“Über ein Kriterium für Ein- oder Zweiertigkeit der Eigenfunctionen in der Wellenmechanik,” Helv. Phys. Acta **12** (1939), 147-167.

On a criterion for one- or two-valuedness of eigenfunctions in wave mechanics.

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(Received 22 December 1938)

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In the present note, the following criterion will be proposed for resolving the question of whether a certain wave equation physically admits single-valued or double-valued wave functions: A single application of the angular impulse operator to a given system of regularly- integrable (square-integrable, resp.) eigen-solutions cannot produce something that is outside of that system for the same value of the total angular impulse quantum number *j*; i.e., the new solutions that are thus-obtained must be linearly expressible in terms of the original ones. As a basis for that criterion, it will be shown that when it is not fulfilled, no one-to-one correspondence would exist between the operator calculus and the matrix calculus for the angular impulse quantities. The application to the scalar wave equation yields the necessity of single-valued wave functions, while for the Schrödinger form of the Dirac equation in polar coordinates, the criterion will lead to the necessity of double-valued solutions. Both results are consistent with experiments. The generalization of the formulation of the criterion for finite rotations will be given, and the one for the full rotation group of spherical space will be mentioned.

1. Problem statement. Formulation of the criterion.

As the author already emphasized on a previous occasion ([1]), there is no argument that is valid *a priori* for saying that the solutions of the wave equation that describe physical behavior of a system quantum-theoretically must necessarily be single-valued. Namely, for the single-valuedness of physical quantities that are always bilinear in the wave function and its complex conjugate, it will suffice that all admissible eigen-solutions should get multiplied by a factor $e^{i\alpha}$ of magnitude 1 when one travels around certain closed paths, and that the factor should depend upon only the path in question, but be independent of the eigen-solution that has been chosen. However, the further treatment of that question in *loc. cit.* soon proved to be insufficient, since among the multi-valued eigen-solutions, in general, there were also ones that satisfied all of the regularity requirements. That was also the case for the multi-valued spherical functions that were treated in *loc. cit.* as solutions of the ordinary non-relativistic wave equation of a particle.

([1]) Cf., Handbuch d. Physik, v. XXIV/1, 2nd ed., Berlin 1933, pp. 126.

In the meantime, the problem that was just spoken of was treated in the literature on several occasions ([1]); in particular, E. SCHRÖDINGER made some essential progress in regard to it. He first remarked that the equivalence of past and future (reversibility of time) for the evolution of physical quantities is true only when the wave functions are one or two-valued, in particular, and of them, the two-valued ones will simply change their sign under the aforementioned orbits. For that reason, as well as for the sake of simplicity, in what follows, we will mainly discuss only those two possibilities. Moreover, starting from his previous formulation of the Dirac equations of the electron in arbitrary coordinates ([2]), SCHRÖDINGER discovered a case in which the solutions of the wave equation must necessarily be assumed to be two-valued if the result is to remain in agreement with experiments. Indeed, he then next treated a new way of representing Dirac's relativistic wave equation for the electron in polar coordinates in ordinary flat space. That state of affairs allowed a serious doubt to arise concerning whether one could find an adequate physical basis for the resolution of the question of the one- or two-valuedness of the solutions of a given wave equation at all.

In contrast to that, in this note, it will be shown that there should be no room for such doubt, and (unlike the situation for the symmetry classes of many-electron problems) a theoretical criterion for the resolution of the question in one or the other sense can, in fact, be given. Admittedly, it does not suffice to investigate the regularity of the eigen-solutions alone if one is to do that, but it is essential that the Hamiltonian operator must admit a transformation group. We restrict the present examination to the groups of ordinary rotations in flat space, and indeed, on the one hand, for the relativistic scalar wave equation of a particle, and on the other hand, for the relativistic wave equation of the spin electron. As is known, that group gives rise to the existence of the three angular impulse operators P_1, P_2, P_3, which always take an eigen-solution to another eigen-solution for a centrally-symmetric problem, since they will then commute with the Hamiltonian operator. Furthermore, any of the three quantities P_k (k = 1, 2, 3) will commute with the square of the total angular impulse:

$$P^2 = P_1^2 + P_2^2 + P_3^2, \tag{1}$$

which is known to possess the eigenvalue $j\,(j + 1)$; one should especially investigate when the half-integer values of j are excluded and when the whole-integer values are. To that end, we start with a system of regular eigen-solutions $u_{j,m}$ of the operator P^2, for which one will then have:

([1]) A. S. EDDINGTON, *Relativity Theory of Protons and Electrons*, Cambridge, 1936, pp. 60 and 150, as well as the older literature that was cited in it. On two-valued spherical functions as solutions of the non-relativistic wave equations, cf., also F. MÖGLICH, Zeit. Phys. **110** (1938), 1. However, eq. (2a) in that paper contains an essential oversight, in that (as will be shown in § 2 of this note) the integrals of the calculated matrix elements of the angular impulse components over the spherical surface will no longer satisfy the demand that they must commute with the matrix of the square of the total angular impulse vector.

On the question of the reversibility of time, cf., E. SCHRÖDINGER, Ann. Phys. (Leipzig) (5) **32** (1938), 49, and for a thorough discussion of multi-valued solutions of the relativistic wave equation of the electron, see his article in Commentationes Pontificia Academia Scientiarum **2** (1938), 321. (Cited as "P. A." in what follows.)

([2]) E. SCHRÖDINGER, Berl. Ber. phys. u. math. Klasse (1932), pp. 105.

$$P^2 u_{j,m} = j(j+1)\, u_{j,m} . \tag{1a}$$

(As usual, we do not explicitly write out any spin indices that might possibly be present.) For a given value of *j*, there are always only finitely many regular eigen-solutions, and it is, moreover, inessential for the application of the criterion whether one does or does not count eigen-solutions that are possibly no longer regular, but still square-integrable, as being present in the system considered. However, if we consider all possible (either integer or half-integer) values of *j* then in the latter case, the system of eigen-solutions might be chosen such that the functions in the system that belong to different *j*-values will fulfill the condition of orthogonality.

We will now pose the following additional physical requirement: *The application of the angular impulse operator P_k to a given finite system of regular (or only square-integrable) eigen-solutions of P^2 with the same value of j shall not produce something that does not belong to that system.*

When that is expressed in a positive way, the new eigenfunctions $P_k\, u_{j,m}$ shall be linearly-expressible in terms of the old ones:

$$P_k\, u_{j,m} = \sum_{m'} c^k_{m\,m'}\, u_{m',\,j} . \tag{2}$$

Obviously, our requirement includes the idea that the new eigen-solutions should also be regular (square-integrable, resp.) The fact that only eigenfunctions with equal values of *j* appear in the left and right-hand sides of (2) is connected with the fact that the P_k commute with all P^2.

Moreover, if one chooses the eigenfunctions $u_{j,m}$ especially such that one of the angular impulse components – say, P_3 – is also brought into diagonal form then the known selection rules for P_k will be valid, and in general at most two of the terms on the right-hand side of (2) will be non-zero. (If the eigenfunctions were normalized then the $c^k_{m\,m'}$ would, in fact, represent the matrix elements of P_k .)

In the following § 2, it will next be shown that the criterion that was given is sufficient in the case of scalar wave equations, as well as in spinor ones (e.g., the Dirac equation), for one to resolve uniquely the alternative of whether a single-valued or a double-valued wave function is admissible. Furthermore, an important result (§ 2) is that in the case for which the criterion is not fulfilled, *some of the new eigenfunctions $P_k\, u_{j,m}$ are no longer orthogonal to a family of the original $u_{j',\,m'}$* with fixed m' and variable j', while $j \neq j'$. That will yield the physical necessity of fulfilling our criterion. Otherwise, the matrix elements of P_k that are calculated in the usual way would no longer be all diagonal in *j*, which would contradict the commutability of all P_k with P^2. One can then also formulate the result in such a way that if our criterion were violated then the usual connection between matrices and operators for the angular impulse components would break down, which would obviously be physically inadmissible.

