Symmetric Euler Angle Decomposition
of the Two-Electron Fixed-Nucleus Problem

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I. INTRODUCTION

The decomposition of the Laplacian operator,
\[
\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2},
\]
where the coefficient of the second term is proportional to the square of the angular momentum operator, is the basic relation between energy and angular momentum in the quantum mechanics of the one body problem (or the relative motion of two particles).

When acting on a wave function which is an eigenfunction of total angular momentum \( l \), the Laplacian simplifies to
\[
\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{l(l + 1)}{r^2}
\]
in which form it is clear that the effect of this decomposition is to reduce the Schrödinger equation from a three dimensional partial differential equation to a one dimensional (ordinary) differential equation. As such this relation is of fundamental mathematical importance and is familiar to everyone who utilizes quantum mechanics at all.

The analogous procedure when more than one particle is
involved, in particular two identical particles in an external force field, although known, is not as well known, nor is it as well developed. When the external field is that of a fixed nucleus, the wave function is expanded in eigenfunctions of the total angular momentum of the two particles multiplied by functions of the three remaining independent variables. The total angular momentum eigenfunctions are functions of the three Euler angles only. These angles are not unique, but in some way they must describe the orientation of the instantaneous plane formed by the two particles and the center of coordinates (nucleus) in space. The remaining three coordinates then describe the positions of the particles in this plane, and the functions of these variables are the generalized radial functions. Hylleraas' original papers in effect contained the reduced or radial equations for total S states in terms of the residual coordinates $r_1, r_2, r_{12}$. In this case, the total orbital angular momentum is a constant function, and hence the reduction of a six-dimensional to a three-dimensional partial differential equation is independent of how one defines the Euler angles.

The standard treatment of the general problem is due to Breit, He used the Euler angles that Hylleraas originally introduced: namely the two spherical angles of one of the particles in the space fixed coordinate system and a second azimuthal angle between the $r_1 - z$ plane and the $r_2 - r_1$ plane. Breit's remaining coordinates were chosen as $r_1$, $r_2$, and $\Theta_{12}$, the latter being the angle between
If, however, one wants to describe two electron atoms or ions in the approximation that the nuclei are fixed, then one has an additional requirement of which there is no analogue in the one-body problem. And that is the Pauli principal: the requirement that the spatial function be either symmetric or antisymmetric under the exchange of the particle coordinates. It is clear that the Hylleraas-Breit choice of Euler angles (which we hereinafter refer to as the Hylleraas-Breit angles), being quite unsymmetrical with respect to the two particles, is not optimum in this respect. In fact the construction of linear combinations of angular momentum functions with the appropriate exchange properties is a very difficult task which depends not only on the Euler angles but on θ₁₂ as well. It is not surprising, therefore, that Breit's original work was limited to P-states, and work thereafter has always been limited to specific angular momentum states.

However, a treatment by Holmberg using a symmetrical choice of Euler angles (which we shall call Holmberg's angles) has in the interim been carried out. With these angles the description of exchange as well as parity (which latter property is also simply describable with the H-B angles) is simple (although these properties are only alluded to in Holmberg's paper). One of the purposes of the present paper is to examine these properties and relate them more clearly to the construction of the total wave function.
and further clarify other aspects of Holmberg's important paper. Principally, however, we shall derive the general radial equations for arbitrary angular momentum ($\ell$) for the case of two identical particles in an external field. Holmberg's treatment applies to three particles of the same mass.

It is clear that in treating three particles of equal mass Holmberg had in mind the three nucleon problem whereas we are interested in two-electron atoms, ions, and diatomic molecules. The application of this formalism to two electron atoms and ions is clear, and the decomposition amounts to a rigorous reduction of the Schrödinger equation. It should only be remarked here that the scattering of electrons from one electron atoms and ions is also a special class of these problems. We have therefore worked out the connection between the boundary conditions for electron-atom scattering and Holmberg's angles (Section VIII).

Inasmuch as Holmberg's paper refers to the three nucleon problem, reference should also be made to the papers of Derrick and Blatt. These papers deal much more realistically with the three nucleon problem in that full account is taken of an internucleon potential which is considerably more complicated than a central potential. As regards the actual choice of coordinates, Derrick and Blatt define axes along the moments of inertia of the three-body system. As such they will depend on the lengths of the interparticle distances and therefore are quite different from Holmberg's angles (Section II).
II. HOLMBERG'S ANGLES

Figure 1 contains a perspective drawing of Holmberg's angles which define the particle plane with respect to the space fixed \( x, y, \) and \( z \) axes. The rotated axes \( x', y', z' \) are then defined by

\[
\mathbf{z'} = \frac{\mathbf{z}_1 \times \mathbf{z}_2}{|\mathbf{z}_1 \times \mathbf{z}_2|} \quad (1)
\]

\[
\mathbf{z} = \frac{\mathbf{z}_2 \times \mathbf{z}'}{|\mathbf{z}_2 \times \mathbf{z}'|} \quad (2)
\]

\[
\mathbf{y'} = \mathbf{z}_2 \times \mathbf{z} \quad (3)
\]

The Holmberg Euler angles are then

\[
\theta = \text{angle between } \mathbf{z} \text{ and } \mathbf{z}' \quad (4)
\]

\[
\phi = \text{angle between } \mathbf{z}' \text{ and } \mathbf{z} \quad (5)
\]

\[
\psi = \text{angle between } \mathbf{z}' \text{ and } (\mathbf{z}_2 - \mathbf{z}_1) \quad (6)
\]

The ranges and planes of these angles are:

\[
0 \leq \theta \leq \pi \quad \text{in } z-z' \text{ plane}
\]

\[
0 \leq \phi \leq \pi \quad \text{in } x-y \text{ plane}
\]

\[
0 \leq \psi \leq 2\pi \quad \text{in } x'-y' \text{ plane}
\]

As is usual a cap on a vector is used to represent a unit vector in the given direction. In particular \( \mathbf{i}, \mathbf{j}, \mathbf{k} \) are the three unit vectors along the (space fixed) \( x, y, \) and \( z \) axes respectively,
and thus are synonymous with \( \hat{z}, \hat{y}, \) and \( \hat{z}. \) Similarly \( \hat{i}', \hat{j}', \hat{k}', \) and \( \hat{x}', \hat{y}', \hat{z}' \) are identical.

It is clear from the figure that \( \hat{x}' \), being in the x-y plane has components:

\[
\hat{x}' = \hat{z} \cos \phi + \hat{y} \sin \phi
\]  
(7)

Since \( \hat{x}' \) is perpendicular to the z-z' plane, it is perpendicular to every line in that plane going through the origin. This includes specifically the line of intersection of the z-z' plane with the x-y plane. However the azimuthal angle of that intersecting line is the azimuth of \( \hat{z}' \) itself, and since \( \hat{z}' \) has azimuth \( \phi \), \( \hat{x}' \) has azimuth \( \frac{3\pi}{2} + \phi \) (cf. figure 1). The polar angle of \( \hat{x}' \) is clearly \( \theta \), therefore we have the important relation:

\[
\hat{x}' = \hat{z} \sin \theta \sin \phi - \hat{y} \sin \theta \cos \phi + \hat{z} \cos \theta
\]  
(8)

The relations between Holmberg's angles and the spherical angles of the individual particles are obtained by substituting Eqs. (7) and (8) into the lhs of Eqs. (1) and (2) and using the ordinary decomposition of \( \vec{x}_1 \) and \( \vec{x}_2 \) in the rhs:

\[
\hat{\vec{x}}_1 = \hat{\vec{z}} \sin \phi \cos \phi + \hat{\vec{y}} \sin \phi \sin \phi + \hat{\vec{z}} \cos \phi,
\]

\[
\hat{\vec{x}}_2 = \hat{\vec{z}} \sin \phi \cos \phi + \hat{\vec{y}} \sin \phi \sin \phi + \hat{\vec{z}} \cos \phi.
\]

One obtains
The latter relation is, of course, the well known expansion for the angle between two vectors.

It is also of interest to give the vectors \( \hat{r}_1 \) and \( \hat{r}_2 \) in the particle plane: (primed co-ordinate system):

\[
\begin{align*}
\hat{r}_1 &= \hat{e} \sin (\Psi - \frac{1}{2} \Theta_{12}) - \hat{e}' \cos (\Psi - \frac{1}{2} \Theta_{12}) \\
\hat{r}_2 &= \hat{e} \sin (\Psi + \frac{1}{2} \Theta_{12}) - \hat{e}' \cos (\Psi + \frac{1}{2} \Theta_{12}) \\
\hat{r}_z &= \hat{e} \sin \Theta + \hat{e}' \cos \Theta
\end{align*}
\]
\[ \hat{r}_1 = \hat{r} \cos \phi + \hat{\phi} \sin \theta \cos \phi \]  
(18)

\[ \hat{r}_2 = \hat{r} \cos \phi - \hat{\phi} \sin \theta \sin \phi + \hat{\phi} \sin \theta \sin \phi \]  
(19)

The following relations which are also very useful can now simply be derived by computing \((\hat{r}_1 \cdot \hat{z})\) and \((\hat{r}_2 \cdot \hat{z})\) in the primed system.

\[ \cos \theta_1 = -\sin \theta \cos (\psi - \frac{1}{2} \theta_{1z}) \]  
(20a)

\[ \cos \theta_2 = -\sin \theta \cos (\psi + \frac{1}{2} \theta_{1z}) \]  
(20b)

\[ \sin \theta_1 \cos \phi = \cos \phi \sin \left(\psi - \frac{1}{2} \theta_{1z}\right) - \cos \theta \sin \phi \cos \left(\psi - \frac{1}{2} \theta_{1z}\right) \]  
(21a)

\[ \sin \theta_2 \cos \phi = \cos \phi \sin \left(\psi + \frac{1}{2} \theta_{1z}\right) - \cos \theta \sin \phi \cos \left(\psi + \frac{1}{2} \theta_{1z}\right) \]  
(21b)

\[ \sin \theta_1 \sin \phi = \sin \phi \sin \left(\psi - \frac{1}{2} \theta_{1z}\right) - \cos \theta \cos \phi \cos \left(\psi - \frac{1}{2} \theta_{1z}\right) \]  
(22a)

\[ \sin \theta_2 \sin \phi = \sin \phi \sin \left(\psi + \frac{1}{2} \theta_{1z}\right) - \cos \theta \cos \phi \cos \left(\psi + \frac{1}{2} \theta_{1z}\right) \]  
(22b)

