

serious is the assumption that the ejected electron finds itself in the field of a purely neutral chlorine atom, or in reality, of four such atoms. Another potential source of error may occur in the approximation leading to the additive result in Eq. (1). It was estimated by Petersen<sup>15</sup> that a double summation, quite laborious to evaluate, which takes account of molecular configuration, could be neglected, leading to this additive result.

Digermane represents an interesting case in that one would expect to see results similar to the Kossel structure peak of  $\text{GeH}_4$  and at the same time at least a single Kronig structure peak as found for  $\text{Cl}_2$  or  $\text{Br}_2$ . The experimental curve shows a peak at the same energy position as found for  $\text{GeH}_4$ , but it is of greater width with two "steps" suggesting a washed out structure. Any Kronig structure contribution can only be a small, wide maximum.

Structure for the two germanium halides presents similar features; but the positions of the structure are closer together for the tetrabromide (Table II), and the amplitudes for the latter are in general smaller. While it is true that the more massive bromine atoms ought to scatter more effectively, the increase in internuclear

distance leads to the reverse effect. Until the correct fields of the bromine atoms in  $\text{GeBr}_4$  are known, the fine structure cannot be calculated and so the experimental results are not compared with theory.

In view of the results obtained, it appears that the theory needs revision before it can be relied upon for quantitative predictions. The theoretical value of the ratio of the average absorption coefficient of Ge in the polyatomic molecule,  $\text{GeCl}_4$ , to that of the isolated atom is too high; the number and positions of the theoretically predicted maxima and minima are not in agreement with experiment. In addition the correct location of the position of the Ge edge and the determination of its width require first a resolution and analysis of the experimental curve.

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## Particle Spin and Rotation

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It is proposed to treat the spin of a particle phenomenologically by considering the particle as a small rotating sphere, the rotation of which is described by euler parameters. If the rotation is quantized in the space of the euler parameters, one obtains both integral and half-integral values for the spin. In this way one arrives at a formalism in which the spin components can be represented as differential operators in the Schrodinger representation.

FROM the standpoint of group theory, the spin of an electron is connected with the two-valued representations of the rotation group in three dimensions. In the present paper an attempt is made to investigate some properties of a model in which this connection is used.

### 1. ROTATION PARAMETERS

Let us consider a free particle with spin as a small rotating rigid sphere. Let us take two cartesian coordinate systems with origins at the center of the sphere, one,  $XYZ$ , with axes having fixed directions in space, the other,  $X'Y'Z'$ , rigidly attached to the sphere. To describe the rotation of the sphere one can make use of the euler angles  $\theta, \varphi, \psi$ , where  $\theta$  is the angle between the  $Z$  and  $Z'$  axes,  $\varphi$  is the angle between the  $Y$  axis and the intersection of the  $XY$  and  $X'Y'$  planes, and  $\psi$  is the angle between the latter and the  $Y'$  axis. However, for

the present purpose we shall introduce instead the euler parameters<sup>1</sup> defined by the relations

$$\begin{aligned}\xi &= \sin \frac{1}{2} \theta \sin \frac{1}{2} (\psi - \varphi), \\ \eta &= \sin \frac{1}{2} \theta \cos \frac{1}{2} (\psi - \varphi), \\ \zeta &= \cos \frac{1}{2} \theta \sin \frac{1}{2} (\psi + \varphi), \\ \chi &= \cos \frac{1}{2} \theta \cos \frac{1}{2} (\psi + \varphi),\end{aligned}\quad (1)$$

so that

$$\xi^2 + \eta^2 + \zeta^2 + \chi^2 = 1. \quad (2)$$

In terms of these parameters, the direction cosines of the  $X'Y'Z'$  axes relative to the  $XYZ$  axes are homogeneous quadratic functions,<sup>1</sup> so that changing the signs of all the parameters leaves the orientation of the sphere unchanged.

