_2) is

$$\xi_1 R_{nl_1}(\xi_1) \mathcal{Y}_{l_1 l_2 LM} ,$$

where R_{nl_1} is the hydrogenic radial wave function. This is the asymptotic solution for $\phi \to 90°$. It is our intention to generalize this hydrogenic solution to the small-R region. To do this, we examine the ϕ dependence in the $R = 0$ limit which is given by the hyperspherical harmon-

ics. Following Lin[15] it is clear that one should multiply a factor $(\sin\phi)^{l_2+1}$ by the hydrogenic function such that our analytical channel function in the β set is

$$\Phi_j^{(\beta)} = CR_{nl_1}(\xi_1)\xi_1(\sin\phi)^{l_2+1}\mathcal{Y}_{l_1l_2LM}/(\cos\phi\sin\phi) , \quad (38)$$

where $C = C(R)$ is a normalization constant.

With this choice of basis functions, we expect that only a few analytical channel functions are needed in the calculation of channel functions for those states which dissociate to $1 + (23)$. Notice that the states which are well represented by the expansion (38) are those which lie in the potential well along $\phi^\beta = 90°$ in Figs. 2–5. Those states which dissociate as $(13) + 2$ correspond to states concentrate near the hole, i.e., in the $(\phi^\beta = \phi_0, \theta = 0)$ region in Figs. 2–5. These latter states are better expressed in the γ set where they would lie in the potential well along $\phi^\gamma = 90°$.

E. A mixed basis function for solving the channel functions

We have now discussed the advantages of various sets of hyperspherical angles for describing states in the three-body system in each limited region of space. Unfortunately, a full solution requires us to deal with the whole space. A possible basis set in the solution of the channel function is then to express the channel function as

$$\Phi_\mu = \sum_i g_i^{(\alpha)}Y_{[K_i]}(\Omega^\alpha) + \sum_j g_j^{(\beta)}\Phi_j^{(\beta)}(R;\Omega^{(\beta)})$$
$$+ \sum_k g_k^{(\gamma)}\phi_k^{(\gamma)}(R;\Omega^{(\gamma)}) . \quad (39)$$

This expansion has been expressed specifically for the Coulombic three-body systems where there are no $(1 + 2)$ bound states in the asymptotic region. The hyperspherical harmonics in the α set are added in the expansion only to account for possible slow convergence in the small-R region. Our preliminary calculations indicated that these functions are not necessary, but definite conclusion cannot be made until full calculations have been carried out. In generalizing (39) to other three-body systems where the pair interactions among the particles are all attractive, as in most triatomic molecules, the α-set hyperspherical harmonics will be replaced by the channel functions describing the bound state of the $(1 + 2)$ pair.

The expansion (39) requires some modifications in the presence of identical particles in the system. For AAC systems, the symmetry condition is properly enforced in the α-set hyperspherical harmonics by limiting the values of l_1. For the β set, we note that the interchange of 1 and 2 gives a set similar to that of the γ set except that ρ_1 goes from 1 to 3 instead of from 3 to 1. A symmetric solution can be constructed from

$$[\Phi_j^{(\beta)}(1,2,3) + \Phi_j^{(\beta)}(2,1,3)]$$

$$= [\Phi_j^{(\beta)}(1,2,3) + (-1)^{l_1^\beta}\Phi_j^{(\gamma)}(1,2,3)] , \quad (40)$$

where the last line follows from the inversion properties of the wave function of the (23) system. To put Eq. (40) in a more general form, if particles 1 and 2 are spin-$\frac{1}{2}$ fermions, then the proper basis functions are

$$[\Phi_j^{(\beta)}(1,2,3) + (-1)^{S+l_1^\beta}\Phi_j^{(\gamma)}(1,2,3)] , \quad (41)$$

and (39) is replaced by

$$\Phi_\mu = \sum_i g_i^{(\alpha)}Y_{[K_i]}(\Omega^\alpha)$$
$$+ \sum_j g_j^{(\beta)}[\Phi_j^{(\beta)} + (-1)^{S+l_1^\beta}\Phi_j^{(\gamma)}] . \quad (42)$$

Here i denotes the set of $l_1^{(\alpha)}, l_2^{(\alpha)}, m^{(\alpha)}$ quantum numbers; j, the set of $n^{(\beta)}, l_1^{(\beta)}, l_2^{(\beta)}$ quantum numbers; and S is the total spin of the two identical particles.

