Approach to the Bound-State Three-Body Problem with Application to the Helium-Like Atom*

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A technique is presented for treating a general type of three-body bound-state problem for situations where the interaction may be written as the sum of three pair potentials. The method is based on the work of Eyges and consists of writing the total wave function for the three-body problem in a special form, i.e., as the sum of three different parts or "orbitals" defined in a natural way from the integral equation by using the appropriate symmetrized or antisymmetrized Green's function. A set of three integral equations for the three orbitals is derived: first for the situation where each particle is distinguishable, and then for situations where two or all of the three particles are identical. It is found that, when some of the particles are identical and the Pauli principle is incorporated into the formulation, the number of independent orbitals can be reduced. Some simple one-dimensional applications involving δ-function pair potentials are examined. The helium atom is discussed from a three-body point of view in order to illustrate our general apporach to the above-mentioned set of coupled integral equations. Each orbital is expanded into a complete set of two-body Sturmian functions for the Coulomb potential. For states in atomic helium of the form $L=0$, the equations assume a simplified form. For these states, the infinite set of integral equations in one variable generated by the expansion is truncated at several orders and solved numerically. Rapid convergence is demonstrated for low-lying states of the helium-like atoms using this method. In particular, results are reported for the $1s1s^1S$, $1s2s^1S$, and $2s2s^1S$ states of He, Li^+, and H^-. The technique is not based upon a perturbation expansion or a variational principle.

I. INTRODUCTION

IT would be impractical to review adequately all of the literature on the three-body problem here. However, we will mention the most important papers which relate to our method for treating the bound-state three-body problem in a general way. Eyges has shown the advantages of writing the wavefunction for the three-body problem as a sum of three parts or "orbitals" defined in a natural way from the Green's function and resulting integral equation.[1] Faddeev picked up this idea and wrote a T matrix for the three-body scattering problem which was free from the difficulties encountered by a Lippmann–Schwinger approach to the problem.[2] There have been a number of other treatments of special three-body scattering problems in nuclear physics (usually for separable potentials) either using the Faddeev equations or working with the ordinary integral equations for scattering in momentum space.[3] Rotenberg pointed out the fact that the Sturmian set for the analogous two-body problem forms a natural basis for three-body expansions.[4] There have also been several attempts to set up a general technique for dealing with three-body, bound-state problems.[5]

The plan of our paper is as follows. In Sec. II we derive a set of three coupled integral equations for the bound-state solutions of three distinguishable particles interacting with each other through pair potentials. In Sec. III we re-examine the three-body problem when two or all of the particles become identical and introduce appropriately symmetrized Green's functions to take this into account. This gives a generalized set of coupled integral equations for the three-body problem where correlation and exchange effects are properly treated. In Sec. IV we examine the angular-momentum properties of the wave function when written in this special form and show how to construct an eigenfunction for any total L and M. We also examine the parity of these solutions and show that for each set of quantum numbers for $L\geqq 1$ we have both an even- and an odd-parity state. In Sec. V we treat several problems involving δ-function potentials in one dimension which give us some insight into problems of more general interest. In Sec. VI we discuss the helium-like atom from a three-body point of view. Here we demonstrate the general technique for treating the coupled set of integral equations by applying the method to this problem. The method consists of an expansion of each orbital into the Sturmian set for the analogous two-body problem. The explicit appearance of the pair potentials may be eliminated and the resulting set of infinite coupled integral equations is then truncated at some order and solved by numerical methods. The energies and wave functions for some states of the

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form $L=0$ in the helium-like atom are calculated, and rapid convergence is demonstrated.

II. FORMULATION OF THE THREE-BODY PROBLEM FOR DISTINGUISHABLE PARTICLES

A. Jacobi Coordinates and the Associated Green's Functions for the Problem

Three-body problems governed by the following Hamiltonian are investigated:

$$H=\sum_{i=1}^{3}\frac{p_i^2}{2m_i}+\sum_{i<j}V_{ij}(|\,\mathbf{r}_i-\mathbf{r}_j\,|). \tag{1}$$

It has been shown by Eyges[1] that it is convenient to use Jacobi coordinates in dealing with three-body problems where all three particles have identical masses. For the same reasons given by him it is also convenient to use the full Jacobi coordinates when the three masses are not equal. The three sets of Jacobi coordinates are given by

$$\mathbf{R}=(m_i\mathbf{r}_i+m_j\mathbf{r}_j+m_k\mathbf{r}_k)/(m_i+m_j+m_k),$$

$$\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j, \qquad \boldsymbol{\varrho}_k=\mathbf{r}_k-(m_i\mathbf{r}_i+m_j\mathbf{r}_j)/(m_i+m_j),$$

where the different sets are generated by i, j, and k assuming the values 1, 2, and 3 in cyclical permutation. We note, of course, that these representations are not independent and linear relations between them can be found. In any one of the three frames the Schrödinger equation with the center-of-mass motion separated out is

$$\left\{\frac{1}{2}\left(\frac{m}{m_i}+\frac{m}{m_j}\right)\nabla_{\mathbf{r}_{ij}}^2+\frac{1}{2}\left(\frac{m}{m_i+m_j}+\frac{m}{m_k}\right)\nabla_{\boldsymbol{\varrho}_k}^2-(v_{ij}+v_{jk}+v_{ki})\right\}\Psi=K^2\Psi, \tag{2}$$

where $K^2=m\,|\,E\,|/\hbar^2$, $v_{ij}=mV_{ij}/\hbar^2$, and the choice of m fixes the mass scale. We now imagine a six-dimensional configuration space defined by any one of the three sets of Jacobi coordinates. Let us represent a general point in this six-dimensional space by the vector $\mathbf{P}$ so that Ψ, in general, will be a function of $\mathbf{P}$.

Each of the three relations embodied in Eq. (2) may be converted to an integral equation for Ψ of the following form:

$$\Psi(\mathbf{P})=-\int d\mathbf{P}'\,\Psi(\mathbf{P}')v_t(\mathbf{P}')G(\mathbf{P}-\mathbf{P}'), \tag{3}$$

where v_t is the total potential and G, the Green's function, is the solution to the following differential equation:

$$L_{ij}G_{ij}\equiv(\alpha_{ij}\nabla_{\mathbf{r}_{ij}}^2+\beta_k\nabla_{\boldsymbol{\varrho}_k}^2-K^2)G_{ij}(\mathbf{r}_{ij}-\mathbf{r}_{ij}',\ \boldsymbol{\varrho}_k-\boldsymbol{\varrho}_k')$$
$$=-\delta(\mathbf{r}_{ij}-\mathbf{r}_{ij}')\delta(\boldsymbol{\varrho}_k-\boldsymbol{\varrho}_k').$$

The subscripts on G refer to the Green's function expressed in a particular set of Jacobi coordinates. G may be represented in integral form as

$$G_{ij}=\frac{1}{(2\pi)^6}\iint d\mathbf{k}\,d\boldsymbol{\kappa}\,\frac{\exp[i\mathbf{k}\cdot(\mathbf{r}_{ij}-\mathbf{r}_{ij}')+i\boldsymbol{\kappa}\cdot(\boldsymbol{\varrho}_k-\boldsymbol{\varrho}_k')]}{\alpha_{ij}k^2+\beta_k\kappa^2+K^2}. \tag{4}$$

Each of the three Green's functions will have a similar form, i.e., that of Eq. (4), and the constants α_{ij} and β_k may be read off from Eqs. (2). It is easy to show that all the G's are identical by considering the proper transformations of the variables of integration $\mathbf{k}$ and $\boldsymbol{\kappa}$. Since the three Green's functions are identical, one is to regard the subscripts as referring to G expressed in a particular Jacobi frame.

B. The Form of the Wave Function

Eyges has shown that it is advantageous to write the wave function for a three-body problem as a sum of three "orbitals" when all the particles have the same mass.[1] Faddeev has also used a similar form in writing a T matrix for three-body scattering problems.[2]

Following Eyges, let us write Ψ as a sum of three parts where each part, or orbital, is associated with one term of the three-body potential:

$$\Psi(\mathbf{P})=\psi_{12}(\mathbf{P})+\psi_{23}(\mathbf{P})+\psi_{31}(\mathbf{P}), \tag{5}$$

where the individual orbitals are defined with regard to each part of the three-body potential

$$\psi_{ij}(\mathbf{P})\equiv-\int d\mathbf{P}'\Psi(\mathbf{P}')v_{ij}(\mathbf{P}')G_{ij}(\mathbf{P}-\mathbf{P}'). \tag{6}$$

We may easily verify that the form of $\Psi(\mathbf{P})$ given in Eq. (5) satisfies the differential equation by substituting Eq. (5) into Eq. (3) and operating on both sides by L. The Green's functions in Eqs. (6) are each expressed in terms of the natural variables of the particular orbital. For example, when $i=1$ and $j=2$, ψ_{12} is the orbital associated with the potential v_{12} and G_{12} would be written as

$$G_{12}=\frac{1}{(2\pi)^6}\iint d\mathbf{k}\,d\boldsymbol{\kappa}\,\frac{\exp[i\mathbf{k}\cdot(\mathbf{r}_{12}-\mathbf{r}_{12}')+i\boldsymbol{\kappa}\cdot(\boldsymbol{\varrho}_3-\boldsymbol{\varrho}_3')]}{\alpha_{12}k^2+\beta_3\kappa^2+K^2}$$

since the natural variable of v_{12} is $\mathbf{r}_{12}$.

C. The General Set of Coupled Equations for Three Distinguishable Particles

In the first two sections we have introduced the three sets of Jacobi coordinates as possible representations of the three-body problem, and also discussed a special form for $\Psi(\mathbf{P})$ which arises naturally when we recast the differential equation for the three-body problem into an integral form. We are now in a position to derive a general set of coupled integral equations which, if solved analytically, would give the complete solution to the three-body problem. If Eq. (5) is substituted in the right-hand side of Eqs. (6) and the natural variables

for each orbital and its associated Green's function are used, we obtain in mixed notation

$$\psi_{12}(\mathbf{r}_{12}, \boldsymbol{\varrho}_3) = -\iint d\mathbf{r}_{12}' d\boldsymbol{\varrho}_3' \,[\psi_{12}(\mathbf{r}_{12}', \boldsymbol{\varrho}_3') + \psi_{23}(\mathbf{r}_{23}', \boldsymbol{\varrho}_1') + \psi_{31}(\mathbf{r}_{31}', \boldsymbol{\varrho}_2')] v_{12}(\mathbf{r}_{12}') G_{12}(\mathbf{r}_{12} - \mathbf{r}_{12}', \boldsymbol{\varrho}_3 - \boldsymbol{\varrho}_3'), \tag{7a}$$

$$\psi_{23}(\mathbf{r}_{23}, \boldsymbol{\varrho}_1) = -\iint d\mathbf{r}_{23}' d\boldsymbol{\varrho}_1' \,[\psi_{12}(\mathbf{r}_{12}', \boldsymbol{\varrho}_3') + \psi_{23}(\mathbf{r}_{23}', \boldsymbol{\varrho}_1') + \psi_{31}(\mathbf{r}_{31}', \boldsymbol{\varrho}_2')] v_{23}(\mathbf{r}_{23}') G_{23}(\mathbf{r}_{23} - \mathbf{r}_{23}', \boldsymbol{\varrho}_1 - \boldsymbol{\varrho}_1'), \tag{7b}$$

$$\psi_{31}(\mathbf{r}_{31}, \boldsymbol{\varrho}_2) = -\iint d\mathbf{r}_{31}' d\boldsymbol{\varrho}_2' \,[\psi_{12}(\mathbf{r}_{12}', \boldsymbol{\varrho}_3') + \psi_{23}(\mathbf{r}_{23}', \boldsymbol{\varrho}_1') + \psi_{31}(\mathbf{r}_{31}', \boldsymbol{\varrho}_2')] v_{31}(\mathbf{r}_{31}') G_{31}(\mathbf{r}_{31} - \mathbf{r}_{31}', \boldsymbol{\varrho}_2 - \boldsymbol{\varrho}_2'). \tag{7c}$$

The constants α_{ij} and β_k occurring in the G_{ij} may be written down by inspection from Eqs. (2) as

$$\alpha_{12} = \frac{1}{2}\left(\frac{m}{m_1} + \frac{m}{m_2}\right), \qquad \alpha_{23} = \frac{1}{2}\left(\frac{m}{m_2} + \frac{m}{m_3}\right), \qquad \alpha_{31} = \frac{1}{2}\left(\frac{m}{m_1} + \frac{m}{m_3}\right),$$

$$\beta_3 = \frac{1}{2}\left(\frac{m}{m_1+m_2} + \frac{m}{m_3}\right), \qquad \beta_1 = \frac{1}{2}\left(\frac{m}{m_2+m_3} + \frac{m}{m_1}\right), \qquad \beta_2 = \frac{1}{2}\left(\frac{m}{m_1+m_3} + \frac{m}{m_2}\right).$$

Several remarks are in order about Eqs. (7a), (7b), and (7c). They are a coupled set of three integral equations where each orbital is coupled to itself and the other two. We also observed that, in each equation, the natural coordinates of the two-body potential are used. For example, in Eq. (7a), the terms inside the brackets on the right-hand side are evaluated in terms of the Jacobi coordinates $\mathbf{r}_{12}'$ and $\boldsymbol{\varrho}_3'$. In other words, when it comes to simplifying the right-hand side of Eq. (7a), the orbitals ψ_{23} and ψ_{31} are written as functions of $\mathbf{r}_{12}'$ and $\boldsymbol{\varrho}_3'$ by using the relationships between the different Jacobi coordinate systems

$$\psi_{23}(\mathbf{r}_{23}', \boldsymbol{\varrho}_1') = \psi_{23}\left\{-\frac{m_1}{m_1+m_2}\,\mathbf{r}_{12}' - \boldsymbol{\varrho}_3', \left[1 - \frac{m_1 m_3}{(m_2+m_3)(m_1+m_2)}\right]\mathbf{r}_{12}' - \frac{m_3}{m_2+m_3}\,\boldsymbol{\varrho}_3'\right\},$$

$$\psi_{31}(\mathbf{r}_{31}', \boldsymbol{\varrho}_2') = \psi_{31}\left\{-\frac{m_2}{m_1+m_2}\,\mathbf{r}_{12}' + \boldsymbol{\varrho}_3', \left[\frac{m_2 m_3}{(m_1+m_3)(m_1+m_2)} - 1\right]\mathbf{r}_{12}' - \frac{m_3}{m_1+m_3}\,\boldsymbol{\varrho}_3'\right\}.$$

