A SYMMETRIC DECOMPOSITION OF THE TWO–ELECTRON WAVE EQUATION FOR FINITE NUCLEAR MASS

By T. M. Kalotas*

[*Manuscript received June* 25, 1965]

Summary

A complete classification of the state of two-electron atoms is given in terms of a set of symmetrized Euler-angle functions, and the matrix of the kinetic energy derived for this choice of states. For a state of given L, π, P_S the non-relativistic Schrödinger equation reduces to a finite set of coupled equations in the internal coordinates r_1, r_2, r_{12}; these equations are given for arbitrary L, π, P_S. The results apply to atomic two-electron systems with nuclei of finite mass, and more generally to any non-relativistic three-body system in which two of the particles have equal mass.

I. Introduction

Recently (Kalotas and Delves 1964) a complete classification of the states of the three-nucleon system in terms of a set of symmetrized spin-isospin Euler-angle functions Y_i has been given. Such a classification has the advantage that for a state of given total angular momentum J, parity π, and neutron excess T_z, the wave function ψ has the form

$$\psi^{J,\pi,T_z} = \sum_i f_i(r_{12}, r_{23}, r_{31}) Y_i \, . \tag{1}$$

The sum in (1) is *finite* and so the non-relativistic Schrodinger equation for ψ in the centre-of-mass system, reduces from a six-dimensional to a *finite* set of three-dimensional coupled equations, with consequent overwhelming saving in labour.

A similar classification is possible for the two-electron system, which in general aspects is simpler. The non-relativistic Hamiltonian for two electrons in the Coulomb field of a nucleus is spin independent; hence we need not consider the electron spins. We give then a complete symmetric classification of the Euler-angle states of the two electrons, together with the resulting set of differential equations for the internal functions f_i of equation (1).

There is no unique choice of Euler-angle functions; however, it is desirable that any choice made should take note of the exact constants of motion for the problem. These constants of motion include

(i) the orbital angular momentum L and projection m_L,

(ii) the parity π,

(iii) the symmetry P_S of the space state under permutation of the two electrons. Here a symmetric space function is associated with a singlet (para) spin function and an antisymmetric space function with a triplet (ortho) spin function.

* Physics Laboratory, University of Sussex, Falmer, Brighton, Sussex, England.

The standard classification of two-electron states is due to Breit (1930), who wrote an expression of the form (1) for P-states. However, his choice of Euler angles was quite unsymmetrical, making the construction of eigenfunctions with the correct symmetry very difficult. With our choice of Euler angles each term in (1) will have the appropriate symmetry and we shall therefore be able to deal with the state of general (L, π, P_S). Recently, Bhatia and Temkin (1964) have made an analysis similar to ours but assumed the nucleus to be fixed. Although their method of construction of the Euler-angle functions is different, the actual Euler angles they use are only trivially different and our results reduce to theirs in the limit of infinite nuclear mass.

In the following section we define our choice of Euler angles and construct a set of angular eigenfunctions Y_i of L^2 and L_Z with appropriate behaviour under the operations of time reversal, parity, and particle permutation. In Section III we give the kinetic energy operator in terms of the triangle Euler-angle coordinates and calculate the internal kinetic energy matrix.

II. The Choice of Body Axes and the Symmetrized Euler-angle Functions

The configuration of two-electron atoms in the centre-of-mass system, is determined by the six coordinates in $\mathbf{r}_1$, $\mathbf{r}_2$ representing the electron positions relative to the nucleus, or alternatively by the triangle Euler-angle coordinates r_1, r_2, r_{12}, α, β, γ. These coordinates are defined by

$$r_1 = |\mathbf{r}_1|, \qquad r_2 = |\mathbf{r}_2|, \qquad r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|,$$

while we define the Euler angles α, β, γ as in Derrick and Blatt (1958); that is, a set of body vectors $\mathbf{b}_1$, $\mathbf{b}_2$ giving the positions of the electrons relative to body axes, are related to the vectors $\mathbf{r}_1$, $\mathbf{r}_2$ in the space frame by