If the two identical particles are bosons, such as the two deuterons in the $d^+d^+\mu^-$ system, we require that the total wave functions be symmetric. Since each deuteron has spin 1, the total spin of the two deuterons can be 0, 1, and 2. The spin function for the total spin-1 state is antisymmetric so that the spatial wave function should be antisymmetric. The spin functions for total spin-0 and spin-2 states are symmetric so that the spatial functions are symmetric. Therefore, the basis expansion (42) can be applied to $d^+d^+\mu^-$ system as well. In the present approximation we consider only the Coulomb interactions between the particles, thus the spin-0 and -2 states are degenerate.

F. Practical problems in the numerical calculations

The mixed-base expansions in (39) or (42) would allow us to use a small number of functions in the solution of the channel wave functions. In practical calculations there are a number of complications. Firstly, the analytical channel function at each R has to be normalized. This poses additional problems for the basis functions in (42) since one is required to evaluate overlap integrals of basis functions between the β-set and γ-set coordinates. Secondly, the analytical channel functions are not orthogonal. Thirdly, we need to face the difficulty of calculating matrix elements of the types

$$\langle Y_{[K]}(\Omega^\alpha) | V | \Phi_j^{(\beta)} \rangle ,$$

$$\langle Y_{[K]}(\Omega^\alpha) | V | \Phi_k^{(\gamma)} \rangle , \quad (43)$$

$$\langle \Phi_j^{(\beta)} | V | \Phi_k^{(\gamma)} \rangle .$$

This is the price we have to pay for insisting on using a small basis set. On the whole we still believe that this is a more practical approach since we can use our physical understanding of the two-body problems in choosing basis functions.

The evaluation of matrix elements in (43) is carried out with the aid of the transformation bracket[16] of hyperspherical harmonics. To evaluate the first matrix element of (43), for example, we can expand the α-set hyperspherical harmonics in terms of β-set hyperspherical harmonics and then the matrix elements are evaluated in β-set coordinates. There are no intrinsic approximations used

in the calculation of this matrix element. Similarly, this can be done for the second matrix elements. For the third matrix element of (43) we first expand $\phi_k^{(\gamma)}$ in terms of γ-set hyperspherical harmonics,

$$\phi_K^{(\gamma)}=\sum_m C_m Y_{[l_1 l_2 m]}^{(\gamma)} \ . \tag{44}$$

Note that the values of l_1 and l_2 are fixed in this expansion. The γ-set hyperspherical harmonics can be transformed to β-set hyperspherical harmonics using the transformation bracket. The resulting integral is then evaluated in β-set coordinates. The major approximation in this approach is the truncated expansion in (44). The truncation error is more serious in the large-R region. However, at large R the overlap as well as the matrix elements of the type in (43) become smaller since in the dissociation limit the different breakup channels do not overlap significantly.

G. Merits and intrinsic limitations of the method

It is appropriate to comment on the merits and the intrinsic limitations of the method proposed here, in particular, in its comparison with other existing methods in the literature for the solution of three-body Coulomb problems in hyperspherical coordinates. Firstly, the present method is applicable directly to states of arbitrary total orbital angular momentum L of the three-body system and to a wide range of masses for the three particles. The (anti)symmetrization of the total wave function for systems with identical particles can be easily implemented. Secondly, the method can be generalized to molecular and nuclear three-body problems straightforwardly. The method takes advantage of the known analytical or semi-analytical solutions of the two-body system in each dissociation channel, thus the basis functions needed in the calculation can be chosen intelligently in accordance with the physical system under consideration.