A similar procedure is used when we evaluate the right-hand sides of Eqs. (7b) and (7c). An advantageous way to simplify the set of integral equations, where some of the functions appear evaluated at transformed arguments, is to work with the Fourier transforms of the orbitals and re-express the three-body problem in a six-dimensional momentum space. Accordingly, we define the Fourier transform pair for each orbital by the standard relations

$$\psi_{ij}(\mathbf{r}_{ij}, \boldsymbol{\varrho}_k) \equiv \frac{1}{(2\pi)^3}\iint d\mathbf{k} d\boldsymbol{\kappa}\, \phi_{ij}(\mathbf{k}, \boldsymbol{\kappa}) \exp(i\mathbf{k}\cdot\mathbf{r}_{ij} + i\boldsymbol{\kappa}\cdot\boldsymbol{\varrho}_k),$$

$$\phi_{ij}(\mathbf{k}, \boldsymbol{\kappa}) \equiv \frac{1}{(2\pi)^3}\iint d\mathbf{r}_{ij} d\boldsymbol{\varrho}_k\, \psi_{ij}(\mathbf{r}_{ij}, \boldsymbol{\varrho}_k) \exp(-i\mathbf{k}\cdot\mathbf{r}_{ij} - i\boldsymbol{\kappa}\cdot\boldsymbol{\varrho}_k).$$

We are now able to Fourier-transform the set of three coupled equations in coordinate space to an analogous set of three coupled equations for the "momentum orbitals" in momentum space. If the integral representations of the appropriate Green's functions and the Fourier transforms of the coordinate orbitals are substituted in the right-hand side of Eqs. (7a), (7b), and (7c), and the whole set is then Fourier-transformed, we will obtain equations for the momentum orbitals on the left-hand side in terms of an eightfold integration on the right-hand side. Upon simplification the resulting equations are

$$\phi_{12}(\mathbf{k}, \boldsymbol{\kappa}) = -[(2\pi)^3(\alpha_{12}k^2 + \beta_3\kappa^2 + K^2)]^{-1}\iint d\mathbf{r}_{12}' d\mathbf{k}'\, v_{12}(\mathbf{r}_{12}')$$

$$\times \left\{\phi_{12}(\mathbf{k}', \boldsymbol{\kappa}) \exp i\mathbf{r}_{12}'\cdot(\mathbf{k}'-\mathbf{k}) + \phi_{23}\left(-\frac{m_3}{m_2+m_3}\,\mathbf{k}', \mathbf{k}' - \frac{m_2+m_3}{m_3}\,\boldsymbol{\kappa}\right)\exp i\mathbf{r}_{12}'\cdot\left[\mathbf{k}'-\mathbf{k}-\left(\frac{m_2+m_3}{m_3} - \frac{m_1}{m_1+m_2}\right)\boldsymbol{\kappa}\right]\right.$$

$$\left. + \phi_{31}\left(\frac{m_3}{m_1+m_3}\,\mathbf{k}', \mathbf{k}' - \frac{m_1+m_3}{m_3}\,\boldsymbol{\kappa}\right)\exp i\mathbf{r}_{12}'\cdot\left[-\mathbf{k}'-\mathbf{k}+\left(\frac{m_1+m_3}{m_3} - \frac{m_2}{m_1+m_2}\right)\boldsymbol{\kappa}\right]\right\}, \tag{8a}$$

$$\phi_{23}(\mathbf{k},\kappa)=-[(2\pi)^3(\alpha_{23}k^2+\beta_1\kappa^2+K^2)]^{-1}\iint d\mathbf{r}_{23}'d\mathbf{k}'\,v_{23}(\mathbf{r}_{23}')$$
$$\times\left\{\phi_{23}(\mathbf{k}',\kappa)\,\exp i\mathbf{r}_{23}'\cdot(\mathbf{k}'-\mathbf{k})+\phi_{31}\left(-\frac{m_1}{m_1+m_3}\mathbf{k}',\mathbf{k}'-\frac{m_1+m_3}{m_1}\kappa\right)\exp i\mathbf{r}_{23}'\cdot\left[\mathbf{k}'-\mathbf{k}-\left(\frac{m_1+m_3}{m_1}-\frac{m_2}{m_2+m_3}\right)\kappa\right]\right.$$
$$\left.+\phi_{12}\left(\frac{m_1}{m_1+m_2}\mathbf{k}',\mathbf{k}'-\frac{m_1+m_2}{m_1}\kappa\right)\exp i\mathbf{r}_{23}'\cdot\left[-\mathbf{k}'-\mathbf{k}+\left(\frac{m_1+m_2}{m_1}-\frac{m_3}{m_2+m_3}\right)\kappa\right]\right\},\tag{8b}$$

$$\phi_{31}(\mathbf{k},\kappa)=-[(2\pi)^3(\alpha_{31}k^2+\beta_2\kappa^2+K^2)]^{-1}\iint d\mathbf{r}_{31}'d\mathbf{k}'\,v_{31}(\mathbf{r}_{31}')$$
$$\times\left\{\phi_{31}(\mathbf{k}',\kappa)\,\exp i\mathbf{r}_{31}'\cdot(\mathbf{k}'-\mathbf{k})+\phi_{12}\left(-\frac{m_2}{m_1+m_2}\mathbf{k}',\mathbf{k}'-\frac{m_1+m_2}{m_2}\kappa\right)\exp i\mathbf{r}_{31}'\cdot\left[\mathbf{k}'-\mathbf{k}-\left(\frac{m_1+m_2}{m_2}-\frac{m_3}{m_1+m_3}\right)\kappa\right]\right.$$
$$\left.+\phi_{23}\left(\frac{m_2}{m_2+m_3}\mathbf{k}',\mathbf{k}'-\left(\frac{m_2+m_3}{m_2}\right)\kappa\right)\exp i\mathbf{r}_{31}'\cdot\left[-\mathbf{k}'-\mathbf{k}+\left(\frac{m_2+m_3}{m_2}-\frac{m_1}{m_1+m_3}\right)\kappa\right]\right\}.\tag{8c}$$

Equations (8a), (8b), and (8c) are the basic set of coupled integral equations for three distinguishable particles interacting with each other by two-body forces.

III. GENERALIZATION TO INCLUDE IDENTICAL PARTICLES

A. Two Identical Fermions and One Different Particle

Now we wish to discuss the problem of two identical fermions and a third particle which is different. The Jacobi coordinates satisfy the following relations upon exchange of the two identical particles:

$$\mathbf{R}\to\mathbf{R},$$
$$\mathbf{r}_{12}\to-\mathbf{r}_{23},\quad \mathbf{r}_{23}\to-\mathbf{r}_{12},\quad \mathbf{r}_{31}\to-\mathbf{r}_{31},$$
$$\boldsymbol{\varrho}_3\to\boldsymbol{\varrho}_1,\quad \boldsymbol{\varrho}_1\to\boldsymbol{\varrho}_3,\quad \boldsymbol{\varrho}_2\to\boldsymbol{\varrho}_2.$$

Since we have chosen particles one and three as the identical pair, we may write the three-body potential as

$$v_t=v_1(\mathbf{r}_{12})+v_1(-\mathbf{r}_{23})+v_2(\mathbf{r}_{31}),\tag{9}$$

where v_2 must be an even function of its argument. We note that no restriction need be placed on the form of v_1 which is the pair potential between the second particle and either one of the two identical particles. The Hamiltonian operators defined from Eqs. (2) and the **L** operators corresponding to the differential equations for the Green's functions expressed in each Jacobi frame, have the following properties upon exchange of the two identical particles:

$$\mathbf{H}_{12}\to\mathbf{H}_{23},\quad \mathbf{H}_{23}\to\mathbf{H}_{12},\quad \mathbf{H}_{31}\to\mathbf{H}_{31},$$
$$\mathbf{L}_{12}\to\mathbf{L}_{23},\quad \mathbf{L}_{23}\to\mathbf{L}_{12},\quad \mathbf{L}_{31}\to\mathbf{L}_{31}.$$

Here, the subscripts refer to the operators expressed in a particular set of coordinates. All of the **H**'s and all of the **L**'s are, of course, identical.

Rather than satisfy the Pauli principle by explicitly symmetrizing the wave function, we choose to work with a symmetrized and antisymmetrized Green's function. The symmetrized Green's function in the Jacobi frame defined by $(\mathbf{r}_{12},\boldsymbol{\varrho}_3)$ satisfies

$$(\alpha_{12}\nabla_{\mathbf{r}_{12}}^2+\beta_3\nabla_{\boldsymbol{\varrho}_3}^2-K^2)G_{12}^{S,A}$$
$$=-\tfrac{1}{2}[\delta(\mathbf{r}_{12}-\mathbf{r}_{12}')\delta(\boldsymbol{\varrho}_3-\boldsymbol{\varrho}_3')\pm\delta(-\mathbf{r}_{23}-\mathbf{r}_{12}')\delta(\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_3')].$$

Similar relations hold for G expressed in the other two Jacobi frames. It is easy to show that there is only one G^S and one G^A for the problem. In the Jacobi frame $(\mathbf{r}_{12},\boldsymbol{\varrho}_3)$ the two functions are

$$G_{12}^{S,A}=\tfrac{1}{2}G_{12}(\mathbf{r}_{12}-\mathbf{r}_{12}',\boldsymbol{\varrho}_3-\boldsymbol{\varrho}_3')$$
$$\pm\tfrac{1}{2}G_{12}(-\mathbf{r}_{23}-\mathbf{r}_{12}',\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_3'),\tag{10}$$

where the G_{12} is the previous unsymmetrized Green's function given by Eq. (4). Again, similar relations hold for G expressed in the other two center-of-mass frames. We may now write three new equations for the orbitals in terms of the symmetrized Green's functions:

$$\psi_{12}(\mathbf{r}_{12},\boldsymbol{\varrho}_3)=-\iint d\mathbf{r}_{12}'d\boldsymbol{\varrho}_3'\{\psi_{12}(\mathbf{r}_{12}',\boldsymbol{\varrho}_3')+\psi_{23}(\mathbf{r}_{23}',\boldsymbol{\varrho}_1')+\psi_{31}(\mathbf{r}_{31}',\boldsymbol{\varrho}_2')\}$$
$$\times v_1(\mathbf{r}_{12}')[\tfrac{1}{2}G_{12}(\mathbf{r}_{12}-\mathbf{r}_{12}',\boldsymbol{\varrho}_3-\boldsymbol{\varrho}_3')\pm\tfrac{1}{2}G_{12}(-\mathbf{r}_{23}-\mathbf{r}_{12}',\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_3')],\tag{11a}$$

$$\psi_{23}(\mathbf{r}_{23},\boldsymbol{\varrho}_1)=-\iint d\mathbf{r}_{23}'d\boldsymbol{\varrho}_1'\{\psi_{12}(\mathbf{r}_{12}',\boldsymbol{\varrho}_3')+\psi_{23}(\mathbf{r}_{23}',\boldsymbol{\varrho}_1')+\psi_{31}(\mathbf{r}_{31}',\boldsymbol{\varrho}_2')]\}$$
$$\times v_1(-\mathbf{r}_{23}')[\tfrac{1}{2}G_{23}(\mathbf{r}_{23}-\mathbf{r}_{23}',\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_1')\pm\tfrac{1}{2}G_{23}(-\mathbf{r}_{12}-\mathbf{r}_{23}',\boldsymbol{\varrho}_3-\boldsymbol{\varrho}_1')],\tag{11b}$$

$$\psi_{31}(\mathbf{r}_{31},\boldsymbol{\varrho}_2)=-\iint d\mathbf{r}_{31}'d\boldsymbol{\varrho}_2'\{\psi_{12}(\mathbf{r}_{12}',\boldsymbol{\varrho}_3')+\psi_{23}(\mathbf{r}_{23}',\boldsymbol{\varrho}_1')+\psi_{31}(\mathbf{r}_{31}',\boldsymbol{\varrho}_2')\}$$
$$\times v_2(\mathbf{r}_{31}')[\tfrac{1}{2}G_{31}(\mathbf{r}_{31}-\mathbf{r}_{31}',\boldsymbol{\varrho}_2-\boldsymbol{\varrho}_2')\pm\tfrac{1}{2}G_{31}(-\mathbf{r}_{31}-\mathbf{r}_{31}',\boldsymbol{\varrho}_2-\boldsymbol{\varrho}_2')].\tag{11c}$$

In Eq. (11a) we make the coordinate transformation $\mathbf{r}_{12}'\to-\mathbf{r}_{23}'$; $\boldsymbol{\rho}_3'\to\boldsymbol{\rho}_1'$ to obtain

$$\psi_{12}(\mathbf{r}_{12},\boldsymbol{\rho}_3)=-\iint d\mathbf{r}_{23}'d\boldsymbol{\rho}_1'\{\psi_{12}(-\mathbf{r}_{23}',\boldsymbol{\rho}_1')+\psi_{23}(-\mathbf{r}_{12}',\boldsymbol{\rho}_3')+\psi_{31}(-\mathbf{r}_{31}',\boldsymbol{\rho}_2')\}$$
$$\times v_1(-\mathbf{r}_{23}')[\tfrac{1}{2}G_{12}(\mathbf{r}_{12}+\mathbf{r}_{23}',\boldsymbol{\rho}_3-\boldsymbol{\rho}_1')\pm\tfrac{1}{2}G_{12}(-\mathbf{r}_{23}+\mathbf{r}_{23}',\boldsymbol{\rho}_1-\boldsymbol{\rho}_1')].$$

The symmetrized Green's function now requires that each orbital be either symmetric or antisymmetric upon exchange of the two identical particles. Therefore, we have

$$\psi_{12}(\mathbf{r}_{12},\boldsymbol{\rho}_3)=-\iint d\mathbf{r}_{23}'d\boldsymbol{\rho}_1'(\pm)\{\psi_{12}(\mathbf{r}_{12}',\boldsymbol{\rho}_3')+\psi_{23}(\mathbf{r}_{23}',\boldsymbol{\rho}_1')+\psi_{31}(\mathbf{r}_{31}',\boldsymbol{\rho}_2')\}$$
$$\times v_1(-\mathbf{r}_{23}')[\tfrac{1}{2}G_{12}(\mathbf{r}_{12}+\mathbf{r}_{23}',\boldsymbol{\rho}_3-\boldsymbol{\rho}_1')\pm\tfrac{1}{2}G_{12}(-\mathbf{r}_{23}+\mathbf{r}_{23}',\boldsymbol{\rho}_1-\boldsymbol{\rho}_1')].$$

Invoking the property that the G_{ij} depend only on the magnitude of their arguments gives

$$\psi_{12}(-\mathbf{r}_{23},\boldsymbol{\rho}_1)=-(\pm)\iint d\mathbf{r}_{23}'d\boldsymbol{\rho}_1'\{\psi_{12}(\mathbf{r}_{12}',\boldsymbol{\rho}_3')+\psi_{23}(\mathbf{r}_{23}',\boldsymbol{\rho}_1')+\psi_{31}(\mathbf{r}_{31}',\boldsymbol{\rho}_2')\}$$
$$\times v_1(-\mathbf{r}_{23}')[\tfrac{1}{2}G_{12}(\mathbf{r}_{23}-\mathbf{r}_{23}',\boldsymbol{\rho}_1-\boldsymbol{\rho}_1')\pm\tfrac{1}{2}G_{12}(-\mathbf{r}_{12}-\mathbf{r}_{23}',\boldsymbol{\rho}_3-\boldsymbol{\rho}_1')].$$

Since $m_1=m_3$ we note that the form of G_{12} is identical with that of G_{23}. Comparing the above equation to Eq. (11b), we see that

$$\psi_{12}(-\mathbf{r}_{23},\boldsymbol{\rho}_1)=\pm\psi_{23}(\mathbf{r}_{23},\boldsymbol{\rho}_1).$$