Another formulation of our criterion that is equivalent to the original one will be given § 3, which will be perhaps most intuitive, but less suitable for practical computations. It is based upon the fact that the angular impulse operators are associated with infinitesimal rotations and that by iterating them an operation must arise that permits one to obtain a new eigen-solution of the wave equation from any eigen-solution under a *finite* rotation of the coordinate system. As a result of the arbitrariness in the choice of the axes of a polar coordinate system, all of those eigen-solutions will be physically equivalent. However, the version of our criterion that arises when one passes from infinitesimal rotations to the finite ones (in truth, it is equivalent to the original version and contains no stronger demand) will say just that here, as well, the new eigen-solutions $v_{j,m}(x)$ must be linearly-expressible in terms of the old ones $u_{j,m}(x)$ that belong to the same j.

However, the definition of the operation that produces $v_{j,m}(x)$ from $u_{j,m}(x)$ demands a somewhat more detailed argument. Initially, it is very simple for the scalar wave equation, since that is directly invariant under rotation of the coordinate axes. One will then get the $v_{j,m}(x)$ from $u_{j,m}(x)$ when one next replaces the old polar angles ϑ, φ with the new ones ϑ', φ' without changing the form of the function $u_{j,m}(x)$, and then replaces them with the old ones ϑ, φ, and expresses the three rotation parameters (e.g., the three Euler angles), which might be briefly denoted by a here, by way of:

$$u_{j,m}(\vartheta, \varphi; a) = u_{j,m}(\vartheta', \varphi'). \tag{3}$$

By our criterion, it will be required here that:

$$u_{j,m}(\vartheta', \varphi') = \sum_{m'} C_{mm'}(a) \cdot u_{j,m}(\vartheta, \varphi), \tag{4}$$

and that can obviously be fulfilled only for single-valued wave functions u. By contrast, the double-valued wave function $u_{j,m}(\vartheta', \varphi')$ obviously cannot be expressed linearly in terms of the $u_{j,m}(\vartheta, \varphi)$ with the same j and constant coefficients, since the $u_{j,m}(\vartheta, \varphi)$ will change sign when one orbits around the point $\vartheta = 0$, but the $u_{j,m}(\vartheta', \varphi')$ will change sign when one orbits around the point $\vartheta' = 0$, which is different from the latter; i.e., there is no "addition theorem" for double-valued spherical functions.

On the same basis, the application of our criterion to the usual Dirac wave equation for the electron will lead inevitably to single-valued solutions. Namely, in order to arrive at the $u_{j,m}$ from the $v_{j,m}$, here one must perform an S-transformation of the spin indices with constant coefficients, in addition to the substitution of the ϑ', φ' with ϑ, φ.

However, things are not the same for the form of the Dirac equation in polar coordinates that was presented by SCHRÖDINGER. That equation is not simply invariant under a transition from one system of axes to another, but in order to again represent the wave equation in the new coordinates, one must append an S-transformation of the spin indices that *depends upon* ϑ, φ. (By the way, that is characteristic of the general covariant form for the Dirac equation that SCHRÖDINGER represented.) In that case, one then obtain a new solution $\chi(\vartheta, \varphi, a)$ from an arbitrary solution $\psi(\vartheta, \varphi)$ by way of:

$$\chi(\vartheta, \varphi, a) = S(\vartheta, \varphi, a) \cdot \psi(\vartheta', \varphi'), \tag{3a}$$

in which the S-matrix acts upon the spin indices (which are not given explicitly here) in the usual way. Instead of (4), our criterion then says:

$$S\,(\vartheta,\,\varphi,\,a)\cdot u_{j,\,m}\,(\vartheta',\,\varphi') = \sum_{m'} C_{m\,m'}(a)\,u_{j,m}(\vartheta,\varphi)\,. \tag{4a}$$

As will be shown in § 3, in the Schrödinger case, the matrix S will depend upon ϑ, φ in such a way that it will change its sign for a closed path on the sphere that goes around $\vartheta = 0$ and leaves $\vartheta' = 0$ outside of it, as well as for a closed path that goes around $\vartheta' = 0$ and leaves $\vartheta = 0$ outside. In that case, eq; (4a) will be possibly true only when $u_{j,\,m}\,(\vartheta,\,\varphi)$ is double-valued, but will not be possibly true when $u_{j,\,m}\,(\vartheta,\,\varphi)$ is single-valued.

Knowing the matrix $S\,(\vartheta,\,\varphi,\,a)$ would then make calculating with the angular impulse operators P_k (which emerge from S by specializing the a for infinitesimal rotations, moreover) to a certain extend superfluous. However, applying the criterion for infinitesimal rotations seems to preserve its self-explanatory meaning on different grounds. First of all, only in the latter version does the importance of the criterion for the self-consistent connection between operator calculus and matrix calculus come to light. Furthermore, directly ascertaining the S-matrix without taking recourse to other forms of the wave equation seems to be truly confusing for finite transformations of a group, namely, for more general groups.

As we have mentioned already, here we restrict ourselves to the case of flat space and the usual three-dimensional rotation group, since the main idea in our argument is already clear in that case. However, that argument can be easily generalized to the wave equations of spherical space, in which the six-parameter rotation group with the six operators M_k, N_k (k = 1, 2, 3) will enter in place of the three-parameter rotation group with the three P_k, the eigenvalues of $\sum_k (M_k^2 + N_k^2)$, in place of those of $\sum_k P_k^2$, and two quantum numbers, in place of m ([1]). In the infinitesimal version, our criterion then once more expresses the idea that the $(M_k\,u)$, $(N_k\,u)$ can be expressed linearly in terms of those of the original regular eigenfunctions (one of which is u) that belong to the same eigenvalue of:

$$\sum_k (M_k^2 + N_k^2)$$

as u does. Moreover, it is precisely the eigenfunctions in spherical space that SCHRÖDINGER ultimately ascertained ([2]) that stand in contradiction to that criterion. That criterion also seems to prove its merit in the ascertainment of the correct eigenfunctions for another choice of coordinates in spherical space.

([1]) See SCHRÖDINGER, P. A., § 4.
([2]) P. A., § 8.

§ 2. The application of the angular impulse operators to the eigen-functions.

a) *The scalar wave equation.*

We consider a centrally-symmetric potential and think of the factor $u(\vartheta, \varphi)$ in the wave function that depends upon polar coordinates as being separated out. As is known, it will satisfy the wave equation:

$$P^2 u \equiv -\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial u}{\partial\vartheta}\right)-\frac{1}{\sin^2\vartheta}\frac{\partial^2 u}{\partial\varphi^2} = j\,(j+1)\,u, \tag{5}$$

in which we have denoted the eigenvalue of P^2 by $j\,(j + 1)$. It is convenient to consider the following linear combinations of the angular impulse components:

$$P_+ = P_1 + i\,P_2 = e^{i\varphi}\left(\frac{\partial}{\partial\vartheta}+i\frac{\cos\vartheta}{\sin\vartheta}\frac{\partial}{\partial\varphi}\right), \tag{6a}$$

$$P_- = P_1 - i\,P_2 = e^{-i\varphi}\left(-\frac{\partial}{\partial\vartheta}+i\frac{\cos\vartheta}{\sin\vartheta}\frac{\partial}{\partial\varphi}\right), \tag{6b}$$

$$P_3 = -i\,\frac{\partial}{\partial\varphi}. \tag{6c}$$

As usual, we consider the eigen-solutions of P_3, whose eigenvalues differ from whole numbers only by a common constant. For the sake of clarity, in what follows, we shall always understand m to mean a non-negative number and distinguish between the eigen-solutions:

$$u^+_{j,m}(\vartheta, \varphi) = f_{j,m}(\cos\vartheta)\,e^{im\varphi}, \tag{7a}$$

$$u^-_{j,m}(\vartheta, \varphi) = f_{j,m}(\cos\vartheta)\,e^{-im\varphi}. \tag{7b}$$