$$\mathbf{b}_k = A(\alpha)B(\beta)C(\gamma)\mathbf{r}_k; \qquad k = 1, 2,$$

where A, B, C are elementary rotation matrices given by

$$A(\alpha) = \begin{bmatrix} \cos\alpha & \sin\alpha & . \\ -\sin\alpha & \cos\alpha & . \\ . & . & 1 \end{bmatrix}, \qquad B(\beta) = \begin{bmatrix} 1 & . & . \\ . & \cos\beta & \sin\beta \\ . & -\sin\beta & \cos\beta \end{bmatrix},$$

$$C(\gamma) = A(\gamma).$$

The criteria for a useful set of body axes are:

(*a*) simple behaviour of the angular functions Y_i of (1) under operations of parity and electron exchange,

(*b*) simple form for the kinetic energy.

We shall choose the body axes in the following way.

(i) The two electrons lie in the body x–y plane with the nucleus at the origin.

(ii) The positive body x-axis bisects the smaller angle θ_{12} subtended at the nucleus by the two electrons.

(iii) Particle numbering is such that a rotation from 1 to 2 is clockwise when looking along the positive body z-axis.

A typical triangle body axis configuration is shown in Figure 1.

The above specification of coordinates is unique except when the nucleus and the two electrons lie in a straight line, in which case the body axes and hence the Euler angles remain undefined. The singular region of phase space requires special care in calculations involving the above coordinates. As in the three-nucleon case, this imposes restrictions on the form of the internal functions f_i in this region; these restrictions will be considered in later work.

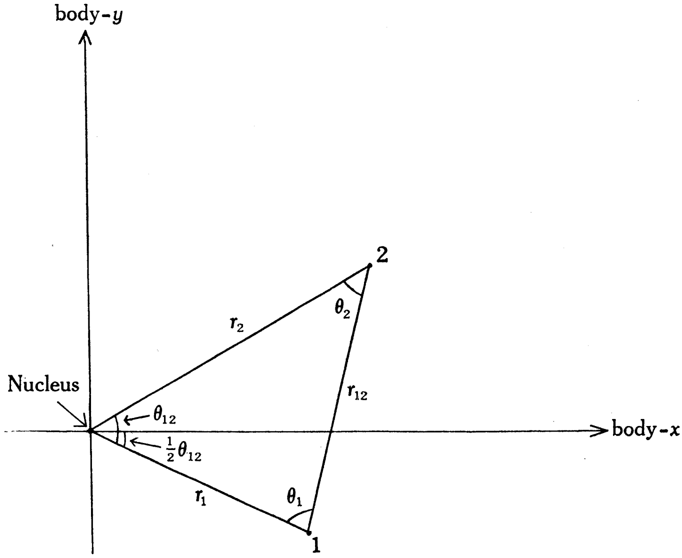

Fig. 1.—A typical configuration showing the position of the body axes.

We now proceed, as in Kalotas and Delves (1964) to construct a set of symmetrized Euler-angle functions of given angular momentum L and z component m_L. Explicitly we define the function

$$Y^L_{m_L}(P_E,|\mu|,(\pi)) = \mathrm{i}^{|\mu|+\bar{P}_E}\{(2L+1)^{\frac{1}{2}}/4\pi\}\epsilon_{\mu,0}\times[D^L_{|\mu|,m_L}(\alpha,\beta,\gamma)+(-1)^{L+\bar{P}_E}D^L_{-|\mu|,m_L}(\alpha,\beta,\gamma)]. \tag{2}$$

Here the $D^L_{\kappa\nu}(\alpha,\beta,\gamma)$ are the representation coefficients of the three-dimensional rotation group appearing in Kalotas and Delves (1964). Further

$$\begin{aligned}\bar{P}_E &= 0, \qquad \text{if } P_E = \text{symmetric } (s),\\ &= 1, \qquad \text{if } P_E = \text{antisymmetric } (a),\\ \epsilon_{\mu,\nu} &= 1/\sqrt{(2^{\delta_{\mu,\nu}})}.\end{aligned}$$

π is a superfluous index denoting the parity and is $+$ $(-)$ if μ is even (odd). Thus of the $2L+1$ functions Y_i of fixed L and m_L, $L+1$ (or L) are of even parity if L is even (or odd) and the remainder have odd parity.

