

quantum mechanically, provided care is taken with the order of the operators. The only change necessary is that \mathbf{C} must be symmetrized so that

$$\mathbf{C} = \hat{r} + \frac{1}{2Ze^2m}(\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) - \frac{1}{2Ze}(\mathbf{r} \times \mathbf{E}) \times \mathbf{r}.$$

ACKNOWLEDGMENTS

The author would like to thank Dr. B. A. Lippmann for first suggesting that the Runge-Lenz vector might provide a suitable starting point for the problem of a hydrogenic atom in an external electric field, and for his encouragement thereafter.

Remarks on the Relativistic Kepler Problem. II. Approximate Dirac-Coulomb Hamiltonian Possessing Two Vector Invariants*

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(Received 23 August 1963)

The Dirac-Coulomb Hamiltonian is shown to contain a "fine structure interaction" which, when removed, defines a new Hamiltonian differing from the Dirac-Coulomb Hamiltonian in order $(\alpha Z)^2/|\kappa|$. The solutions of this new Hamiltonian, as well as its complete set of invariant operators, are explicitly given. This "symmetric Hamiltonian" possesses a larger symmetry group than the R_4 group structure of the nonrelativistic Coulomb Hamiltonian. The simplicity of the complete orthonormal set of solutions of the symmetric Hamiltonian lends itself to several useful applications which are briefly indicated. The relation between the solutions of this new Hamiltonian and the Sommerfeld-Maue-Meixner-Furry wave functions is discussed.

I. INTRODUCTION

IN a previous paper¹ the structure of the eigenfunctions for a Dirac electron in a pure Coulomb field has been discussed by means of a new representation that diagonalizes the operator Γ . The operator Γ is the analog, for the Dirac-Coulomb problem, of the angular momentum operator $\rho_3 K$ in the free Dirac electron problem. In the new representation the Dirac-Coulomb problem becomes formally similar in structure to the plane-wave problem; the nonintegral "angular momentum" $\rho_3 \Gamma \rightarrow \gamma = |[(j + \frac{1}{2})^2 - (\alpha Z)^2]^{1/2}|$ is not sharp and γ mixes with $\gamma - 1$ analogous to the mixing of angular momenta l and $l - 1$ in the plane-wave problem. In both problems there exists a scalar invariant—the Lippmann-Johnson² operator, which, in a spherical representation, plays the role of the defining radial differential operator for the radial functions.

It was noted in the discussion of the Lippmann-Johnson operator in I Sec. IV that the results presented there led in a natural way to consideration of a third problem intermediate in complexity between the Dirac-Coulomb problem and the plane-wave problem. It is the purpose of the present paper to discuss this inter-

mediate problem, the "symmetric Coulomb-field problem" as we propose to call it.

A basic motivation behind the present work derives from various physical problems involving the interaction of relativistic electrons and radiation in the presence of (nuclear) Coulomb fields (for example, bremsstrahlung, internal conversion, nuclear excitation). Invariably one is led to technically intractable results involving complicated radial integrals suitable only for numerical treatment (or by approximations lacking a critical error assessment). This situation is to be contrasted to similar calculations carried out within a nonrelativistic framework: the famous Sommerfeld integration in closed form of the dipole bremsstrahlung energy loss is a striking example. The naive question therefore suggests itself—why should the introduction of relativistic effects, even when small, lead to such an inordinate increase in complication?

An immediate answer—but one which requires rather much amplification—is this: The nonrelativistic Coulomb field possesses the symmetry³ of the four-dimensional rotation group R_4 . It is well known that relativity spoils this symmetry.⁴ The loss of symmetry thus occurs at the classical level and is not primarily a property of the spin.⁵

* Work was supported in part by the U. S. Army Research Office (Durham) and by the National Science Foundation.

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¹ L. C. Biedenharn, Phys. Rev. **126**, 845 (1962). We shall, hereafter, refer to this as I. References to the very extensive literature on this problem are contained in paper I.

² M. H. Johnson and B. A. Lippmann, Phys. Rev. **78**, 329 (1950).

³ V. Fock, Z. Physik **98**, 145 (1935); V. Bargmann, *ibid.* **99**, 576 (1936); W. Pauli, *ibid.* **36**, 336 (1926).

⁴ There remains, however, the degeneracy of states having opposite signs for the Dirac operator K characterized by the Lippmann-Johnson operator (see Ref. 2).