In order for $f_{j,m}$ to be regular for $\vartheta = 0$ and $\vartheta = \pi$, one must necessarily have:

$$j - m \text{ integer and non-negative.} \tag{8}$$

In this case, the known representations of spherical functions with:

$$z = \cos\vartheta \tag{9}$$

will yield:

$$f_{j,m}(z) = (1 - z^2)^{-m/2}\left(\frac{d}{dz}\right)^{j-m}(1 - z^2)^{j}, \tag{10}$$

$$m = \alpha + \text{integer}, \qquad 0 \leq \alpha \leq 1, \tag{11a}$$

$$\alpha \leq m \leq j. \tag{11b}$$

Normalizing those eigen-solutions will not be required for what follows. In that way, one will get all *regular* solutions of the differential equation that follows from (9):

$$-\frac{d}{dz}\left[(1-z^2)\frac{df}{dz}\right] + \frac{m^2}{1-z^2}\,f = j\,(j+1)\,f. \tag{12}$$

The cases $\alpha = 0$ (viz., integer j and m) and $\alpha = 1/2$ (viz., half-integer j and m) will have especial interest in what follows. For $\alpha = 1/2$, the solutions:

$$f_{j,-m}(z) = (1-z^2)^{m/2}\left(\frac{d}{dz}\right)^{j+m}(1-z^2)^j \tag{13}$$

will be singular. By contrast, the case of j and m integer is especially distinguished by the fact that:

$$f_{j,-m}(z) = \text{const.}\, f_{j,m}(z), \qquad \text{for } j, m \text{ integer}, \tag{14}$$

while for m non-integer, from the singularity of at the locations $z = \pm 1$, one must recognize that $f_{j,-m}$ must be a completely different solution from $f_{j,m}$.

In order to prove (14) for integer j and m, we can infer the following representation of $f_{j,m}$ from (10) directly by means of a complex integral that is also otherwise useful:

$$f_{j,m}(z) = (1-z^2)^{-m/2}\frac{(j-m)!}{2\pi i}\int_{K_0}\frac{[1-(z+t)^2]^j}{t^{j-m+1}}\,dt\,. \tag{15}$$

Here, the path of integration is a circle around the zero point. Since the integrand still possesses branch loci for $t = 1 - z$ and $t = -(1 + z)$ for non-integer j (and m), in that case, it must be expressly added that they should lie outside the circle K_0 :

$$|\,t\,| < |\,1-z\,| \text{ and } |\,t\,| < |\,1+z\,| \text{ on } K_0 \text{ for non-integer } j, m; \tag{15a}$$

it is only for integer j, m that the quantity is that quantity indifferent to the circle K_0. The expression for $f_{j,-m}(z)$:

$$f_{j,-m}(z) = (1-z^2)^{m/2}\frac{(j+m)!}{2\pi i}\int_{K_0}\frac{[1-(z+t)^2]^j}{t^{j+m+1}}\,dt \tag{16}$$

can now be converted by the substitution:

$$t \to -\frac{1-z^2}{t}$$

into:

$$f_{j,-m}(z) = (1-z^2)^{-m/2} e^{-2\pi im} \frac{(j+m)!}{2\pi i} \int_{K_0} \frac{[1-(z+t)^2]^j}{t^{j-m+1}} dt, \tag{16}$$

in which we now have:

$$|t| > |1-z|, \quad |t| > |1+z| \text{ on } K_1. \tag{16b}$$

It is only for integer j and m that the circle K_1 can be continuously deformed to the circle K_0 and the relation (14) will then be true.

We further show that the regular eigenfunction:

$$u^+_{j,\frac{1}{2}}(\vartheta, \varphi) = f_{j,\frac{1}{2}}(z) e^{i\varphi/2}$$

is not generally orthogonal to the singular [but still square-integrable, as is easy to see from (10)] eigenfunction:

$$u^+_{j',-\frac{1}{2}}(\vartheta, \varphi) = f_{j',-\frac{1}{2}}(z) e^{i\varphi/2}.$$

(Naturally, the same thing will be true for $u^-_{j,\frac{1}{2}}$ and $u^-_{j',-\frac{1}{2}}$.) On initially has:

$$\frac{1}{4\pi} \int \left(u^+_{j,\frac{1}{2}}\right)^* u^+_{j',-\frac{1}{2}} \sin\vartheta \, d\vartheta \, d\varphi = \frac{1}{2} \int_{-1}^{+1} f_{j,\frac{1}{2}} f_{j',-\frac{1}{2}} dz.$$

It follows further from (12) that:

$$[j(j+1) - j'(j'+1)] = \frac{1}{2} \left| (1-z^2) \left(f_{j',-\frac{1}{2}} \frac{df_{j,\frac{1}{2}}}{dz} - f_{j,\frac{1}{2}} \frac{df_{j',-\frac{1}{2}}}{dz} \right) \right|_{-1}^{+1}.$$

Now, the right-hand side is finite at each of the limits $z = +1$ and $z = -1$ precisely, and the contributions of those two limits will then have the same sign when $j - j'$ is odd, while they will cancel in any other case. In fact, for half-integer m and j, the functions $f_{j,\frac{1}{2}}$ and $f_{j',-\frac{1}{2}}$ will both be even or both odd in z only for odd $j - j'$. Our result is then:

$$\int \left(u^\pm_{j,\frac{1}{2}}\right)^* u^\pm_{j',-\frac{1}{2}} \sin\vartheta \, d\vartheta \, d\varphi \neq 0 \qquad \text{for odd } j - j' \text{ and } j, j' \text{ half-integer.} \tag{17}$$

We now apply the operators P_+ and P_- to the eigen-solutions and show that:

$$P_+(f_{j,m} e^{im\varphi}) = \text{const.}\, f_{j,m+1} e^{i(m+1)\varphi}, \qquad P_-(f_{j,m} e^{im\varphi}) = \text{const.}\, f_{j,m-1} e^{i(m-1)\varphi}, \tag{18a}$$

$$P_+(f_{j,m} e^{-im\varphi}) = \text{const.}\, f_{j,m-1} e^{-i(m-1)\varphi}, \qquad P_-(f_{j,m} e^{-im\varphi}) = \text{const.}\, f_{j,m+1} e^{-i(m+1)\varphi}. \tag{18b}$$

Moreover, $f_{j,\,j+1}$ must always be set to zero identically in this for the boundary value $j = m$. In fact, (6) and (15) implies that, e.g.:

$$P_+ f_{j,\,m}\, e^{im\varphi} = e^{i\,(m+1)\,\varphi} \left[-(1-z^2)\frac{df_{j,m}}{dz} - \frac{mz}{(1-z^2)^{1/2}}\, f_{j,m} \right]$$

$$= e^{i(m+1)\varphi}(1-z^2)^{-(m+1)/2}\frac{(j-m)!}{2\pi i}\int_{K_0}\{2j(1-z^2)(z+t)[1-(z+t)^2]^{j-1} - 2mz[1-(z+t)^2]^j\}\frac{dt}{t^{j-m+1}}\,.$$

The integrand can be converted into:

$$(j + m + 1)\,[1 - (z + t)^2]^{\,j}\, t^{\,-(j-m)} - \{[1 - (z + t)^2]^{\,j}\,(2z + t)\, t^{-(j-m)}\}.$$