III. PROPERTIES UNDER PARITY AND EXCHANGE

The operation of parity corresponds to the simultaneous inversion of both particles; coordinates: \(r_1 \rightarrow -\hat{r}_1, r_2 \rightarrow -\hat{r}_2\). It can be seen from figure 1 that this places \(r_1\) and \(r_2\) facing the opposite direction, but the cross product and hence \(\hat{z}'\) will not
change as a result of this operation. Thus the z-z' plane will
not change and \( \hat{z} \) will not change. On the other hand \((\hat{z}_2-\hat{z}_1)\)
goes into the negative of itself, so that \(\Psi\) gets increased by \(\pi\).
In other words under parity

\[
\begin{align*}
\theta & \rightarrow \theta \\
\Phi & \rightarrow \Phi \\
\Psi & \rightarrow \Psi + \pi
\end{align*}
\]

(23)

Exchange corresponds to the transformation \(\Pi \rightarrow \Pi_2\). From the
analytical definitions \(\hat{z}'\) and \(\hat{x}'\), Eqs. (1) and (2), the new primed axes
will go into the negative of themselves. Also \((\hat{z}_2-\hat{z}_1)\) goes into
negative of itself. Clearly the inversion of the z' axis corre-
ponds to the transformation \(\theta \rightarrow \pi - \theta\). Noting that \(\Phi\) is the
angle in the x-y plane and measured as positive with respect
to the z axis, which is fixed, we see that \(\Phi \rightarrow \pi + \Phi\) . The
simultaneous inversion of \(\hat{z}'\) and \((r_2-r_1)\) means that the modulus
of the angle \(\Psi\) remains the same. However, since \(\Psi\) is an angle
in the x'-y' plane, it is measured as positive with respect to the
z' axis. Since the latter goes into the negative itself, it
becomes clear that \(\Psi \rightarrow 2\pi - \Psi\) . Thus we have under exchange

\[
\begin{align*}
\theta & \rightarrow \pi - \theta \\
\Phi & \rightarrow \Phi + \pi \\
\Psi & \rightarrow 2\pi - \Psi
\end{align*}
\]

(24)
The significance of these transformations relates to the transformation properties of the vector spherical harmonics under the same operation. These functions, which are the eigenfunctions of the angular momentum (next section), are the basic functions in terms of which the complete wave function is expanded. They can be written

\[ J_{l}^{m,k}(\theta, \phi, \psi) = \frac{\sqrt{(2l+1)} e^{i(m \phi + k \psi)}}{4\pi} Y_{l}^{m,k}(\theta) \]  

(25)

where the normalization has been so chosen that the function is identical with what is given in section IV and the \( d_{l}^{m,k}(\theta) \) agree with those given by Wigner 8. Only the dependence on \( \theta \) is non-trivial; for \( m \gamma \theta \gamma 0 \)

\[ d_{l}^{m,k}(\theta) = \sqrt{\frac{(l+m)! (l-k)!}{(l-m)! (l+k)!}} \cdot C_{l}^{m+k-m} (l, m, k, \theta) \]

(26)

\( F(a, b; c; z) \) is the hypergeometric function in the notation of Magnus and Oberhettinger 9. The important property of \( d_{l}^{m,k}(\theta) \), proved in Wigner's book 8, is:

\[ d_{l}^{m,k}(\pi - \theta) = (-1)^{l} d_{l}^{m,-k}(\theta) \]

(27)

Letting \( P \) and \( E_{12} \) represent parity and exchanges we have from (23) and (24):

\[ P J_{l}^{m,k}(\theta, \phi, \psi) = J_{l}^{m,k}(\theta, \phi, \psi + \pi) \]

\[ E_{12} J_{l}^{m,k}(\theta, \phi, \psi) = J_{l}^{m,k}(\pi - \theta, \phi + \pi, 2\pi - \psi) \]
which using (27) reduce to

\[ \rho \mathcal{D}_{k}^{m,k}(\theta, \phi, \psi) = (-1)^{k} \mathcal{D}_{k}^{m,k}(\theta, \phi, \psi) \]  

(28)

\[ \mathcal{E}_{11} \mathcal{D}_{k}^{m,k}(\theta, \phi, \psi) = (-1)^{l} \mathcal{D}_{k}^{m,k}(\theta, \phi, \psi) \]  

(29)

The simplicity of Eq. (29) is the essential feature which recommends Holmberg's angles to the description of the two electron problem.

IV. ANGULAR MOMENTUM

The components of the total angular momentum are readily expressed in terms of the particles' spherical angles. Thus, for example

\[ -i \frac{\hbar}{\hbar} \mathbf{M}_x = \sum \hat{q}_i \frac{\partial}{\partial \hat{\sigma}_i} + \cot \hat{\eta}_1 \cos \hat{\varphi}_1 \frac{\partial}{\partial \hat{\varphi}_1} + \sum \hat{q}_2 \frac{\partial}{\partial \hat{\varphi}_2} \]

\[ + \cot \hat{\vartheta}_2 \cos \hat{\varphi}_2 \frac{\partial}{\partial \hat{\varphi}_2} \]  

(30)

The particles' angles \( \hat{\eta}_1, \hat{\varphi}_1, \hat{\vartheta}_2, \hat{\varphi}_2 \) via (9) - (14) are implicit functions of the four angles \( \theta, \phi, \psi, \theta_{12} \). Thus the problem of finding \( \mathbf{M}_x \) in these angles is a straightforward problem of partial differentiation. We can write

\[ -i \frac{\hbar}{\hbar} \mathbf{M}_x = A_{\theta} \frac{\partial}{\partial \theta} + A_{\phi} \frac{\partial}{\partial \phi} + A_{\psi} \frac{\partial}{\partial \psi} + A_{\theta_{12}} \frac{\partial}{\partial \theta_{12}} \]

where

\[ A_{\theta} = \sum \hat{q}_i \frac{\partial}{\partial \hat{\sigma}_i} + \sum \hat{q}_2 \frac{\partial}{\partial \hat{\varphi}_2} + \cot \hat{\eta}_1 \cos \hat{\varphi}_1 \frac{\partial}{\partial \hat{\varphi}_1} + \cot \hat{\vartheta}_2 \cos \hat{\varphi}_2 \frac{\partial}{\partial \hat{\varphi}_2} \]

\[ + \cot \hat{\varphi}_2 \cos \hat{\varphi}_2 \frac{\partial}{\partial \hat{\varphi}_2} \]  

(31)
and \( \varphi \) can be anyone of the angles \( \theta, \phi, \psi, \) or \( \theta_{12} \). Using then Eqs. (9) - (14), one finds that the following relations fall out quite easily:

\[
A_{\theta_{12}} = 0 \tag{32}
\]

\[
A_{\theta} = -\cos \phi \tag{33}
\]

\[
A_{\phi} = \sin \phi \cos \theta \tag{34}
\]

\[
A_{\psi} = -\frac{\sin \phi}{\sin \theta} \tag{35}
\]

Thus

\[
M_{x} = \frac{\hbar}{\gamma} \left[ \cos \phi \frac{\partial}{\partial \theta} - \sin \phi \cos \theta \frac{\partial}{\partial \phi} + \frac{\sin \phi}{\sin \theta} \frac{\partial}{\partial \psi} \right]. \tag{36}
\]

One can, of course, proceed in a completely analogous way to get the remaining components of the angular momentum, however, let us note from Eqs. (20) that

\[
\frac{\partial \psi_{1}}{\partial \phi} = \frac{\partial \psi_{2}}{\partial \phi} = 0 \tag{37}
\]

and from (10) and (11)

\[
\frac{\partial \phi_{1}}{\partial \phi} = \frac{\partial \phi_{2}}{\partial \phi} = 1 \tag{38}
\]
Since
\[ \frac{\partial}{\partial \phi} = \sum_{j} \left( \frac{\partial}{\partial \phi} \right) \frac{\partial}{\partial \theta} \right) \]
substitution of (37) and (38) yields
\[ \frac{\partial}{\partial \phi} = \frac{\partial}{\partial \theta} + \frac{\partial}{\partial \varphi} \]
However, since
\[ M_z = \frac{\hbar}{i} \left( \frac{\partial}{\partial \theta} + \frac{\partial}{\partial \varphi} \right) \]
we therefore have the z-component of \( M \):
\[ M_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \] (39)

The remaining component of the angular momentum may be derived from the commutation relation \( [M_\theta, M_\phi] = i \hbar M_y \)
Straightforward substitution yields:
\[ M_y = \frac{\hbar}{i} \left[ \sin \phi \frac{\partial}{\partial \theta} + \cos \phi \cot \theta \frac{\partial}{\partial \varphi} - \frac{\cos \phi}{\sin \theta} \frac{\partial}{\partial \psi} \right] \] (40)

These relations are independent of \( \theta_{12} \) corresponding to the statement that the angular momentum only depends on the (three) Euler angles \( \Theta, \Phi, \Psi \). The forms of the three operators is the same as one gets with the Hylleraas-Breit angles. The square of the angular momentum is likewise the same. One finds directly
from the sum of the squares that
\[ M^2 = -h^2 \left[ (1 + \cot \theta) \frac{\partial^2}{\partial \Phi^2} + \frac{\partial^2}{\partial \Theta^2} + \frac{1}{\sin \Theta} \frac{\partial}{\partial \Phi} \psi \right. \]
\[ \left. - 2 \cot \theta \frac{\partial \psi}{\sin \Theta \partial \Phi} + \cot \theta \frac{\partial}{\partial \Theta} \right] \]