This relation, together with the fact that each orbital is itself either symmetric or antisymmetric upon exchange of the identical particles allows us to write the space part of the total wave function as

$$\Psi^{S,A}=\psi_{12}{}^{e,o}(\mathbf{r}_{12},\boldsymbol{\rho}_3)+\psi_{12}{}^{e,o}(\mathbf{r}_{23},\boldsymbol{\rho}_1)+\psi_{31}{}^{e,o}(\mathbf{r}_{31},\boldsymbol{\rho}_2),\tag{12}$$

where the superscript e means an even function of the $\mathbf{r}_{ij}$ argument and corresponds to the symmetric solution (Ψ^S) and the superscript o means an odd function of the $\mathbf{r}_{ij}$ argument and corresponds to the antisymmetric solution (Ψ^A). The even and odd orbitals are now given by the following coupled equations:

$$\psi_1{}^{e,o}(\mathbf{r}_{12},\boldsymbol{\rho}_3)=-\iint d\mathbf{r}_{12}'d\boldsymbol{\rho}_3'\{\psi_1{}^{e,o}(\mathbf{r}_{12}',\boldsymbol{\rho}_3')+\psi_1{}^{e,o}(\mathbf{r}_{23}',\boldsymbol{\rho}_1')+\psi_2{}^{e,o}(\mathbf{r}_{31}',\boldsymbol{\rho}_2')\}v_1(\mathbf{r}_{12}')G_{12}(\mathbf{r}_{12}-\mathbf{r}_{12}',\boldsymbol{\rho}_3-\boldsymbol{\rho}_3'),\tag{13a}$$

$$\psi_2{}^{e,o}(\mathbf{r}_{31},\boldsymbol{\rho}_2)=-\iint d\mathbf{r}_{31}'d\boldsymbol{\rho}_2'\{\psi_1{}^{e,o}(\mathbf{r}_{12}',\boldsymbol{\rho}_3')+\psi_1{}^{e,o}(\mathbf{r}_{23}',\boldsymbol{\rho}_1')+\psi_2{}^{e,o}(\mathbf{r}_{31}',\boldsymbol{\rho}_2')\}v_2(\mathbf{r}_{31}')G_{31}(\mathbf{r}_{31}-\mathbf{r}_{31}',\boldsymbol{\rho}_2-\boldsymbol{\rho}_2'),\tag{13b}$$

where we define $\psi_1{}^{e,o}\equiv\psi_{12}{}^{e,o}$ and $\psi_2{}^{e,o}\equiv\psi_{31}{}^{e,o}$. The G_{ij} here are the unsymmetrized functions given by Eq. (4). Equations (13a) and (13b) include all effects due to correlation and exchange which are often treated approximately by perturbation theory or by variational techniques. For example, the $1s2s$ states of the helium atom divide into two classes. One has a symmetric space part and the other antisymmetric with a different energy.

In momentum space we may write Eqs. (13a) and (13b) as

$$\phi_1{}^{e,o}(\mathbf{k},\boldsymbol{\kappa})=-[(2\pi)^3(\alpha_{12}k^2+\beta_3\kappa^2+K^2)]^{-1}\iint d\mathbf{k}'d\mathbf{r}\,v_1(\mathbf{r})\{\phi_1{}^{e,o}(\mathbf{k}',\boldsymbol{\kappa})\exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k})$$
$$+\phi_1{}^{e,o}(-b\mathbf{k}',\mathbf{k}'-(\boldsymbol{\kappa}/b))\exp i\mathbf{r}\cdot[\mathbf{k}'-\mathbf{k}-(b^{-1}-b)\boldsymbol{\kappa}]+\phi_2{}^{e,o}(\tfrac{1}{2}\mathbf{k}',\mathbf{k}'-2\boldsymbol{\kappa})\exp i\mathbf{r}\cdot[-\mathbf{k}'-\mathbf{k}+(2-a)\boldsymbol{\kappa}]\},\tag{14a}$$

$$\phi_2{}^{e,o}(\mathbf{k},\boldsymbol{\kappa})=-[(2\pi)^3(\alpha_{31}k^2+\beta_2\kappa^2+K^2)]^{-1}\iint d\mathbf{k}'d\mathbf{r}\,v_2(\mathbf{r})\{\phi_2{}^{e,o}(\mathbf{k}',\boldsymbol{\kappa})\exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k})$$
$$+\phi_1{}^{e,o}(a\mathbf{k}',\mathbf{k}'-(\boldsymbol{\kappa}/a))\exp i\mathbf{r}\cdot[-\mathbf{k}'-\mathbf{k}+(a^{-1}-\tfrac{1}{2})\boldsymbol{\kappa}]+\phi_1{}^{e,o}(-a\mathbf{k}',\mathbf{k}'-(\boldsymbol{\kappa}/a))\exp i\mathbf{r}\cdot[\mathbf{k}'-\mathbf{k}-(a^{-1}-\tfrac{1}{2})\boldsymbol{\kappa}]\}.\tag{14b}$$

The constants appearing in these equations are given by

$$\alpha_{12}=\tfrac{1}{2}a^{-1},\quad \beta_3=\tfrac{1}{2}(1+b),\quad \alpha_{31}=1,\quad \beta_2=\tfrac{1}{2}(a^{-1}-\tfrac{1}{2}),$$
$$a=M/(m+M),\quad b=m/(m+M).$$

Here, we have set $m_1=m_3=m$ and $m_2=M$.

B. Three Identical Spinless Particles

For the case of three identical bosons the total wave function must be symmetric under an exchange of any pair of particles, i.e.,

$$\Psi(1,2,3)=\Psi(1,3,2)=\Psi(2,1,3)=\Psi(3,2,1).$$

For an exchange of particles one and two,

$$\mathbf{r}_{12}\leftrightarrow-\mathbf{r}_{12},\quad \mathbf{r}_{31}\leftrightarrow-\mathbf{r}_{23},$$
$$\boldsymbol{\rho}_3\leftrightarrow\boldsymbol{\rho}_3,\quad \boldsymbol{\rho}_2\leftrightarrow\boldsymbol{\rho}_1;$$

and for an exchange of particles two and three,

$$\mathbf{r}_{23}\leftrightarrow-\mathbf{r}_{23},\quad \mathbf{r}_{12}\leftrightarrow-\mathbf{r}_{31},$$
$$\boldsymbol{\rho}_1\leftrightarrow\boldsymbol{\rho}_1,\quad \boldsymbol{\rho}_3\leftrightarrow\boldsymbol{\rho}_2.$$

Using arguments similar to those of Sec. III A we may show that $\varphi_{12}=\varphi_{23}=\varphi_{31}$. Thus we have

$$\phi^{e,o}(\mathbf{k},\boldsymbol{\kappa})=-[(2\pi)^3(k^2+\tfrac{3}{4}\kappa^2+K^2)]^{-1}\iint d\mathbf{r}d\mathbf{k}'\, v(\mathbf{r})\{\phi^{e,o}(\mathbf{k}',\boldsymbol{\kappa})\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k})$$
$$+\phi^{e,o}(\tfrac{1}{2}\mathbf{k}',\mathbf{k}'-2\boldsymbol{\kappa})\ \exp i\mathbf{r}\cdot(-\mathbf{k}'-\mathbf{k}+\tfrac{3}{2}\boldsymbol{\kappa})+\phi^{e,o}(-\tfrac{1}{2}\mathbf{k}',\mathbf{k}'-2\boldsymbol{\kappa})\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k}-\tfrac{3}{2}\boldsymbol{\kappa})\}. \quad (15)$$

We have used the fact that when all the masses become equal:

$$\alpha_{12}=\alpha_{23}=\alpha_{31}=1,$$
$$\beta_3=\beta_1=\beta_2=\tfrac{3}{4}.$$

Equation (15) is the same as the one derived by Eyges[1] whose starting point was a three-body system of particles with the same mass.

IV. ANGULAR MOMENTUM AND PARITY CONSIDERATIONS

A. Angular Momentum and the General Expansion for φ_{ij}

The general expression for the angular momentum operator for three particles of arbitrary mass in a Cartesian coordinate system is $\mathbf{L}=(L_x, L_y, L_z)$, where

$$L_x=-i\hbar\sum_{n=1}^{3}\left(y_n\frac{\partial}{\partial z_n}-z_n\frac{\partial}{\partial y_n}\right).$$

The other two components of $\mathbf{L}$ are given by cyclical permutations of x, y, and z. It can be shown that the expression for the angular-momentum operator for three particles of different mass in each Jacobi frame is given by $\mathbf{L}=(L_x, L_y, L_z)$, where

$$L_x=-i\hbar\left\{R_y\frac{\partial}{\partial R_z}-R_z\frac{\partial}{\partial R_y}\right.$$
$$\left.+y_{ij}\frac{\partial}{\partial z_{ij}}-z_{ij}\frac{\partial}{\partial y_{ij}}+\rho_{ky}\frac{\partial}{\partial \rho_{kz}}-\rho_{kz}\frac{\partial}{\partial \rho_{ky}}\right\}$$

and where the components of $\mathbf{R}$, $\mathbf{r}_{ij}$, and $\boldsymbol{\varrho}_k$ are given by

$$\mathbf{R}=(R_x, R_y, R_z),\quad \mathbf{r}_{ij}=(x_{ij}, y_{ij}, z_{ij}),\quad \boldsymbol{\varrho}_k=(\rho_{kx}, \rho_{ky}, \rho_{kz}).$$

Similar expressions hold for L_y and L_z. We note that the form of $\mathbf{L}$ is the same in each Jacobi frame and is also the same as $\mathbf{L}$ expressed in Cartesian coordinates. If we require that $\Psi(\mathbf{r}_{ij}, \boldsymbol{\varrho}_k)$ is an eigenstate of both the total angular momentum and the total Z component of angular momentum, we may then deduce that each orbital is also an eigenstate of $\mathbf{L}$ and $\mathbf{M}$. Let $\mathbf{L}_{ijk}$ denote $\mathbf{L}$ expressed in a particular Jacobi frame, then $\mathbf{L}_{ijk}=\mathbf{L}_{jki}=\mathbf{L}_{kij}$. Since the most general form of the total wave function is that given by Eq. (5), we may write

$$\mathbf{L}_{ijk}\Psi=\mathbf{L}_{ijk}\psi_{ij}(\mathbf{r}_{ij}, \boldsymbol{\varrho}_k)+\mathbf{L}_{jki}\psi_{jk}(\mathbf{r}_{jk}, \boldsymbol{\varrho}_i)+\mathbf{L}_{kij}\psi_{ki}(\mathbf{r}_{ki}, \boldsymbol{\varrho}_j).$$

We see that for particles of arbitrary mass each orbital must be an eigenstate of $\mathbf{L}$ and $\mathbf{M}$.

The most general expansion for a function of two vectors may be written as

$$\phi_{ij}(\mathbf{k},\boldsymbol{\kappa})=\sum_{nlm}a_{nlm}(\boldsymbol{\kappa})S_{nl}(k)Y_l^m(\Omega_k), \quad (16)$$

where $S_{nlm}(\mathbf{k})$ form a complete set of functions and the coefficients $a_{nlm}(\boldsymbol{\kappa})$ are unknown functions of the vector $\boldsymbol{\kappa}$. If we impose the condition that each orbital must be an eigenstate of $\mathbf{L}$ and $\mathbf{M}$, then

$$\phi_{ij}^{LM}(\mathbf{k},\boldsymbol{\kappa})=\sum_{nll'}{}_{LM}f_{l'}^{nl}(\kappa)S_{nl}(k)$$
$$\times\sum_{mm'}C_{ll'}(L,M,m,m')Y_{l'}^{m'}(\Omega_\kappa)Y_l^m(\Omega_k), \quad (17)$$

where $C_{ll'}(L, M, m, m')$ is the Clebsch–Gordan coefficient. This is the most general expansion for an arbitrary orbital where the $f_{l'}^{nl}(\kappa)$ are regarded as unknown functions of κ. For $L=0$ and $M=0$ the Clebsch–Gordan coefficients vanish for $l\neq l'$ and for $m\neq -m'$. The remaining coefficients are just $(-1)^m$. For these states we have

$$\phi_{ij}(\mathbf{k},\boldsymbol{\kappa})=\sum_{nlm}(-1)^m f_{nl}(\kappa)S_{nl}(k)Y_l^{-m}(\Omega_\kappa)Y_l^m(\Omega_k).$$

For these $Y_l^m(\Omega)$,

$$Y_l^{m*}(\Omega)=(-1)^m Y_l^{-m}(\Omega),$$

we obtain

$$\phi_{ij}(\mathbf{k},\boldsymbol{\kappa})=\sum_{nlm}f_{nl}(\kappa)S_{nl}(k)Y_l^{m*}(\Omega_\kappa)Y_l^m(\Omega_k). \quad (18)$$

Or, in more compact notation,

$$\phi_{ij}(\mathbf{k},\boldsymbol{\kappa})=\sum_{nlm}f_{nlm}{}^*(\boldsymbol{\kappa})S_{nlm}(\mathbf{k}).$$

B. Parity Considerations

Under a parity transformation all the coordinates are inverted through the origin. In Cartesian coordinates this transformation for three particles is

$$\mathbf{r}_1\rightarrow-\mathbf{r}_1,\qquad \mathbf{r}_2\rightarrow-\mathbf{r}_2,\qquad \mathbf{r}_3\rightarrow-\mathbf{r}_3.$$

In each of our Jacobi coordinate frames the parity transformation is written as

$$\mathbf{R}\rightarrow-\mathbf{R},\qquad \mathbf{r}_{ij}\rightarrow-\mathbf{r}_{ij},\qquad \boldsymbol{\varrho}_k\rightarrow-\boldsymbol{\varrho}_k.$$

Now we wish to examine the properties of our solutions under this transformation.

For solutions with $L=0$ we see that, for two identical particles and a third different particle, the equations for the orbitals divide into two classes. They are the symmetric space solutions where the $\varphi_{ij}(\mathbf{k},\boldsymbol{\kappa})$ are even in $\mathbf{k}$ and the antisymmetric space solutions where the $\varphi_{ij}(\mathbf{k},\boldsymbol{\kappa})$ are odd in $\mathbf{k}$. Since these solutions are expanded into complete sets with terms containing

$Y_l^{m*}(\Omega_\kappa)Y_l^m(\Omega_k)$, they will have the parity of $(-1)^{2l}$ and will always be even.