The second term will vanish when one integrates over the circle K_0 and it will yield:

$$P_+ f_{j,\,m}\, e^{im\varphi} = (j + m + 1)\,(j - m)\, f_{j,\,m+1}\, e^{\,i\,(m+1)\varphi}.$$

Moreover, one finds in a rather simple way that:

$$\begin{aligned} P_- f_{j,\,m}\, e^{im\varphi} &= e^{\,i\,(m-1)\varphi}\left[(1-z^2)\frac{df_{j,m}}{dz} - \frac{mz}{(1-z^2)^{1/2}}\, f_{j,m}\right], \\ &= e^{\,i\,(m-1)\varphi}\,(1-z^2)^{-(m-1)/2}\,\frac{d}{dz}\left[f_{j,m}(1-z^2)^{m/2}\right], \\ &= e^{\,i\,(m-1)\varphi}\,(1-z^2)^{-(m-1)/2}\left(\frac{d}{dz}\right)^{j-m+1}(1-z^2)^j\,, \\ &= e^{\,i\,(m-1)\varphi} f_{j,\,m-1}\,. \end{aligned}$$

The relations (18b) can be calculated in an entirely analogous way. Now, for us, it is important, in particular, that the singular solution $f_{j,-\frac{1}{2}}$ should appear as a result in the relations:

$$P_-\left(f_{j,\frac{1}{2}}\, e^{i\varphi/2}\right) = \text{const. } f_{j,-\frac{1}{2}}\, e^{-i\varphi/2}, \qquad P_+\left(f_{j,\frac{1}{2}}\, e^{-i\varphi/2}\right) = \text{const. } f_{j,-\frac{1}{2}}\, e^{+i\varphi/2},$$

whereas for integer j, m, from (14), one will have:

$$P_-\, f_{j,\,0} = \text{const. } f_{j,\,-1}\, e^{-i\varphi} = \text{const. } f_{j,\,1}\, e^{-i\varphi} = \text{const. } u^-_{j,1}(\vartheta, \varphi).$$

For half-integer j, m, the application of the angular impulse operators to our system (7), (10) of eigenfunctions, which has (17) as a consequence, will, in fact, lead to the fact that the angular impulse matrices that are calculated from the integrals in the usual way for $m = 1/2$ will no longer be diagonal in j, as we had in § 1. From our criterion, those half-integer spherical functions must then be excluded here.

b) *The wave equation of the spinning electron.*

Here, we shall begin with the form of the Dirac equation in polar coordinates that SCHRÖDINGER presented as a special case of his general theory of a spinning electron in a gravitational field. The explanation for the connection between this representation of the theory and the usual one shall be postponed to the following §.

We write the Schrödinger equation in the form ([1]):

$$\frac{1}{c}\frac{\partial\psi}{\partial t}-i\varphi_0\psi+\alpha_1\frac{1}{r}\frac{1}{\sqrt{\sin\vartheta}}\frac{\partial}{\partial\vartheta}(\sqrt{\sin\vartheta}\,\psi)+\alpha_2\frac{1}{r\sin\vartheta}\frac{\partial\psi}{\partial\varphi}+\alpha_3\frac{1}{r}\frac{\partial(r\psi)}{\partial r}+i\frac{mc}{h}\beta\psi=0, \quad (20)$$

in which the matrices α_k, β satisfy the well-known Dirac commutation relations, and φ_0 means a scalar potential field (multiplied by e / hc) that is assumed to be centrally-symmetric.

One then obtains the angular impulse components from the usual method when one extends the corresponding expressions (6) by terms that commute with the Hamiltonian operator. In that way, one will get:

$$P_+ = P_1 + i\,P_2 = e^{i\varphi}\left(\frac{\partial}{\partial\vartheta}+\frac{i\cos\vartheta}{\sin\vartheta}\frac{\partial}{\partial\varphi}+\frac{1}{2}\frac{s_3}{\sin\vartheta}\right), \quad (21a)$$

$$P_- = P_1 - i\,P_2 = e^{-i\varphi}\left(-\frac{\partial}{\partial\vartheta}+\frac{i\cos\vartheta}{\sin\vartheta}\frac{\partial}{\partial\varphi}+\frac{1}{2}\frac{s_3}{\sin\vartheta}\right), \quad (21a)$$

$$P_3 = -\,i\,\frac{\partial}{\partial\varphi}, \quad (21c)$$

with the abbreviation $s_3 = -\,i\,\alpha_1\,\alpha_2$ (and cyclic permutations). Deviating from the usual form of the theory, here, the component P_3 has no additional term, while the matrix s_3 appears in the additional terms in P_1 and P_2, instead of in the P_3, as usual.

Another operator that commutes with the Hamiltonian operator, as well as with the P_k, is defined by:

$$K\,\psi = \beta\,\alpha_3\left(\frac{\alpha_1}{\sqrt{\sin\vartheta}}\frac{\partial}{\partial\vartheta}\sqrt{\sin\vartheta}+\frac{\alpha_2}{\sin\vartheta}\frac{\partial}{\partial\varphi}\right)\psi. \quad (22)$$

The total square of the P_k can be expressed in terms of the square of K by way of:

([1]) SCHRÖDINGER, P. A., eq. (5.12) and (8.1) in the limit $R \to \infty$. Here, we have introduced the new notation α_1, α_2, α_3, β for the matrices that SCHRÖDINGER denoted by $i\alpha_4\,\alpha_2$, $i\alpha_4\,\alpha_3$, $i\alpha_4\,\alpha_1$, $-\,\alpha_4$. That is justified by the fact that the Dirac commutation relations will also follow for those matrices if they were true for the original α_1, …, α_4 . Furthermore, from time to time, SCHRÖDINGER introduced the abbreviation $\omega = r\,\sqrt{\sin\vartheta}\,\psi$, but that would not be convenient for what follows here.

$$P^2 \equiv P_1{}^2 + P_2{}^2 + P_3{}^2 = K^2 - \tfrac{1}{4}. \tag{23}$$

Therefore, if j (j + 1) are the eigenvalues of P^2 then $k = \pm (j + \frac{1}{2})$ will be the eigenvalues of K. As is well-known, the signed quantum number k plays a very decisive role in the fine structure of the H-atom.

For the further integration, one can make the Ansatz for, e.g., the matrices α_k , β:

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{24}$$

with

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

from which, it follows that:

$$s_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix} \qquad \text{with} \quad k = 1, 2, 3, \tag{24a}$$

moreover. Furthermore, if ψ is decomposed into one factor that depends upon only ϑ, φ and one that depends upon r:

$$\psi = \chi(r)\, u(\vartheta, \varphi), \tag{25}$$

in which:

$$K\, u = k\, u, \tag{26}$$

and with:

$$\frac{\partial}{\partial t} = -\, i\, v,$$

then one will have:

$$-\, i\left(\frac{v}{c} + \varphi_0\right)\chi + \frac{1}{r}\alpha_3\, \beta k \chi + \alpha_3 \frac{1}{r}\frac{\partial(r\chi)}{\partial r} + i\frac{mc}{h}\beta\chi = 0. \tag{27}$$

(22) will yield the first two components of $u(\vartheta, \varphi)$:

$$k\, u = \frac{i\sigma_2}{\sqrt{\sin\vartheta}}\frac{\partial}{\partial\vartheta}(\sqrt{\sin\vartheta}\, u) - \frac{i\sigma_1}{\sin\vartheta}\frac{\partial u}{\partial\varphi}, \tag{28}$$

and corresponding equations for u_3, u_4 in which k is replaced with $-k$. One will get the solution of those equations by changing the sign of one of the components in the pair; e.g., u_2 . One will then ultimately get the solution:

$$\psi_1 = F(r)\, u_1(\vartheta, \varphi), \quad \psi_2 = F(r)\, u_2(\vartheta, \varphi), \quad \psi_3 = i\, G(r)\, u_1(\vartheta, \varphi),$$
$$\psi_4 = -\, i\, G(r)\, u_2(\vartheta, \varphi). \tag{29}$$

(27) implies that F and G must satisfy:

$$\left(\frac{v}{c}+\varphi_0\right)F+\frac{1}{r}kG-\frac{1}{r}\frac{d(rG)}{dr}-\frac{mc}{h}F=0, \tag{30a}$$

$$\left(\frac{v}{c}+\varphi_0\right)G+\frac{1}{r}kF+\frac{1}{r}\frac{d(rF)}{dr}+\frac{mc}{h}G=0. \tag{30b}$$

The last equations agree with the ones that are derived in the textbooks, and will not be dealt with further here.