⁵ That is to say, a spinless charged-particle problem would show a similar loss of symmetry when subjected to relativistic effects. [Relativistic spin-orbit effects are, however, not trivial. Indeed the

In the classical problem it is quite possible to re-introduce the degeneracy (closed orbits) by considering an appropriately rotating coordinate system. The transformation, called S in paper I, which diagonalized Γ , was shown to be in a qualitative sense the analog, in the classical limit, of the classical rotating coordinate system. One is thus led purely formally to investigate the meaning of closed orbits (orbits of nonrelativistic form) in the frame of reference defined by the transformation S . In this way one is led to define a new type of Coulomb problem—the symmetric Coulomb problem—which has the Hamiltonian \bar{H} given in Sec. III. As we shall prove later, the symmetry group of this Hamiltonian is characterized by the two vector invariants \mathbf{J} and \mathbf{K} which are the analogs of \mathbf{L} and \mathbf{A} of the spinless nonrelativistic problem.⁶

As will be demonstrated in Sec. III the symmetric Hamiltonian, H_{sym} , is an approximation to the Dirac-Coulomb Hamiltonian, in which the approximation consists in “turning off” the fine structure. (It seems remarkable that this “turning off” has such a simple form.) One already knows the existence of several approximations to the Dirac-Coulomb *wave functions*—these are the Sommerfeld-Maue-Meixner-Furry (S-M-M-F) functions.⁷ It is probably no surprise that the solutions of the symmetric Hamiltonian are closely related to the S-M-M-F functions, since both are $(\alpha Z)^2$ approximations to the exact Dirac-Coulomb functions. This relationship will be discussed in Sec. III.

The fact that a Hamiltonian basis (in Dirac four-component form) exists for the solutions to H_{sym} —in contrast to the S-M-M-F functions—is of considerable value. Not only are these functions now seen to be complete and orthonormal and possessing bound states, but a systematic expansion of these, directly in the fine structure splitting $(\alpha Z)^2/\kappa$, is now possible.

The usefulness of H_{sym} is further enhanced by the fact that the integration of the symmetric Coulomb problem is completely expressed in terms of the operators \mathbf{J} and \mathbf{K} , precisely as in the nonrelativistic case. In consequence *matrix elements over these basis functions are purely geometric in character*. This is especially clear for the bound states.

In Sec. II we shall, as a preliminary, discuss the case of the nonrelativistic spin- $\frac{1}{2}$ particle in a Coulomb field, and introduce the symmetric Hamiltonian in Sec. III. Sections IV and V will be devoted to the investigation of the eigenfunctions and eigenvalues of this Hamiltonian. In the concluding section, Sec. VI, we shall present explicit invariant operators of this Hamiltonian and examine its group structure. We hope to discuss in a future paper questions related to the separation of the

adjunction of a Pauli spin in the nonrelativistic problem is a great convenience in solving the nonrelativistic Coulomb problem (see Sec. II).]

⁶ L. C. Biedenharn, J. Math. Phys. 2, 433 (1961).

⁷ A. Sommerfeld and A. W. Maue, Ann. Physik 22, 629 (1935); W. Furry, Phys. Rev. 36, 391 (1934); J. Meixner, Z. Physik 90, 312 (1934).

differential equation in parabolic coordinates, the momentum-space wave functions, the Hartree-Fock wave functions, and other applications.

II. NONRELATIVISTIC SPIN- $\frac{1}{2}$ PARTICLE IN A COULOMB FIELD

It is an interesting fact that it is considerably easier to discuss the motion in a Coulomb field of a Pauli particle (nonrelativistic spin- $\frac{1}{2}$ particle with dynamically independent spin) than the motion of a spinless particle.⁸ It is particularly important that we avail ourselves of this simplicity since the detailed considerations of Sec. IV are based directly upon introducing such wave functions for the “big” and “little” spinors in ρ space. The spin-angular part of the wave functions are easily handled by the methods of Wigner algebra. The coupled spin-angle functions are defined by¹

$$\phi_{\pm\kappa}^{\mu} = i^{l(\pm\kappa)} X_{\pm\kappa}^{\mu} = \sum_{\tau} C(l(\pm\kappa), \frac{1}{2}, |\kappa| - \frac{1}{2}; \mu \mp \tau, \pm\tau, \mu) \times Y_{l(\pm\kappa), \mu \mp \tau} i^{l(\pm\kappa)} X_{1/2}^{\pm\tau} \quad (1)$$