There are two other methods which have been applied to the solution of the channel equation (24) for arbitrary L's of which we are aware. In the work of Botero and Greene,[19] the solution in (24) is expanded in terms of hyperspherical harmonics in α-set coordinates (see Sec. III C). The slow convergence of this method is well known, and it is difficult to apply the method to systems where m/m_3 ($m=m_1=m_2$) is much greater than unity, such as $d^+\mu^-d^+$, for example. In the other limit where m_3/m (m is m_1 or m_2) is very small, i.e., the "molecular limit" such as H_2^+ and HD^+, the channel function has been solved in powers of m_3/m to first order by Macek and Jerjian.[21] If one is limited to $L=0$ states, then a method similar to the present one has been applied by Botero and Greene[22] to $e^-e^+e^-$ by using the same analytical channel functions as ours. Their method reduces the evaluation of matrix elements to two-dimensional integrals since no Euler angles are presented for $L=0$ states. Other forms of basis functions can be used for expansion in the solution of (24). For example, Botero[23] introduced Hylleraas-type functions and calculated the lowest potential curves for $d^+\mu^-t^+$ and $d^+\mu^-d^+$ systems variationally. Generalization of these

two methods to states with $L\neq0$ becomes quite complicated and has not been implemented so far.

There are a number of potential intrinsic limitations on the present method which should be addressed. It is known that the adiabatic basis functions converge slowly in the asymptotic region[24] (large R). How serious is this in scattering problems has to be addressed in the future in actual calculations, but methods for matching solutions to the independent-particle coordinates exist.[25] The basis functions used in our present method are nonorthogonal. In calculations where a large basis set is employed, one may question the possibility of numerical linear dependence. This possibility is reduced by the fact that the analytical basis functions used here are intended such that a "minimum" basis set is to be employed. The linear dependence can be avoided also by a judicious choice of basis functions. Since the basis set is expected to be small, this can be easily done. In the present approach, the rearrangement coupling is evaluated using transformation brackets of hyperspherical harmonics. Since these integrals are of a short-range nature this has not limited the accuracy of our calculations severely. These rearrangement integrals can be calculated[26] by a two-dimensional numerical integration similar to those used by Botero and Greene[22] for any L's, but similar numerical difficulty exists at large R.

IV. APPLICATIONS

To test the utility of analytical channel functions and the method discussed in this article for the solution of the adiabatic potential curves, in this section we present calculations for a number of Coulombic three-body systems using only one basis function for AAC systems and two basis functions for ABC systems. For AAC systems, the basis function is

$$\Phi=\phi^{(\beta)}+(-1)^{S+l_1}\phi^{(\gamma)} \ ,$$
$$\phi^{(\beta)}=CR_{1s}(\xi_1)(\sin\phi)^{l_2}\mathcal{Y}_{l_1 l_2 LM}(\hat{\xi}_1,\hat{\xi}_2) \ , \tag{45}$$

where

$$R_{1s}(\xi_1)=\exp(-\sqrt{\mu_1\mu}Z_2 Z_3\xi_1) \tag{46}$$

is the hydrogenic 1s ($l_1=0$) radial wave function, C is a normalization constant, and all the labels refer to β-set coordinates. The potential curve obtained corresponds to the lowest curve for the symmetry considered. For ABC systems, we include two basis functions, one in the β set and another in the γ set

$$\Phi=A_\beta\phi^{(\beta)}+A_\gamma\phi^{(\gamma)} \ , \tag{47}$$

where $\phi^{(\gamma)}$ has the same form as $\phi^{(\beta)}$. The two resulting potential curves correspond to the lowest curve in each of the $A+(BC)$ and $B+(AC)$ dissociation limits. In the evaluation of matrix elements involving functions from different sets of Jacobi coordinates, we need to expand the analytical channel function in terms of hyperspherical harmonics [see Eq. (44)]. In the present work we limit the expansion to the lowest 13 functions, i.e., with $m=0,1,2,\ldots,12$. The convergence of this expansion is

excellent for small R and adequate for large R. We note again that we need to do this expansion only when evaluating integrals involving functions from two different sets of coordinates. At large R, such integrals are small and thus the truncation error is not significant.

In the following we present some typical results. It is not our intention to discuss each system in detail here since we have only performed simple calculations so far. More complete calculations including doubly excited states for each system are underway and the results from those studies will be reported in due time. However, the present simple calculations do display how the behaviors of the physical systems evolve as the masses of the particles are varied.