The vector spherical harmonics, which have been given for
the restricted range \( m \geq k \geq 0 \) in Eq. (25), are the simultaneous
eigenfunctions of \( M^2 \) with eigenvalue \( \ell^2 (\ell + 1) \) and \( \pm m \)
\[ M^2 \mathcal{S}_l^m (\theta, \Phi, \Psi) = \ell^2 (\ell + 1) \mathcal{S}_l^m (\theta, \Phi, \Psi) \]  \( (42) \)
\[ M^2 \mathcal{J}_l^m (\theta, \Phi, \Psi) = \pm m \mathcal{J}_l^m (\theta, \Phi, \Psi) \]  \( (43) \)

They are given in a completely general, normalized form in Pauling
and Wilson \( 1^\text{0} \):
\[ \mathcal{S}_l^m (\theta, \Phi, \Psi) = N_{l,m,k} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cdot \mathcal{F}(-\ell + \nu \beta - 1, \ell + \nu \beta, l + k - m, \sin^2 \frac{\theta}{2}) \]

where
\[ \nu = \frac{|k + m| + |k - m| + 2}{2} \]

and the normalization constant is
\[ N_{l,m,k} = \left[ \frac{(2 \ell + 1) (\ell + \frac{1}{2} |k + m| + \frac{1}{2} |k - m|)! (\ell - \frac{1}{2} |k + m| + \frac{1}{2} |k - m|)! \sigma^2 (\ell - \frac{1}{2} |k + m| - \frac{1}{2} |k - m|)! (\ell + \frac{1}{2} |k + m| - \frac{1}{2} |k - m|)! (|k - m|)!}{\sigma^2 (\ell - \frac{1}{2} |k + m| - \frac{1}{2} |k - m|)! (\ell + \frac{1}{2} |k + m| - \frac{1}{2} |k - m|)! (|k - m|)!} \right]^\frac{1}{2} \]  \( (46) \)
In addition to the usual magnetic quantum number $m$, the vector spherical harmonics depend on the quantum number $k$, an integer whose range of values is the same as $m$: $-l \leq m, k \leq l$.

The physical significance of $k$ derives from the fact that the $\mathcal{L}^{m,k}_l$ are the eigenfunctions of the spherical top (for which (42) is the Schrödinger equation), and $k$ is the angular momentum quantum number about the body-fixed axis of rotation. With regard to the applications that we contemplate here, $k$ can be considered a degeneracy label which must be adjusted such that other requirements are fulfilled.

V. CONSTRUCTION OF THE TOTAL WAVE FUNCTION

We shall confine ourselves here strictly to the atomic problem which implies that the potential energy as well as the kinetic energy commutes with the total angular momentum. In this case the total wave function for a given $l$ must be a linear superposition of the degenerate $\mathcal{L}^{m,k}_l$. In addition, $m$ will be fixed for a given magnetic substate and the "radial" equations will be independent of $m$ (cf. Appendix II).

Considering, for the moment, the residual coordinates as $r_1, r_2, \theta_{12}$, we can therefore expand the total wave function in the form:

$$\Psi_{l,m}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{k=-l}^{l} \mathcal{L}^{m,k}_l(r_1, r_2, \theta_{12}) \mathcal{L}^{m,k}_l(\theta, \phi, \psi)$$ (47)
The parity operations, Eq. (23), only effects the Euler angles, and from Eq. (28) it only multiplies the \( S_{l}^{m} \) function by \((-1)^{k}\). Therefore by restricting the sum to even and odd values of \( k \), we guarantee that the superpositions have even and odd parity respectively:

\[
\Psi_{\ell m}^{\text{even}}(\varrho_{1}, \varrho_{2}) = \sum_{k \text{ even}}^{n} \int_{l}^{k} (\varrho_{1}, \varrho_{2}, \theta_{12}) S_{l}^{m} (\theta, \phi, \psi) \tag{48a}
\]

\[
\Psi_{\ell m}^{\text{odd}}(\varrho_{1}, \varrho_{2}) = \sum_{k \text{ odd}}^{n} \int_{l}^{k} (\varrho_{1}, \varrho_{2}, \theta_{12}) S_{l}^{m} (\theta, \phi, \psi) \tag{48b}
\]

where the double prime on the summation emphasizes that the sum goes over every other value of \( k \).

In deriving the radial equations (next section) we shall exploit the invariance of the radial equations with respect to \( m \), by choosing \( m = 0 \). When the Hamiltonian is written in terms of the Euler angles and the remaining variables, there will occur terms involving \( \frac{\partial}{\partial \phi} \) and \( \frac{\partial}{\partial \psi} \). By virtue of \( m = 0 \), the former terms vanish, but the latter terms would bring down the imaginary coefficient \( ik \). In order to avoid complex equations, it is therefore convenient to construct real angular momentum functions. Let

\[
S_{l}^{X+} = \frac{1}{\sqrt{2}} (S_{l}^{o} X_{+} + S_{l}^{o} X_{-}) = \frac{\sqrt{2l+1}}{2\pi} \cos X \psi d_{l}^{o} X (\theta) \tag{49a}
\]

\[
S_{l}^{X-} = \frac{i}{\sqrt{2}} (S_{l}^{o} X_{+} - S_{l}^{o} X_{-}) = \frac{\sqrt{2l+1}}{2\pi} \sin X \psi d_{l}^{o} X (\theta) \tag{49b}
\]
for \( \kappa > 0 \), where
\[
\kappa = |k|
\]
(50)

and for \( \kappa = 0 \) define
\[
\mathcal{J}^0_+ = \mathcal{J}^0_0, \quad \mathcal{J}^0_- = 0
\]
(49c)

This then constitutes a set of real, orthonormal vector spherical harmonics (note \( d_{\ell}^0; x = d_{\ell}^0; -k \)). These real vector spherical harmonics are still eigenfunctions of parity with eigenvalue \((-1)^\kappa\).

The property of exchange is a mite more complicated than parity in the sense that it affects not only the Euler angles, but the residual coordinates as well. The beauty and importance of Holmberg's angles, however, is that there is no mixing, and independent of whether we consider the residual variables \( r_1, r_2, \theta_{12} \) or \( r_1, r_2, r_{12} \), the effect of exchange on the residual coordinates is simply \( r_1 \leftarrow r_2 \).

Finally then, if we construct
\[
\psi_{\ell_0}^{(r, \theta)} = \sum_{\kappa} \left[ \Psi^{+}_{\kappa} (r_1, r_2, \theta_{12}) \mathcal{J}^+ (\theta, \phi, \psi) + \Psi^{-}_{\kappa} (r_1, r_2, \theta_{12}) \mathcal{J}^- (\theta, \phi, \psi) \right] ,
\]
(51)

the operation of exchange on this sum then gives, with the use of (29), :
Thus if

\[ f^+_\ell (r_1, r_2, \theta_1, \theta_2) = \pm (-1)^\ell f^+_\ell (r_1, r_2, \theta_1, \theta_2) \]  (52a)

\[ f^-\ell (r_1, r_2, \theta_1, \theta_2) = \pm (-1)^{\ell+1} f^-\ell (r_1, r_2, \theta_1, \theta_2) \]  (52b)

the function \( \psi_{l0} \) of Eq. (51) is a real, space symmetric (upper sign) or space antisymmetric (lower sign), eigenfunction of \( M_z^2 \) and \( M_z \) corresponding to the quantum numbers \( l \) and \( m \) with \( m = 0 \). The space symmetric and antisymmetric solutions correspond to singlet and triplet spin states respectively. Furthermore the restriction to \( m = 0 \) is sufficient for deriving the radial equations.

We have shown that the \( m = 0 \) function can be written in manifestly real form, Eq. (51). However in that form, it is not obvious what the generalization is to arbitrary \( m \) states. The generalization is nevertheless simply obtained. Let

\[ \mathcal{D}_\ell^\kappa = \frac{1}{\sqrt{2}} \left( f^+\ell - i f^-\ell \right) \quad \kappa \neq 0 \]  (53)
then the form (51) reduces to that of Eq. (47) for \( m = 0 \). For arbitrary \( m \) one then need only replace the \( \mathcal{G}_l^{m,\mp} \) functions by the appropriate \( \mathcal{G}_l^{m,\pm} \) functions, the radial \( f_l \) functions remaining the same.

Alternatively one can define generalizations of the \( \mathcal{L}_l^{x\pm} \), Eq. (49), for arbitrary \( m \).

\[
\mathcal{G}_l^{m,x\pm} = \begin{cases} 
\frac{1}{\sqrt{2}} \left( \mathcal{G}_l^{m,x} + \mathcal{G}_l^{m,-x} \right) & x \neq 0, m \neq 0 \\
\mathcal{G}_l^{m,x} & x = 0
\end{cases}
\]  

with

\[
\mathcal{G}_l^{(m,o)} \equiv \begin{cases} 
\mathcal{G}_l^{x\pm} & x = 0 \text{ for } m = 0.
\end{cases}
\]

The complete function for arbitrary \( m \) can then be written

\[
\Psi_{\ell m}(r, \theta) = \sum_{x} \left[ f_{\ell}^{x+} \mathcal{G}_l^{m,x+} + f_{\ell}^{x-} \mathcal{G}_l^{m,x-} \right]
\]

In this case the "radial" functions \( f_{\ell}^{x\pm} \) are the same as in (51), hence real; whereas the angular functions become altered. Note for \( m \neq 0 \), however, that the modified spherical harmonics, \( \mathcal{G}_l^{(m,x)} \), are no longer real.

VI. THE KINETIC ENERGY

Just as in the case of the angular momentum, the kinetic energy can be obtained by a straightforward process of partial differentiation.
In this case, however, since second partial derivatives are involved, the differentiation is a much longer job, and, as we shall see, the partial derivatives involving \( \theta_{12} \) no longer cancel out.

We start then with the kinetic energy in spherical coordinates

\[
\nabla_1^2 + \nabla_2^2 = \frac{1}{r_1 \sin \theta_1} \frac{\partial^2}{\partial r_1^2} + \frac{1}{r_2 \sin \theta_2} \frac{\partial^2}{\partial r_2^2} + \frac{1}{r_1} \left[ \frac{1}{\sin \theta_1} \frac{\partial}{\partial \theta_1} \frac{2}{\partial \phi_1} \right] \sin \theta_1 \frac{\partial^2}{\partial \phi_1^2} + \frac{1}{r_2} \left[ \frac{1}{\sin \theta_2} \frac{\partial}{\partial \theta_2} \frac{2}{\partial \phi_2} \right] \sin \theta_2 \frac{\partial^2}{\partial \phi_2^2}
\]

The first two terms are, of course, unaffected by the transformation.