If we now set, in analogy to what we did with the scalar wave equation (28):

$$u^{+}_{1;k,m}=f_{k,m}(\cos\vartheta)\,e^{im\varphi}, \qquad u^{+}_{2;k,m}=g_{k,m}(\cos\vartheta)\,e^{im\varphi}, \tag{31}$$

in which we understand k and m to mean negative numbers, then it will follow from (28) that f and g must satisfy ([1]):

$$\frac{1}{\sqrt{\sin\vartheta}}\frac{d}{d\vartheta}(\sqrt{\sin\vartheta}\,g)+\frac{m}{\sin\vartheta}g-kf=0, \tag{32a}$$

$$\frac{1}{\sqrt{\sin\vartheta}}\frac{d}{d\vartheta}(\sqrt{\sin\vartheta}\,f)-\frac{m}{\sin\vartheta}f+kg=0. \tag{32b}$$

The further solutions then follow immediately from that:

$$u^{-}_{1;k,m}=g_{k,m}\,e^{-im\varphi}, \qquad u^{-}_{2;k,m}=-f_{k,m}\,e^{-im\varphi}, \tag{31}$$

$$f_{-k,m}=f_{k,m}, \qquad g_{-k,m}=-g_{k,m}. \tag{33}$$

The regular solutions of equations (32) were given by SCHRÖDINGER ([2]), in which he employed some previous results of WEYL. If we again set:

$$z=\cos\vartheta \tag{34}$$

then we must set:

$$k-m-\tfrac{1}{2}\geq 0 \quad \text{and } k>0 \text{ is integer}, \tag{35}$$

and we will get:

([1]) The notation in SCHRÖDINGER is somewhat different, since we write the quantities that he denoted by (f, g) as: $i\sqrt{\sin\vartheta}\,f$, $\sqrt{\sin\vartheta}\,g$, resp.

([2]) P. A., § 7.

$$f_{k,m}(z) = (1+z)^{-\frac{1}{2}(m+\frac{1}{2})}(1-z)^{-\frac{1}{2}(m-\frac{1}{2})}\left(\frac{d}{dz}\right)^{k-m-\frac{1}{2}}(1+z)^{k}(1-z)^{k-1}, \tag{36a}$$

$$g_{k,m}(z) = (1+z)^{-\frac{1}{2}(m-\frac{1}{2})}(1-z)^{-\frac{1}{2}(m+\frac{1}{2})}\left(\frac{d}{dz}\right)^{k-m-\frac{1}{2}}(1+z)^{k-1}(1-z)^{k}, \tag{36a}$$

in which we will discuss the cases k integer, m half-integer and k half-integer, m integer separately. According to (33), it suffices to restrict to positive k. (For $k = 0$, there are no regular solutions for $z = +1$ and $z = -1$.)

The solutions:

$$u^{(-)}_{1;k,-m} = f_{k,-m}\,e^{-im\varphi}, \qquad u^{(-)}_{2;k,-m} = g_{k,-m}\,e^{-im\varphi}, \tag{31a–}$$

and

$$u^{+}_{1;k,-m} = g_{k,-m}\,e^{im\varphi}, \qquad u^{+}_{2;k,-m} = -f_{k,-m}\,e^{im\varphi}, \tag{31a+}$$

which emerge from (36) when one formally replaces m with $-m$, will demand a more precise discussion.

Analogous to § 1, we next show that the case of k integer, m half-integer is distinguished in particular by the fact that:

$$\left.\begin{matrix} f_{k,-m} \\ g_{k,-m} \end{matrix}\right\} = \text{const.}\left\{\begin{matrix} g_{k,m} \\ -f_{k,m} \end{matrix}\right. \quad \text{for } k \text{ integer, } m \text{ half-integer;} \tag{37}$$

i.e., in that case, the regular solutions (31) can also be obtained by formally replacing m with $-m$ in (31) and (36a, b). When one introduces a circle K_0 around the zero point as the integration path in the complex t-plane, one can next write:

$$f_{k,m}(z) = (1+z)^{-\frac{1}{2}(m+\frac{1}{2})}(1-z)^{-\frac{1}{2}(m-\frac{1}{2})}\frac{(k-m-\frac{1}{2})!}{2\pi i}\int_{K_0}\frac{dt}{t^{k-m+\frac{1}{2}}}(1+z+t)^{k}(1-z-t)^{k-1}, \tag{38a}$$

$$g_{k,m}(z) = (1+z)^{-\frac{1}{2}(m-\frac{1}{2})}(1-z)^{-\frac{1}{2}(m+\frac{1}{2})}\frac{(k-m-\frac{1}{2})!}{2\pi i}\int_{K_0}\frac{dt}{t^{k+m+\frac{1}{2}}}(1+z+t)^{k-1}(1-z-t)^{k}, \tag{38b}$$

in place of (36). For integer $k \geq 1$, the quantity in the integral is indifferent to the circle K_0, while in the other cases, one should especially observe that the branching loci $t = -(1 + z)$ and $t = 1 - z$ lie outside the circle:

$$|\,t\,| < |\,1+z\,| \text{ and } |\,t\,| < |\,1-z\,| \text{ on } K_0 \text{ for } k, m - \text{are not integer.} \tag{39}$$

In the expressions for $f_{k,-m}$ and $g_{k,-m}$:

$$f_{k,-m}(z) = (1+z)^{\frac{1}{2}(m-\frac{1}{2})}(1-z)^{\frac{1}{2}(m+\frac{1}{2})}\frac{(k+m-\frac{1}{2})!}{2\pi i}\int_{K_0}\frac{dt}{t^{k+m+\frac{1}{2}}}(1+z+t)^{k}(1-z-t)^{k-1}, \tag{40a}$$

$$g_{k,-m}(z) = (1+z)^{\frac{1}{2}(m+\frac{1}{2})}(1-z)^{\frac{1}{2}(m-\frac{1}{2})}\frac{(k+m-\frac{1}{2})!}{2\pi i}\int_{K_0}\frac{dt}{t^{k+m+\frac{1}{2}}}(1+z+t)^{k-1}(1-z-t)^{k}\,, \qquad (40a)$$

we now make the substitution:

$$t \to -\frac{1-z^2}{t}\,,$$

which will give:

$$f_{k,-m}(z)$$
$$= (1+z)^{-\frac{1}{2}(m-\frac{1}{2})}(1-z)^{-\frac{1}{2}(m+\frac{1}{2})}e^{-i\pi(m-\frac{1}{2})}\frac{(k+m-\frac{1}{2})!}{2\pi i}\int_{K_0}\frac{dt}{t^{k-m+\frac{1}{2}}}(1+z+t)^{k-1}(1-z-t)^{k}\,, \qquad (41a)$$

$$g_{k,-m}(z)$$
$$= -(1+z)^{-\frac{1}{2}(m+\frac{1}{2})}(1-z)^{-\frac{1}{2}(m-\frac{1}{2})}e^{-i\pi(m-\frac{1}{2})}\frac{(k+m-\frac{1}{2})!}{2\pi i}\int_{K_0}\frac{dt}{t^{k-m+\frac{1}{2}}}(1+z+t)^{k}(1-z-t)^{k-1}\,, \qquad (41a)$$

in which now:

$$|\,t\,| > |\,1+z\,|, \quad |\,t\,| > |\,1-z\,| \text{ on } K_1\,. \qquad (42)$$

However, since the circle K_1 can be continuously deformed into the circle K_0 for integer k and integer $m-\frac{1}{2}$, the relation (37) is proved for that special case.