For the sake of greater generality and convenience, let us now take four new parameters  $\xi_k$  ( $k=1, 2, 3, 4$ )

<sup>1</sup> E. T. Whittaker, *Analytical Dynamics* (Cambridge University Press, London, 1937, or New York, 1944), pp. 8-16.

defined by

$$\xi = \xi_1/\rho, \quad \eta = \xi_2/\rho, \quad \zeta = \xi_3/\rho, \quad \chi = \xi_4/\rho, \quad (3)$$

where

$$\rho = (\sum \xi_k^2)^{1/2}. \quad (4)$$

Summations, unless otherwise indicated, are to be taken over the values 1 to 4. The space spanned by these parameters will be referred to as  $\xi$ -space.

From the properties of the euler angles and parameters<sup>1</sup> it is found that the components of angular velocity of the sphere with respect to  $XYZ$  are given by

$$\omega_i = 2(\xi_4 \dot{\xi}_i - \xi_i \dot{\xi}_4 + \xi_k \dot{\xi}_l - \xi_l \dot{\xi}_k)/\rho^2, \quad (ikl) = (123), \quad (5)$$

where the relation  $(ikl) = (123)$  means that  $(i, k, l)$  form a cyclic permutation of  $(1, 2, 3)$  and a dot denotes differentiation with respect to the time. Similarly, the components of angular velocity with respect to  $X'Y'Z'$  are given by

$$\omega'_i = 2(\xi_4 \dot{\xi}'_i - \xi'_i \dot{\xi}_4 - \xi_k \dot{\xi}'_l + \xi_l \dot{\xi}'_k)/\rho^2, \quad (ikl) = (123). \quad (6)$$

The square of the angular velocity is then given by

$$\begin{aligned} \omega^2 &= 4 \sum_{i < k} (\xi_i \dot{\xi}_k - \xi_k \dot{\xi}_i)^2 / \rho^2 \\ &= 4(\sum \dot{\xi}_i^2 - \dot{\rho}^2) / \rho^2. \end{aligned} \quad (7)$$

If the sphere representing the particle is assumed to have a moment of inertia  $I$  about any axis through its center, then its kinetic energy is given by

$$T = \frac{1}{2} I \omega^2 = 2I(\sum \dot{\xi}_i^2 - \dot{\rho}^2) / \rho^2. \quad (8)$$

The generalized momentum components are given by

$$\pi_i = \partial T / \partial \dot{\xi}_i = 4I(\rho \dot{\xi}_i - \xi_i \dot{\rho}) / \rho^3, \quad (9)$$

whence

$$\sum \pi_i^2 = 4I^2 \omega^2 / \rho^2. \quad (10)$$

The angular momentum components of the sphere relative to  $XYZ$  and  $X'Y'Z'$ , respectively, are

$$M_i = I \omega_i, \quad M'_i = I \omega'_i \quad (i = 1, 2, 3), \quad (11)$$

so that the square of the angular momentum is given by

$$M^2 = I^2 \omega^2 = \frac{1}{4} \rho^2 \sum \pi_i^2. \quad (12)$$

On the other hand, one can define in the  $\xi$ -space generalized angular momentum components

$$\mu_{ij} = \xi_i \pi_j - \xi_j \pi_i = 4I(\xi_i \dot{\xi}_j - \xi_j \dot{\xi}_i) / \rho^2, \quad (13)$$

so that Eqs. (5) and (6) can be written

$$\begin{aligned} \omega_i &= (\mu_{4i} + \mu_{ki}) / 2I, \\ \omega'_i &= (\mu_{4i} - \mu_{ki}) / 2I, \quad (ikl) = (123). \end{aligned} \quad (5a)$$