The various functions Y_i are orthonormal, that is,

$$\int \mathrm{d(Euler)}\; Y^{L*}_{m_L}(P_E,|\mu|,(\pi))\,Y^{L'}_{m_{L'}}(P'_E,|\mu'|,(\pi')) = \delta_{L,L'}\,\delta_{m_L,m_{L'}}\,\delta_{|\mu|,|\mu'|}\,\delta_{P_E,P_E'},$$

and satisfy the time reversal reality condition

$$UY^L_{m_L}(P_E,|\mu|,(\pi)) = (-1)^{L-m_L}Y^L_{m_L}(P_E,|\mu|,(\pi)). \tag{3}$$

The functions are either symmetric or antisymmetric under interchange of the two electrons (the mixed representation is irrelevant to our case)

$$P_{12}Y^L_{m_L}(P_E,|\mu|,(\pi)) = (-1)^{\bar{P}_E}Y^L_{m_L}(P_E,|\mu|,(\pi)).$$

Hence any wave function of orbital angular momentum L, z component m_L, parity π, and permutation symmetry P_S, may be written in the form

$$\psi^L_{m_L}(P_S,\pi) = \sum_{P_E,|\mu|} f^L_{m_L}(P_R,|\mu|,(\pi))\,Y^L_{m_L}(P_E,|\mu|,(\pi)). \tag{4}$$

In the sum (4) the number μ is restricted to even (odd) values according as π is $+$ $(-)$. The symmetry P_R of the internal functions must be chosen so that

$$P_R \times P_E = P_S.$$

Hence the internal functions have the same (or opposite) symmetry as the corresponding Euler-angle functions for para (or ortho) states. Equation (4) constitutes our symmetric decomposition of the two-electron wave function.

In the work of Bhatia and Temkin (1964), the body axes are defined in a different way to ours but their Euler angles θ, ϕ, ψ are nevertheless closely related to our α, β, γ through

$$\alpha = \psi - \tfrac{1}{2}\pi; \qquad \beta = \theta; \qquad \gamma = \phi.$$

This leads to symmetrized angle functions that are very similar to our Y_i.

III. The Kinetic Energy

For the situation corresponding to two electrons each of mass m and a nucleus of mass M, the kinetic energy operator in the centre-of-mass system may be written

$$T = -(\hbar^2/2\mu)(\nabla_1^2+\nabla_2^2)-(\hbar^2/M)\nabla_1 . \nabla_2. \tag{5}$$

Here μ is the reduced electron mass $mM/(m+M)$, while for $k = 1, 2$

$$\nabla_k \equiv \partial/\partial \mathbf{r}_k$$

We give here the form of the kinetic energy in triangle Euler-angle coordinates.

In the fixed nucleus approximation $M \to \infty$ and

$$T \to -(\hbar^2/2m)(\nabla_1^2+\nabla_2^2).$$

For energy calculations of the helium isoelectronic series it is reasonable to consider the mass polarization operator $-(\hbar^2/M)\nabla_1 . \nabla_2$ as a perturbation term. We shall treat this term exactly but for convenience deal separately with the two operators

$$T_0 \equiv (\nabla_1^2+\nabla_2^2),$$
$$T_{12} \equiv \nabla_1 . \nabla_2.$$

As the transformations are lengthy, we give only the final results. For convenience we give also the matrix elements of these operators defined by

$$\Omega_{ij} \equiv \int \mathrm{d(Euler)}\, Y_i^* \,\Omega Y_j, \tag{6}$$

where Ω is any operator in general. The essential results are given below.