Things are different in the case of k half-integer, m integer. The solutions (36a), (36b) will then be regular for $m > 0$ only at the two places $z = -1$ and $z = +1$, while the solutions (31a) are singular for $-m \leq 0$. For $m = 0$, they will still be square-integrable in z. However, it is noteworthy that for $m = 0$, we will get two different solutions from (36) and (37). First:

$$u^{\mathrm{I}}_{1;k,0} = f_{k,0}\,, \qquad u^{\mathrm{I}}_{2;k,0} = g_{k,0}\,, \qquad (43a)$$

and second:

$$u^{\mathrm{II}}_{1;k,0} = g_{k,0}\,, \qquad u^{\mathrm{II}}_{2;k,0} = -f_{k,0}\,. \qquad (43b)$$

We further show that these two families of solutions are not orthogonal to each other when $k - k'$ is odd. With $m \geq 0$ and k half-integer, we even have, more generally:

$$\frac{1}{4\pi}\sum_{\rho=1,2}\int u^{+*}_{\rho;k,m}u^{+}_{\rho;k',-m}\sin\vartheta\, d\vartheta\, d\varphi$$
$$= -\frac{1}{4\pi}\sum_{\rho=1,2}\int u^{-*}_{\rho;k,m}u^{-}_{\rho;k',-m}\sin\vartheta\, d\vartheta\, d\varphi$$
$$= \tfrac{1}{2}\int_{-1}^{+1}(f_{k;m}\,g_{k',-m} - g_{k;m}\,f_{k',-m})\,dz = \neq 0 \quad \text{for } k-k' \text{ odd}, \qquad (45)$$

which is a result that is analogous to § 1, eq. (17). Moreover, one can deduce from (36) that the integral in (45) is even in z when k is half-integer and $k - k'$ is odd, while the integrand is odd in z for even $k - k'$, so the integrand will vanish then.

In order to prove (45), we infer from (32a, b) that:

$$(k - k') \int_{-1}^{+1} (f_{k,m}\, g_{k',-m} - g_{k,m}\, f_{k',-m})\, dz = \tfrac{1}{2} \Big| (1-z^2)^{1/2} (f_{k,m}\, f_{k',-m} + g_{k,m}\, g_{k',-m}) \Big|_{-1}^{+1}.$$

The application of the operators P_+ and P_- that are defined by (21a, b) to the eigenfunctions will further give the result:

$$P_+ \begin{cases} f_{k,m}\, e^{im\varphi} \\ g_{k,m}\, e^{im\varphi} \end{cases} = \text{const.} \begin{cases} f_{k,m+1}\, e^{i(m+1)\varphi} \\ g_{k,m+1}\, e^{i(m+1)\varphi} \end{cases}, \tag{46a}$$

$$P_- \begin{cases} f_{k,m}\, e^{im\varphi} \\ g_{k,m}\, e^{im\varphi} \end{cases} = \text{const.} \begin{cases} f_{k,m-1}\, e^{i(m-1)\varphi} \\ g_{k,m-1}\, e^{i(m-1)\varphi} \end{cases}, \tag{46b}$$

$$P_+ \begin{cases} g_{k,m}\, e^{-im\varphi} \\ -f_{k,m}\, e^{-im\varphi} \end{cases} = \text{const.} \begin{cases} g_{k,m-1}\, e^{-i(m-1)\varphi} \\ -f_{k,m-1}\, e^{-i(m-1)\varphi} \end{cases}, \tag{46c}$$

$$P_- \begin{cases} g_{k,m}\, e^{-im\varphi} \\ -f_{k,m}\, e^{-im\varphi} \end{cases} = \text{const.} \begin{cases} g_{k,m+1}\, e^{-i(m+1)\varphi} \\ -f_{k,m+1}\, e^{-i(m+1)\varphi} \end{cases}, \tag{46c}$$

which is analogous to (18) in § 1. The bright-hand side of (46a) and (46d) must be set to identically zero for the boundary value $m = k - \frac{1}{2}$.

In fact, if one recalls (21) and (24a) then one will next get from (36a, b) that:

$$\begin{aligned}
P_- (f_{k,m}\, e^{im\varphi}) &= e^{i(m-1)\varphi} (1 - z^2)^{1/2} \left[\frac{df_{k,m}}{dz} - \frac{mz}{1-z^2} f_{k,m} + \tfrac{1}{2} \frac{1}{1-z^2} f_{k,m} \right] \\
&= e^{i(m-1)\varphi} (1 - z^2)^{1/2} \left[\frac{df_{k,m}}{dz} + \tfrac{1}{2}(m + \tfrac{1}{2}) \frac{f_{k,m}}{1+z} - \tfrac{1}{2}(m - \tfrac{1}{2}) \frac{f_{k,m}}{1-z} \right] \\
&= e^{i(m-1)\varphi}\, (1+z)^{-\frac{1}{2}(m-\frac{1}{2})} (1+z)^{-\frac{1}{2}(m-\frac{1}{2})} \frac{d}{dz} \left[f_{k,m} (1+z)^{\frac{1}{2}(m+\frac{1}{2})} (1-z)^{\frac{1}{2}(m-\frac{1}{2})} \right] \\
&= e^{i(m-1)\varphi} f_{k,m-1},
\end{aligned}$$

and likewise:

$$\begin{aligned}
P_- (g_{k,m}\, e^{im\varphi}) &= e^{i(m-1)\varphi} (1 - z^2)^{1/2} \left[\frac{dg_{k,m}}{dz} - \frac{mz}{1-z^2} g_{k,m} - \tfrac{1}{2} \frac{1}{1-z^2} g_{k,m} \right] \\
&= e^{i(m-1)\varphi} (1 - z^2)^{1/2} \left[\frac{dg_{k,m}}{dz} + \tfrac{1}{2}(m - \tfrac{1}{2}) \frac{g_{k,m}}{1+z} - \tfrac{1}{2}(m + \tfrac{1}{2}) \frac{g_{k,m}}{1-z} \right]
\end{aligned}$$

$$= e^{i\,(m-1)\,\varphi}\,(1+z)^{-\frac{1}{2}(m-\frac{3}{2})}(1-z)^{-\frac{1}{2}(m-\frac{1}{2})}\,\frac{d}{dz}\Big[\,g_{k,m}(1+z)^{\frac{1}{2}(m-\frac{1}{2})}(1-z)^{\frac{1}{2}(m+\frac{1}{2})}\Big]$$
$$= e^{i\,(m-1)\,\varphi}\,g_{k,\,m-1}\,.$$

Furthermore, by means of the integral representation (38), one will get:

$$P_+\,(f_{k,\,m}\,e^{im\,\varphi}) = e^{i\,(m+1)\,\varphi}\,(1-z^2)^{1/2}\left[-\frac{df_{k,m}}{dz}+\tfrac{1}{2}(m+\tfrac{1}{2})\frac{f_{k,m}}{1-z}-\tfrac{1}{2}(m-\tfrac{1}{2})\frac{f_{k,m}}{1-z}\right]$$

$$= e^{i\,(m+1)\,\varphi}\,(1+z)^{-\frac{1}{2}(m+\frac{3}{2})}(1-z)^{-\frac{1}{2}(m+\frac{3}{2})}\cdot\frac{(k-m-\frac{1}{2})!}{2\pi i}$$
$$+\int_{K_0}\frac{dt}{t^{k-m+\frac{1}{2}}}\{-(1-z^2)k(1+z+t)^{k-1}(1-z-t)^{k-1}$$
$$+\,(1-z^2)(k-1)(1+z+t)^k\cdot(1-z-t)^{k-2}$$
$$+\,[(m+\tfrac{1}{2})\,(1-z)-(m-\tfrac{1}{2})\,(1+z)]\,(1+z+t)^k\,(1-z-t)^{k-1}\}.$$