and these satisfy the equations:

$$(\boldsymbol{\sigma} \cdot \mathbf{L} + 1)\phi_{\kappa}^{\mu} = -\kappa\phi_{\kappa}^{\mu}, \quad (2)$$

$$\boldsymbol{\sigma} \cdot \hat{r}\phi_{\kappa}^{\mu} = iS(-\kappa)\phi_{-\kappa}^{\mu}, \quad (3)$$

where \hat{r} is the unit vector \mathbf{r}/r , $S(\kappa)$ denotes the sign of κ , and

$$\mathbf{J}^2\phi_{\kappa}^{\mu} = j(j+1)\phi_{\kappa}^{\mu}, \quad (4)$$

$$J_z\phi_{\kappa}^{\mu} = \mu\phi_{\kappa}^{\mu}, \quad (5)$$

$$(\phi_{\kappa}^{\mu'}, \phi_{\kappa}^{\mu}) = \delta_{\kappa\kappa'}\delta_{\mu\mu'}, \quad (6)$$

$$T\phi_{\kappa}^{\mu} = (-)^{j+\mu}\phi_{\kappa}^{-\mu}, \quad (7)$$

where T is the time reversal operator.

In Eq. (6) the scalar product involves summation over spin coordinates in addition to integration over the angles. For each κ there are $2|\kappa|$ eigenfunctions having the projection quantum numbers $\mu = -j, -j+1, \dots, +j$ because $|\kappa| = j + \frac{1}{2}$. T in Eq. (7) stands for the time reversal operator $i\sigma_y K_0$ with K_0 being complex conjugation. The choice of $(-)^{j+\mu}$ rather than $(-)^{j-\mu}$ is

motivated by the fact that f or $\chi_{1/2}^{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $\chi_{1/2}^{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ the ϕ_{κ}^{μ} obey this choice using $i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

Consider next the NR problem which has the Hamiltonian

$$H_{\text{NR}} = -\frac{1}{2m}\nabla^2 - \frac{Z\alpha}{r}, \quad (8)$$

⁸ We shall refer to this problem hereafter as the NRS problem for brevity and indicate by NR the nonrelativistic problem without spin.

with eigenvalue

$$|\epsilon_{NR}| = |E_{NR}|/m = \frac{1}{2}(\alpha Z/N)^2. \quad (9)$$

As has been shown by Pauli³—and others—this Hamiltonian has two vector invariants \mathbf{L} and \mathbf{A} , which is defined (with suitable normalization) as:

$$\mathbf{A} = [-2mH_{NR}]^{-1/2} \{ \alpha Z \hat{r} m + \frac{1}{2}(\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) \}, \quad (10)$$

$$\mathbf{A} \cdot \mathbf{L} = \mathbf{L} \cdot \mathbf{A} = 0, \quad (11)$$

$$\mathbf{A} \times \mathbf{A} = i\mathbf{L}; \quad \mathbf{L} \times \mathbf{L} = i\mathbf{L}, \quad (12)$$

$$\mathbf{A} \times \mathbf{L} + \mathbf{L} \times \mathbf{A} = 2i\mathbf{A}. \quad (13)$$

These relations are the generator relations for the R_4 group.

The spin vector $\boldsymbol{\sigma}$ commutes with the Runge-Lenz vector \mathbf{A} . The scalar product $\boldsymbol{\sigma} \cdot \mathbf{A}$ defines the ‘‘Coulomb Helicity Operator’’ for the NRS system as follows:

$$\begin{aligned} \boldsymbol{\sigma} \cdot \mathbf{A}' &= [N^2 - (\boldsymbol{\sigma} \cdot \mathbf{L} + 1)^2]^{-1/2} [-2mH_{NR}]^{-1/2} \\ &\quad \times \{ \boldsymbol{\sigma} \cdot \hat{r} \alpha Z m - i(\boldsymbol{\sigma} \cdot \mathbf{L} + 1) \boldsymbol{\sigma} \cdot \mathbf{p} \} \\ &= [N^2 - (\boldsymbol{\sigma} \cdot \mathbf{L} + 1)^2]^{-1/2} \boldsymbol{\sigma} \cdot \mathbf{A}. \end{aligned} \quad (14)$$