It follows then that

$$\begin{aligned} M_i &= \frac{1}{2}(\mu_{4i} + \mu_{ki}), \\ M'_i &= \frac{1}{2}(\mu_{4i} - \mu_{ki}), \quad (ikl) = (123), \end{aligned} \quad (14)$$

and

$$M^2 = \frac{1}{4} \sum_{i < j} \mu_{ij}^2. \quad (15)$$

To quantize the system in the  $\xi$ -space, one introduces commutation relations

$$\xi_k \pi_l - \pi_l \xi_k = i\hbar \delta_{kl}. \quad (16)$$

It follows from this that the  $\mu_{ij}$  obey the usual commutation relations for angular momentum

$$\mu_{jk} \mu_{lm} - \mu_{lm} \mu_{jk} = i\hbar(\mu_{jl} \delta_{km} + \mu_{km} \delta_{jl} - \mu_{jm} \delta_{kl} - \mu_{kl} \delta_{jm}). \quad (17)$$

From Eqs. (14) and (17) it follows that the components  $M_j$  satisfy the usual commutation relations

$$M_j M_k - M_k M_j = i\hbar M_l, \quad (jkl) = (123). \quad (18)$$

On the other hand, for the components  $M'_j$  one obtains commutation relations of the form<sup>2</sup>

$$M'_j M'_k - M'_k M'_j = -i\hbar M'_l, \quad (jkl) = (123). \quad (19)$$

The components  $M_j$  and  $M'_k$  commute, for all values of  $j$  and  $k$ .

## 2. POLAR COORDINATES

To investigate the quantization of the rotation in  $\xi$ -space it is desirable to introduce polar coordinates. Several different polar coordinate systems suggest themselves, but perhaps one of the most convenient is given by the relations:

$$\begin{aligned} \xi_1 &= \rho \sin \alpha \cos \beta, \\ \xi_2 &= \rho \sin \alpha \sin \beta, \\ \xi_3 &= \rho \cos \alpha \sin \gamma, \\ \xi_4 &= \rho \cos \alpha \cos \gamma, \end{aligned} \quad (20)$$

where  $0 \leq \alpha \leq \pi/2$ ,  $0 \leq \beta < 2\pi$ ,  $0 \leq \gamma < 2\pi$ . Comparing this set of equations with Eq. (1), we see that

$$\alpha = \theta/2, \quad \beta = \frac{1}{2}(\varphi - \psi + \pi), \quad \gamma = \frac{1}{2}(\varphi + \psi). \quad (21)$$

The substitution of (20) into (8) gives for the classical kinetic energy

$$T = 2I(\dot{\alpha}^2 + \dot{\beta}^2 \sin^2 \alpha + \dot{\gamma}^2 \cos^2 \alpha). \quad (22)$$

From this, by the usual procedure for the case of curvilinear coordinates, one obtains as the Schrodinger equation

$$\nabla^2 \Psi = -K^2 \Psi, \quad (23)$$

where

$$K^2 = 8IT_e/\hbar^2 = 4(M^2)_e/\hbar^2, \quad (24)$$

the subscript  $e$  indicating the eigenvalue of the quantity in question, and

$$\begin{aligned} \nabla^2 \Psi &= \frac{1}{\sin \alpha \cos \alpha} \left[ \frac{\partial}{\partial \alpha} \left( \sin \alpha \cos \alpha \frac{\partial \Psi}{\partial \alpha} \right) \right. \\ &\quad \left. + \cot \alpha \frac{\partial^2 \Psi}{\partial \beta^2} + \tan \alpha \frac{\partial^2 \Psi}{\partial \gamma^2} \right]. \end{aligned} \quad (25)$$

Separating variables and imposing on  $\Psi$  the conditions of finiteness, continuity, and single-valuedness

<sup>2</sup> O. Klein, Z. Physik 58, 730 (1929).

in the  $\xi$ -space, one gets as a solution

$$\Psi = G(\alpha) \sin^{|m|} \alpha \cos^{|n|} \alpha e^{i(m\beta + n\gamma)}, \quad (26)$$

where  $m, n = 0, \pm 1, \pm 2, \dots$ , and

$$G(\alpha) = F(a, b; c; \sin^2 \alpha), \quad (27)$$

where  $F$  is the hypergeometric function,

$$\begin{aligned} a &= \frac{1}{2} [|m| + |n| + 1 + (K^2 + 1)^{\frac{1}{2}}], \\ b &= \frac{1}{2} [|m| + |n| + 1 - (K^2 + 1)^{\frac{1}{2}}], \\ c &= |m| + 1, \end{aligned} \quad (28)$$