For the most general situation, where $L\neq 0$ and the individual orbitals are expanded by Eq. (17), we see that each term in the φ_{ij} will contain factors like $Y_{l'}^{m'}(\Omega_\kappa)Y_l^m(\Omega_k)$ and will have the parity $(-1)^{l+l'}$. Since l and l' may assume all integral values, the parity of each term in the expansion may be either even or odd. The parity operator $\mathbf{P}$ commutes with the Hamiltonian; therefore we may require that each eigenstate be constructed with a definite parity. For states where $L\neq 0$ we may have eigenstates with either even or odd parity. For example, for $L=1$ we know from the addition of angular momenta that

$$|l-l'|\leqq L\leqq l+l'$$

and we may form $L=1$ with terms like $l=1$, $l'=1$; $l=2$, $l'=2$; etc. or with terms like $l=1$, $l'=0$; $l=0$, $l'=1$; $l=2$, $l'=1$; $l=1$, $l'=2$; etc. The first set will form an orbital with even parity and the second set will give an orbital with odd parity. The complete set of commuting operators is then $\mathbf{H}$, $\mathbf{L}$, $\mathbf{M}$, $\mathbf{P}$, $\mathbf{O}$, $\mathbf{O}_S$, $\mathbf{S}$, and $\mathbf{M}_S$, where $\mathbf{S}$ and $\mathbf{M}_S$ are included separately in nonrelativistic mechanics as the spin parts. The operators $\mathbf{O}$ and $\mathbf{O}_S$ are the space-exchange and the spin-exchange operators. Our set of eigenvectors may be written as

$$|ELMPOO_SSM_S\rangle=\Psi_{ELMPO}(\mathbf{r}_{ij},\varrho_k)\,|SM_S\rangle,$$

where it is understood that the antisymmetric combination of the space part and the spin part is taken. The total space part of the wave function is

$$\Psi_{ELMPO}(\mathbf{r}_{ij},\varrho_k)$$
$$=\psi_{ijELMPO}(\mathbf{r}_{ij},\varrho_k)+\psi_{jkELMPO}(\mathbf{r}_{jk},\varrho_i)+\psi_{kiELMPO}(\mathbf{r}_{ki},\varrho_j).$$

V. SOME ONE-DIMENSIONAL APPLICATIONS INVOLVING DELTA-FUNCTION POTENTIALS

In Sec. III we have seen how identical particles can be treated in this formulation of the three-body problem. In Sec. IV we found that each orbital must have the same angular momentum properties as the total wave function. The general equations for distinguishable particles simplify to Eqs. (14a) and (14b) for two identical particles, and to Eq. (15) for three identical particles. Now we wish to examine some artificial one-dimensional problems in order to gain insight into problems of more general interest.

We first consider the ground state of three identical spinless particles which attract each other with one-dimensional δ-function potentials. The total potential is

$$v_t=-S\delta(x_1-x_2)-S\delta(x_2-x_3)-S\delta(x_3-x_1),$$

where S is the strength of the δ function. This problem was studied by McGuire[6] using ray-tracing techniques and by Eyges[1] working with Eq. (15). For completeness, we wish to summarize Eyges's results. The ground state of this system is represented by the one-dimensional analog of Eq. (15):

$$\phi^e(k,\kappa)=\frac{S}{(2\pi)(k^2+\frac{3}{4}\kappa^2+K^2)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dk'dx\,\delta(x)$$
$$\times\{\phi^e(k',\kappa)\,\exp ix(k'-k)+\phi^e(\tfrac{1}{2}k',k'-2\kappa)[\exp ix(k'-k-\tfrac{3}{2}\kappa)+\exp ix(-k'-k+\tfrac{3}{2}\kappa)]\}.$$

Performing the integral on x and dropping the superscript e gives

$$\phi(k,\kappa)=\frac{S}{(2\pi)(k^2+\frac{3}{4}\kappa^2+K^2)}\int_{-\infty}^{\infty}dk'\{\phi(k',\kappa)+2\phi(\tfrac{1}{2}k',k'-2\kappa)\}.$$

We note that the right-hand side is only a function of κ and so we make the following substitution:

$$\phi(k,\kappa)=g(\kappa)/(k^2+\tfrac{3}{4}\kappa^2+K^2).$$

The resulting integral equation for $g(\kappa)$ is

$$g(\kappa)\left[1-\frac{S}{2(\frac{3}{4}\kappa^2+K^2)^{1/2}}\right]=\frac{S}{\pi}\int_{-\infty}^{\infty}d\kappa'\,\frac{g(\kappa')}{\frac{1}{4}(\kappa'+2\kappa)^2+\frac{3}{4}\kappa'^2+K^2}.$$

If we substitute

$$g(\kappa)=1/(\kappa^2+\alpha^2)$$

the integral on κ' may be done by extending the integration to the complex plane. This satisfies the above integral equation for $g(\kappa)$ if $\alpha=K=S$. The exact total wave function in momentum space (unnormalized) may then be written as

$$\Phi(k,\kappa)=\phi(k,\kappa)+\phi(-\tfrac{1}{2}k+\tfrac{3}{4}\kappa,-k-\tfrac{1}{2}\kappa)+\phi(-\tfrac{1}{2}k-\tfrac{3}{4}\kappa,k-\tfrac{1}{2}\kappa),$$

$$\Phi(k,\kappa)=(k^2+\tfrac{3}{4}\kappa^2+K^2)^{-1}\{(k^2+K^2)^{-1}+[(k+\tfrac{1}{2}\kappa)^2+K^2]^{-1}+[(k-\tfrac{1}{2}\kappa)^2+K^2]^{-1}\}.$$

[6] J. B. McGuire, J. Math. Phys. 5, 622 (1963).

TABLE I. One-dimensional δ-function potentials ($m_1=m_3\ll m_2$).

Potential (v_t)	Energy ($-K^2$)	$g_1(\kappa)$ approx.	$g_2(\kappa)$ approx.
$-\delta(x_{12})-\delta(x_{23})-\delta(x_{31})$	-1.664 ± 0.002	$+2.25/(\kappa^2+2.25)\pm0.05$	$+0.680[5.05/(\kappa^2+5.05)]\pm0.05$
$-\delta(x_{12})-\delta(x_{23})+\delta(x_{31})$	-0.648 ± 0.001	$+0.55/(\kappa^2+0.55)\pm0.05$	$-0.310[2.80/(\kappa^2+2.80)]\pm0.05$
$-\delta(x_{12})-\delta(x_{23})+\frac{1}{2}\delta(x_{31})$	-0.789 ± 0.001	$+0.575/(\kappa^2+0.575)\pm0.05$	$-0.200[3.35/(\kappa^2+3.35)]\pm0.05$

In coordinate space we may also show that the total unnormalized wave function is

$$\Psi(x_{12}, y_3)=\exp\{-\tfrac{1}{2}K[\,|\,x_{12}\,|+|\,\tfrac{1}{2}x_{12}+y_3\,|+|\,\tfrac{1}{2}x_{12}-y_3\,|\,]\},$$

$$\Psi(x_1, x_2, x_3)=\exp\{-\tfrac{1}{2}K[\,|\,x_1-x_2\,|+|\,x_2-x_3\,|+|\,x_3-x_1\,|\,]\}.$$

We now turn to a more general case where two of the particles are identical and the third particle is different. We may also imagine that two identical particles (one and three) repel each other as long as the total system remains bound. Therefore, we consider a one-dimensional, three-body problem where the potential is given by

$$v_t=-S_1\delta(x_1-x_2)-S_1\delta(x_2-x_3)\mp S_2\delta(x_3-x_1),$$

where we may consider either an attractive or repulsive interaction between particles one and three. The motive for studying an artificial three-body problem like this is to learn about the effect of a repulsive part of the total potential on the total solution, provided that the system remains bound. Substituting these two types of potentials into the one-dimensional analogs of Eqs. (14a) and (14b) and performing the integrations over the δ-function potentials we obtain

$$\phi_1(k,\kappa)=\frac{S_1}{(2\pi)(\alpha_{12}k^2+\beta_3\kappa^2+K^2)}\int_{-\infty}^{\infty}dk'\,\{\phi_1(k',\kappa)+\phi_1(-bk',k'-\kappa/b)+\phi_2(\tfrac{1}{2}k',k'-2\kappa)\},$$

$$\phi_2(k,\kappa)=\frac{\pm S_2}{(2\pi)(\alpha_{31}k^2+\beta_2\kappa^2+K^2)}\int_{-\infty}^{\infty}dk'\,\{\phi_2(k',\kappa)+\phi_1(ak',k'-\kappa/a)+\phi_1(-ak',k'-\kappa/a)\}.$$

Making the following substitutions for φ_1 and φ_2:

$$\phi_1(k,\kappa)=g_1(\kappa)/(\alpha_{12}k^2+\beta_3\kappa^2+K^2),\qquad \phi_2(k,\kappa)=g_2(\kappa)/(\alpha_{31}k^2+\beta_2\kappa^2+K^2),$$

and simplifying the resulting equations for $g_1(\kappa)$ and $g_2(\kappa)$ gives

$$g_1(\kappa)\left[\frac{2\pi}{S_1}-\frac{\pi}{(\alpha_{12}\beta_3\kappa^2+\alpha_{12}K^2)^{1/2}}\right]=\int_{-\infty}^{\infty}dy\left\{\frac{g_1(y)}{\alpha_{12}(by+\kappa)^2+\beta_3y^2+K^2}+\frac{g_2(y)}{\alpha_{31}(\frac{1}{2}y+\kappa)^2+\beta_2y^2+K^2}\right\},\tag{19a}$$

$$g_2(\kappa)\left[\pm\frac{\pi}{S_2}-\frac{\pi}{2(\alpha_{31}\beta_2\kappa^2+\alpha_{31}K^2)^{1/2}}\right]=\int_{-\infty}^{\infty}dy\,\frac{g_1(y)}{\alpha_{12}(ay+\kappa)^2+\beta_3y^2+K^2}.\tag{19b}$$

An exact solution for this set of coupled integral equations for $g_1(\kappa)$ and $g_2(\kappa)$ would solve the problem of two identical particles and a third particle interacting through δ-function pair potentials. At present, we have not been able to find exact solutions to Eqs. (19a) and (19b). We have been able to solve them on the IBM 7044 computer and obtain an approximate eigenvalue and eigenvector for the ground state of the system. We are particularly interested in examining the numerical solutions when the masses of the two identical particles are much smaller than the mass of the third particle. In that case

$$a\to1,\qquad b\to0,$$

$$\alpha_{12}\to\tfrac{1}{2},\qquad \beta_3=\tfrac{1}{2},\qquad \alpha_{31}=1,\qquad \beta_2=\tfrac{1}{4},$$

and Eqs. (19a) and (19b) become

$$g_1(\kappa)\left[\frac{2\pi}{S_1}-\frac{2\pi}{(\kappa^2+2K^2)^{1/2}}\right]=\int_{-\infty}^{\infty}dy\left\{\frac{g_1(y)}{\frac{1}{2}\kappa^2+\frac{1}{2}y^2+K^2}+\frac{g_2(y)}{(\frac{1}{2}y+\kappa)^2+\frac{1}{4}y^2+K^2}\right\},$$

$$g_2(\kappa)\left[\pm\frac{\pi}{S_2}-\frac{\pi}{(\kappa^2+4K^2)^{1/2}}\right]=\int_{-\infty}^{\infty}dy\,\frac{g_1(y)}{\frac{1}{2}(y+\kappa)^2+\frac{1}{2}y^2+K^2}.$$

We found one eigenvalue and the associated eigenfunction representing the ground state of the system

for each of several combinations of values for S_1 and S_2. The results for the ground-state energy and approximate functions for $g_1(\kappa)$ and $g_2(\kappa)$ are shown in Table I. The approximate functions for $g_1(\kappa)$ and $g_2(\kappa)$ in Table I are included only to give the reader a feeling for the numerical results. In order to obtain more accurate functions, more complicated terms would have to be included in a curve-fitting procedure. The machine results for $g_1(\kappa)$ and $g_2(\kappa)$ are plotted in Figs. 1(a), 1(b), and 1(c) and have about the same accuracy as the computed values for the energy listed in Table I. Since $g_1(\kappa)$ and $g_2(\kappa)$ are even functions, only the values for positive κ are shown. We may write the total unnormalized wave function in momentum space by recalling that

$$\Phi(k,\kappa)\equiv(2\pi)^{-1}\iint dx_{12}dy_3\,\Psi(x_{12},y_3)\,\exp(ikx_{12}+i\kappa y_3).$$

Substituting the orbitals in coordinate space for $\Psi(x_{12},y_3)$ and transforming to the appropriate Jacobi frame for each term of the integral gives

$$\Phi(k,\kappa)=\iint\psi_1(x_{12},y_3)\,\exp(ikx_{12}+i\kappa y_3)\,dx_{12}dy_3$$

$$+\iint\psi_1(x_{23},y_1)\,\exp[iky_1+i\kappa(-x_{23})]dx_{23}dy_1$$

$$+\iint\psi_2(x_{31},y_2)\,\exp[ik(-\tfrac{1}{2}x_{31}-y_2)+i\kappa(\tfrac{1}{2}x_{31}-y_2)]dx_{31}dy_2,$$

$$\Phi(k,\kappa)=\phi_1(k,\kappa)+\phi_1(-\kappa,k)+\phi_2(-\tfrac{1}{2}k+\tfrac{1}{2}\kappa,\,-k-\kappa).$$

For this problem the orbitals are given by

$$\phi_1(k,\kappa)=g_1(\kappa)/(\tfrac{1}{2}k^2+\tfrac{1}{2}\kappa^2+K^2)$$
$$\phi_2(k,\kappa)=g_2(\kappa)/(k^2+\tfrac{1}{4}\kappa^2+K^2).$$

Several comments are in order about these results. We recall that when all three particles are identical and interact through attractive δ-function potentials the exact energy of the ground state was $-K^2=-S^2\equiv-1$. We see that when two of the particles are identical and much lighter than the third, the binding energy increases. We also find that if the light pair of particles repel one another the binding energy decreases from that of the previous case as expected. Another feature which appears is a negative sign in the second term of the total wave function for the orbital representing the repulsive pair of particles. In addition, a decrease in the relative strength of the repulsive interaction is seen to increase the binding energy as expected.

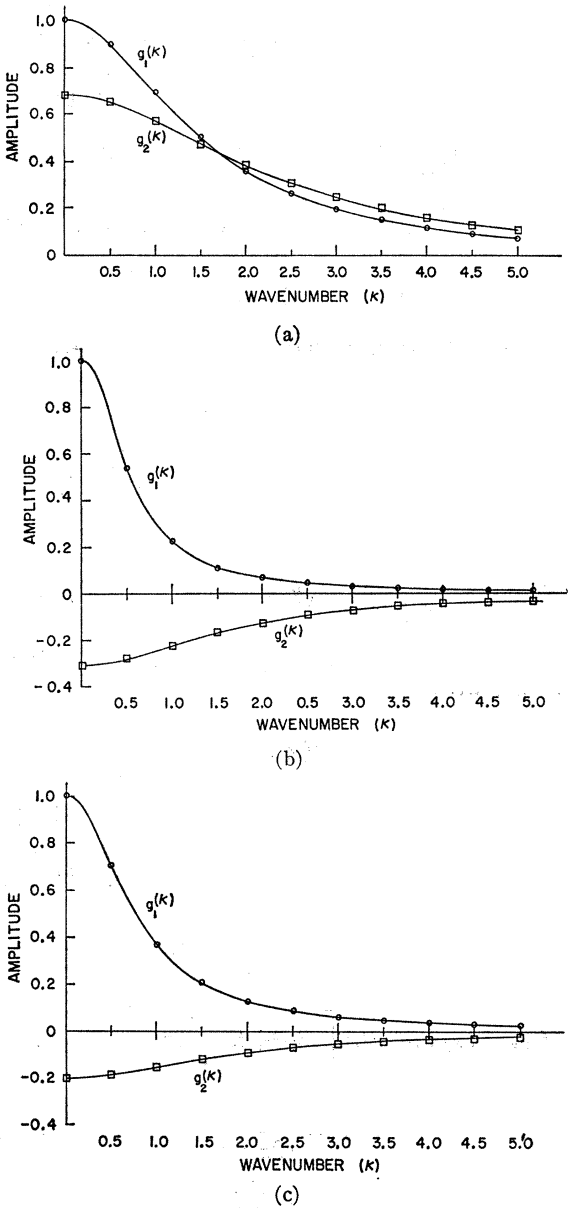

FIG. 1. (a) The functions g_1 and g_2 for $v_t=-\delta(x_{12})-\delta(x_{23})-\delta(x_{31})$ and $m_1=m_3\ll m_2$; (b) the functions g_1 and g_2 for $v_t=-\delta(x_{12})-\delta(x_{23})+\delta(x_{31})$ and $m_1=m_3\ll m_2$; (c) the functions g_1 and g_2 for $v_t=-\delta(x_{12})-\delta(x_{23})+\frac{1}{2}\delta(x_{31})$ and $m_1=m_3\ll m_2$.