This pseudoscalar operator anticommutes with $\boldsymbol{\sigma} \cdot \mathbf{L} + 1$ as can be verified directly. By means of this anti-commutation property one can formally factorize the operator \tilde{N}^2 of the NR problem. That is

$$\begin{aligned} \tilde{N}^2 &= (\alpha Z)^2 m^2 [-2mH_{NR}]^{-1} = A^2 + L^2 + 1 \quad (15) \\ &= (\boldsymbol{\sigma} \cdot \mathbf{A} + \boldsymbol{\sigma} \cdot \mathbf{L} + 1)^2. \end{aligned} \quad (16)$$

A new linear operator can, therefore, be defined by

$$\tilde{N} = \alpha Z m [-2mH_{NR}]^{-1/2} = (\boldsymbol{\sigma} \cdot \mathbf{A} + \boldsymbol{\sigma} \cdot \mathbf{L} + 1). \quad (17)$$

Like the Weyl equation, to which it is formally similar, this eigenvalue system $\tilde{N} \rightarrow N$ is *not* acceptable as a factorization of the NR Hamiltonian.

The eigenfunctions of the NR Hamiltonian are well known to be (apart from a normalization constant)

$$\langle r \theta \phi | N l m \rangle = F_{Nl}(r) i^l Y_l^m(\theta, \varphi), \quad (18)$$

where the radial function is given in terms of the confluent hypergeometric function

$$\begin{aligned} F_{Nl}(r) &= C e^{-1/2(2k_{NR}r)} (2k_{NR}r)^l \\ &\quad \times {}_1F_1(- (N-l-1), 2l+1; 2k_{NR}r), \quad (19) \\ k_{NR} &= (\alpha Z/N)m, \end{aligned}$$

and is normalized as

$$\int_0^\infty F_{Nl}^2 r^2 dr = 1.$$

It follows that the eigenfunctions for the NRS system are of the form

$$\langle r \theta \phi \sigma_z | N \kappa \mu \rangle = F_{Nl}(r) \phi_{\kappa \mu}. \quad (20)$$

The operator $\boldsymbol{\sigma} \cdot \mathbf{A}$ when expressed in this representation, as was done in Eq. (14), has the property of reversing

the sign of κ :

$$\boldsymbol{\sigma} \cdot \mathbf{A}' | N \kappa \mu \rangle = iS(\kappa) | N - \kappa \mu \rangle, \quad (21)$$

a result which can be easily established by means of the two operator relations

$$(\boldsymbol{\sigma} \cdot \mathbf{A} + \boldsymbol{\sigma} \cdot \mathbf{L} + 1)^2 = A^2 + L^2 + 1 = N^2, \quad (16)$$

$$[\boldsymbol{\sigma} \cdot \mathbf{A}, \boldsymbol{\sigma} \cdot \mathbf{L} + 1]_{\pm} = 0, \quad (22)$$

and also the fact that \mathbf{A} and $\boldsymbol{\sigma}$ commute with \tilde{N}^2 .

From the formal point of view the NRS system has the abstract group structure $SU_2 \times SU_2 \times SU_2$. In order to see this let us note that the NRS system has, as generators, the three commuting ‘‘angular-momentum operators’’

$$\mathbf{j}_1 = \frac{1}{2}(\mathbf{L} + \mathbf{A}), \quad (23)$$

$$\mathbf{j}_2 = \frac{1}{2}(\mathbf{L} - \mathbf{A}), \quad (24)$$

$$\mathbf{j}_3 = \frac{1}{2}\boldsymbol{\sigma}, \quad (25)$$

with

$$\mathbf{j}_i \times \mathbf{j}_i = i\mathbf{j}_i. \quad (26)$$

To complete the synopsis of the NRS system, let us obtain explicit operators which raise and lower the value of κ .