The angular differentiations then involve the transformation from the variables \( \theta_1, \varphi_1, \theta_2, \varphi_2 \) to \( \theta, \varphi, \psi, \) and \( \theta_{12} \).

Consider the coefficient of the \( r_1^{-2} \) term. After some regrouping, we can write

\[
\frac{1}{r_1 \sin \theta_1} \frac{\partial^2}{\partial r_1^2} \frac{2}{\partial \phi_1^2} \left[ \sin \theta_1 \frac{\partial^2}{\partial \phi_1^2} \right] \frac{2}{\partial \phi_1^2} = \sum \left[ \frac{2}{\partial \phi_1^2} \left( \frac{2}{\partial \phi_1^2} \right) \right] \frac{2}{\partial \phi_1^2}
\]

where for \( \alpha = 1, 2, 3, 4, \) \( \chi_\alpha \) refers to \( \theta, \varphi, \psi, \theta_{12} \). The problem thus reduces to finding each of the square brackets separately in terms of the Euler angles and \( \theta_{12} \). The results are given in Table I.

The kinetic energy thus becomes

\[
\nabla_1^2 + \nabla_2^2 = \sum \left\{ \frac{1}{r_1} \frac{2}{\partial r_1^2} + \frac{1}{r_2} \frac{2}{\partial r_2^2} + \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{1}{\sin \theta_{12}} \frac{2}{\partial \theta_{12}} \right\} + \frac{F_1}{r_1^2} + \frac{F_2}{r_2^2}
\]
where

\[ F_1 = \frac{1}{\sin^2 \theta_{12}} \left[ \sin^2 \left( \frac{\psi + \theta_{12}}{2} \right) \frac{2}{\sin^2 \theta} + \cos^2 \left( \frac{\psi + \theta_{12}}{2} \right) \cot \theta \frac{2}{\partial \theta} \right. \]

\[ + \cos \left( \frac{\psi + \theta_{12}}{2} \right) \frac{2}{\sin^2 \theta} \frac{\partial^2}{\partial \theta \partial \bar{\psi}} + \sin \left( \frac{2\psi + \theta_{12}}{2} \right) \cot \theta \frac{2}{\sin \theta} \frac{\partial}{\partial \bar{\theta}} \]

\[ - \sin \left( \frac{2\psi + \theta_{12}}{2} \right) \frac{2}{\sin \theta} \frac{\partial}{\partial \bar{\theta}} \frac{\partial}{\partial \bar{\psi}} + \sin \left( \frac{2\psi + \theta_{12}}{2} \right) \cot \theta \frac{2}{\sin \theta} \frac{\partial}{\partial \theta} \frac{\partial}{\partial \bar{\psi}} \]

\[ - 2 \cos \frac{1}{2} \left( \frac{\psi + \theta_{12}}{2} \right) \cot \theta \frac{2}{\sin \theta} \frac{\partial}{\partial \theta} \frac{\partial}{\partial \bar{\psi}} \] \[ = \frac{1}{2} + A_1 \frac{2}{\partial \psi} + B_1 \frac{2}{\partial \theta} \]

and

\[ A_1 = \frac{1}{4} + \frac{\cot \theta \cos \left( \frac{\psi + \theta_{12}}{2} \right)}{\sin^2 \theta_{12}} \] \[ (60) \]

\[ B_1 = - \cos \psi \frac{\sin \left( \frac{\psi + \theta_{12}}{2} \right)}{\sin^2 \theta_{12}} - \cot \theta \frac{\sin \left( \frac{2\psi + \theta_{12}}{2} \right)}{\sin^2 \theta_{12}} \]

\[ + \cos \frac{\theta_{12}}{2} \frac{1}{\sin \theta_{12} \frac{\partial}{\partial \psi}} \left( 1 - \frac{1}{\cos \theta_{12}} \right) \] \[ (61) \]

The expressions for \( F_2, A_2 \) and \( B_2 \) can be obtained by replacing \( \theta_{12} \) by \( - \theta_{12} \) in the above formulae (including the appropriate partial derivatives):

\[ F_2 (\theta, \psi, \psi, \theta_{12}) = F_1 (\theta, \psi, \psi, - \theta_{12}) \] \[ (62) \]

It is clear, since all the coefficients are independent of \( \bar{\psi} \), that \( M_2 \) commutes with the kinetic energy. We have also explicitly
verified that \[ [M_x', \nabla_1^2 + \nabla_2^2] = 0. \]

Note that the partial derivative involving \( \theta_{12} \) and no other angles has been placed in the curly brackets with the radial derivatives. This is because this term, as the radial derivatives themselves, do not affect the orbital angular momentum, and are the only terms which act on total \( S \) states \(^1,2,3\).

In fact, in the action of the remaining terms on the angular momentum eigenfunction rests the bulk of the reduction of the Schrödinger equation to its 3-dimensional "radial" form. With this reduction in mind (cf. next section), it is convenient to write \( F_1 \) in terms of operators whose effect on the angular momentum eigenfunctions is particularly simple. One can show

\[ F_1 = \frac{1}{2} \sin 2\theta_{12} \left[ - \frac{1}{\hbar^2} M^2 + \cos \theta_{12} (\sin 2\psi \Lambda_2 - \cos 2\psi \Lambda_1) \right. \]
\[ + \sin \theta_{12} (\sin 2\psi \Lambda_1 + \cos 2\psi \Lambda_2) \left. \right] \]
\[- \frac{\hbar^2}{\partial \theta_{12}} \partial \psi + \left( \frac{1}{4} - \frac{1}{2} \sin^2 \theta_{12} \right) \frac{\partial^2}{\partial \psi^2} \]
\[ + \left( \cot \theta_{12} - \cot \theta_{12} - \frac{1}{2 \sin \theta_{12}} \right) \frac{\partial}{\partial \psi} \]

where

\[ \Lambda_1 = 2 \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial \psi^2} + \frac{1}{\hbar^2} M^2 \]
\[ \Lambda_2 = \frac{2 \cot \theta}{\sin \theta} \frac{\partial}{\partial \phi} - \frac{2 \cot \theta}{\sin \theta} \frac{\partial^2}{\partial \theta \partial \phi} + \frac{1}{\hbar^2} \cot \theta \frac{\partial^2}{\partial \phi^2} \]
\[ - \left( 1 + 2 \cot \theta \right) \frac{\partial}{\partial \psi} \]
and $\hat{M}^2$ is the total angular momentum squared operator given in Eq. (41). $F_2$ is again derivable from $F_1$ by replacing $\Theta_{12}$ by $-\Theta_{12}$.

VII. THE REDUCED OR RADIAL EQUATIONS, ATOMIC CASE

The essential properties of the combinations of the operators appearing in $F_1$ and $F_2$, Eq. (62), are the following (cf. Appendix I):

\begin{align}
(S_m 2 \psi \Lambda_2 - \cos 2 \psi \Lambda_1) \hat{J}_{\ell}^{(x^+)} &= -2 \pi (x-1) B_{\ell x} (1 - \delta_{0, x}) \hat{J}_{\ell}^{(x^+)} + \delta_{1, x} (1 - 2 A_x^e) \hat{J}_{\ell}^{(x-2)^+} \\
&\quad - \frac{(1 + 3 \delta_{0, x})}{[1 + \delta_{0, x}(12-1)]} A_x^e A_{x+1}^e \frac{1}{2 B_{\ell x}^{(x+2)}} \hat{J}_{\ell}^{(x+2)^+} \tag{65a}
\end{align}

\begin{align}
(S_m 2 \psi \Lambda_1 + \cos 2 \psi \Lambda_2) \hat{J}_{\ell}^{(x^-)} &= -2 \pi (x-1) B_{\ell x} (1 - \delta_{0, x}) (1 - \delta_{0, x}) \hat{J}_{\ell}^{(x-2)^-} \\
&\quad - S_{1, x} (1 - 2 A_x^e) \hat{J}_{\ell}^{(x^-)} + \frac{(1 + 3 \delta_{0, x})}{[1 + \delta_{0, x}(12-1)]} A_x^e A_{x+1}^e \frac{1}{2 B_{\ell x}^{(x+2)}} \hat{J}_{\ell}^{(x+2)^-} \tag{65b}
\end{align}

\begin{align}
(S_m 2 \psi \Lambda_2 - \cos 2 \psi \Lambda_1) \hat{J}_{\ell}^{(x^-)} &= -2 \pi (x-1) B_{\ell x} (1 - \delta_{3, x}) (1 - \delta_{0, x}) \hat{J}_{\ell}^{(x-2)^-} \\
&\quad - S_{1, x} (1 - 2 A_x^e) \hat{J}_{\ell}^{(x^-)} - \frac{(1 - \delta_{0, x})}{[1 + \delta_{0, x}(12-1)]} A_x^e A_{x+1}^e \frac{1}{2 B_{\ell x}^{(x+2)}} \hat{J}_{\ell}^{(x+2)^-} \tag{66a}
\end{align}

\begin{align}
(S_m 2 \psi \Lambda_1 + \cos 2 \psi \Lambda_2) \hat{J}_{\ell}^{(x^-)} &= 2 \pi (x-1) B_{\ell x} (1 - \delta_{0, x}) \hat{J}_{\ell}^{(x-2)^+} \\
&\quad - S_{1, x} (1 - 2 A_x^e) \hat{J}_{\ell}^{(x^+)} - \frac{(1 - \delta_{0, x})}{[1 + \delta_{0, x}(12-1)]} A_x^e A_{x+1}^e \frac{1}{2 B_{\ell x}^{(x+2)}} \hat{J}_{\ell}^{(x+2)^+} \tag{66b}
\end{align}
where
\[ A^\ell_x = \frac{(x-l)(x+\ell+1)}{2(x+1)} \tag{67} \]

and
\[ B^\ell_x = \frac{(l-x+1)(l-x+2)(x+l)(l+x-1)}{4x(x-1)} \tag{68} \]