and where, to make  $\Psi$  well-behaved, one must have

$$b = -p \quad (p = 0, 1, 2, \dots), \quad (29)$$

or, setting  $L = |m| + |n| + 2p$ ,

$$K^2 = L(L + 2). \quad (30)$$

Writing  $L = 2S$  and using (24), we get

$$(M^2)_e = \hbar^2 S(S + 1), \quad (31)$$

where  $S = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ . If the value of  $S$  is given, then  $m$  and  $n$  must satisfy the condition

$$S - \frac{1}{2} (|m| + |n|) = p. \quad (32)$$

Representing the  $\mu_{jk}$  by operators, we have

$$\mu_{12}\Psi = -i\hbar\partial\Psi/\partial\beta = m\hbar\Psi, \quad (33)$$

$$\mu_{43}\Psi = -i\hbar\partial\Psi/\partial\gamma = n\hbar\Psi,$$

so that, by (14),

$$M_z\Psi = \frac{1}{2}\hbar(m+n)\Psi. \quad (34)$$

If, for  $(M_z)_e$ , the eigenvalue of  $M_z$ , we write  $M_s\hbar$ , then it follows that

$$M_s = \frac{1}{2}(m+n). \quad (35)$$

Similarly, if for  $(M_z')_e$  we write  $M_s'\hbar$ , then

$$M_s' = \frac{1}{2}(n-m), \quad (36)$$

so that

$$m = M_s - M_s', \quad n = M_s + M_s'. \quad (37)$$

From (32) it follows that for a given value of  $S$

$$M_s, M_s' = S, S-1, \dots, -S+1, -S. \quad (38)$$

There are  $2S+1$  different values of  $M_s$ , and for each such value there are  $2S+1$  different states characterized by different values of  $M_s'$ , giving a total of  $(2S+1)^2$  states.

If one changes the signs of all four  $\xi$ -coordinates, the orientation of  $X'Y'Z'$  relative to  $XYZ$  is left unchanged. Such a change of signs is brought about in the polar coordinate system by changing  $\beta$  to  $\beta + \pi$ ,  $\gamma$  to  $\gamma + \pi$ . Now, if  $S$  is zero or an integer,  $m$  and  $n$  are both odd or both even, and  $\Psi$  remains unchanged; if  $S$  is a half-odd-integer, either  $m$  or  $n$  only is odd, and  $\Psi$  changes sign. Hence  $\Psi$ , as a function of ordinary space, is single-valued in the first case and double-valued in the second. In the first case the wave functions and

eigenvalues are essentially the same as those obtained in the "symmetrical top" calculations<sup>3</sup> for the sphere.

The fact that, for  $S$  a half-odd-integer, the wave functions are double-valued functions in ordinary space does not appear to cause any difficulty.<sup>4</sup> It can be readily shown that if one operates on a wave function characterized by  $L, M_s, M_s'$  with a component  $M_j$  one obtains a linear combination of wave functions with the same  $L$  and  $M_s'$ , but various values of  $M_s$ . Hence the criterion of acceptability proposed by Pauli is fulfilled.

### 3. CASE $S = \frac{1}{2}$

As a simple example, consider the case (say that of the electron)  $S = \frac{1}{2}$ , for which  $M_s, M_s' = \pm \frac{1}{2}$ . One readily obtains for this case the following four wave functions:

$$\begin{aligned} M_s = +\frac{1}{2}, M_s' = +\frac{1}{2}: & \Psi_1 = \cos\alpha e^{i\gamma}/\pi, \\ = -\frac{1}{2}, & = +\frac{1}{2}: \Psi_2 = i \sin\alpha e^{-i\beta}/\pi, \\ = +\frac{1}{2}, & = -\frac{1}{2}: \Psi_3 = i \sin\alpha e^{i\beta}/\pi, \\ = -\frac{1}{2}, & = -\frac{1}{2}: \Psi_4 = \cos\alpha e^{-i\gamma}/\pi, \end{aligned} \quad (39)$$