Let us first notice that the vector operator $\boldsymbol{\sigma} \times \mathbf{L}$, which acts on the spin-angle functions $\phi_{\kappa \mu}$, is perpendicular to the angular momentum vector \mathbf{J} . It therefore cannot connect states of the same $|\kappa|$. Since \mathbf{L}^2 commutes with \mathbf{L} we see readily that $\boldsymbol{\sigma} \times \mathbf{L}$ commutes with \mathbf{L}^2 ; thus it leaves $l(l+1) = \kappa(\kappa+1)$ invariant. Since $\boldsymbol{\sigma} \times \mathbf{L}$ cannot change the ‘‘ l ’’ value of the spinors $\phi_{\kappa \mu}$, it must therefore connect either κ or $(-\kappa-1)$. The first possibility is already removed by the perpendicularity, hence $\boldsymbol{\sigma} \times \mathbf{L} \Rightarrow \kappa, -\kappa-1$. Since we already know that the Coulomb helicity operator reverses the sign κ , we can then readily verify the following explicit relations;

$$\begin{aligned} \boldsymbol{\sigma} \cdot \mathbf{A}' (\boldsymbol{\sigma} \times \mathbf{L})_q | N \kappa \mu \rangle &= iS(-\kappa-1) C(j(\kappa), 1, j(\kappa+1); \mu, q, \mu+q) \\ &\quad [\kappa(2\kappa+1)]^{1/2} | N \kappa+1 \mu+q \rangle, \end{aligned} \quad (27)$$

$$\begin{aligned} (\boldsymbol{\sigma} \times \mathbf{L})_q \boldsymbol{\sigma} \cdot \mathbf{A}' | N \kappa \mu \rangle &= iS(\kappa) C(j(\kappa), 1, j(\kappa-1); \mu, q, \mu+q) \\ &\quad \times [\kappa(2\kappa-1)]^{1/2} | N \kappa-1 \mu+q \rangle. \end{aligned} \quad (28)$$

III. THE INTRODUCTION OF THE SYMMETRIC HAMILTONIAN

The symmetric Hamiltonian, to be introduced in this section, constitutes a Dirac Hamiltonian which approximates, with an error of the order of $(\alpha Z)^2/\kappa$, the exact Dirac Hamiltonian with the Coulomb potential. It is logically correct simply to define the symmetric Hamiltonian—out of thin air as it were—and demonstrate that the assertions to be made are correct. Such a procedure, even though valid, is not very satisfying if physical insight is desired and we will accordingly attempt to present the actual motivation that led to the introduction of this symmetric Hamiltonian. Our point

of view will be qualitative and interpretive, for we recognize that a really precise treatment would be excessively involved. Every critical result will be proved directly in succeeding sections.

In order to do this, we need first to summarize some of the main viewpoints and results of paper I. In that paper we demonstrated that there existed a new frame of reference {defined by the transformation $S = \exp[-\frac{1}{2}\rho_2\sigma\cdot\hat{r}\tanh^{-1}(\alpha Z/K)]$ } in which the new "big" and "little" spinors assumed precisely the form of the (two-component) wave functions, in a spherical representation, of the NRS system, with the single distinction that the integer angular momentum l (of the Pauli particle) now became the noninteger angular momentum $\gamma = |\kappa^2 - (\alpha Z)^2|^{1/2}$. The definition of the transformation consisted, in fact, of requiring that this occur. Let us next recall that Sommerfeld obtained his famous energy levels of the hydrogen atom by transforming to a rotating coordinate system in which the relativistic precession (the familiar "rosette" motion) was eliminated and closed orbits occur. The transformation S was shown to be a Lorentz transformation in some sense analogous to the Sommerfeld's transformation.^{9,10}

The coordinate system defined by S is thus that frame of reference in which the relativistic Kepler motion appears most closely similar to the non-relativistic Kepler motion. It is a very natural step then to ask: What are the consequences of assuming that in this special frame the motion is precisely nonrelativistic? The symmetric Hamiltonian is found to emerge as an answer.

In order to obtain this Hamiltonian it suffices to recall that there exists, for the relativistic Kepler problem, a scalar constant of the motion—the Lippmann-Johnson invariant—which (in the coordinate frame S) constitutes the defining differential operator for the radial Coulomb functions, and thus defines radial functions for all limiting cases (NR case and plane-wave case). To define the symmetric Hamiltonian, therefore, one would need only to use the (Lippmann-Johnson) operator in nonrelativistic form—that is, $l(\gamma) \rightarrow l(\kappa)$ or $|\gamma| \rightarrow |\kappa|$. The desired Hamiltonian then results from Eq. (24a) of I with $|\gamma| \rightarrow |\kappa|$ and $m \rightarrow -m$.¹¹

This leads to the Hamiltonian

$$\tilde{H} = S_1^2 H_p = \{ \exp[-\rho_2\sigma\cdot\hat{r}\sinh^{-1}(\alpha Z/K)] \} \times (\rho_1\sigma\cdot\mathbf{p} - \rho_3 m_0). \quad (29)$$

The Hamiltonian is not Hermitian and is, of course,

⁹ A. Sommerfeld, *Atomic Structure and Spectral Lines* (E. P. Dutton & Company Inc., New York, 1931), p. 254.