Recall that \( x \) is the absolute value of \( k \), Eq. (50). We have explicitly verified that these relationships are not altered if one replaces the \( \mathcal{Y}^x \) functions by the \( \mathcal{Y}_l \) functions of Eq. (54). (cf. Appendix II)

This is, of course, necessary for the radial equations to be independent of \( m \). With these relationships, it becomes quite simple to derive the reduced equations from the original Schrödinger equation

\[ H \Psi \xi_o = E \Psi \xi_o \quad \tag{69} \]

where the wave function \( \Psi \xi_o \) is expanded in Eq. (51). One obtains

\[
\begin{aligned}
&\left[ L_{\xi_1} + \frac{2m}{\hbar^2} (E-V) \right] f^x_\ell - \left( \frac{1}{l^x_\ell} + \frac{1}{l^x_{\ell+1}} \right) \left[ \left\{ \frac{\ell(\ell+1)-x^2}{2\sin \theta_{12}} + \frac{x^2}{4} - \cot \theta_{12} \delta_{1,x} - \right\} \frac{A^\ell_{x-1} A^\ell_{x-1} f^x_\ell}{B^x_\ell} \right] \\
&+ \frac{\cosec \theta_{12} (x+1)(x+2) B^x_\ell f^x_\ell}{4\sin \theta_{12}} + \frac{\cosec \theta_{12}}{4\sin \theta_{12}} \frac{1 + 3 \delta_{0,x-2}}{\left[ 1 + \Delta_{2,x-1}(1^2) \right]} \frac{A^\ell_{x-2} A^\ell_{x-1} f^x_\ell}{B^x_\ell} \\
&+ \left( \frac{1}{l^x_\ell} - \frac{1}{l^x_{\ell+1}} \right) \left[ x \left( c_{x=0} \cosec \theta_{12} - \cot \theta_{12} - \frac{1}{2\sin \theta_{12}} \right) f^x_\ell - x \frac{\partial f^x_\ell}{\partial \theta_{12}} \right] \\
&- \delta_{1,x} \left( 1 - 2A^\ell_\ell \right) f^x_\ell + \frac{(x+1)(x+2)}{2\sin \theta_{12}} B^x_\ell f^x_\ell \\
&- \delta_{0,x-2} \frac{1}{4\sin \theta_{12}} \frac{A^\ell_{x-1} A^\ell_{x-2} f^x_\ell}{B^x_\ell} \left( 1 + \delta_{0,x-2} \right) \frac{B^x_\ell f^x_\ell}{\Delta_{2,x-1}(1^2)} \right] = 0 \quad \tag{70a}
\end{aligned}
\]
where \( L_{\theta_{12}} \) is the S wave part of the kinetic energy, and only the term containing it survives in the description of S states: \( 1, 2, 3 \)

\[
L_{\theta_{12}} = \frac{1}{\tau_1} \Theta_{1,2} \frac{2}{\tau_2} \Theta_{1,2} + \left( \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_{1,2}} \right) \frac{1}{\Delta \Theta_{1,2}} \Theta_{1,2} \Theta_{1,2}
\]
Eq. (70) are the "radial" equations, which it has been our purpose to derive. They pertain to both types of parity and exchange states. Parity is determined by the eveness or oddness of \( x \).

If, for example, \( \ell \) is even, and we want to describe a state of even parity, Eqs. (70) couple the functions \( \mathcal{f}_x^+ \) and \( \mathcal{f}_x^- \) for \( x = 0, 2, 4 \cdots \ell \). This involves \( \ell/2 \) pairs plus one function (for \( x = 0 \), \( \mathcal{D}_\ell^{0-} \) is zero hence \( \mathcal{f}_\ell^{0-} \) can be taken to be zero) or \( \ell + 1 \) functions. The odd parity equations for the same \( \ell \) correspond to the coupling of the function with \( x = 1, 3, \ldots, \ell - 1 \). This relates \( \ell/2 \) pairs or \( \ell \) functions to each other. Both even and odd parity together therefore involve \((2\ell + 1)\) functions corresponding the \((2\ell + 1)\) degeneracy of the vector spherical harmonics for a given \( m \). For \( \ell \) odd, there are \( \ell \) functions involved in the even parity equations and \( \ell + 1 \) functions in the odd parity equations.

For a given parity and \( \ell \), both singlet and triplet (space symmetric and antisymmetric) states are described by the same set of equations. The differences in the solutions devolve from the different boundary conditions which must be applied, Eqs. (52). One of the key virtues of the functions \( \mathcal{f}_x^\pm (r_1, r_2, \theta_{12}) \) is that they are either symmetric or antisymmetric; thus they may be confined to the region, say \( r_1 \parallel r_2 \). If, for example, \( \ell \) is even so that the exchange character of \( \mathcal{f}_x^+ \) is symmetric (which, according to
(52), implies that $f^+_x$ is antisymmetric, then these properties may be embodied in the boundary conditions:

$$\left[ \frac{2}{\partial n} f^+_x(r_1, r_2, \theta_{12}) \right] = 0 , \quad r_1 = r_2$$

(72)

where $\frac{2}{\partial n}$ represents the normal derivative, and

$$\left[ f^-_x(r_1, r_2, \theta_{12}) \right] = 0 , \quad r_1 = r_2$$

(73)

and the solution from there on involves only the region $r_1 > r_2 > r_1^0$. Such equations have distinct advantages from the point of view of numerical solutions.

One can define, however, an asymmetric function in terms of which the radial equations can be more simply written. Letting

$$F^+_x(r_1, r_2, \theta_{12}) \equiv f^+_x(r_1, r_2, \theta_{12}) + f^-_x(r_1, r_2, \theta_{12})$$

(74)

and

$$\tilde{F}^+_x(r_1, r_2, \theta_{12}) \equiv f^+_x(r_1, r_2, \theta_{12}) - f^-_x(r_1, r_2, \theta_{12})$$

(75)

so that, from Eq. (47),

$$\tilde{F}^x(r_1, r_2, \theta_{12}) = \pm (-1)^x F^+_x(r_1, r_2, \theta_{12})$$

(76)
These equations, depending as they do on $F^x_\ell$ and $F^{x'}_\ell$, are more analogous to the form the $P$-wave equation of Breit. The question may arise in connection with these as well as Breit’s equations, of whether they are well-defined, since they involve two functions $F^x_\ell$ and $F^{x'}_\ell$ and yet there is only one equation (for a given $\chi$). This question, in fact would appear to be particularly relevant as the previous form of our equations, (70) do constitute a coupled set for a given $\chi$. To see that both situations are meaningful and in particular that (77) is well-defined, consider a numerical solution of (77). In that case the space of the independent variables is divided into a grid of points, and $F^x_\ell$ is the collection of numbers associated with these
grid points. $F^X$ can therefore be considered a vector with as many components as there are grid points. The differential equation is replaced by a matrix which operates on the vector $F^X$. Now everytime an $\tilde{F}^X_t$ occurs in the equation, it is completely clear what has to be done: namely one must let the matrix counterpart of its coefficient in the differential equation operate on that component of $F^X$ which is its reflection point defined by (76). This is a completely unambiguous prescription which is tantamount to saying that the set (77) is well defined by itself. The reason that (70) is composed of two equations for each $x$ whereas (77) is not is due to the fact that the functions $\tilde{F}^X_t$ are asymmetric and therefore must be solved for in the whole $x_1, x_2, x_{12}$ space. On the other hand the $F^X_t$ functions are either symmetric or antisymmetric, and therefore they are restricted to the $x_1 \geq x_2, x_{12}$ (or equivalently to the $x_1 \leq x_2, x_{12}$) space. Since this is only half the independent variable space, it is necessary that there be double the number of functions to recover the same information. This is again to say that (70) and (77) are completely equivalent. (Nevertheless a redundant equation with $F^X_t$ and $\tilde{F}^X_t$ interchanged may readily be derived.)

We have stated that (70) has certain advantages from the point of view of numerical integration. However, it should also be stated that the form (77) will probably be more advantageous for ordinary variational calculations. This is because if one adopts a specific
analytic form of $F_0^\times$, one need only interchange $r_1$ and $r_2$ in
the expression to obtain $\tilde{F}_0^\times$.

The differences in the $f_1^\times$ description from that of $F_0^\times$
gives rise to characteristic differences in the formulation of
boundary conditions for scattering problems (cf. the next section).

The restriction of these equations to the atomic case (two
identical particles in a fixed central field) has implicitly been made
by assuming that the potential is a function of the residual coordinates,

$$V = V(r_1, r_2, r_{12}),$$

so that $V$ commutes with the angular momentum and therefore appears
as an additional diagonal term in the radial equations.

The inter-particle distance $r_{12}$ is related to the independent
radial coordinates that we have thus far considered, $r_1$, $r_2$, $\theta_{12}$ via
the law of cosines:

$$r_{12}^2 = r_1^2 + r_2^2 - 2r_1r_2 \cos \theta_{12}.$$  

Alternatively, however, one can consider $r_1$, $r_2$, and $r_{12}$ as the
independent coordinates and derive radial equations involving them.
Those coordinates, in fact, have certain advantages since the three
singularities in the potential occur at their null point. As
such they can describe the wave function in the region of close
interaction very well. These variables, therefore, are particularly
suited to calculation of low-lying bound states of two-electron atoms (where on the whole the electrons are quite close to each other and to the nucleus) and such successful calculations have been done ever since the early work of Hylleraas. 1

When one considers the equation in the form we have previously given them, involving $\theta_{12}$, one is naturally led to expand the "radial" wave function in terms of Legendre polynomials of $\cos \theta_{12}$ 11. The expansion is then truncated after some $P_n(\cos \theta_{12})$ and convergence is sought as a function of $n$. In these classes of two electron problems, this constitutes the idea of configuration interaction in its most general form. Recently this idea has come under some criticism 13,14,15 principally because such a relative partial wave expansion necessarily converges slowly where the electron-electron interaction is large ($r_{12}$ small). The argument is doubtless justified for the above-mentioned low-lying bound states. However the argument can easily get distorted and exaggerated, for instance when applied to the low-energy scattering of electrons from hydrogen. 14 The point there is that the long-range correlation coming from the induced potential in the atom is at least as important as the short range correlations 16 and yet is only poorly approximated by the conventional Hylleraas type of expansion. This situation has been discussed elsewhere 12.