A. H⁻

The center of mass for this system is very close to the proton, and $\rho_1^\gamma \simeq r_1$ and $\rho_1^\beta \simeq -r_2$. Therefore, the basis functions presented here do not differ in any significant way from the ones used previously[15] by assuming the mass of the proton to be infinite. The lowest potential curves for $^{1,3}S^e$ and $^{1,3}P^o$ calculated using the present method reproduced the previous calculations.[15] We just mention that for H⁻ the lowest $^1S^e$ potential curve which supports only one bound state—the ground state of H⁻ is attractive, and that the lowest curves for $^3S^e$, $^1P^o$, and $^3P^o$, are completely repulsive. The readers are referred to Refs. 1 or 15 for details of these curves.

B. $e^-e^-e^+$

Potential curves corresponding to $^1S^e$, $^3S^e$, and $^1P^o$ for this system are shown in Fig. 6. For $^1S^e$, we can compare our one-basis function result with the calculation of Botero and Greene.[22] These authors obtained the potential curve, shown by the dashed-dotted lines, by diagonalizing the Hamiltonian starting with β-set analytical channel functions (similar to ours), but the integrals were evaluated in α-set coordinates. Notice that a single analytical channel function in the β set already provides a very good approximation to the calculation of Botero and Greene. We expect that our results converge with theirs if a few more basis functions are included. The discrepancy is due to the lack of "angular correlation" in the present calculation in that basis sets of p^2 and d^2, i.e., $(l_1, l_2) = (1,1)$ and $(2,2)$ were not included. (A similar study for H⁻ has been reported, see Ref. 27.) This work is in progress and the results will be reported together with the study of doubly excited states of this system.

We have also shown the lowest potential curves for $^3S^e$ and $^1P^o$. Both curves are repulsive and look similar to the corresponding ones in H⁻. Except for the mass scaling, we note that there is no drastic difference in the potential curves between H⁻ and $e^-e^-e^+$. Such mass scaling has been studied recently in a Hylleraas-type calculation.[28]

C. $d^+d^+\mu^-$

This system has been studied quite extensively in conjunction with the interest in muon-catalyzed fusion. The
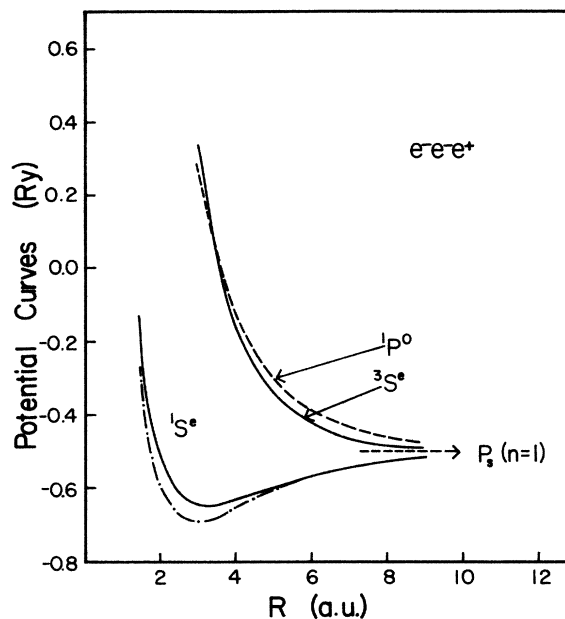

FIG. 6. Adiabatic potential curves for $e^-e^+e^-$ calculated with a single analytical channel function for $^1S^e$, $^3S^e$, and $^1P^o$ symmetries. The dashed-dotted line is from the calculation of Ref. 22.

lowest $^1S^e$ potential curve calculated with one basis function is shown in Fig. 7. The potential curve is normalized so that it approaches -1.0 Ry in the dissociation limit [absolute energy scale is obtained by (multiplied by) the reduced mass of the $(d\mu)$ pair]. To demonstrate that diagonalization in the α-set hyperspherical harmonics gives very slow convergence, we also indicate in Fig. 7 in dashed-dotted lines the potential curve obtained by di-
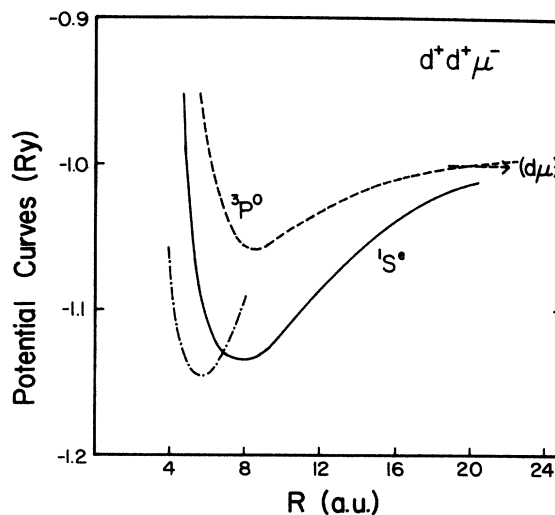