(a) The Transformed Operators T_0, T_{12}

(i) We find that the operator T_0 takes the following form in triangle Euler-angle coordinates

$$T_0 = T_0^1+T_0^2+T_0^3+T_0^4,$$

where

$$T_0^1 = \frac{\partial^2}{\partial r_1^2}+\frac{\partial^2}{\partial r_2^2}+2\frac{\partial^2}{\partial r_{12}^2}+2\cos\theta_1\frac{\partial^2}{\partial r_1\partial r_{12}}+2\cos\theta_2\frac{\partial^2}{\partial r_2\partial r_{12}}+\frac{2}{r_1}\frac{\partial}{\partial r_1}+\frac{2}{r_2}\frac{\partial}{\partial r_2}+\frac{4}{r_{12}}\frac{\partial}{\partial r_{12}}, \tag{7}$$

$$T_0^2 = \frac{(r_1^2-r_2^2)\sin\theta_{12}}{r_1 r_2 r_{12}}\left(\frac{\partial}{\partial r_{12}}\right)\left(\frac{L_z^B}{-i\hbar}\right), \tag{8}$$

$$T_0^3 = \frac{R^2\cos^2\frac{1}{2}\theta_{12}}{4\Delta^2}\left(\frac{L_x^B}{-i\hbar}\right)^2+\frac{R^2\sin^2\frac{1}{2}\theta_{12}}{4\Delta^2}\left(\frac{L_y^B}{-i\hbar}\right)^2+\frac{R^2}{4r_1^2r_2^2}\left(\frac{L_z^B}{-i\hbar}\right)^2$$
$$+\frac{(r_2^2-r_1^2)}{4r_1r_2\Delta}\left\{\left(\frac{L_x^B}{-i\hbar}\right)\left(\frac{L_y^B}{-i\hbar}\right)+\left(\frac{L_y^B}{-i\hbar}\right)\left(\frac{L_x^B}{-i\hbar}\right)\right\}, \tag{9}$$

$$T_0^4 = \frac{(r_1^2-r_2^2)\cos\theta_{12}}{4r_1r_2\Delta}\left(\frac{L_z^B}{-i\hbar}\right). \tag{10}$$

The components of the angular momentum operator $\mathbf{L}^B$ appearing in the above expressions, are discussed in the Appendix. We have also used the notation

$$R^2 \equiv r_1^2+r_2^2,$$
$$\Delta \equiv \text{triangle area} = \tfrac{1}{2}r_1r_2\sin\theta_{12},$$

while θ_1 and θ_2 are angles defined through Figure 1. T_0^1 is a pure S-state operator, while T_0^2, T_0^3, and T_0^4 contain angular derivatives and so give zero when applied to S-state functions.

(ii) Similarly we find that T_{12} takes the form

$$T_{12} = T_{12}^1+T_{12}^2+T_{12}^3,$$

where

$$T_{12}^1 = -\frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}-\frac{\partial^2}{\partial r_{12}^2}-\cos\theta_1\frac{\partial^2}{\partial r_1\partial r_{12}}-\cos\theta_2\frac{\partial^2}{\partial r_2\partial r_{12}}+\cos\theta_{12}\frac{\partial^2}{\partial r_1\partial r_2}, \tag{11}$$

$$T_{12}^2 = \frac{\Delta}{r_1r_2}\left\{\frac{1}{r_1}\frac{\partial}{\partial r_2}-\frac{1}{r_2}\frac{\partial}{\partial r_1}+\frac{(r_2^2-r_1^2)}{r_1r_2r_{12}}\frac{\partial}{\partial r_{12}}\right\}\left(\frac{L_z^B}{-i\hbar}\right), \tag{12}$$

$$T_{12}^{3}=\frac{\cos\theta_{12}}{4r_1r_2}\left(\frac{L_z^B}{-i\hbar}\right)^2-\frac{r_1r_2}{16\Delta^2}\left\{\left(\frac{L_+^B}{-i\hbar}\right)^2+\left(\frac{L_-^B}{-i\hbar}\right)^2\right\}-\frac{r_1r_2\cos\theta_{12}}{16\Delta^2}$$
$$\times\left\{\left(\frac{L_+^B}{-i\hbar}\right)\left(\frac{L_-^B}{-i\hbar}\right)+\left(\frac{L_-^B}{-i\hbar}\right)\left(\frac{L_+^B}{-i\hbar}\right)\right\}. \tag{13}$$

T_{12}^1 is here the S-state part of T_{12}.