VI. THE HELIUM-LIKE ATOM

A. Formulation for States of the Form $L=0$

In previous sections we have seen how the three-body problem for particles of arbitrary mass may be formulated in momentum space. We also have shown how to deal with situations where some or all of the particles are identical and obey either Fermi–Dirac or Einstein–Bose statistics. We have examined the angular momentum and parity properties of these solutions and seen how to expand the orbitals for states of arbitrary L and M. Now we turn to a realistic problem and demonstrate our general method by treating the ground state and some excited states of the helium-like atom. From our discussion in Sec. III and IV we note that solutions to Eqs. (14a) and (14b) are divided into two classes for states of the form $L=0$. In our derivation we will carry both the even and odd l so that both

solutions to these equations can be examined. For states of this type, we may expand the two orbitals $\varphi_1(\mathbf{k}, \boldsymbol{\kappa})$ and $\varphi_2(\mathbf{k}, \boldsymbol{\kappa})$ in the following way, where the sum on l is restricted to either both even l or both odd l:

$$\phi_1(\mathbf{k}, \boldsymbol{\kappa}) = \sum_{nlm} f_{nl}{}^{\alpha}(\kappa)\, Y_l{}^{m*}(\Omega_\kappa)\, S_{nl}{}^{\alpha}(k)\, Y_l{}^{m}(\Omega_k), \quad (20a)$$

$$\phi_2(\mathbf{k}, \boldsymbol{\kappa}) = \sum_{nlm} f_{nl}{}^{\beta}(\kappa)\, Y_l{}^{m*}(\Omega_\kappa)\, S_{nl}{}^{\beta}(k)\, Y_l{}^{m}(\Omega_k). \quad (20b)$$

The total potential for the helium atom is

$$v_t = S_1 u(\mathbf{r}_1-\mathbf{r}_2) + S_1 u(\mathbf{r}_2-\mathbf{r}_3) + S_2 u(\mathbf{r}_3-\mathbf{r}_1),$$

where

$$S_1 = 2e^2 m_e/\hbar^2,$$
$$S_2 = -e^2 m_e/\hbar^2, \qquad u(\mathbf{r}_i-\mathbf{r}_j) = -1/|\,\mathbf{r}_i-\mathbf{r}_j\,|.$$

We note that the third term in the potential is the electron-electron repulsion and is positive. The functions $S_{nl}{}^{\alpha}(k)$ and $S_{nl}{}^{\beta}(k)$ will be chosen as the Sturmian set of strength α^2 and β^2 for the analogous two-body problem. Some of the properties of the Sturmian set for the Coulomb potential are discussed in Appendix A. Substituting the expansion (20a) in Eq. (14a) and rearranging slightly gives

$$(\alpha_1 k^2+\beta_1\kappa^2+K^2)\sum_{nlm} f_{nlm}{}^{\alpha*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\alpha}(\mathbf{k}) = \frac{-S_1}{(2\pi)^3}\iint d^3k'd^3r\; u(\mathbf{r})$$
$$\times\{\sum_{nlm} f_{nlm}{}^{\alpha*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\alpha}(\mathbf{k}')\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k}) + \sum_{nlm} f_{nlm}{}^{\beta*}(\mathbf{k}'-2\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\tfrac{1}{2}\mathbf{k}')\ \exp i\mathbf{r}\cdot[-\mathbf{k}'-\mathbf{k}+(2-a)\boldsymbol{\kappa}]$$
$$+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/b)\, S_{nlm}{}^{\alpha}(-b\mathbf{k}')\ \exp i\mathbf{r}\cdot[\mathbf{k}'-\mathbf{k}-(1/b-b)\boldsymbol{\kappa}]\}.$$

Here, we have written the expansion of $\varphi_1(\mathbf{k}, \boldsymbol{\kappa})$ in more compact notation. For the second integral equation we may also write

$$(\alpha_2 k^2+\beta_2\kappa^2+K^2)\sum_{nlm} f_{nlm}{}^{\beta*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\mathbf{k}) = \frac{-S_2}{(2\pi)^3}\iint d^3k'd^3r\; u(\mathbf{r})$$
$$\times\{\sum_{nlm} f_{nlm}{}^{\beta*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\mathbf{k}')\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k}) + \sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(-a\mathbf{k}')\ \exp i\mathbf{r}\cdot[\mathbf{k}'-\mathbf{k}-(a^{-1}-\tfrac{1}{2})\boldsymbol{\kappa}]$$
$$+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(a\mathbf{k}')\ \exp i\mathbf{r}\cdot[-\mathbf{k}'-\mathbf{k}+(a^{-1}-\tfrac{1}{2})\boldsymbol{\kappa}]\}.$$

We may now multiply the first equation by $S_{n'l'm'}{}^{\alpha*}(\mathbf{k})\, Y_{l'}{}^{m'}(\Omega_\kappa)$, the second by $S_{n'l'm'}{}^{\beta*}(\mathbf{k})\, Y_{l'}{}^{m'}(\Omega_\kappa)$, and integrate with respect to $\mathbf{k}$ to obtain

$$\sum_n f_{nl'm'}{}^{\alpha*}(\boldsymbol{\kappa})\, Y_{l'}{}^{m'}(\Omega_\kappa)\left[(\beta_1\kappa^2+K^2)\int dk\; k^2 S_{n'l'}{}^{\alpha}(k)\, S_{nl'}{}^{\alpha}(k) + \alpha_1\int dk\; k^4 S_{n'l'}{}^{\alpha}(k)\, S_{nl'}{}^{\alpha}(k)\right]$$
$$= \frac{-S_1}{(2\pi)^3}\int d^3k'\left\{\iint d^3k d^3r\; u(\mathbf{r})\, S_{n'l'm'}{}^{\alpha*}(\mathbf{k})\, Y_{l'}{}^{m'}(\Omega_\kappa)\left[\sum_{nlm} f_{nlm}{}^{\alpha*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\alpha}(\mathbf{k}')\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k})\right.\right.$$
$$+\sum_{nlm} f_{nlm}{}^{\beta*}(\mathbf{k}'-2\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\tfrac{1}{2}\mathbf{k}')\ \exp i\mathbf{r}\cdot(-\mathbf{k}'-\mathbf{k}+(2-a)\boldsymbol{\kappa})$$
$$\left.\left.+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/b)\, S_{nlm}{}^{\alpha}(-b\mathbf{k}')\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k}-(b^{-1}-b)\boldsymbol{\kappa})\right]\right\}.$$

For the second equation we have

$$\sum_n f_{nl'm'}{}^{\beta*}(\boldsymbol{\kappa})\, Y_{l'}{}^{m'}(\Omega_\kappa)\left[(\beta_2\kappa^2+K^2)\int dk\; k^2 S_{n'l'}{}^{\beta}(k)\, S_{nl'}{}^{\beta}(k) + \alpha_2\int dk\; k^4 S_{n'l'}{}^{\beta}(k)\, S_{nl'}{}^{\beta}(k)\right]$$
$$= \frac{-S_2}{(2\pi)^3}\int d^3k'\left\{\iint d^3k d^3r\; u(\mathbf{r})\, S_{n'l'm'}{}^{\beta*}(\mathbf{k})\, Y_{l'}{}^{m'}(\Omega_\kappa)\left[\sum_{nlm} f_{nlm}{}^{\beta*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\mathbf{k}')\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k})\right.\right.$$
$$+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(-a\mathbf{k}')\ \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k}-(a^{-1}-\tfrac{1}{2})\boldsymbol{\kappa})$$
$$\left.\left.+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(a\mathbf{k}')\ \exp i\mathbf{r}\cdot(-\mathbf{k}'-\mathbf{k}+(a^{-1}-\tfrac{1}{2})\boldsymbol{\kappa})\right]\right\}.$$

From our discussion in Appendix A we see that the Sturmian set in momentum space obeys the following double integral equation:

$$S_{nlm}{}^{\alpha*}(\mathbf{k}') = \frac{-2\alpha\lambda_n}{(2\pi)^3(k'^2+\alpha^2)} \iint d^3k d^3r\, u(\mathbf{r})\, S_{nlm}{}^{\alpha*}(\mathbf{k})\, \exp i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k}),$$

where α^2 is the two-body energy, or strength, of the set and the $\{\lambda_n\}$ are just the positive integers. We may also write

$$S_{nlm}{}^{\alpha*}(-\mathbf{k}'+(2-a)\boldsymbol{\kappa}) = \frac{-2\alpha\lambda_n}{(2\pi)^3[(-\mathbf{k}'+(2-a)\boldsymbol{\kappa})^2+\alpha^2]} \iint d^3k d^3r\, u(\mathbf{r})\, S_{nlm}{}^{\alpha*}(\mathbf{k})\, \exp i\mathbf{r}\cdot(-\mathbf{k}'+(2-a)\boldsymbol{\kappa}-\mathbf{k}).$$

Using this property of the Sturmian set, we may eliminate the integration over the potential on the right-hand side of each of the two equations. This gives

$$\sum_n f_{nl'm'}{}^{\alpha*}(\boldsymbol{\kappa})\, Y_{l'}{}^{m'}(\Omega_\kappa)[(\beta_1\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\alpha}+\alpha_1\gamma_{n'l'nl'}{}^{\alpha}]$$

$$= S_1 \int d^3k'\, Y_{l'}{}^{m'}(\Omega_\kappa) \left\{ \sum_{nlm} f_{nlm}{}^{\alpha*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\alpha}(\mathbf{k}')\, \frac{(k'^2+\alpha^2)}{2\alpha\lambda_{n'}}\, S_{n'l'm'}{}^{\alpha*}(\mathbf{k}') \right.$$

$$+ \sum_{nlm} f_{nlm}{}^{\beta*}(\mathbf{k}'-2\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\tfrac{1}{2}\mathbf{k}') \left[\frac{(-\mathbf{k}'+(2-a)\boldsymbol{\kappa})^2+\alpha^2}{2\alpha\lambda_{n'}}\right] S_{n'l'm'}{}^{\alpha*}(-\mathbf{k}'+(2-a)\boldsymbol{\kappa})$$

$$\left. + \sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/b)\, S_{nlm}{}^{\alpha}(-b\mathbf{k}') \left[\frac{(\mathbf{k}'-(b^{-1}-b)\boldsymbol{\kappa})^2+\alpha^2}{2\alpha\lambda_{n'}}\right] S_{n'l'm'}{}^{\alpha*}(\mathbf{k}'-(b^{-1}-b)\boldsymbol{\kappa}) \right\},$$

and for the second equation

$$\sum_n f_{nl'm'}{}^{\beta*}(\boldsymbol{\kappa})\, Y_{l'}{}^{m'}(\Omega_\kappa)[(\beta_2\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\beta}+\alpha_2\gamma_{n'l'nl'}{}^{\beta}]$$

$$= S_2 \int d^3k'\, Y_{l'}{}^{m'}(\Omega_\kappa) \left\{ \sum_{nlm} f_{nlm}{}^{\beta*}(\boldsymbol{\kappa})\, S_{nlm}{}^{\beta*}(\mathbf{k}')\, \frac{(k'^2+\beta^2)}{2\beta\lambda_{n'}}\, S_{n'l'm'}{}^{\beta}(\mathbf{k}') \right.$$

$$+ \sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(-a\mathbf{k}') \left[\frac{(\mathbf{k}'-(1/a-\frac{1}{2})\boldsymbol{\kappa})^2+\beta^2}{2\beta\lambda_{n'}}\right] S_{n'l'm'}{}^{\beta*}(\mathbf{k}'-(1/a-\tfrac{1}{2})\boldsymbol{\kappa})$$

$$\left. + \sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(a\mathbf{k}') \left[\frac{(-\mathbf{k}'+(1/a-\frac{1}{2})\boldsymbol{\kappa})^2+\beta^2}{2\beta\lambda_{n'}}\right] S_{n'l'm'}{}^{\beta*}(-\mathbf{k}'+(1/a-\tfrac{1}{2})\boldsymbol{\kappa}) \right\}.$$

The following constants have been defined:

$$\epsilon_{n'l'nl'}{}^{\alpha,\beta} \equiv \int dk\, k^2 S_{n'l'}{}^{\alpha,\beta}(k)\, S_{nl'}{}^{\alpha,\beta}(k); \qquad \gamma_{n'l'nl'}{}^{\alpha,\beta} \equiv \int dk\, k^4 S_{n'l'}{}^{\alpha,\beta}(k)\, S_{nl'}{}^{\alpha,\beta}(k).$$

These integrals are all trivial and may be easily computed. Utilizing the orthogonality relation in momentum space derived in Appendix A gives

$$\sum_n f_{nl'm'}{}^{\alpha*}(\boldsymbol{\kappa})\, Y_{l'}{}^{m'}(\Omega_\kappa)[(\beta_1\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\alpha}+\alpha_1\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}(S_1\alpha)\delta_{nn'}]$$

$$= \frac{S_1}{2\alpha\lambda_{n'}} \int d^3k'\, Y_{l'}{}^{m'}(\Omega_\kappa) \{ \sum_{nlm} f_{nlm}{}^{\beta*}(\mathbf{k}'-2\boldsymbol{\kappa})\, S_{nlm}{}^{\beta}(\tfrac{1}{2}\mathbf{k}')[(\mathbf{k}'-(2-a)\boldsymbol{\kappa})^2+\alpha^2](-1)^{l'} S_{n'l'm'}{}^{\alpha*}(\mathbf{k}'-(2-a)\boldsymbol{\kappa})$$

$$+ \sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/b)\,(-1)^{l} S_{nlm}{}^{\alpha}(b\mathbf{k}')[(\mathbf{k}'-(1/b-b)\boldsymbol{\kappa})^2+\alpha^2] S_{n'l'm'}{}^{\alpha*}(\mathbf{k}'-(1/b-b)\boldsymbol{\kappa}) \}.$$