¹⁰ A transformation to a rotating coordinate frame does not belong to special relativity and the statement made here is not to imply a genuine equivalence but only to mean that the Lorentz transformation S appears to transform to a coordinate system agreeing instantaneously with the rotating system. The total angular momentum in fact commutes with S ; see, for instance, I Sec. B.

¹¹ This latter step is required since Eq. (24a) of I is the Dirac-Coulomb operator in the frame S having negative mass, i.e., SO_{-S}^{-1} of paper I.

not required to be. In order to obtain a Hermitean Hamiltonian we transform \tilde{H} by the operator S_1 and obtain

$$H_{\text{sym}} = S_1^{-1}\tilde{H}S_1 = S_1 H_p S_1 \quad (30)$$

$$= H_{\text{Dirac}} + H_{\text{fs}}, \quad (31)$$

where¹² the fine structure interaction

$$H_{\text{fs}} \equiv \rho_2(\sigma\cdot\hat{r}/r)K\{[1+(\alpha Z/K)^2]^{1/2}-1\}. \quad (32)$$

The first point to note is that the transformation S_1 is not the same as the one which takes the Dirac equation into its "most nonrelativistic" form. The two transformations differ by terms $\mathcal{O}(\alpha Z)^3$. The fact that the two frames S and S_1 differ in $\mathcal{O}(\alpha Z)^3$ has a consequence that any straightforward approximation of the Dirac-Coulomb functions, as an expansion in αZ (the Sommerfeld-Maue definition, for example) inevitably confuses two different effects: the effect of nonrational $l(\gamma)$ and the effect of the different coordinate frames. The result would be literally impossible to untangle.

As was pointed out in the introduction, the S-M-M-F wave functions were first obtained as approximations to the exact Dirac-Coulomb functions. Later Sommerfeld¹³ presented a systematic view which is briefly as follows: The iterated Dirac-Coulomb Hamiltonian contains three terms in $\alpha Z - \alpha Z/r$, $\alpha Z\rho_1(\sigma\cdot\hat{r}/r^2)$, $(\alpha Z/r)^2$ —of which the first (Coulomb) term is considered to belong to the zeroth-order operator, D . Sommerfeld and Maue expressed the solution Ψ to the iterated equation as a power series in αZ

$$\Psi = \Phi_0 + (\alpha Z)\Phi_1 + (\alpha Z)^2\Phi_2 + \dots,$$

and the projected component $D\Psi$ (in their notation) was the solution to the linear (Dirac) equation. Apart from the fact that even the first approximation Φ_1 contains a factor which has to be determined differently for different applications, the projected component $D\Psi$, accurate only up to $\mathcal{O}(\alpha Z)$, is not of particular simplicity. The function $\Phi_0 + \alpha Z\Phi_1$ is usually referred to as the "Sommerfeld-Maue function." For such a function, defined as part of a series expansion, the question of a Hamiltonian basis is not relevant. This is in sharp contrast to the solutions of H_{sym} , which clearly are also solutions of the iterated equation. In point of fact $\Phi_0 + \alpha Z\Phi_1$ fails [in order $(\alpha Z)^2$] to satisfy the iterated Dirac-Coulomb equation, either in the zeroth order (D of Sommerfeld) or even when the "spin-correction term" $\alpha Z\rho_1(\sigma\cdot\hat{r}/r^2)$ is included. The origin of this behavior may be traced to the fact that the spin-dependent perturbation in the S-M method really belongs to the zeroth-order system in the appropriate frame of reference, as does a part of the $(\alpha Z/r)^2$ term. The essential "perturbation" in the Dirac-Coulomb Hamiltonian is the "fine structure interaction" as shown

¹² L. C. Biedenharn, *Bull. Am. Phys. Soc.* **7**, 314 (1962).

¹³ A. Sommerfeld, *Atombau und Spektrallinien* (F. Vieweg & Sohn, Braunschweig, 1960), p. 408.

above. This distinguishes our approach from that of Sommerfeld-Maue.