where the functions have been normalized and the phases chosen so that the matrices of the angular momentum components are given by

$$2M_j/\hbar = \sigma_j = -i\alpha_k\alpha_l, \quad (jkl) = (123), \quad (40)$$

the  $\sigma$ 's being the doubled Pauli spin matrices and the  $\alpha$ 's the Dirac matrices. With these functions one finds that the matrices of the  $M_i'$  are given by

$$\begin{aligned} 2M_x'/\hbar &= -i\alpha_1\alpha_2\alpha_3, & 2M_y'/\hbar &= -\alpha_1\alpha_2\alpha_3\alpha_4, \\ 2M_z'/\hbar &= \alpha_4. \end{aligned} \quad (41)$$

If one is concerned only with the components  $M_i$ , then one can take a set of states associated with a single eigenvalue  $M_s'$ . For instance, one can take only  $\Psi_1$  and  $\Psi_2$  and thus obtain the two-rowed Pauli spin matrices. On the other hand, if one takes all four  $\Psi$ 's, then one can form the above six four-rowed matrices which, together with their products, formally give the full set of Dirac matrices.

### 4. EXTERNAL FIELD AND PARTICLE MOTION

Let us assume that the particle has a magnetic moment associated with its spin, so that the magnetic moment is given by  $\lambda\mathbf{M}$ . If it is situated in a uniform magnetic field  $\mathfrak{H}$ , then the hamiltonian describing the rotation of the sphere in this field will be

$$H = T - \lambda\mathbf{M} \cdot \mathfrak{H}, \quad (42)$$

or, if one takes the  $Z$  axis in the direction of  $\mathfrak{H}$ ,

$$H = T - \lambda\mathfrak{H}M_z. \quad (43)$$

It is evident that, if one sets up a Schrodinger equation

<sup>3</sup> F. Reiche and H. Rademacher, Z. Physik **39**, 444 (1926).

<sup>4</sup> E. Schrodinger, Ann. Physik **32**, 49 (1938); W. Pauli, Helv. Phys. Acta **12**, 147 (1939).

for this case, the solution for  $\Psi$  will be the same as was obtained above in the absence of a field and the change in the energy due to the field will be given by  $-\lambda\hbar\Phi M_s$ .

Thus far we have considered the sphere as rotating about a fixed center, i.e., the particle as being at rest. To take account of the motion of the particle, one sets up a Schrodinger equation with a hamiltonian that includes both translational and rotational kinetic and potential energy, associated with the position and momentum of the particle as well as its spin. The difference between the present procedure and the usual one (Pauli) lies in the fact that spin components are here represented by differential operators instead of matrices. Substituting  $\pi_k = -i\hbar\partial/\partial\xi_k$  in (14), one obtains the spin components in the operator form. Alternatively, in terms of the polar variables  $\alpha, \beta, \gamma$  one finds

$$\begin{aligned}
 (M_x + iM_y)\Psi &= \frac{-i\hbar}{2} e^{i(\beta+\gamma)} \\
 &\quad \times \left( \frac{\partial\Psi}{\partial\alpha} + i \cot\alpha \frac{\partial\Psi}{\partial\beta} - i \tan\alpha \frac{\partial\Psi}{\partial\gamma} \right), \\
 (M_x - iM_y)\Psi &= \frac{-i\hbar}{2} e^{-i(\beta+\gamma)} \\
 &\quad \times \left( \frac{\partial\Psi}{\partial\alpha} - i \cot\alpha \frac{\partial\Psi}{\partial\beta} + i \tan\alpha \frac{\partial\Psi}{\partial\gamma} \right), \\
 M_z\Psi &= \frac{-i\hbar}{2} \left( \frac{\partial\Psi}{\partial\beta} + \frac{\partial\Psi}{\partial\gamma} \right), \\
 (M_x' + iM_y')\Psi &= \frac{-i\hbar}{2} e^{i(\beta-\gamma)} \\
 &\quad \times \left( \frac{\partial\Psi}{\partial\alpha} + i \cot\alpha \frac{\partial\Psi}{\partial\beta} + i \tan\alpha \frac{\partial\Psi}{\partial\gamma} \right), \\
 (M_x' - iM_y')\Psi &= \frac{-i\hbar}{2} e^{i(\gamma-\beta)} \\
 &\quad \times \left( \frac{\partial\Psi}{\partial\alpha} - i \cot\alpha \frac{\partial\Psi}{\partial\beta} - i \tan\alpha \frac{\partial\Psi}{\partial\gamma} \right), \\
 M_z'\Psi &= \frac{-i\hbar}{2} \left( \frac{\partial\Psi}{\partial\gamma} - \frac{\partial\Psi}{\partial\beta} \right).
 \end{aligned} \tag{44}$$