FIG. 7. Adiabatic potential curves for $^1S^e$ and $^3P^o$ symmetries of the $d^+d^+\mu^-$ system calculated with a single analytical channel function. The energy scale is normalized to -1.0 Ry asymptotically, see text. The dashed-dotted line is obtained by diagonalization in a set of 39 hyperspherical harmonics in α-set coordinates (see text).

agonalizing in a basis of 39 hyperspherical harmonics. The hyperspherical harmonics chosen are (l,l,m) $=(0,0,m)$, $m =0,1,\ldots,8$; $(2,2,m)$, $m =0,1,2,\ldots,6$; $(4,4,m)$, $m =0,1,2,3$; $(6,6,m)$, $m =0,1$; $(l,l,0)$, $l =8,10,12,14$. We note that diagonalization using hyperspherical harmonics gives better results at small R, but becomes less accurate than the result obtained from a single analytical channel basis function at moderate and large values of R.

In Fig. 7 we also show the $^3P^o$ curve. This curve is to be compared with the $^3P^o$ curve in H^- or in $e^-e^-e^+$. In spite of the different statistics and corresponding spins, the spatial functions for the $^3P^o$ states of these systems are antisymmetric. (Since deuterons are bosons with spin 1, the spin function correspond to this state is antisymmetric, i.e., $S =1$.) We note that this curve has an *attractive* potential well with a repulsive barrier at large R (varies as $2/R^2$), in contrast with the complete repulsive curves in H^- and in $e^-e^-e^+$. In other words, we witnessed a drastic change in the shape of potential curves, and thus the spectra, as the mass ratio of the system is changed. We comment that there are two bound states known to exist for this curve.[29-32] To get accurate quantitative results, we would need to perform calculations in a larger basis set. We only demonstrate that a single basis function calculation is already capable of exhibiting the major features of this three-body system.

D. $p^+p^+\mu^-$

We have calculated the lowest potential curves for both $^1S^e$ and $^{1,3}P^o$ symmetries. The $^1S^e$ potential curve, as shown in Fig. 8, is very similar to the one shown for

the $d^+d^+\mu^-$ system. In terms of the normalized energy scale explained in Sec. IV C, we note that the minimum value of the potential curve in this case is slightly lower than that in $d^+d^+\mu^-$. One has to remember though that the hyperspherical radius is mass-weighted so that it is not the internuclear separation. We emphasize here that the $^1P^o$ curve is completely repulsive and the $^3P^o$ curve shows an attractive potential well at small R, similar to the one shown for $d^+d^+\mu^-$.

We stress here that both of the $L =1$ curves are completely repulsive for H^- and for $e^-e^-e^+$, but one of the $L =1$ curves show an attractive potential well at small R for $p^+p^+\mu^-$ and for $d^+d^+\mu^-$. In the future it would be desirable to investigate the minimum value of m_1/m_3 which would result in at least one bound state for $L =1$. Similar questions can be raised for other L's.