The integrand can be converted into:

$$(k+m+\tfrac{1}{2})\;t^{-(k-m-\frac{1}{2})}(1+z+t)^k\,(1-z-t)^{k-1}$$
$$-\frac{d}{dt}\,[\,t^{-(k-m-\frac{1}{2})}(2z+t)\,(1+z+k)^k\,(1-z-t)^{k-1}].$$

The second term will vanish when one integrates over the circle K_0 , and that will give:

$$P_+\,(f_{k,\,m}\,e^{im\,\varphi}) = (k+m+\tfrac{1}{2})\,(k-m-\tfrac{1}{2})\,f_{k,\,m+1}\,e^{\,i\,(m+1)\,\varphi}.$$

One will likewise get:

$$P_+\,(g_{k,\,m}\,e^{im\,\varphi}) = e^{i\,(m+1)\,\varphi}\,(1-z^2)^{1/2}\left[-\frac{dg_{k,m}}{dz}+\tfrac{1}{2}(m-\tfrac{1}{2})\frac{g_{k,m}}{1-z}-\tfrac{1}{2}(m+\tfrac{1}{2})\frac{g_{k,m}}{1-z}\right]$$

$$= e^{i\,(m+1)\,\varphi}\,(1+z)^{-\frac{1}{2}(m+\frac{3}{2})}(1-z)^{-\frac{1}{2}(m+\frac{3}{2})}\cdot\frac{(k-m-\frac{1}{2})!}{2\pi i}$$
$$+\int\frac{dt}{t^{k-m+\frac{1}{2}}}\{-(1-z^2)(k-1)(1+z+t)^{k-2}(1-z-t)^{k-1}$$
$$+\,(1-z^2)k(1+z+t)^{k-1}(1-z-t)^{k-1}$$
$$+\,[(m-\tfrac{1}{2})\,(1-z)-(m+\tfrac{1}{2})\,(1+z)]\,(1+z+t)^{k-1}\,(1-z-t)^k\}.$$

The integrand can be converted into:

$$(k+m+\tfrac{1}{2})\;t^{-(k-m-\frac{1}{2})}(1+z+t)^{k-1}\,(1-z-t)^k$$

$$-\frac{d}{dt}\left[t^{-(k-m-\frac{1}{2})}(2z+t)(1+z+k)^{k-1}(1-z-t)^k\right],$$

and the integration over the circle K_0 will yield:

$$P_+(g_{k,m}\,e^{im\varphi}) = (k+m+\tfrac{1}{2})(k-m-\tfrac{1}{2})\,g_{k,m+1}\,e^{i(m+1)\varphi}.$$

The calculation of (46c) and (46d) proceeds analogously.

It is especially important for the application of our criterion to know that singular solutions will appear in the case of k half-integer, m integer in the relations:

$$P_-\begin{cases} f_{k,1}\,e^{i\varphi} \\ g_{k,1}\,e^{i\varphi}\end{cases} = \text{const.}\begin{cases} f_{k,0} \\ g_{k,0}\end{cases}, \qquad P_+\begin{cases} g_{k,1}\,e^{-i\varphi} \\ -f_{k,1}\,e^{-i\varphi}\end{cases} = \text{const.}\begin{cases} g_{k,0} \\ -f_{k,0}\end{cases},$$

$$P_-\begin{cases} f_{k,0} \\ g_{k,0}\end{cases} = \text{const.}\begin{cases} f_{k,-1}\,e^{-i\varphi} \\ g_{k,-1}\,e^{-i\varphi}\end{cases}, \qquad P_+\begin{cases} g_{k,0} \\ -f_{k,0}\end{cases} = \text{const.}\begin{cases} g_{k,-1}\,e^{i\varphi} \\ -f_{k,-1}\,e^{i\varphi}\end{cases}$$

as a result. Therefore, our criterion demands *the exclusion of the case k half-integer, m integer.* In fact, in that case, one will always get contradictions for the angular impulse matrices that are calculated from the integrals in the usual way. If one computes, on the one hand, one of the two solutions ($f_{k,0}$, $g_{k,0}$) *or* ($g_{k,0}$, $-f_{k,0}$) in the original system of solutions then, according to (45), (45a), some of the calculated matrix elements will be non-diagonal in k, which would contradict the commutation of the operators P_+ and P_- with the operator K that is defined by (22). On the other hand, if one were to not count the (non-regular, but still square-integrable) solutions for $m = 0$ among the allowable eigen-solutions ([1]) then, since the solutions for $m = 0$ would then be orthogonal to the all of the original allowable solutions, from (46), pieces would be cut out of the boundary by the matrix elements of P_+ and P_-, which would interfere with the validity of the commutation relations that would be necessary for those matrices.

By contrast, in the case of k integer ($\neq 0$), m half-integer, as a consequence of (37), the application of the operators P_+ and P_- to the original orthogonal system $u^+_{k,m}(\vartheta, \varphi)$, $u^-_{k,m}(\vartheta, \varphi)$, with $\frac{1}{2} \leq m \leq k - \frac{1}{2}$, would not produce something out of that system, as our criterion demands, such that this case would then deliver the physically-correct eigen-solutions.

([1]) Cf. SCHRÖDINGER, P. A., rem. by the editor at the conclusion.

§ 3. Connection between Schrödinger's form of the Dirac equation and the usual form. Behavior of the solutions for finite rotations.

Let Ψ satisfy the usual Dirac equation:

$$\frac{1}{c}\frac{\partial\Psi}{\partial t} - i\varphi_0\Psi + \sum_{k=1}^{3}\alpha_k\frac{\partial\Psi}{\partial x_k} + i\frac{mc}{h}\beta\Psi = 0, \tag{47}$$

while ψ fulfills equation (20) in polar coordinates:

$$x_1 = r\sin\vartheta\cos\varphi, \qquad x_2 = r\sin\vartheta\sin\varphi, \qquad x_3 = r\cos\vartheta, \tag{48}$$

which we can write as:

$$\frac{1}{c}\frac{\partial\psi}{\partial t} - i\varphi_0\psi + \alpha_1\frac{1}{r}\left(\frac{\partial\psi}{\partial\vartheta} + \frac{1}{2}\frac{\cos\vartheta}{\sin\vartheta}\psi\right) + \alpha_2\frac{1}{r\sin\vartheta}\frac{\partial\psi}{\partial\varphi} + \alpha_3\left(\frac{\partial\psi}{\partial r} + \frac{1}{r}\psi\right) + \frac{imc}{h}\beta\psi = 0. \tag{49}$$

The transition from Ψ to ψ will now be mediated by the unitary matrix $R(\vartheta, \varphi)$, which is independent of ϑ, φ, and is defined in terms of the spin matrices that are defined by:

$$s_1 = -i\,\alpha_2\,\alpha_3, \qquad s_2 = -i\,\alpha_3\,\alpha_1, \qquad s_3 = -i\,\alpha_1\,\alpha_2, \tag{50}$$

and the identity matrix, which are combined linearly according to the formula ([1]):

$$R(\vartheta, \varphi) = e^{is_2\frac{\vartheta}{2}} \cdot e^{is_2\frac{\varphi}{2}}$$
$$= \cos\frac{\vartheta}{2}\sin\frac{\varphi}{2}I - i\sin\frac{\vartheta}{2}\sin s_1\frac{\varphi}{2} + i\sin\frac{\vartheta}{2}\cos\frac{\varphi}{2}\cdot s_2 + i\cos\frac{\vartheta}{2}\sin\frac{\varphi}{2}\cdot s_3. \tag{51}$$