(b) *The Matrix Elements of* T_0 *and* T_{12}

As noted above, the orthogonality of the Euler-angle functions allows us to integrate out the Euler-angle dependence. We give here the reduced matrices of the operators T_0 and T_{12} as defined by equation (6).

(i) We let i, j stand for the groups of indices L, m_L, $|\mu|$, P_E and L, m_L, $|\mu'|$, P_E' respectively and calculate the matrix elements T_{0ij}^w for $w=1, 2, 3, 4$. Since L^2 and L_z commute with the kinetic energy, L and m_L are taken the same in i and j. Thus we get

$$T_{0ij}=\sum_{w=1}^{4}T_{0ij}^w,$$

with

$$T_{0ij}^1=\delta_{|\mu|,|\mu'|}\,\delta_{P_E,P_E'}\,T_0^1, \tag{14}$$

$$T_{0ij}^2=\delta_{|\mu|,|\mu'|}\,\delta_{P_E,\bar{P}_E'}\left\{(-1)^{\bar{\bar{P}}_E}|\mu|\frac{(r_1^2-r_2^2)\sin\theta_{12}}{r_1r_2r_{12}}\frac{\partial}{\partial r_{12}}\right\}, \tag{15}$$

$$\begin{aligned}T_{0ij}^3=\;&\delta_{|\mu|,|\mu'|}\,\delta_{P_E,P_E'}\left\{\frac{R^2\{|\mu|^2-L(L+1)\}}{8\Delta^2}-\frac{R^2|\mu|^2}{4r_1^2r_2^2}\right\}\\
&+\delta_{|\mu|,|\mu'|+2}\,\delta_{P_E,P_E'}\left\{\epsilon_{|\mu|,2}\,N_L(-|\mu|)\frac{R^2\cos\theta_{12}}{16\Delta^2}\right\}\\
&+\delta_{|\mu|,|\mu'|-2}\,\delta_{P_E,P_E'}\left\{\epsilon_{\mu,0}\,N_L(|\mu|)\frac{R^2\cos\theta_{12}}{16\Delta^2}\right\}\\
&+\delta_{|\mu|,2-|\mu'|}\,\delta_{P_E,P_E'}\left\{\epsilon_{\mu,0}\,\epsilon_{|\mu|,2}\,(-1)^{L+|\mu|+\bar{P}_E}N_L(-|\mu|)\frac{R^2\cos\theta_{12}}{16\Delta^2}\right\}\\
&+\delta_{|\mu|,|\mu'|+2}\,\delta_{P_E,\bar{P}_E'}\left\{\epsilon_{|\mu|,2}\,(-1)^{\bar{\bar{P}}_E}N_L(-|\mu|)\frac{r_2^2-r_1^2}{8r_1r_2\Delta}\right\}\\
&+\delta_{|\mu|,|\mu'|-2}\,\delta_{P_E,\bar{P}_E'}\left\{\epsilon_{\mu,0}\,(-1)^{\bar{P}_E}N_L(|\mu|)\frac{r_2^2-r_1^2}{8r_1r_2\Delta}\right\}\\
&+\delta_{|\mu|,2-|\mu'|}\,\delta_{P_E,\bar{P}_E'}\left\{\epsilon_{\mu,0}\,\epsilon_{|\mu|,2}\,(-1)^{L+|\mu|}N_L(-|\mu|)\frac{r_2^2-r_1^2}{8r_1r_2\Delta}\right\},\end{aligned} \tag{16}$$

$$T_{0ij}^4=\delta_{|\mu|,|\mu'|}\,\delta_{P_E,\bar{P}_E'}\left\{(-1)^{\bar{\bar{P}}_E}|\mu|\frac{(r_1^2-r_2^2)\cos\theta_{12}}{4r_1r_2\Delta}\right\}. \tag{17}$$