These reservations notwithstanding, however, it is nevertheless true that the most accurate three body calculations have been made using the $r_1$, $r_2$, $r_{12}$ coordinates, or linear combinations of them17,
on the low-lying states of helium and its isoelectronic ions. We therefore give below the radial equations in terms of $r_1$, $r_2$, $r_{12}$. The equations are in their asymmetric form corresponding to Eq. (77), since it is assumed that they will be utilized in connection with variational calculations with analytic expansions of the radial wave functions.

\[
\begin{align*}
\left[ L_{\ell \gamma_1} + \frac{2m}{\hbar^2} (E - V) \right] F_\ell^- &= \left( \frac{1}{\gamma_1^-} + \frac{1}{\gamma_2^-} \right) \left[ \left( \frac{\ell + 1}{r} \right)^2 \right] \left\{ \left[ \frac{F_{\ell 1}^{x^2} + F_{\ell 2}^{x^2}}{\rho^2} \right] F_{\ell}^- \right. \\
&- \delta_{\ell \gamma_1^-} \left( 1 - 2 A_{\gamma_1^-} \right) \left[ \gamma_1^{x^2} + \gamma_2^{x^2} - \gamma_{12}^{x^2} \right] \frac{r_1 r_2}{\rho^2} \frac{\tilde{F}_{\ell}^-}{r_1 r_2} \\
&+ (\lambda + 1)(\lambda + 2) B_{\ell \lambda + 2} \left( \gamma_1^{x^2} + \gamma_2^{x^2} - \gamma_{12}^{x^2} \right) \frac{2 \gamma_1^- \gamma_2^-}{\rho^2} \left\{ \frac{F_{\ell 1}^{x^2} + F_{\ell 2}^{x^2}}{\rho^2} - \delta_{\ell \gamma_1^-} \left( \frac{F_{\ell 1}^{x^2} - F_{\ell 1}^{x^2}}{2} \right) \right\} \\
&+ \frac{A_{\ell - 2} A_{\ell - 2} (- \gamma_1^{x^2} + \gamma_2^{x^2} - \gamma_{12}^{x^2}) \gamma_1^{- \gamma_2^{-}}}{2 B_{\ell \lambda} \left[ 1 + \delta_{\ell \lambda} - (\lambda - 1) \right] \rho^2} \\
&+ (\lambda + 1)(\lambda + 2) B_{\ell \lambda + 2} \frac{2 \gamma_1^- \gamma_2^-}{\rho^2} \left\{ \frac{F_{\ell 1}^{x^2} + F_{\ell 2}^{x^2}}{\rho^2} - \delta_{\ell \gamma_1^-} \left( \frac{F_{\ell 1}^{x^2} - F_{\ell 1}^{x^2}}{2} \right) \right\} \\
&+ \frac{A_{\ell - 2} A_{\ell - 2} \gamma_1^{- \gamma_2^{-}}}{2 B_{\ell \lambda} \left[ 1 + \delta_{\ell \lambda} - (\lambda - 1) \right]} \frac{1}{\rho^2} \left\{ \frac{F_{\ell 1}^{x^2} + F_{\ell 2}^{x^2}}{\rho^2} - \delta_{\ell \gamma_1^-} \left( \frac{F_{\ell 1}^{x^2} - F_{\ell 1}^{x^2}}{2} \right) \right\} \\
- \delta_{\ell \gamma_1^-} \left( 1 - 2 A_{\gamma_1^-} \right) \frac{r_1 r_2}{\rho^2} F_{\ell}^- &= 0 \\
\end{align*}
\]
Here

\[ \mathcal{F} = \left[ \frac{1}{2} \mathbf{r}_1^2 - (\mathbf{r}_1 - \mathbf{r}_2)^2 \right] + 2 \mathbf{r}_1 \cdot \left( \mathbf{r}_1^2 + \mathbf{r}_2^2 \right) \]

(80)

The quantity whose square root \( \mathcal{F} \) is can easily be shown to be positive definite. In the equation (68) the \( F_\mathcal{F} \) \( \mathcal{F} \) is understood to be a function of \( r_1, r_2, r_{12} \):

\[ F_\mathcal{F} = F_\mathcal{F}(r_1, r_2, r_{12}) \]

In addition \( L_{\sigma_1} \) is the kinetic energy counterpart of the S-wave \( L_{\sigma_2} \) in terms of \( r_1, r_2, r_{12} \):

\[ L_{\sigma_1} = \frac{1}{r_1} \frac{\partial^2 r_1}{\partial r_1^2} + \frac{1}{r_2} \frac{\partial^2 r_2}{\partial r_2^2} + \frac{2}{r_{12}} \frac{\partial^2 r_{12}}{\partial r_{12}^2} \]

\[ + \frac{r_1^2 + r_2^2 - r_{12}^2}{r_1 r_2} \frac{\partial^2 r_1}{\partial r_1 \partial r_2} \]

\[ + \frac{r_1^2 + r_2^2 - r_{12}^2}{r_1 r_2} \frac{\partial^2 r_2}{\partial r_1 \partial r_2} \]

(81)

The equations (79) can readily be put in the form of coupled equations for a given \( \chi \). In that form they would be closest to the form originally given by Holmberg, \(^6\), (although as we have stated his equations apply to three equal mass particles). One salient difference between the two sets of equations, however, is that the present ones are manifestly real, whereas one term in Holmberg's equations is imaginary. \(^6\). It is clear that the equations as well as the solutions must be reducible to completely real form for any given angular momentum state. The accomplishment of this in the
present case comes from the explicit construction of real vector spherical harmonics, Eq. (49).

VIII BOUNDARY CONDITIONS FOR SCATTERING

In this section we derive the asymptotic forms of the radial functions corresponding to the scattering of an electron from a one electron atom in its ground state. The Coulomb modifications when the target system is an ion instead of an atom can readily be made and will have no effect on the angular integrations with which we are here concerned.

As we have seen in the foregoing sections culminating in the last section, the selection of a symmetric choice of Euler angles (Hönlberg's angles) has allowed for a completely general derivation of the radial equations. From the point of view of a scattering problem, however, a symmetric choice of angles is not the most advantageous since here we are concerned with an intrinsically asymmetric situation. Thus if we consider that region of configuration space where \( r_1 \) is large and \( r_2 \) small, corresponding to electron 1 being scattered from the atom to which electron 2 is bound, the wave function in this region alone will not be symmetric. However, in terms of the Hylleraas-Breit angles, the spherical angles of one of the particles being defined as two of the Euler angles, the wave function in this asymmetric region is easier to describe. Nevertheless this is a complication of detail only, since all the angular integrations may readily be performed as we shall now show.
We start with the statement that the complete wave function must have the asymptotic form:

\[
\lim_{r_1 \to \infty} \Psi_{l0}(r_1, r_2) = \frac{\sum \left( \kappa r_1 + \delta \ell - \frac{\ell \pi}{2} \right) Y_{l0}(\Omega_1)}{r_1} P_{l0}(r_1) Y_{\Omega_0}(\Omega_2) \tag{82}
\]

where \((R_{1s}(r_2)/r_2) Y_{\Omega_0}(\Omega_1)\) is the ground state of the one-electron atom (hydrogen). On the other hand, from Eq. (51),

\[
\lim_{r_1 \to \infty} \Psi_{e0}(r_1, r_2) = \frac{\sum \left( \kappa r_1 + \delta \ell - \frac{\ell \pi}{2} \right) R_{1s}(r_1) \sum \left[ \alpha_2 \right]}{r_1} \tag{83}
\]

where

\[
\alpha_2 = \int_{0}^{\pi} \int_{0}^{\pi} \int_{0}^{2\pi} \left[ \int \right] \sin \theta \ d\theta \ d\phi \ d\psi
\tag{84}
\]

It should be noted that (82) refers to the state of parity \((-1)^\ell\) as long as we are considering elastic scattering from the ground \((1s)\) state. This then defines the evenness or oddness of the values over which \(\kappa\) goes in the summation in Eq. (83).

The quadrature in (84) can readily be performed by recalling from Section II that \(\theta_1\) is the angle between \(\hat{z}_2\) and \(\hat{z}_1\), whose spherical angles in the primed coordinate systems are given in Eq. (20). One can then use these spherical angles to expand \(P\left(\cos \Theta_1\right)\) via the addition theorems for spherical harmonics.
In its real form this gives in the present case
\[
\rho^m_\ell (\theta) = \rho^m_\ell (\pi/2) \rho^m_\ell (\theta) + 2 \sum_{m=1}^{\ell} (-1)^m \binom{\ell - m}{m} \rho^m_\ell (\pi/2) \rho^m_\ell (\theta) \cos \left( m\left( \frac{1}{2} \theta_{12} \right) \right)
\] 
(85)

In (85) we have written both the Legendre and associated Legendre polynomials as functions of the angle but what we mean in all cases is that the angle is to be substituted into the transcendental form of the function. For example \( P_1 (\beta) = \cos \beta \) and not \( P_1 (\beta) = \beta \). The sign of the \( P_\ell^m \) is that of Magnus and Oberhettinger (which differs by \((-1)^m\) from that of Morse and Feshbach). To complete the quadrature in (84) we note that

\[
\alpha_{\ell}^\infty (\theta) = (-1)^\ell \left[ \frac{(l-x)!}{(l+x)!} \right]^{\ell/2} \rho_{\ell}^\infty (\theta)
\] 
(86)

Substitution into (84) now yields the desired result:

\[
\alpha_{\ell}^{x^+} (\theta_{12}) = \rho_{\ell}^{x^+} \left( \frac{\pi}{2} \right) \left[ \frac{(l-x)!}{(l+x)!} \right]^{\ell/2} \left\{ S_{\ell, x} + (1 - S_{\ell, x}) \cos \frac{l}{2} \theta_{12} \right\}
\] 
(87a)

\[
\alpha_{\ell}^{x^-} (\theta_{12}) = \rho_{\ell}^{x^-} \left( \frac{\pi}{2} \right) \left[ \frac{(l-x)!}{(l+x)!} \right]^{\ell/2} \left\{ (1 - S_{\ell, x}) \sin \frac{l}{2} \theta_{12} \right\}
\] 
(87b)

The radial function themselves thus approach

\[
\lim_{\gamma \to \infty} f_{\ell}^{\pm} (r_1, r_2, \theta_{12}) = \frac{s_{\ell} (k \gamma + \epsilon \gamma^2 - \epsilon \pi \gamma)} {r_1} \frac{R_{15} (r_2)} {r_2^2} \alpha_{\ell}^{x^\pm} (\theta_{12})
\] 
(88)
in which form we see that \( r_1, r_2 \) dependence of all the \( f_{r_x} \) functions is independent of \( \Omega \), so that none of them vanishes in the asymptotic region. Since in all cases the \( \Theta_{12} \) dependence is trivial, it may be worthwhile to define new functions whose asymptotic behaviour is strictly the \( r_1, r_2 \) dependence in (88).