The second equation for the electron–electron orbital is

$$\sum_n f_{nl'm'}{}^{\beta*}(\boldsymbol{\kappa})\, Y_{l'}{}^{m'}(\Omega_\kappa)[(\beta_2\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\beta}+\alpha_2\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}(S_2\beta)\delta_{nn'}] = \frac{S_2}{2\beta\lambda_{n'}} \int d^3k'\, Y_{l'}{}^{m'}(\Omega_\kappa)$$

$$\times \{ \sum_{nlm} [(-1)^l+(-1)^{l'}] f_{nlm}{}^{\alpha*}(\mathbf{k}'-\boldsymbol{\kappa}/a)\, S_{nlm}{}^{\alpha}(a\mathbf{k}')[(\mathbf{k}'-(1/a-\tfrac{1}{2})\boldsymbol{\kappa})^2+\beta^2] S_{n'l'm'}{}^{\beta*}(\mathbf{k}'-(1/a-\tfrac{1}{2})\boldsymbol{\kappa}) \}.$$

The quantity $(-1)^{l'}$ may be factored out since l and l' are either both even or both odd. Making the appropriate transformation of variables on the right-hand side of these two equations leads to a more simplified result:

$$\sum_n f_{nl'm'}{}^{\alpha*}(\kappa)\,Y_{l'}{}^{m'}(\Omega_\kappa)\left[(\beta_1\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\alpha}+\alpha_1\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}(S_1\alpha)\delta_{n'n}\right]$$

$$=\frac{S_1}{2\alpha\lambda_{n'}}(-1)^{l'}\int d^3x\,Y_{l'}{}^{m'}(\Omega_\kappa)\Big\{\sum_{nlm} f_{nlm}{}^{\beta*}(\mathbf{x})\,S_{nlm}{}^{\beta}(\tfrac{1}{2}\mathbf{x}+\boldsymbol{\kappa})\left[(\mathbf{x}+a\boldsymbol{\kappa})^2+\alpha^2\right]S_{n'l'm'}{}^{\alpha*}(\mathbf{x}+a\boldsymbol{\kappa})$$
$$+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{x})\,S_{nlm}{}^{\alpha}(b\mathbf{x}+\boldsymbol{\kappa})\left[(\mathbf{x}+b\boldsymbol{\kappa})^2+\alpha^2\right]S_{n'l'm'}{}^{\alpha*}(\mathbf{x}+b\boldsymbol{\kappa})\Big\}.$$

For the second equation

$$\sum_n f_{nl'm'}{}^{\beta*}(\kappa)\,Y_{l'}{}^{m'}(\Omega_\kappa)\left[(\beta_2\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\beta}+\alpha_2\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}S_2\beta\delta_{n'n}\right]$$

$$=\frac{S_2}{\beta\lambda_{n'}}(-1)^{l'}\int d^3x\,Y_{l'}{}^{m'}(\Omega_\kappa)\Big\{\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{x})\,S_{nlm}{}^{\alpha}(a\mathbf{x}+\boldsymbol{\kappa})\left[(\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa})^2+\beta^2\right]S_{n'l'm'}{}^{\beta*}(\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa})\Big\}.$$

These two equations are a set of coupled integral equations, where the two different kinds of particles have arbitrary masses. The equations simplify if we let the mass ratio of the electron to the nucleus go to zero. The error introduced by this approximation is of the order of 1 part in 8000 for the helium atom. There is really no loss of generality in doing this since the equations are still tractable if this approximation is not made. However, it does simplify the computational aspects of the problem. In this limit the constants appearing in these equations are

$$\alpha_1\to\tfrac{1}{2},\qquad \beta_1\to\tfrac{1}{2},\qquad \alpha_2=1,\qquad \beta_2\to\tfrac{1}{4},\qquad a\to 1,\qquad b\to 0.$$

Substituting, we obtain

$$\sum_n f_{nl'm'}{}^{\alpha*}(\kappa)\,Y_{l'}{}^{m'}(\Omega_\kappa)\left[(\tfrac{1}{2}\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\alpha}+\tfrac{1}{2}\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}(S_1\alpha)\delta_{n'n}\right]$$

$$=\frac{S_1}{2\alpha\lambda_{n'}}(-1)^{l'}\int d^3x\,Y_{l'}{}^{m'}(\Omega_\kappa)\Big\{\sum_{nlm} f_{nlm}{}^{\beta*}(\mathbf{x})\,S_{nlm}{}^{\beta}(\tfrac{1}{2}\mathbf{x}+\boldsymbol{\kappa})\left[(\mathbf{x}+\boldsymbol{\kappa})^2+\alpha^2\right]S_{n'l'm'}{}^{\alpha*}(\mathbf{x}+\boldsymbol{\kappa})$$
$$+\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{x})\,S_{nlm}{}^{\alpha}(\boldsymbol{\kappa})\,(x^2+\alpha^2)\,S_{n'l'm'}{}^{\alpha*}(\mathbf{x})\Big\}.$$

For the second equation

$$\sum_n f_{nl'm'}{}^{\beta*}(\kappa)\,Y_{l'}{}^{m'}(\Omega_\kappa)\left[(\tfrac{1}{4}\kappa^2+K^2)\epsilon_{n'l'nl'}{}^{\beta}+\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}(S_2\beta)\delta_{n'n}\right]$$

$$=\frac{+S_2}{\beta\lambda_{n'}}(-1)^{l'}\int d^3x Y_{l'}{}^{m'}(\Omega_\kappa)\Big\{\sum_{nlm} f_{nlm}{}^{\alpha*}(\mathbf{x})\,S_{nlm}{}^{\alpha}(\mathbf{x}+\boldsymbol{\kappa})\left[(\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa})^2+\beta^2\right]S_{n'l'm'}{}^{\beta*}(\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa})\Big\}.$$

Now we may sum both sides of these two equations on m' and integrate with respect to Ω_κ:

$$\sum_{n,m'} f_{nl'}{}^{\alpha}(\kappa)\left[(K^2+\tfrac{1}{2}\kappa^2)\epsilon_{n'l'nl'}{}^{\alpha}+\tfrac{1}{2}\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}(S_1\alpha)\delta_{n'n}\right]$$

$$=\frac{S_1}{2\alpha\lambda_{n'}}(-1)^{l'}\int dx\,x^2\iint d\Omega_{\mathbf{x}}d\Omega_\kappa\Big\{\sum_{nlmm'} f_{nl}{}^{\alpha}(x)\,S_{nl}{}^{\alpha}(\kappa)\,Y_l{}^{m*}(\Omega_{\mathbf{x}})\,Y_l{}^{m}(\Omega_\kappa)\,(x^2+\alpha^2)\,S_{n'l'}{}^{\alpha}(x)\,Y_{l'}{}^{m'*}(\Omega_{\mathbf{x}})\,Y_{l'}{}^{m'}(\Omega_\kappa)$$
$$+\sum_{nlmm'} f_{nl}{}^{\beta}(x)\,S_{nl}{}^{\beta}(|\,\tfrac{1}{2}\mathbf{x}+\boldsymbol{\kappa}\,|)\,Y_l{}^{m*}(\Omega_{\mathbf{x}})\,Y_l{}^{m}(\Omega_{1/2\mathbf{x}+\kappa})\left[(\mathbf{x}+\boldsymbol{\kappa})^2+\alpha^2\right]S_{n'l'}{}^{\alpha}(|\,\mathbf{x}+\boldsymbol{\kappa}\,|)\,Y_{l'}{}^{m'*}(\Omega_{\mathbf{x}+\kappa})\,Y_{l'}{}^{m'}(\Omega_\kappa)\Big\}.$$

For the second equation we also obtain

$$\sum_{nm'} f_{nl'}{}^{\beta}(\kappa)\left[(K^2+\tfrac{1}{4}\kappa^2)\epsilon_{n'l'nl'}{}^{\beta}+\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}(S_2\beta)\delta_{nn'}\right]=\frac{+S_2}{\beta\lambda_{n'}}(-1)^{l'}\int dx\,x^2\iint d\Omega_{\mathbf{x}}d\Omega_\kappa$$
$$\times\Big\{\sum_{nlmm'} f_{nl}{}^{\alpha}(x)\,S_{nl}{}^{\alpha}(|\,\mathbf{x}+\boldsymbol{\kappa}\,|)\,Y_l{}^{m*}(\Omega_{\mathbf{x}})\,Y_l{}^{m}(\Omega_{\mathbf{x}+\kappa})\left[(\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa})^2+\beta^2\right]S_{n'l'}{}^{\beta}(|\,\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa}\,|)\,Y_{l'}{}^{m'*}(\Omega_{\mathbf{x}+1/2\kappa})\,Y_{l'}{}^{m'}(\Omega_\kappa)\Big\}.$$

The additional theorem for spherical harmonics is

$$\sum_{m=-l}^{l} Y_l^{m*}(\Omega_1)\, Y_l^{m}(\Omega_2) = \frac{2l+1}{4\pi} P_l(\cos\gamma),$$

where γ is the angle between the directions Ω_1 and Ω_2. Using this theorem and the fact that the cosine of the angle between any two vectors **A** and **B** is $\mathbf{A}\cdot\mathbf{B}/|\,\mathbf{A}\,||\,\mathbf{B}\,|$, we may simplify our equations to give

$$\sum_n (2l'+1) f_{nl'}{}^{\alpha}(\kappa)\left[(K^2+\tfrac{1}{2}\kappa^2)\epsilon_{n'l'nl'}{}^{\alpha}+\tfrac{1}{2}\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}(S_1\alpha)\delta_{n'n}\right]$$

$$= \frac{S_1}{2\alpha\lambda_{n'}}(-1)^{l'}\int dx\, x^2 \iint d\Omega_x d\Omega_\kappa \left\{\sum_{nl} f_{nl}{}^{\alpha}(x)\, S_{nl}{}^{\alpha}(\kappa)\,(x^2+\alpha^2)\, S_{n'l'}{}^{\alpha}(x)\,\frac{(2l+1)}{4\pi} P_l(\cos\gamma)\,\frac{(2l'+1)}{4\pi} P_{l'}(\cos\gamma)\right.$$

$$\left. +\sum_{nl} f_{nl}{}^{\beta}(x)\, S_{nl}{}^{\beta}(|\,\tfrac{1}{2}\mathbf{x}+\boldsymbol{\kappa}\,|)\left[(\mathbf{x}+\boldsymbol{\kappa})^2+\alpha^2\right] S_{n'l'}{}^{\alpha}(|\,\mathbf{x}+\boldsymbol{\kappa}\,|)\,\frac{(2l+1)}{4\pi} P_l\left(\frac{\frac{1}{2}x+\kappa\cos\gamma}{|\,\frac{1}{2}\mathbf{x}+\boldsymbol{\kappa}\,|}\right)\frac{(2l'+1)}{4\pi} P_{l'}\left(\frac{\kappa+x\cos\gamma}{|\,\mathbf{x}+\boldsymbol{\kappa}\,|}\right)\right\}.$$

For the second equation

$$\sum_n (2l'+1) f_{nl'}{}^{\beta}(\kappa)\left[(K^2+\tfrac{1}{4}\kappa^2)\epsilon_{n'l'nl'}{}^{\beta}+\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}(S_2\beta)\delta_{n'n}\right] = +\frac{S_2}{\beta\lambda_{n'}}(-1)^{l'}\int dx\, x^2 \iint d\Omega_x d\Omega_\kappa$$

$$\times\left\{\sum_{nl} f_{nl}{}^{\alpha}(x)\, S_{nl}{}^{\alpha}(|\,\mathbf{x}+\boldsymbol{\kappa}\,|)\left[(\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa})^2+\beta^2\right] S_{n'l'}{}^{\beta}(|\,\mathbf{x}+\tfrac{1}{2}\boldsymbol{\kappa}\,|)\,\frac{(2l+1)}{4\pi} P_l\left(\frac{x+\kappa\cos\gamma}{|\,\mathbf{x}+\boldsymbol{\kappa}\,|}\right)\frac{(2l'+1)}{4\pi} P_{l'}\left(\frac{x\cos\gamma+\frac{1}{2}\kappa}{|\,\mathbf{x}+\frac{1}{2}\boldsymbol{\kappa}\,|}\right)\right\}.$$

We may now choose the z axis to be along the vector **x** and do some of the integrals over the angles to obtain

$$\sum_n f_{nl'}{}^{\alpha}(\kappa)\left[(K^2+\tfrac{1}{2}\kappa^2)\epsilon_{n'l'nl'}{}^{\alpha}+\tfrac{1}{2}\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}(S_1\alpha)\delta_{n'n}\right] = \frac{S_1}{4\alpha\lambda_{n'}}(-1)^{l'}$$

$$\times\int_0^\infty dx\, x^2\left\{\sum_n 2 f_{nl'}{}^{\alpha}(x)\, S_{nl'}{}^{\alpha}(\kappa)\,(x^2+\alpha^2)\, S_{n'l'}{}^{\alpha}(x)+\int_{-1}^{1} dz \sum_{nl} f_{nl}{}^{\beta}(x)\, S_{nl}{}^{\beta}\left[(\tfrac{1}{4}x^2+\kappa^2+x\kappa z)^{1/2}\right]\left[x^2+\kappa^2+2x\kappa z+\alpha^2\right]\right.$$

$$\left.\times S_{n'l'}{}^{\alpha}\left[(x^2+\kappa^2+2x\kappa z)^{1/2}\right](2l+1) P_l\left[\frac{\frac{1}{2}x+\kappa z}{(\frac{1}{4}x^2+\kappa^2+x\kappa z)^{1/2}}\right] P_{l'}\left[\frac{\kappa+xz}{(x^2+\kappa^2+2x\kappa z)^{1/2}}\right]\right\}. \tag{21a}$$

For the second equation we have

$$\sum_n f_{nl'}{}^{\beta}(\kappa)\left[(K^2+\tfrac{1}{4}\kappa^2)\epsilon_{n'l'nl'}{}^{\beta}+\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}(S_2\beta)\delta_{n'n}\right]$$

$$= \frac{S_2}{2\beta\lambda_{n'}}(-1)^{l'}\int_0^\infty dx\, x^2\int_{-1}^{1} dz \sum_{nl} f_{nl}{}^{\alpha}(x)\, S_{nl}{}^{\alpha}\left[(x^2+\kappa^2+2x\kappa z)^{1/2}\right]\left[x^2+\tfrac{1}{4}\kappa^2+x\kappa z+\beta^2\right]$$

$$\times S_{n'l'}{}^{\beta}\left[(x^2+\tfrac{1}{4}\kappa^2+x\kappa z)^{1/2}\right](2l+1) P_l\left[\frac{x+\kappa z}{(x^2+\kappa^2+2x\kappa z)^{1/2}}\right] P_{l'}\left[\frac{\frac{1}{2}\kappa+xz}{(x^2+\frac{1}{4}\kappa^2+x\kappa z)^{1/2}}\right], \tag{21b}$$

where z has been substituted for $\cos\gamma$. We note that all the integrals over z can be done because of the special form of the P_l and the associated S_{nl}. These integrals will just be sums of polynomials in x and κ multiplied by integrals of the type

$$g_{ij}{}^{k} = \int_{-1}^{1} dz\, \frac{z^k}{(az+b)^i (cz+d)^j},$$

where a, b, c, and d are simply polynomials in the x and κ and the i, j, and k take on integral values.[7] We define the following two symbols:

$$H_{n'l'nl}{}^{\alpha\beta} \equiv x^2\int_{-1}^{1} dz\,\left[x^2+\kappa^2+2x\kappa z+\alpha^2\right]$$

$$\times S_{n'l'}{}^{\alpha}\left[(x^2+\kappa^2+2x\kappa z)^{1/2}\right] S_{nl}{}^{\beta}\left[(\tfrac{1}{4}x^2+\kappa^2+x\kappa z)^{1/2}\right] P_l\left[\frac{\frac{1}{2}x+\kappa z}{(\frac{1}{4}x^2+\kappa^2+x\kappa z)^{1/2}}\right] P_{l'}\left[\frac{\kappa+xz}{(x^2+\kappa^2+2x\kappa z)^{1/2}}\right],$$

$$H_{n'l'nl}{}^{\beta\alpha} \equiv x^2\int_{-1}^{1} dz\,\left[x^2+\tfrac{1}{4}\kappa^2+x\kappa z+\beta^2\right]$$

$$\times S_{n'l'}{}^{\beta}\left[(x^2+\tfrac{1}{4}\kappa^2+x\kappa z)^{1/2}\right] S_{nl}{}^{\alpha}\left[(x^2+\kappa^2+2x\kappa z)^{1/2}\right] P_l\left[\frac{x+\kappa z}{(x^2+\kappa^2+2x\kappa z)^{1/2}}\right] P_{l'}\left[\frac{\frac{1}{2}\kappa+xz}{(x^2+\frac{1}{4}\kappa^2+x\kappa z)^{1/2}}\right].$$

[7] W. Gröbner and N. Hofreiter, *Integraltafel Erster Teil Unbestimmte Integrale* (Springer-Verlag, Wien, 1965), Vol. I, p. 10.