We have used the shorthand

$$N_L(\mu)\equiv[(L-\mu)(L+\mu+1)(L-\mu-1)(L+\mu+2)]^{\frac{1}{2}}.$$

Also

$$\widetilde{P}_E \equiv \text{adjoint symmetry of } P_E = a, \qquad \text{if } P_E = s,$$
$$= s, \qquad \text{if } P_E = a.$$

(ii) With i, j as in (a) above, we write the matrix elements $T^w_{12\,ij}$ for $w = 1$, 2, 3 as

$$T^1_{12\,ij} = \delta_{|\mu|,|\mu'|}\,\delta_{P_E,P_E'}\,T^1_{12}, \tag{18}$$

$$T^2_{12\,ij} = \delta_{|\mu|,|\mu'|}\,\delta_{P_E,\tilde{P}_E'}\left\{(-1)^{\bar{\tilde{P}}_E}|\mu|\frac{\Delta}{r_1 r_2}\left(\frac{1}{r_1}\frac{\partial}{\partial r_2}-\frac{1}{r_2}\frac{\partial}{\partial r_1}+\frac{r_2^2-r_1^2}{r_1 r_2 r_{12}}\frac{\partial}{\partial r_{12}}\right)\right\}, \tag{19}$$

$$\begin{aligned} T^3_{12\,ij} = {} & \delta_{|\mu|,|\mu'|}\,\delta_{P_E,P_E'}\left\{|\mu|^2\frac{\cos\theta_{12}}{4r_1 r_2}+\{L(L+1)-|\mu|^2\}\frac{r_1 r_2\cos\theta_{12}}{8\Delta^2}\right\} \\ & +\delta_{|\mu|,|\mu'|+2}\,\delta_{P_E,P_E'}\left\{N_L(-|\mu|)\,\epsilon_{|\mu|,2}\left(-\frac{r_1 r_2}{16\Delta^2}\right)\right\} \\ & +\delta_{|\mu|,|\mu'|-2}\,\delta_{P_E,P_E'}\left\{N_L(|\mu|)\,\epsilon_{\mu,0}\left(-\frac{r_1 r_2}{16\Delta^2}\right)\right\} \\ & +\delta_{|\mu|,2-|\mu'|}\,\delta_{P_E,P_E'}\left\{(-1)^{L+|\mu|+\bar{P}_E}N_1(-|\mu|)\,\epsilon_{|\mu|,2}\,\epsilon_{\mu,0}\left(\frac{-r_1 r_2}{16\Delta^2}\right)\right\}. \end{aligned} \tag{20}$$

IV. The Coupled Equations for the Internal Functions

The non-relativistic Hamiltonian for two-electron atoms has the form

$$H = \frac{-\hbar^2}{2\mu}T_0-\frac{\hbar^2}{M}T_{12}+e^2\left(\frac{1}{r_{12}}-\frac{Z}{r_1}-\frac{Z}{r_2}\right), \tag{21}$$

where Z is the nuclear charge parameter and $-e$ the electron charge. We decompose the wave function in the form (4) above and write

$$i = L,\ m_L,\ |\mu|,\ P_E,$$
$$j = L,\ m_L,\ |\mu'|,\ P_E'.$$

Then for any operator Ω we may write

$$\Omega\psi = \Omega\left(\sum_i f_i Y_i\right)$$
$$= \sum_j \sum_i \Omega_{ji} f_i Y_j,$$

where Ω_{ji} is the reduced matrix of the operator Ω as defined by (6). In $\sum_i$, i runs over a set of variables V, determined by specified L, m_L, P_S, and π. Setting

$$\Omega = T \equiv -\frac{\hbar^2}{2\mu}T_0-\frac{\hbar^2}{M}T_{12}$$

leads to $\Omega_{ij} = 0$, unless j is in the set V and, further, j exhausts V for all non-zero Ω_{ji}. We may thus write the Schrödinger equation in reduced form as