For bound state problems, it is clear that all the radial functions must vanish in all asymptotic regions.

**IX OTHER APPLICATIONS**

In addition to two electron atomic or ionic systems the present equations apply to double mu or pi mesic atoms, although as the mass of the identical particles gets heavier, the correction for the center of mass becomes more important. Also for the spinless bosons (pi mesons) only the space symmetric solutions will presumably be relevant.

The equations can also be applied to two different particles of the same mass (positron-hydrogen scattering, for example). In this case, the potential, \( V \), will no longer be symmetric hence the solutions will not be symmetric which implies that boundary conditions like (72) must be changed to matching conditions of the asymmetric solutions along the line \( r_1 = r_2 \). This has the effect of giving one solution where formerly there were two, in accord with the distinguishability of the particles.

The major extension of this approach is to two-electron diatomic
molecules. In this case, the extension from one\textsuperscript{20} to two electrons is non-trivial. However, the analysis has been completed and will be published elsewhere.\textsuperscript{21}
Appendix I

In this appendix, we prove the Eqs. (65) and (66). For $m = 0$, terms give zero. Therefore, we can write

$$
\Lambda_1 \rightarrow \frac{\partial^2}{\partial \theta^2} \cot \theta - \frac{\partial}{\partial \theta} \cot \frac{\partial}{\partial \psi} \quad (I1)
$$

$$
\Lambda_2 \rightarrow 2 \cot \theta \frac{\partial^2}{\partial \psi \partial \theta} - \frac{\partial}{\partial \psi} - 2 \cot \frac{\partial}{\partial \psi} \quad (I2)
$$

and

$$
\mathcal{J}^x_{\ell} = N_{\ell,x} \cos x \psi \sin \theta F_x \quad (I3)
$$

$$
\mathcal{J}^{-} = N_{\ell,x} \sin x \psi \sin \theta F_x \quad (I4)
$$

where

$$
N_{\ell,x} = \sqrt{\frac{2\ell + 1}{8\pi^2} \cdot \frac{(\ell + \chi)!}{(\ell - \chi)!}} \cdot \frac{1}{2^x} \cdot \frac{1}{x!} \quad (I5)
$$

and

$$
F_x = F(x-\ell, x+\ell+1, 1+\chi, \frac{\omega^2}{2}) \quad (I6)
$$
Now
\[ \Lambda, \mathcal{J}^\ell_\ell = N_{\ell \chi} \cos \chi \psi \left[ 2x(x-1) \sin \theta \cos \theta F_x - x \sin \theta F_x \right. \]
\[ \left. + x \sin \theta \cos \theta A^\ell_\chi F_{x+1} + \sin \theta A^\ell_\chi A^\ell_{\chi+1} F_{x+2} \right] \] (I7)

where we have used the well known relations for the derivatives of hypergeometric functions:
\[ \frac{d}{d\theta} F_x = A^\ell_\chi \sin \theta F_{x+1} \] (I8)
\[ \frac{d^2}{d\theta^2} F_x = A^\ell_\chi \cos \theta F_{x+1} + A^\ell_\chi A^\ell_{\chi+1} \sin \theta F_{x+2} \] (I9)

A relation between \( F_x, F_{x+1} \) and \( F_{x+2} \) can be obtained from the differential equation satisfied by the hypergeometric function
\[ \cos \theta F_{x+1} = F_x - \frac{A^\ell_{\chi+1} \sin \theta}{2(x+1)} F_{x+2} \] (I10)

Using (I10) in (I7), we find
\[ \Lambda, \mathcal{J}^\ell_\ell = N_{\ell \chi} \cos \chi \psi \left[ 2x(x-1) \sin \theta \cos \theta F_x \right. \]
\[ \left. - x \sin \theta F_x + 2x \sin \theta A^\ell_\chi F_x \right. \]
\[ \left. + \left( 1 - \frac{x}{x+1} \right) \sin \theta A^\ell_\chi A^\ell_{\chi+1} F_{x+2} \right] \] (I11)
Similarly, \( \Lambda _{1} (x) \) 

\[
\Lambda _{1} (x) = - \frac{N_{p}}{x} \sin x\psi \left[ 2 x (x-1) \cos^2 \theta F_{x} - x \sin \theta F_{x}ight]
\]

\[
- 2 x A_{x}^{e} \sin \theta F_{x} - \frac{x}{x+1} \sin A_{x} A_{x+1} A_{x+2} F_{x+2}
\]

(II2)

Multiply (II2) by \( \sin 2\psi \) and (II1) by \( \cos 2\psi \) and subtract to get

\[
(\sin 2\psi \Lambda _{2} - \cos 2\psi \Lambda _{1}) \partial _{x} = - \frac{N_{p}}{x} \cos (x-1) \psi G - \frac{N_{p}}{x} \frac{x}{x+1} \sin A_{x} A_{x+1} A_{x+2} F_{x+2}
\]

(II3)

where

\[
G = \left( 2 x (x-1) \sin \theta \cos \theta - x \sin \theta + 2 x \sin \theta A_{x}^{e} \right) F_{x}
\]

(II4)
Let \( x \rightarrow x + 1 \) in (II0), then

\[
\cos \theta \; F_{x+2} = F_{x+1} - \frac{\sin \theta}{2} A_{x+2}^\ell \; F_{x+3}
\]

Substituting in the above for \( F_{x+1} \) and \( F_{x+3} \) by using (II0) we get after some rearrangement

\[
\left[ \cos \theta \left( \frac{x+2}{x+1} \right) \right. + \frac{x+1}{2(x+1)^2} \; \sin \theta \; A_{x+1}^\ell + \frac{\sin \theta}{2} A_{x+2}^\ell \left] \right. \; F_{x+2}
\]

\[
= \frac{\sin \theta}{4} \; A_{x+2}^\ell \cdot A_{x+3}^\ell \; F_{x+4} = \frac{x+2}{x+1} \; F_x
\]

Letting \( x \rightarrow x - 2 \) multiplying by \( 2(\; x - 1 \;)^2 \; \sin^2 \theta \) and rearranging we have for \( x \geq 2 \)

\[
G = 2x(x-1) \; \sin\theta \; F_{x-2} \quad x \neq 0, 1
\]

(II5)

Also we find directly from (II1) and (II2)

\[
G = \frac{1}{2} \; \sin \theta \; A_{x}^\ell \; A_{x}^\ell \; F_x \quad x = 0
\]

(II6)

\[
G = -(1-2 \; A_{1}^\ell) \; \sin \theta \; F_1 \quad x = 1
\]

(II7)

Finally then with the substitution of the above in (II3) we obtain for \( x \geq 2 \).
\[(\sin 2\psi \Lambda_2 - \cos 2\psi \Lambda_1) \mathcal{Y}_\ell^{X^+} = -2\pi (x-1) \mathcal{Y}_\ell^{(x-2)^-} + \frac{1}{4} \mathcal{B}_{\ell X} \mathcal{Y}_\ell^{(x-2)^+} \mathcal{B}_{\ell X+2}\] (II.8)

where \( \mathcal{B}_{\ell X} \) has already been defined in Eq. (68).

The special cases \( x = 0, 1 \) can be determined from (II.3), (II.6), (II.7). With proper normalization

\[\left(\sin 2\psi \Lambda_2 - \cos 2\psi \Lambda_1\right) \mathcal{Y}_\ell^{0^+} = -\sqrt{2} \frac{A_1^\ell A_1^\ell}{\mathcal{B}_{\ell 2}} \mathcal{Y}_\ell^{3^+}\] (II.9)

and

\[\left(\sin 2\psi \Lambda_2 - \cos 2\psi \Lambda_1\right) \mathcal{Y}_\ell^{1^+} = (1-2A_1^\ell) \mathcal{Y}_\ell^{1^+} - \frac{A_1^\ell A_1^\ell}{2\mathcal{B}_{\ell 3}} \mathcal{Y}_\ell^{3^+}\] (II.10)

We can combine (II.8, II.9, II.10) to get Eq. (65a).