Equations (21a) and (21b) now may be written as

$$\sum_n f_{nl'}{}^{\alpha}(\kappa)[(K^2+\tfrac{1}{2}\kappa^2)\epsilon_{n'l'nl'}{}^{\alpha}+\tfrac{1}{2}\gamma_{n'l'nl'}{}^{\alpha}-\tfrac{1}{2}S_1\alpha\delta_{n'n}]$$

$$=\frac{S_1}{4\alpha\lambda_{n'}}(-1)^{l'}\int_0^{\infty}dx\{\sum_n 2x^2 f_{nl'}{}^{\alpha}(x)\,S_{nl'}{}^{\alpha}(\kappa)\,(x^2+\alpha^2)\,S_{n'l'}{}^{\alpha}(x)+\sum_{nl}(2l+1)f_{nl}{}^{\beta}(x)\,H_{n'l'nl}{}^{\alpha\beta}(x,\kappa)\},\quad(22a)$$

$$\sum_n f_{nl'}{}^{\beta}(\kappa)[(K^2+\tfrac{1}{4}\kappa^2)\epsilon_{n'l'nl'}{}^{\beta}+\gamma_{n'l'nl'}{}^{\beta}-\tfrac{1}{2}S_2\beta\delta_{n'n}]=+\frac{S_2}{2\beta\lambda_{n'}}(-1)^{l'}\int_0^{\infty}dx\{\sum_{nl}(2l+1)f_{nl}{}^{\alpha}(x)\,H_{n'l'nl}{}^{\beta\alpha}(x,\kappa)\}.\quad(22b)$$

We have examined the first, second, and fourth truncations of this system of equations for the helium-like atom where l is restricted to the even integers. The truncations are generated by keeping the first, the first and second, and the first four terms in the expansions for the two independent orbitals. For example, the first truncation for even l is

$$f_{10}{}^{\alpha}(\kappa)[2K^2+\alpha^2-2S_1\alpha+\kappa^2]=\frac{16\alpha^4S_1}{\pi}\left\{\frac{2}{(\kappa^2+\alpha^2)^2}\int_0^{\infty}dx\,f_{10}{}^{\alpha}(x)\,\frac{x^2}{(x^2+\alpha^2)}+\left(\frac{\beta}{\alpha}\right)^{5/2}\int_0^{\infty}dx\,f_{10}{}^{\beta}(x)\,I_{1010}{}^{\alpha\beta}(x,\kappa)\right\},\quad(23a)$$

$$f_{10}{}^{\beta}(\kappa)[4K^2+4\beta^2-4S_2\beta+\kappa^2]=\frac{64\beta^4S_2}{\pi}\left(\frac{\alpha}{\beta}\right)^{5/2}\int_0^{\infty}dx\,f_{10}{}^{\alpha}(x)\,I_{1010}{}^{\beta\alpha}(x,\kappa),\quad(23b)$$

where the two I's may be written out explicitly as

$$I_{1010}{}^{\alpha\beta}=\frac{-2x^2}{(\kappa^2-\frac{1}{2}x^2+2\beta^2-\alpha^2)[(\kappa^2+\frac{1}{4}x^2+\beta^2)^2-x^2\kappa^2]}+\frac{2x}{\kappa[\kappa^2-\frac{1}{2}x^2+2\beta^2-\alpha^2]^2}\ln\frac{[(x+\kappa)^2+\alpha^2][(\kappa-\frac{1}{2}x)^2+\beta^2]}{[(x-\kappa)^2+\alpha^2][(\kappa+\frac{1}{2}x)^2+\beta^2]},$$

$$I_{1010}{}^{\beta\alpha}=\frac{4x^2}{(x^2-\frac{1}{2}\kappa^2+2\beta^2-\alpha^2)[(x^2+\kappa^2+\alpha^2)^2-4x^2\kappa^2]}+\frac{x}{\kappa[x^2-\frac{1}{2}\kappa^2+2\beta^2-\alpha^2]^2}\ln\frac{[(x+\frac{1}{2}\kappa)^2+\beta^2][(x-\kappa)^2+\alpha^2]}{[(x-\frac{1}{2}\kappa)^2+\beta^2][(x+\kappa)^2+\alpha^2]}.$$

We note that these functions are well behaved for all values of x and κ. The second and fourth truncations of the system were treated in the same fashion. They will not be developed explicitly here since they are long and involved, but the results (energies and wave functions) are presented in the next section.

B. Results for Helium-Like Atoms

We will not attempt a detailed review of the literature on the helium atom here since there are several excellent references on the subject.[8] There have been some very accurate calculations for the ground state and some excited states of the helium-like atom. Pekeris and co-workers[9] have obtained accuracy up to nine or ten significant figures in the energy eigenvalue by applying the variational principle to a trial function containing, in certain cases, as many as one thousand terms. Our purpose in this paper is to present a general method for three-body problems and show the validity of the approach by considering only enough truncations of the system to demonstrate rapid convergence.

The behavior of the three-body energy as α^2 and β^2 are varied was studied for the first, second, and fourth truncations of the system. Figure 2 shows the ground-state energy in atomic units ($-K^2$) for the second truncation as a function of α^2 and β^2, where α^2 is the strength of the Sturmian set for the electron-nucleus orbital expansion and β^2 is the strength for the electron-electron orbital expansion. The experimental energy in atomic units for the ground state of the helium atom is -2.9037 and is shown by the dotted line in Fig. 2. For the first truncation, $-K^2$ as a function of α^2 and β^2, forms a saddle surface, but for the second and higher truncations an absolute minimum in the energy appears.

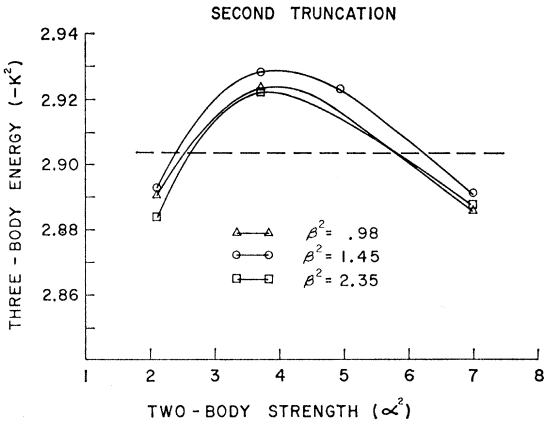

FIG. 2. The ground-state energy in helium for the second truncation as a function of α and β.

[8] See, for example, H. A. Bethe and E. Salpeter, *Quantum Mechancis of One- and Two-Electron Atoms* (Academic Press Inc., New York, 1957); E. A. Hylleraas, *Advances in Quantum Chemistry* (Academic Press Inc., New York, 1964); A. L. Stewart, Advan. Phys. **12**, 299 (1964).

[9] B. Schiff, C. L. Pekeris, and H. Lifson, Phys. Rev. **137**, A1672 (1965); C. L. Pekeris, *ibid.* **115**, 1216 (1959).

TABLE II. Three-body energies for helium-like atoms in atomic units.

Atom	Order of truncation	Our energy $1s^2$	Our energy $1s2s^1S$	Our energy $2s^2$	Comparison energy $1s^2$	Comparison energy $1s2s^1S$	Comparison energy $2s^2$	ΔE $1s^2$	ΔE $1s2s^1S$	ΔE $2s^2$
He	1st	−2.00	...	...	−2.9037[a]	...	...	+3.3%	...	...
He	2nd	−2.928	−2.094	−0.7581	−2.9037	−2.1460[a]	−0.7788[b]	+0.84%	−2.4%	−2.6%
He	4th	−2.9001	−2.1335	−0.7756	−2.9037	−2.1460	−0.7788	−0.12%	−0.58%	−0.41%
H^-	4th	−0.5320		−0.1722	−0.5278[a]	[c]	[c]	+0.79%	...	...
Li^+	4th	−7.2646	−5.0535	−1.8660	−7.2799[a]	−5.0409[a]	[c]	−0.21%	+0.25%	...

[a] A. L. Stewart, Advan. Phys. **12**, 299 (1964) (variational calculations).
[b] A. K. Bhatia and A. Temkin, Bull. Am. Phys. Soc. **11**, 722 (1966) (variational calculation).
[c] To the best of our knowledge there are no other calculations or experimental values for these states.

It should be noted here that this minimum in the energy is not equivalent to a variational minimum, since no variational principle has been employed in our treatment. If we choose β^2 such that $-K^2$ changes the least when small changes are made in β^2, i.e., in regions where

$$\partial\{-K^2(\alpha^2,\beta^2)\}/\partial\beta^2=0,$$

then the energy depends only on α^2. Figure 3 shows these results for the first, second, and fourth truncations of the helium atom in the ground state. We note that for any reasonable choice of the parameter α^2 the maximum difference between the calculated energy and the experimental value is about one part in 30 for the first truncation, one part in 125 for the second truncation, and about one part in 850 for the fourth truncation. From Figs. 2 and 3 we see that the dependence of the energy on α^2 and β^2 rapidly becomes smaller as the order of truncation is increased. For example, in the first truncation the energy changes by $\pm 3\%$ as α^2 and β^2 are varied from 2 to 6.5, while in the fourth truncation the energy varies by about $\pm 0.20\%$ for approximately the same variation in α^2 and β^2. This method produces a rapidly convergent energy as more functions are taken in the expansion of the orbitals, and the energy is seen to converge toward the exact value.

The unknown functions $f_{nl}{}^{\alpha}(\kappa)$ and $f_{nl}{}^{\beta}(\kappa)$ are given as functions of κ for these three truncations in Figs. 4, 5(a) and 5(b), and 6(a), 6(b), 6(c), and 6(d). The stability of the system is seen by noting that small percentage changes in the wave function, produced by taking higher-order terms in the orbital expansions, results in smaller percentage changes in the energy of the system. Each successive order of truncation reproduces the preceeding $f_{nl}{}^{\alpha}(\kappa)$ and $f_{nl}{}^{\beta}(\kappa)$ to within a small percentage, which is also to be expected. The unnormalized wave function in momentum space may be written down for the ground state of the helium atom. We recall that

$$\Phi(\mathbf{k},\boldsymbol{\kappa})\equiv\frac{1}{(2\pi)^3}\iint d\mathbf{r}_{12}d\boldsymbol{\varrho}_3\,\Psi(\mathbf{r}_{12},\boldsymbol{\varrho}_3)\exp(i\mathbf{k}\cdot\mathbf{r}_{12}+i\boldsymbol{\kappa}\cdot\boldsymbol{\varrho}_3).$$

Substituting the orbitals in coordinate space for $\Psi(\mathbf{r}_{12},\boldsymbol{\varrho}_3)$ and transforming to the appropriate Jacobi frame for each term of the integral gives

$$\Phi(\mathbf{k},\boldsymbol{\kappa})$$
$$=\phi_1(\mathbf{k},\boldsymbol{\kappa})+\phi_1(-\boldsymbol{\kappa},\mathbf{k})+\phi_2(-\tfrac{1}{2}\mathbf{k}+\tfrac{1}{2}\boldsymbol{\kappa},-\mathbf{k}-\boldsymbol{\kappa}).$$

For symmetric states of the type $L=0$ we have

$$\Phi(\mathbf{k},\boldsymbol{\kappa})=\phi_1(\mathbf{k},\boldsymbol{\kappa})+\phi_1(\boldsymbol{\kappa},\mathbf{k})+\phi_2(\tfrac{1}{2}\mathbf{k}-\tfrac{1}{2}\boldsymbol{\kappa},\mathbf{k}+\boldsymbol{\kappa}).$$

Energies and wave functions may also be calculated for other helium-like atoms as well as for some excited

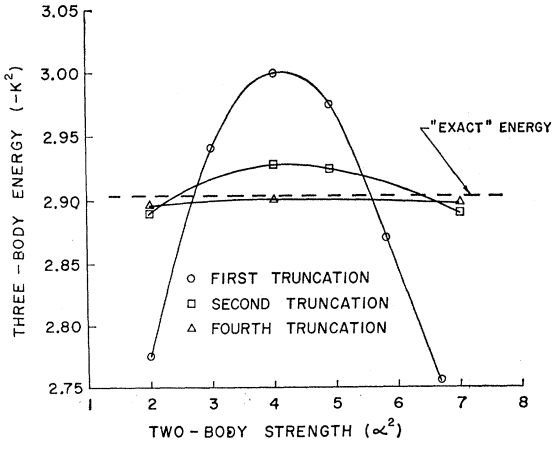

FIG. 3. The ground-state energy in helium for the first, second, and fourth truncations as a function of α.

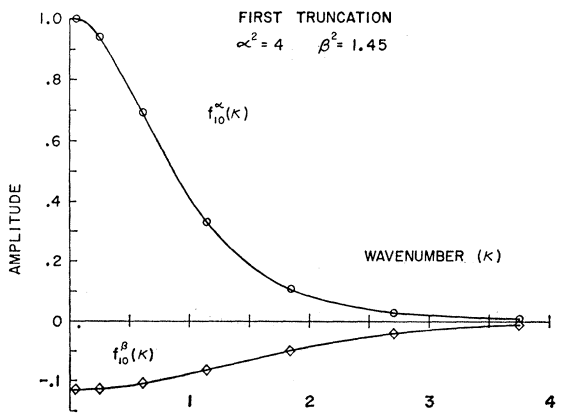

FIG. 4. The functions f_{10} for the ground state of helium in the first truncation.