$$\sum_{i\epsilon v}\left[\sum_{j\epsilon v}\left(-\frac{\hbar^2}{2\mu}T_{0ij}-\frac{\hbar^2}{M}T_{12\,ij}\right)f_j-\left\{e^2\left(\frac{Z}{r_1}+\frac{Z}{r_2}-\frac{1}{r_{12}}\right)+E\right\}f_i\right]Y_i = 0, \tag{22}$$

and hence for all i in V

$$\sum_{j\epsilon v}\left(-\frac{\hbar^2}{2\mu}T_{0ij}-\frac{\hbar^2}{M}T_{12\,ij}\right)f_i-\left\{e^2\left(\frac{Z}{r_1}+\frac{Z}{r_2}-\frac{1}{r_{12}}\right)+E\right\}f_i=0. \qquad (23)$$

Equation (23) constitutes a set of coupled equations for the internal functions f_i. For later convenience we also give here explicitly the form that these coupled equations take on carrying out the implied matrix multiplication, in the limit of infinite nuclear mass (that is, keeping the operator T_0 only). A typical member of the coupled set has the form

$$\begin{aligned}
&\left[T_0^1+\left\{\frac{R^2\{|\mu|^2-L(L+1)\}}{8\Delta^2}-\frac{R^2|\mu|^2}{4r_1^2r_2^2}\right\}+\frac{2me^2}{\hbar^2}\left(\frac{Z}{r_1}+\frac{Z}{r_2}-\frac{1}{r_{12}}\right)+\frac{2mE}{\hbar^2}\right]f^L_{m_L}(P_R,\,|\mu|)\\
&+\left[(-1)^{\bar{P}_E}|\mu|\left(\frac{r_1^2-r_2^2}{r_1r_2}\right)\left\{\frac{\cos\theta_{12}}{4\Delta}+\frac{\sin\theta_{12}}{r_{12}}\frac{\partial}{\partial r_{12}}\right\}\right]f^L_{m_L}(\widetilde{P}_R,\,|\mu|)\\
&+\left[\epsilon_{|\mu|,2}N_L(-|\mu|)\frac{R^2\cos\theta_{12}}{16\Delta^2}\right]f^L_{m_L}(P_R,\,|\mu|-2)\\
&+\left[\epsilon_{\mu,0}N_L(|\mu|)\frac{R^2\cos\theta_{12}}{16\Delta^2}\right]f^L_{m_L}(P_R,\,|\mu|+2)\\
&+\left[(-1)^{L+|\mu|+\bar{P}_E}\,\epsilon_{\mu,0}\,\epsilon_{|\mu|,2}\,N_L(-|\mu|)\frac{R^2\cos\theta_{12}}{16\Delta^2}\right]f^L_{m_L}(P_R,\,2-|\mu|)\\
&+\left[(-1)^{\bar{P}_E}\,\epsilon_{|\mu|,2}\,N_L(-|\mu|)\frac{r_2^2-r_1^2}{8r_1r_2\Delta}\right]f^L_{m_L}(\widetilde{P}_R,\,|\mu|-2)\\
&+\left[(-1)^{\bar{P}_E}\,\epsilon_{\mu,0}\,N_L(|\mu|)\frac{r_2^2-r_1^2}{8r_1r_2\Delta}\right]f^L_{m_L}(\widetilde{P}_R,\,|\mu|+2)\\
&+\left[(-1)^{L+|\mu|}\,\epsilon_{\mu,0}\,\epsilon_{|\mu|,2}\,N_L(-|\mu|)\frac{r_2^2-r_1^2}{8r_1r_2\Delta}\right]f^L_{m_L}(\widetilde{P}_R,\,2-|\mu|)=0. \qquad (24)
\end{aligned}$$

On interpreting this equation, the following points should be noted.

(i) We have used the convention

$$f^L_{m_L}(P_R,\,\kappa)=0, \qquad \text{if } \kappa<0 \text{ or } \kappa>L.$$

(ii) Apparently eight functions are coupled into a single general equation (24) but this is reduced to six when it is noted that if $|\mu|\neq 2$ one of $|\mu|-2$ or $2-|\mu|$ is negative and hence the corresponding two functions are identically zero by (i).