Similarly, we can prove (65a), (66a), (66b).
Appendix II

For \( m \neq 0 \), we get, using Eqs. (44) and (64)

\[
\Lambda_1 \mathcal{G}^{m,k}_{l} = N_{lmk} e^{i(m \Phi + k \Psi)} \frac{\sin \frac{\Theta}{2}}{\sin \frac{\Theta}{2}} \frac{\cos \frac{\Theta}{2}}{\cos \frac{\Theta}{2}} \left\{ \left( m^2 \left( 1 - \sin^2 \frac{\Theta}{2} \right) - 4 m k \cos \Theta \right) \right.
\]

\[
+ k^2 \left( 1 + \cos \Theta - \frac{1}{\sin \Theta} \right) \frac{1}{\sin \Theta} - \frac{k + m}{2} \cos \frac{\Theta}{2} - \frac{k - m}{2} \cot \frac{\Theta}{2}
\]

\[
- \frac{|k - m|}{2} \left\{ F(-l + \frac{\Theta}{2} - 1, \ell + \frac{\Theta}{2}, 1 + |k - m|, \sin \frac{\Theta}{2})
\right.
\]

\[
+ 2 \left( m^2 \cos^2 \frac{\Theta}{2} - |k + m| \sin \frac{\Theta}{2} \right) A^0_{m,k} F(-l + \frac{\Theta}{2}, \ell + \frac{\Theta}{2} + 1, 2 + |k - m|, \sin \frac{\Theta}{2})
\]

\[
+ \sin^2 \Theta A^\ell_{m,k} C^\ell_{m,k} F(-l + \frac{\Theta}{2} + 1, \ell + \frac{\Theta}{2} + 2, 3 + |k - m|, \sin^2 \frac{\Theta}{2}) \right\}
\]

and

\[
\Lambda_2 \mathcal{G}^{m,k}_{l} = i N_{lmk} e^{i(m \Phi + k \Psi)} \frac{\sin \frac{\Theta}{2}}{\sin \frac{\Theta}{2}} \frac{\cos \frac{\Theta}{2}}{\cos \frac{\Theta}{2}} \left\{ \frac{2 m \cos \Theta - k (1 + \cos \Theta)}{\sin^2 \Theta}
\right.
\]

\[
+ \frac{k \cos \Theta - m}{\sin \Theta} \left( |k - m| \cot \frac{\Theta}{2} - |k + m| \tan \frac{\Theta}{2} \right) \right\} \times
\]

\[
F(-l + \frac{\Theta}{2} - 1, \ell + \frac{\Theta}{2}, 1 + |k - m|, \sin \frac{\Theta}{2})
\]

\[
+ 2 (k \cos \Theta - m) A^\ell_{m,k} F(-l + \frac{\Theta}{2}, \ell + \frac{\Theta}{2} + 1, 2 + |k - m|, \sin \frac{\Theta}{2}) \right\}.
\]
where

$$A_{m, k}^\ell = \frac{(-\ell + \beta_{\ell} - 1)(\ell + \beta_{\ell})}{2(1 + |k - m|)}$$  \hspace{1cm} (II3)

$$C_{m, k}^\ell = \frac{(-\ell + \beta_{\ell})(\ell + \beta_{\ell} + 1)}{2(2 + |k - m|)}$$  \hspace{1cm} (II4)

For illustration purposes, let $k - 2 \geq m$. Multiply (II2) by \sin 2\psi and (II1) by \cos 2\psi and subtract to get

$$\left(\sin 2\psi \Lambda_2 - \cos 2\psi \Lambda_1\right) \mathcal{D}_{m, k}^\ell = -N_{\ell m k} \ e^{i m \theta} \ \frac{\sin \theta}{2^k} \ \cot \frac{\theta}{2} \ \left[ e^{i(k+2)\psi} \ \frac{\sin^2 \theta}{2} + e^{i(k-2)\psi} \right.$$

$$\left. A_{m, k}^\ell \ C_{m, k}^\ell \ F(-\ell + k + 2, \ell + k + 1, 2 + k - m, \sin^2 \frac{\theta}{2}) + \right.$$}

$$\left. e^{i(k-2)\psi} \left\{ \left( \frac{2(k \cos \theta - m \cos \theta)(k - 1 - m)}{\sin^2 \theta + \cos \theta (1 + k) - m} \right) A_{m, k}^\ell \right.$$

$$\left. \left. \frac{\sin \theta}{\cos \theta (1 + k) - m} \right) F(-\ell + k, \ell + k + 1, 1 + k - m, \sin^2 \frac{\theta}{2}) + \right.$$}

$$\left. \left( \frac{1 - k \cos \theta + m}{2[(k + \cos \theta - m]} \right) \right.$$}

$$\left. \left. \frac{\sin^2 \theta}{A_{m, k}^\ell \ C_{m, k}^\ell \ F(-\ell + k + 2, \ell + k + 1, 3 + k - m, \sin^2 \frac{\theta}{2})} \right] \right.$$}

where we have used the relation

$$F(-\ell + k + 1, \ell + k + 2, 1 + k - m, \sin^2 \frac{\theta}{2}) = \frac{1 + k - m}{\cos \theta (1 + k) - m} \ F(-\ell + k, \ell + k + 1, 1 + k - m, \sin^2 \frac{\theta}{2})$$
Using this result, (which reduces to (II5) for \( m = 0 \)) in (II5), we obtain for \( k \neq 0,1 \)

\[
\begin{align*}
\left[ 2(k \cos \theta - m)(\cos \theta (k+1) - m) + 2 \frac{\sin^2 \theta (k+1-m)(2k \cos \theta - 2m)}{\cos \theta (k+1) - m} \right] A_{m,k}^l \\
- k \sin^2 \theta F(-l+k, l+k+1, 1+k-m, \sin^2 \frac{\theta}{2}) \\
- \frac{\cos \theta (k+1) - m}{\cos \theta (k+1) - m} \cdot \sin^2 \frac{\theta}{2} A_{m,k}^l C_{m,k}^l F(-l+k+2, l+k+3, 3+k-m, \sin^2 \frac{\theta}{2}) \\
= 2(k-m)(k-1-m) F(-l+k-2, l+k-1, k-m-1, \sin^2 \frac{\theta}{2})
\end{align*}
\]

so that

\[
(S_k \Psi \Lambda_2 - \cos 2\Psi \Lambda_1) \beta_{m,k-l}^{m,l} = -2(k-m)(k-m-1) \beta_{m,k}^l \beta_{m-k+2}^l - \frac{A_{m,k}^l C_{m,k}^l \theta_{m,k+2}^l}{2 \theta_{m,k+2}^l}
\]

where

\[
\beta_{m,k}^l = \frac{N_{m,k}}{4 N_{m,k-2}} = \left[ \frac{(l+k)(l+k-1)(l+k+2)(k-l+1)}{4 (k-m)(k-m-1)} \right]^{1/2}
\]
It is easily verified that

\[(k-m)(k-m-1)B_{\ell k} = k(k-1)B_{\ell k}\]  

(III0)

\[
\frac{A_{m,k} \cdot C_{m,k}}{B_{\ell k+2}} = \frac{A_{k} \cdot A_{k+1}}{B_{\ell k}}
\]  

(III1)

Using (III0) and (III1) in (III8), we find

\[
(Su \cdot 2 \psi A_2 - \cos 2 \psi A_1) \mathcal{D}_{\ell}^{m,k} = -2k(k-1)B_{\ell k} \mathcal{D}_{\ell}^{m,k-2} - \frac{A_{k} \cdot A_{k+1} \mathcal{D}_{\ell}}{2B_{\ell k+2}}
\]  

(III2)

Similarly, we find

\[
(Su \cdot 2 \psi A_2 - \cos 2 \psi A_1) \mathcal{D}_{\ell}^{m,-k} = -2k(k-1)B_{\ell k} \mathcal{D}_{\ell}^{m,-(k-2)} - \frac{A_{k} \cdot A_{k+1} \mathcal{D}_{\ell}}{2B_{\ell k+2}}
\]  

(II13)

Adding (III2) and (II13) and using the definition (54a) we derive finally for \[ \pi \neq 0, 1 \]
\[(\sin \psi \Lambda_{\ell} - \cos \psi \Lambda_{\ell+1}) J^{m, \ell}_{(\ell+1)} = -2 \ell(x-1) B_{2\ell} J^{m, (\ell-2)}_{\ell} - \frac{A_{\ell} A_{\ell+1}}{2 B_{\ell+2}} J^{m, (\ell+2)}_{\ell} \]  

which is identical in form to (11\beta) for \( m = 0 \). Other relations can be proved in the same way, thus the radial equations are in fact independent of \( m \).
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4. U. Fano, private communication. One of us (A.T.) acknowledges valuable discussions with Dr. Fano in 1959 at the outset of the formulation of these ideas.

5. The D-wave equations in Breit's angles have been worked out by H. Feshbach, M. I. T. thesis (1942, unpublished) and by one of us, A. Temkin (1959, unpublished). The wave functions for several states have been derived by C. Schwartz, Phys. Rev. 123, 1700 (1961).


Table 1: Coefficients of the Angular Derivatives in the Kinetic Energy \( a \) Cf. Eq. (49)

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Derivative</th>
<th>Coefficient</th>
<th>Derivative</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sin^2(\gamma + \theta_{12}) )</td>
<td>( \frac{\partial^2}{\partial \gamma^2} )</td>
<td>( \cot \theta_{12} )</td>
<td>( \frac{\partial}{\partial \theta_{12}} )</td>
</tr>
<tr>
<td>( \frac{1}{\sin^2 \theta_{12}} )</td>
<td>( \frac{\partial^2}{\partial \theta_{12}^2} )</td>
<td>( -\sin(2\gamma + \theta_{12}) )</td>
<td>( \frac{\partial^2}{\partial \gamma \partial \theta_{12}} )</td>
</tr>
<tr>
<td>( \frac{\cot \theta \cos^2(\gamma + \theta_{12})}{\sin^2 \theta_{12}} )</td>
<td>( \frac{\partial}{\partial \theta} )</td>
<td>( -2 \cos \theta \cos^2(\gamma + \theta_{12}) )</td>
<td>( \frac{\partial^2}{\partial \gamma \partial \theta_{12}} )</td>
</tr>
<tr>
<td>( \frac{\cos \theta \sin(2\gamma + \theta_{12})}{\sin^2 \theta \sin^2 \theta_{12}} )</td>
<td>( \frac{\partial}{\partial \theta} )</td>
<td>( 0 )</td>
<td>( \frac{\partial^2}{\partial \gamma \partial \theta_{12}} )</td>
</tr>
<tr>
<td>( B_1 )</td>
<td>( \frac{\partial}{\partial \gamma} )</td>
<td>( -1 )</td>
<td>( \frac{\partial^2}{\partial \gamma \partial \theta_{12}} )</td>
</tr>
</tbody>
</table>

\( a \) \( A_1 \) and \( B_1 \) are given in Eqs. (60) and (61).
Figure 1. Perspective drawing of Holmberg's Euler angles and the unit vectors of the problem.