The wave function for a given state will consist of a single component which, however, will depend on the  $\xi$ 's, in addition to the position coordinates.

## 5. DISCUSSION

In discussing the rotating sphere model of the electron, mention might be made of the work of M. H. Payne,<sup>5</sup> in which the electron spin is treated by means of bipolar coordinates, the electron being regarded as a point mass moving on the surface of a sphere. However, not only the model, but also the point of view there are quite different from those of the present work.

The chief purpose of considering the spin as a rotation described by variables in the  $\xi$ -space is to enable one to represent the spin components by operators (in the Schrodinger representation) as well as by matrices. From the formal standpoint this appears desirable, since it permits one to treat all physical variables in a uniform manner. On the other hand, it is well known<sup>6</sup> that in the case of an electron the rotating sphere model leads to serious difficulties if the sphere is taken to have the classical electron radius. These difficulties may be associated with the necessity for changes in some of our physical concepts when we are dealing with very small dimensions. It is possible that, after such changes, the rotating sphere model may nevertheless retain an approximate validity. For the present, at any rate, the spin description considered here has to be regarded as a phenomenological one.

In conclusion, the author wishes to express his indebtedness to Professor E. L. Hill for helpful advice.

## APPENDIX

If one takes a polar coordinate system defined by

$$\begin{aligned}
 \xi_1 &= \rho \sin u \sin v \cos w, \\
 \xi_2 &= \rho \sin u \sin v \sin w, \\
 \xi_3 &= \rho \sin u \cos v, \\
 \xi_4 &= \rho \cos u,
 \end{aligned}$$

where  $0 \leq u \leq \pi$ ,  $0 \leq v \leq \pi$ ,  $0 \leq w < 2\pi$ , then in Eq. (23) one has

$$\nabla^2\Psi = \frac{1}{\sin^2 u} \frac{\partial}{\partial u} \left( \sin^2 u \frac{\partial\Psi}{\partial u} \right) + \frac{1}{\sin^2 u \sin v} \frac{\partial}{\partial v} \left( \sin v \frac{\partial\Psi}{\partial v} \right) + \frac{1}{\sin^2 u \sin^2 v} \frac{\partial^2\Psi}{\partial w^2}.$$

In this case the well-behaved solutions of the equation are found to be

$$\Psi = R(u) P_l(\cos v) e^{imw},$$

where  $l=0, 1, 2, \dots$ ,  $|m|=l, l-1, \dots$ , and

$$R(u) = (\sin u)^{-1} P_{L+\frac{1}{2}}^{l+\frac{1}{2}}(\cos u)$$

in terms of an associated Legendre function with  $L=l, l+1, \dots$ . This can also be written  $\sin^l u Q(\cos u)$ , where  $Q$  is a polynomial of degree  $L-l$ . In terms of  $L, K$  is again given by (30), and the total number of states for a given value of  $L$  is readily counted up to be  $(L+1)^2 = (2S+1)^2$ .

<sup>5</sup> M. H. Payne, Phys. Rev. **65**, 39 (1944).

<sup>6</sup> G. E. Uhlenbeck and S. Goudsmit, Naturwiss. **13**, 953 (1925).