(iii) The set of equations is explicitly real and hence the set of functions f_i may be chosen to be real. This is a consequence of the choice of phase for the Y_i satisfying the time reversal reality condition (3).

V. Acknowledgments

The author is much indebted to his supervisor Dr. L. M. Delves for suggesting the problem and for his willing help and inspiration. Thanks are also greatly due to Dr. G. H. Derrick for making available much of his original work on the ground state of H^3. Finally, the author is grateful for the Australian and British Commonwealth Scholarship which made this research possible.

VI. References

Bhatia, A. K., and Temkin, A. (1964).—*Rev. Mod. Phys.* **35**: 1050.
Breit, G. (1930).—*Phys. Rev.* **35**: 569.
Derrick, G. H., and Blatt, J. M. (1958).—*Nucl. Phys.* **8**: 130.
Goldstein, H. (1959).—"Classical Mechanics." p. 134. (Addison-Wesley: Reading, Mass.)
Kalotas, T., and Delves, L. M. (1964).—*Nucl. Phys.* **60**: 363.

Appendix

Angular Momentum Operators referred to Body Axes

Let $\mathrm{d}\alpha$, $\mathrm{d}\beta$, $\mathrm{d}\gamma$ be infinitesimal increments in the Euler angles α, β, γ and use the vector notation to write

$$\mathbf{da} \equiv \begin{bmatrix} \mathrm{d}\alpha \\ \mathrm{d}\beta \\ \mathrm{d}\gamma \end{bmatrix}; \qquad \frac{\partial}{\partial \mathbf{a}} \equiv \begin{bmatrix} \dfrac{\partial}{\partial \alpha} \\ \dfrac{\partial}{\partial \beta} \\ \dfrac{\partial}{\partial \gamma} \end{bmatrix}.$$

It follows readily (Goldstein 1959) that the resulting infinitesimal rotation referred to body axes is given by

$$\mathrm{d}\boldsymbol{\theta}^B = S\,\mathbf{da},$$

where S is the matrix

$$S = \begin{bmatrix} . & \cos\alpha & \sin\alpha\sin\beta \\ . & -\sin\alpha & \cos\alpha\sin\beta \\ 1 & . & \cos\beta \end{bmatrix}. \tag{A 1}$$

Let $\mathbf{L}$ be the orbital angular momentum for the two electrons (in the space system) and refer it to body axes by

$$\mathbf{L}^B \equiv \begin{bmatrix} \hat{\mathbf{x}}_B \,.\, \mathbf{L} \\ \mathbf{y}_B \,.\, \mathbf{L} \\ \hat{\mathbf{z}}_B \,.\, \mathbf{L} \end{bmatrix},$$

where $\mathbf{x}_B$, $\hat{\mathbf{y}}_B$, $\hat{\mathbf{z}}_B$ are body axis unit vectors. Then it follows, after some elementary analysis that,

$$\mathbf{L}^B = -i\hbar(S^{-1})^T \frac{\partial}{\partial \mathbf{a}}. \tag{A 2}$$

We define the useful operators L_0^B, L_+^B, L_-^B by

$$\left.\begin{aligned} L_0^B &= L_z^B, \\ L_\pm^B &= L_x^B \mp \mathrm{i} L_y^B, \end{aligned}\right\} \tag{A 3}$$

and these operators give the following results when acting on the representation coefficients $D^L_{\mu,m_L}(\alpha, \beta, \gamma)$

$$\left.\begin{aligned} L_0^B D^L_{\mu,m_L} &= \hbar\mu D^L_{\mu,m_L}, \\ L_\pm^B D^L_{\mu,m_L} &= \hbar[(L\mp\mu)(L\pm\mu+1)]^{\frac{1}{2}} D^L_{\mu\pm1,m_L}. \end{aligned}\right\} \tag{A 4}$$