E. $e^+p^+e^-$

We show the two lowest potential curves for $L =0$ and $L =1$, respectively, in Fig. 9. The two $L =0$ curves are almost indistinguishable from the calculation of Pelikan and Klar[33] where they used a large set of hyperspherical harmonics (about 200) to diagonalize the Hamiltonian. The attractive potential wells are not strong enough to support bound states. The two $L =1$ curves are completely repulsive, see Fig. 9.
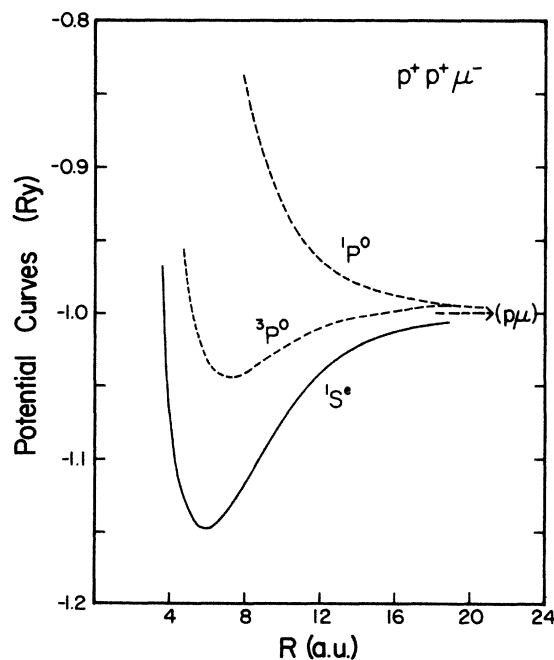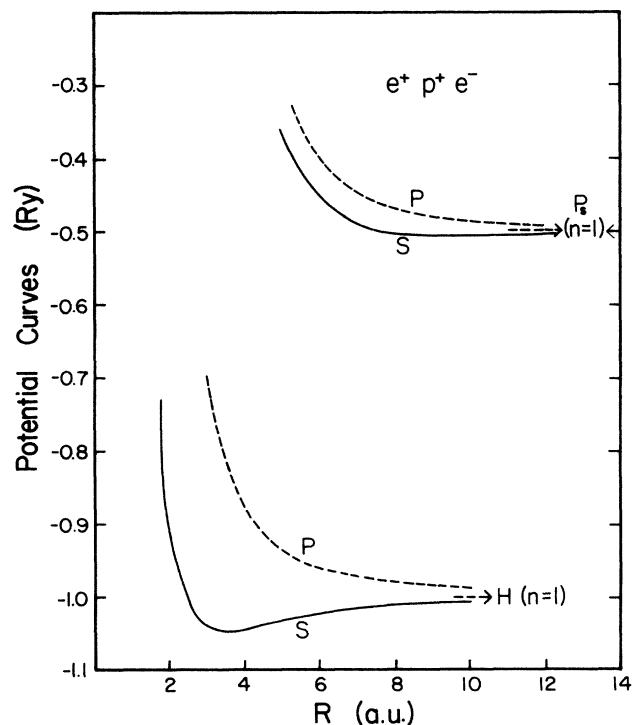

FIG. 8. Adiabatic potential curves for $^1S^e$, $^1P^o$, and $^3P^o$ symmetries of the $p^+p^+\mu^-$ system calculated with a single analytical channel function. The energy scale has been normalized as in Fig. 7.