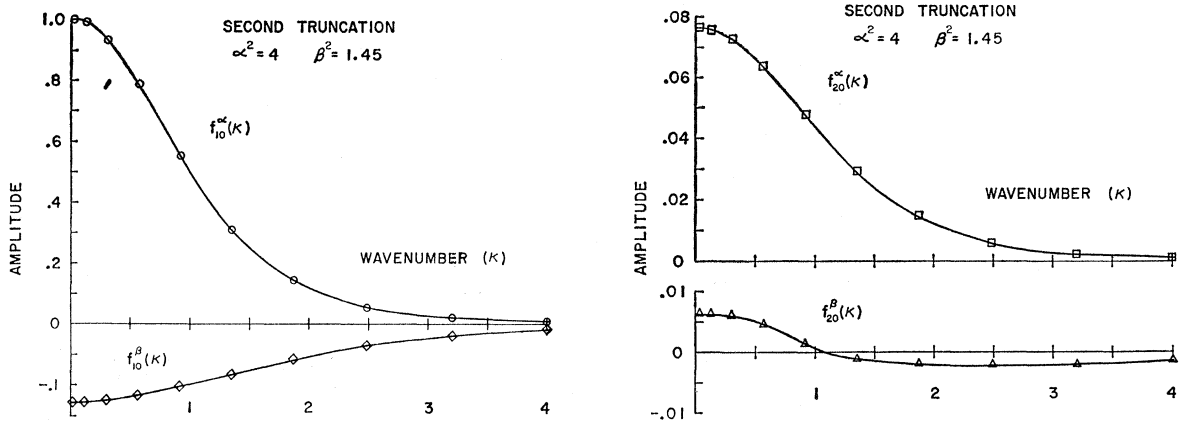

FIG. 5. The functions f_{nl} for the ground state of helium in the second truncation.

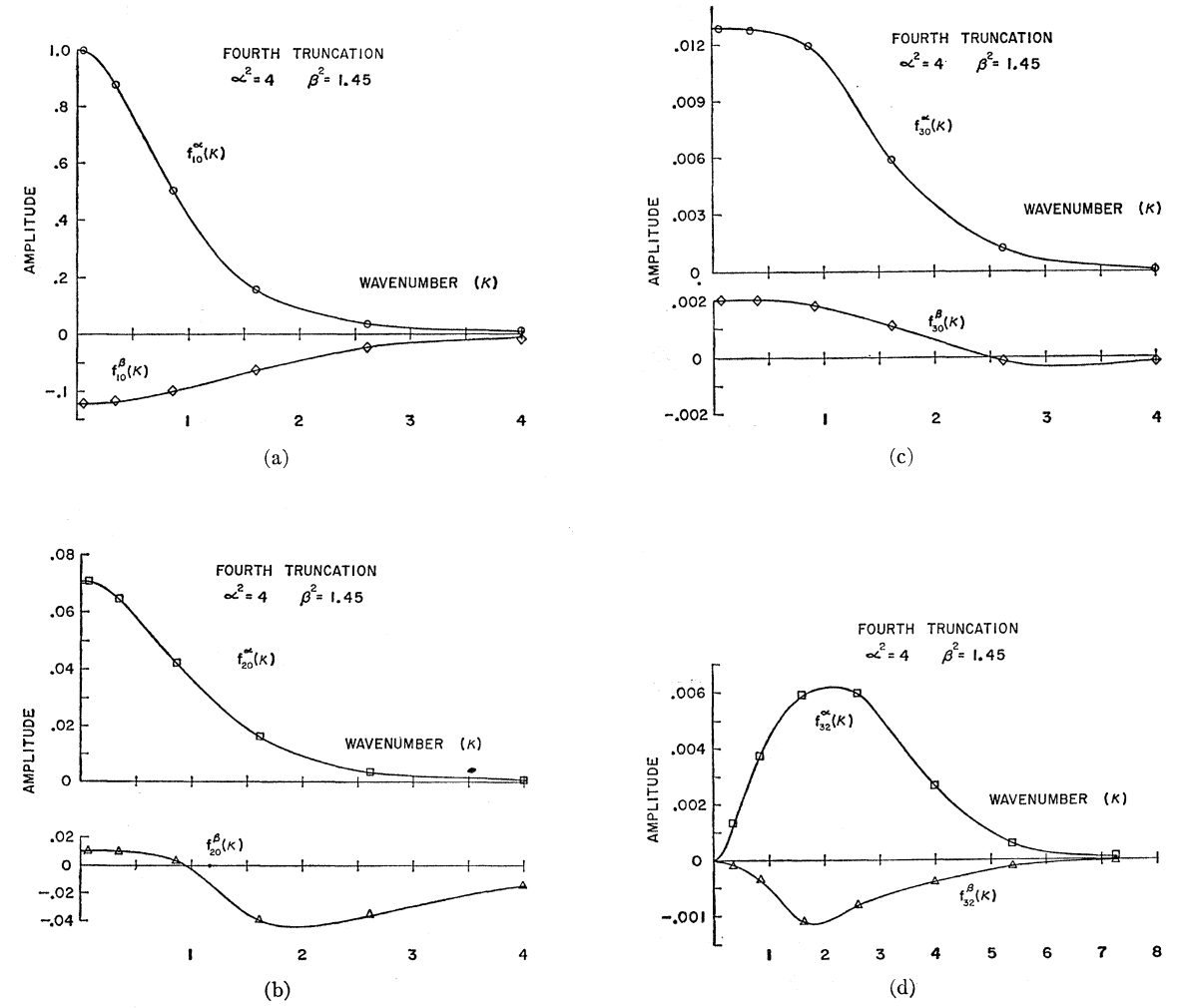

FIG. 6. The functions f_{nl} for the ground state of helium in the fourth truncation.

states of the helium atom itself. By changing the relative values of s_1 and s_2 occurring in the three-body potential, we were able to calculate energies for the H^- atom and the Li^+ atom. These energies along with the results for the helium atom are shown in Table II. The values for our energy shown in the Table are chosen at the absolute minimum of the energy versus α^2 and β^2 surface for the second and fourth truncations of the system of equations. The numbers quoted for "comparison energy" were taken from the literature and represent values which have the accuracy of at least the number of digits carried. In the fourth truncation of the He, Li^+, and H^- atoms as many as nine roots were found for each atom. The problem of identifying all of these is not an easy task since other calculated or experimental energies do not exist for most of them. Since these highly excited states have many nodes, the numerical integrations give energies and wave functions which are less accurate than those for lower states. Because of these difficulties we confine our attention to only a few of the lower-lying states. Again we emphasize that it is not our purpose to obtain highly accurate results in this paper, but to demonstrate the validity of our method.

VII. CONCLUSIONS

We have presented a general method for treating bound-state, three-body problems which does not depend on perturbation theory or a variational principle. We have considered some simple examples involving one-dimensional δ-function potentials. We have also treated the helium-like atom from a three-body point of view and demonstrated that rapid convergence is achieved for bound states of the form $L=0$ when a Sturmian two-body expansion is used. For three-body problems where the two-body Sturmian set cannot be found analytically, machine solutions for the two-body functions can be used. For these situations several expansion techniques may be investigated for performing the angular integration. With the general method presented here, accurate wave functions and energies can be constructed for the bound-state problem of three particles interacting with one another through pair potentials. There are, of course, limitations as to how many excited states can be handled on the present computers.

ACKNOWLEDGMENTS

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APPENDIX: STURMIAN FUNCTIONS

The Sturm–Liouville equation is

$$d\{k(x)(dy/dx)\}/dx+[\lambda g(x)-l(x)]y=0, \quad \text{(A1)}$$

where k, g, and l are real, continuous functions of the real variable x throughout the closed interval $a\leqq x\leqq b$. If $k>0$ and $g>0$ then the Schrödinger equation for the radial function $R(r)$ in three-dimensional problems may be written in this form. Here $g(x)$ depends on the potential, and the energy of the system appears in the function $l(x)$. The normal energy-eigenvalue problem is to find solutions of equation (A1) for the set of values of the energy such that the boundary conditions are met. We may turn this problem around and examine the eigenvalue–eigenvector solutions to this equation when the energy of the system is fixed and the strength of the potential is allowed to vary so that the boundary conditions are met. It can be shown that there will be an infinitely denumerable set of values $\{\lambda_n\}$ and their associated eigensolutions, $y_n(x)$.[10] It can also be shown that this set of functions $\{y_n\}$ may be constructed so as to form a complete set of orthonormal functions on the interval $a\leqq x\leqq b$ with respect to the weighting function $g(x)$.[10] These functions have been called Sturmian functions and form a set closely related to the eigenfunctions in the conventional quantum-mechanical problem where the potential is specified and the energy assumes a set of values.[4] The orthogonality condition for the Sturmian functions may be written as

$$\int_a^b dx\, g(x)y_n^*(x)y_m(x)=\delta_{nm}. \quad \text{(A2)}$$

The two-body Schrödinger equation for a hydrogen-like atom in three dimensions is

$$\{-(\hbar^2/2\mu)\nabla^2+V(\mathbf{r})\}\Psi(\mathbf{r})=E\Psi(\mathbf{r}),$$

where $V(\mathbf{r})$ is the attractive Coulomb potential between the nucleus and the electron. Separating out the angular parts and multiplying through by $-2\mu/\hbar^2$ gives the following equation for the radial part of $\psi(\mathbf{r})$:

$$1/r^2(d/dr)[r^2(d/dr)R]$$
$$-2\alpha u(r)R-[l(l+1)/r^2]R=K_{(2)}{}^2R,$$

where

$$K_{(2)}{}^2=(2\mu/\hbar^2)\,|\,E\,|, \qquad u(r)=-1/r, \qquad \alpha=e^2\mu/\hbar^2.$$

To find the Sturmian set for this equation we consider the differential equation where the potential assumes a set of decreasing values (increasing values of λ) such that the boundary conditions of the problem are satisfied.

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\tilde{S}_{nl}}{dr}\right)-2\alpha\lambda_{nl}u(r)\tilde{S}_{nl}-\frac{l(l+1)}{r^2}\tilde{S}_{nl}=K_{(2)}{}^2\tilde{S}_{nl}.$$

[10] E. L. Ince, *Ordinary Differential Equations* (Dover Publications, Inc., New York, 1926).

The problem is to find the values of λ_{nl} and the functions associated with these values. We choose the first value of λ to be 1 so that the first Sturmian function is a physical ground-state wave function with energy $K_{(2)}^2$. With this choice of units, the constant $K_{(2)}^2$ is determined as α^2. By choosing $\lambda_{10}=1$, it is also easy to show that the λ_{nl} are just the positive integers from 1 to ∞. The corresponding Sturmian functions may be found and are given by [4]

$$\tilde{S}_{nl}(r) = -\left[\frac{\alpha(n-l-1)!}{2(n+l)!^3}\right]^{1/2}(2\alpha)^{l+1}r^l e^{-\alpha r}L_{n+l}^{2l+1}(2\alpha r), \tag{A3}$$

where L_p^q are the associated Laguerre polynomials. A related set of functions has been used by Schull and Löwdin.[11] The $\tilde{S}_{nl}$ have the same form as the ordinary Coulomb functions except that the energy eigenvalues do not appear in the argument of the functions. We also note that the orthogonality integral is different for the Sturmian functions since the weighting function $g(r)$ in Eq. (A2) contains the potential

$$\int_0^\infty dr\, r^2\left(\frac{2}{r}\right)\tilde{S}_{nl}(r)\,\tilde{S}_{n'l}(r) = \alpha\delta_{nn'}.$$

This normalization has been chosen so that the Sturmian set will have the conventional units of probability amplitude. Thus, the complete set of Sturmian functions for the problem in coordinate space is

$$\tilde{S}_{nlm}(\mathbf{r}) = \tilde{S}_{nl}(r)\,Y_l^m(\Omega_r).$$

Taking in the Fourier transform of the differential equation for $\tilde{S}_{nlm}(\mathbf{r})$ gives a double integral equation for the Fourier transform of $\tilde{S}_{nlm}(\mathbf{r})$. In our system of units the integral equation is

$$S_{nlm}(\mathbf{k}) = \frac{-2\alpha\lambda_{nl}}{(2\pi)^3(k^2+\alpha^2)} \times\iint d\mathbf{k}'d\mathbf{r}\, u(\mathbf{r})\,\exp[i\mathbf{r}\cdot(\mathbf{k}'-\mathbf{k})]S_{nlm}(\mathbf{k}'), \tag{A4}$$

where $S_{nlm}(\mathbf{k})$ is the Fourier transform of $\tilde{S}_{nlm}(\mathbf{r})$:

$$S_{nlm}(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}}\int d\mathbf{r}\,\tilde{S}_{nlm}(\mathbf{r})\,\exp(-i\mathbf{k}\cdot\mathbf{r}).$$

For our formulation of the three-body problem we need the Sturmian set for the Coulomb potential in momentum space. This may be calculated by taking the Fourier transform of $\tilde{S}_{nlm}(\mathbf{r})$, where $\tilde{S}_{nl}(r)$ is given by Eq. (A3):

$$S_{nlm}(\mathbf{k}) = \frac{-1}{(2\pi)^{3/2}}\left[\frac{\alpha(n-l-1)!}{2(n+l)!^3}\right]^{1/2}(2\alpha)^{l+1} \times\int d\mathbf{r}\, r^l e^{-\alpha r}L_{n+l}^{2l+1}(2\alpha r)\,\exp(-i\mathbf{k}\cdot\mathbf{r})\,Y_l^m(\Omega_k).$$

Using the plane-wave expansion for $\exp(-i\mathbf{k}\cdot\mathbf{r})$,

$$\exp(-i\mathbf{k}\cdot\mathbf{r}) = 4\pi\sum_l\sum_m(-i)^l j_l(kr)\,Y_l^{m*}(\Omega_r)\,Y_l^m(\Omega_k),$$

and invoking the orthogonality relation for spherical harmonics gives an integral expression for $S_{nl}(k)$:

$$S_{nl}(k) = -\left[\frac{\alpha(n-l-1)!}{\pi(n+l)!^3}\right]^{1/2}(2\alpha)^{l+1} \times\int dr\, r^{l+2}e^{-\alpha r}L_{n+l}^{2l+1}(2\alpha r)j_l(kr).$$

Arbitrary phases have been dropped since we are only interested in the set of functions $\{S_{nl}\}$. This integral may be evaluated in general, giving

$$S_{nl}(k) = 2^{2(l+1)}\left[\frac{\alpha(n-l-1)!}{\pi(n+l)!}\right]^{1/2} nl!\alpha^{l+2} \times\frac{k^l}{(k^2+\alpha^2)^{l+2}}C_{n-l-1}^{l+1}\left(\frac{k^2-\alpha^2}{k^2+\alpha^2}\right), \tag{A5}$$

where C_p^q is the standard Gegenbauer polynomial. The orthogonality condition in momentum space for our choice of units is

$$\int_0^\infty dk\, k^2 S_{nl'}(k)\,(k^2+\alpha^2)\,S_{n'l'}(k) = \delta_{n'n}\alpha^2\lambda_{n'l'}.$$

[11] H. Schull and P.-O. Löwdin, J. Chem. Phys. **30**, 617 (1959).