As one sees, R commutes with the matrix β. On the basis of the known commutation relations for the s_k, one will further easily confirm that one will get the matrix that is inverse to R by switching i with $-i$, as well as the sequence of the two exponential factors:

$$R^{-1}(\vartheta, \varphi) = e^{-is_2\frac{\varphi}{2}} \cdot e^{-is_2\frac{\vartheta}{2}}$$
$$= \cos\frac{\vartheta}{2}\sin\frac{\varphi}{2}I + i\sin\frac{\vartheta}{2}\sin s_1\frac{\varphi}{2} - i\sin\frac{\vartheta}{2}\cos\frac{\varphi}{2}\cdot s_2 - i\cos\frac{\vartheta}{2}\sin\frac{\varphi}{2}\cdot s_3. \tag{51}$$

One can now show, in fact, that the assignments:

([1]) I must thank E. SCHRÖDINGER for his friendly communication of the way of writing $R(\vartheta, \theta)$ as a product of two exponential factors, which is also suitable for the proof of the following relations (53), (55).

$$\psi = R\Psi \qquad \text{or} \qquad \Psi = R^{-1}\,\psi \tag{52}$$

will take one from equation (47) to equation (49), or conversely. That is based upon the relations ([1])

$$R^{-1}\,\alpha_1\,R = \alpha_1 \cos\vartheta\cos\varphi + \alpha_2 \cos\vartheta\cos\varphi - \alpha_3 \sin\vartheta, \tag{53$_1$}$$

$$R^{-1}\,\alpha_2\,R = -\,\alpha_1 \sin\varphi + \alpha_2 \cos\varphi, \tag{53$_2$}$$

$$R^{-1}\,\alpha_3\,R = \alpha_1 \sin\vartheta\cos\varphi + \alpha_2 \sin\vartheta\sin\varphi + \alpha_3 \cos\vartheta, \tag{53$_3$}$$

which follow from (51).

By means of the relations:

$$\frac{\partial}{\partial x_1} = \cos\vartheta\cos\varphi\,\frac{1}{r}\frac{\partial}{\partial\vartheta} - \sin\varphi\left(\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}\right) + \sin\vartheta\cos\varphi\,\frac{\partial}{\partial r},$$

$$\frac{\partial}{\partial x_2} = \cos\vartheta\cos\varphi\,\frac{1}{r}\frac{\partial}{\partial\vartheta} + \cos\varphi\left(\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}\right) + \sin\vartheta\sin\varphi\,\frac{\partial}{\partial r},$$

$$\frac{\partial}{\partial x_3} = -\sin\vartheta\,\frac{1}{r}\frac{\partial}{\partial\vartheta} + \cos\vartheta\,\frac{\partial}{\partial r},$$

it will further follow from (53) that:

$$\sum_{k=1}^{3}\alpha_k\frac{\partial}{\partial x_k} = (R^{-1}\,\alpha_1\,R)\,\frac{1}{r}\frac{\partial}{\partial\vartheta} + (R^{-1}\,\alpha_2\,R)\,\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi} + R^{-1}\,\alpha_3\,R\frac{\partial}{\partial r}\,. \tag{54}$$

Finally, one will find that the matrix X, which is defined by:

$$R^{-1}\,\alpha_1\,\frac{\partial R}{\partial\vartheta} + \frac{1}{\sin\vartheta}\left(R^{-1}\alpha_2\,\frac{\partial R}{\partial\varphi}\right) = R^{-1}\,X\,R,$$

([1]) In order to verify these relations, as well as the following ones (55), one can also start with the special representation (24) of the Dirac matrices, and from (24a) that gives the s_k as simply:

$$\begin{pmatrix}\sigma_k & 0\\ 0 & \sigma_k\end{pmatrix}.$$

From (51), (51a), one will then get:

$$R = \begin{pmatrix}T & 0\\ 0 & T\end{pmatrix},$$

with the two-rowed matrices:

$$T = \begin{pmatrix}\cos\frac{\vartheta}{2}e^{i\varphi/2} & \sin\frac{\vartheta}{2}e^{-i\varphi/2}\\ -\sin\frac{\vartheta}{2}e^{i\varphi/2} & \cos\frac{\vartheta}{2}e^{-i\varphi/2}\end{pmatrix}, \quad T^{-1} = \begin{pmatrix}\cos\frac{\vartheta}{2}e^{-i\varphi/2} & -\sin\frac{\vartheta}{2}e^{-i\varphi/2}\\ \sin\frac{\vartheta}{2}e^{i\varphi/2} & \cos\frac{\vartheta}{2}e^{i\varphi/2}\end{pmatrix},$$

and the relations (53) reduce to the simpler ones in which R has been replaced with T, and the α_k have been replaced with the s_k .

will be:

$$X = \alpha_1 \frac{\partial R}{\partial \vartheta} R^{-1} + \frac{1}{\sin\vartheta}\alpha_2 \frac{\partial R}{\partial \varphi} R^{-1} = -\left(\frac{1}{2}\frac{\cos\vartheta}{\sin\vartheta}\alpha_1 + \alpha_3\right). \tag{55}$$

One finally arrives at the Schrödinger form (49) from the original Dirac equation (47) from (54) and (55), by means of the substitution (52).

Although we shall not go into the details here, the angular impulse operators in equation (49) that are defined by (21) can also be obtained from the usual angular impulse operators:

$$P_1^0 = \frac{1}{i}\left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2}\right) + \tfrac{1}{2} s_1, \ \ldots \qquad \text{(and cyclic permutations)} \tag{56}$$

in equation (47) by recomputing in terms of the *R*-matrix.

We can also now resolve the question that was discussed in § 1 regarding the behavior of the solutions of (49) for finite rotations of the polar axis, since that question reverts to the known behavior of the solutions of (47) under the matrix *R*. If we then once more consider a finite rotation of the coordinate system that is characterized by three parameters *a*, which will determine new coordinates x'_k (polar angles ϑ', φ', resp.) as functions of the old coordinates x_k (angles ϑ, φ, resp.) and the *a*. For a spherically-symmetric potential $\varphi_0 = \varphi_0(r)$ in the usual system (47) of Dirac equations, one will get a new solution $X(x, a)$ of the equations in the x_k from an arbitrary solution $\Psi(x)$ of the same equations when one first replaces the *x* with x' while leaving the functional form of Ψ unaltered and expressing the x' in terms of the *x* and *a*, and secondly, performing an *S*-transformation with *constant* coefficients that depends upon *a*:

$$X(x, a) = S^0(a)\, \Psi(x'). \tag{57}$$

(Here, we do not write out the spin indices explicitly, as usual.) The matrix $S^0(a)$ is known from the theory of spinors, and does not need to be specified in detail here.

We now get the corresponding relation directly:

$$\chi(\vartheta, \varphi, a) = S(\vartheta, \varphi, a)\, \psi(\vartheta', \varphi'), \tag{58}$$

which associates any arbitrary solution ψ of (49) with a new solution χ of (49) by way of the connection (52):

$$\Psi(x') = R^{-1}(\vartheta', \varphi')\, \psi(\vartheta', \varphi'), \qquad \chi = R(\vartheta, \varphi)\, X,$$

which will give the matrix $S(\vartheta, \varphi, a)$ as:

$$S(\vartheta, \varphi, a) = R(\vartheta, \varphi) \cdot S^0(a) \cdot R^{-1}(\vartheta', \varphi'), \tag{59}$$

in which ϑ', φ' are to be thought of as functions of ϑ, φ, and *a*.