FIG. 9. The two lowest potential curves for $L =0$ and $L =1$ of $e^+p^+e^-$ system calculated with one analytical channel function in β-set coordinates and one in γ-set coordinates. One of the curves for each L converges to the ground state of H and another to the ground state of positronium.
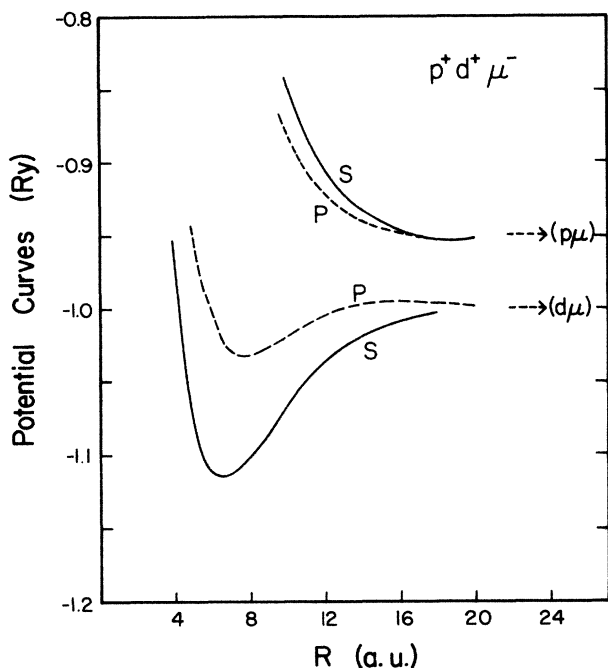
FIG. 10. The same as Fig. 9 but for the $p^+d^+\mu^-$ system. The lower pair of curves converge to the ground state of $(d^+\mu^-)$ and the upper pair of curves to the ground state of $(p^+\mu^-)$. The energy scale has been normalized as in Fig. 7.
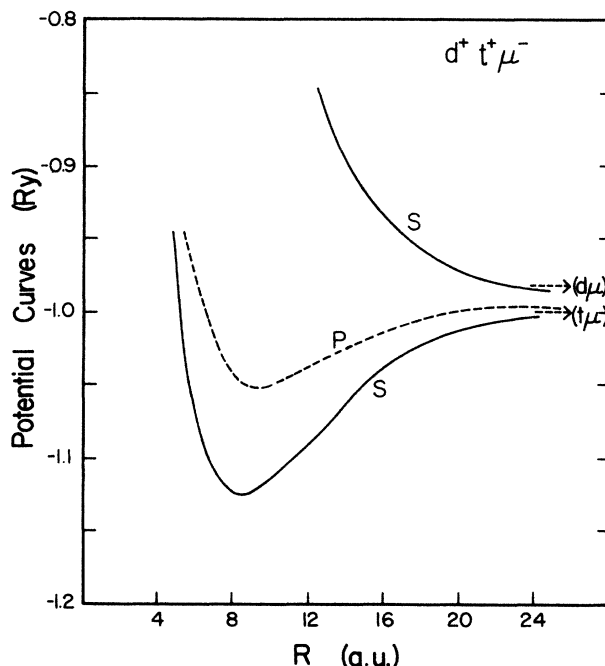
FIG. 11. The two lowest $L=0$ curves and the lowest curve for $L=1$ of the $d^+t^+\mu^-$ system. The second repulsive $L=1$ curve is not shown. The energy scale has been normalized as in Fig. 7.

F. $p^+d^+\mu^-$

The two lowest potential curves for $L=0$ and $L=1$ are shown in Fig. 10. It is normalized such that the asymptotic limit of the lowest curve is -1.0 Ry. The special feature for this system is that the lowest $L=1$ curve exhibits a potential well at small R and a potential barrier at large R where the potential behaves asymptotically like $2/R^2$. This is quite different from the $e^+p^+e^-$ system where the $L=1$ curves are completely repulsive. On the other hand, we can compare the two $L=1$ curves with the two $L=1$ curves for $p^+p^+\mu^-$. The lowest $L=1$ curve here corresponds to the $^3P^o$ curve for $p^+p^+\mu^-$, and the repulsive $L=1$ curve corresponds to the $^1P^o$ curve for $p^+p^+\mu^-$.

G. $d^+t^+\mu^-$

We show in Fig. 11 the two $L=0$ potential curves and the lowest $L=1$ curve. The $L=1$ curve is of particular interest in the study of muon-catalyzed fusion.[34] It has been shown by other calculations that there are two bound states for $L=1$ and the second state, with binding energy at -0.61 eV, is responsible for the resonant enhancement of the fusion cross section as muon is slowed down in a d-t mixture. Work is in progress to obtain more precise potential curves in order to obtain precise energy values.

We comment here that the present method is not very effective in treating the familiar H_2^+ and HD^+. It turns out that the solution for these systems is highly localized near its singular points (see Table I) and its expansion in terms of hyperspherical harmonics [Eq. (44)] converges slowly. To obtain a converged result would require a much larger set of hyperspherical harmonics in (44) than carried out in the present study.

V. SUMMARY AND DISCUSSION

In this article we have proposed a method of solving Coulombic three-body problems in hyperspherical coordinates. By adopting an adiabatic approximation, we obtain the channel wave functions and channel potential curves. We illustrated how to construct analytical channel functions in different sets of Jacobi coordinates. The use of these different sets of Jacobi coordinates allows us to treat each dissociation channel in its natural coordinate system. This is crucial in applying the present approach to rearrangement scatterings.

We have performed preliminary calculations using the present method on a number of Coulombic three-body systems using only one or two basis functions. These results prove that the method works efficiently and we are currently investigating each system using a larger basis set.

The present method is not limited to Coulombic three-body systems. The method can be easily applied to three-body systems in molecular physics and in nuclear physics.

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