It should be noted that the fine structure interaction is of order $(\alpha Z)^2/|\kappa|$, which indicates that the S-M series in powers of αZ is unduly restrictive, as noted first by Bethe and Maximon.¹⁴ It is clear that the spherical solutions of H_{sym} differ from the exact spherical Dirac-Coulomb functions in the same order¹⁵ $(\alpha Z)^2/|\kappa|$.

IV. SOLUTIONS OF \tilde{H} AND NORMALIZATION

Out of the spherical spinors of Eq. (1) one can easily build the simultaneous eigenvectors of the commuting operators K and $\rho_2 \sigma \cdot \hat{r}$;

$$K \begin{pmatrix} \phi_{-\kappa}^\mu \\ \phi_{\kappa}^\mu \end{pmatrix} = \kappa \begin{pmatrix} \phi_{-\kappa}^\mu \\ \phi_{\kappa}^\mu \end{pmatrix}, \quad (33)$$

$$\rho_2 \sigma \cdot \hat{r} \begin{pmatrix} \phi_{-\kappa}^\mu \\ \phi_{\kappa}^\mu \end{pmatrix} = S(-\kappa) \begin{pmatrix} \phi_{-\kappa}^\mu \\ \phi_{\kappa}^\mu \end{pmatrix}. \quad (34)$$

In order to solve the eigenvalue equation

$$\tilde{H} \Psi_{N\kappa\mu} = E_N \Psi_{N\kappa\mu}, \quad (35)$$

let us rewrite the above equation as

$$[i\rho_2 \sigma \cdot \mathbf{p} + m_0 + E S_1^{-2} \rho_3] \Psi = 0. \quad (36)$$

If we now iterate this equation by multiplying on the left with $(-\rho_2 \sigma \cdot \mathbf{p} + m_0 - E S_1^{-2} \rho_3)$, we get a second-order equation which, when we use the relation

$$[i\rho_2 \sigma \cdot \mathbf{p}, S_1^{-2} \rho_3]_+ = 2\alpha Z/r, \quad (37)$$

reduces to

$$[\nabla^2 + (E^2 - m_0^2) + 2\alpha Z E/r] \Phi = 0; \quad (38)$$

a solution of which is easily written down

$$\Phi = \begin{pmatrix} 0 \\ |N\kappa\mu\rangle \end{pmatrix}. \quad (39)$$

Here we have put $k^2 = m_0^2 - E^2$ in the radial function. Now by a procedure exactly similar to that adopted in paper I Sec. III, one arrives at the solution (unnormalized)

$$\Psi_{N-\kappa\mu} = \begin{pmatrix} k [(N^2/\kappa^2) - 1]^{1/2} |N-\kappa\mu\rangle \\ -(E_N [1 + (\alpha Z/\kappa)^2]^{1/2} + m_0) |N\kappa\mu\rangle \end{pmatrix}. \quad (40)$$

We notice that the factors multiplying the spinors $|N\kappa\mu\rangle$ and $|N-\kappa\mu\rangle$ are not constants, as in the non-

relativistic case, but are functions dependent on N and κ obeying the condition that their ratio is fixed. It is this dynamical coupling of the relativistic particle to the Coulomb field that makes the representation space of the eigenfunctions $\Psi_{N\kappa\mu}$ not a mere doubling of the space of $|N\kappa\mu\rangle$. Since \mathbf{J}^2 , J_z and K commute with \tilde{H} , these solutions have sharp $j = |\kappa| - \frac{1}{2}$ and $\mu = j_z$ and κ . Their parity is $(-)^{l(\kappa)}$.

The transformation S_1 introduces some new features. It is not a unitary operator and, as we have noted earlier, \tilde{H} is not Hermitean although H_{sym} is. In fact we have

$$S_1^{-1} = \rho_3 S_1 + \rho_3 \neq S_1^{-1}. \quad (41)$$

In order to make the charge of the particle invariant it is necessary to normalize the eigenfunctions such that

$$(\Psi_{N\kappa\mu}, S_1^{-2} \Psi_{N\kappa\mu}) = 1. \quad (42)$$

This ensures the invariance of the eigenvalue E_N . Remembering that \tilde{H} is a transform of the Hermitean Hamiltonian H_{sym} we see readily

$$\tilde{H} = S_1 H_{\text{sym}} S_1^{-1}, \quad (43)$$

$$\Psi_{N\kappa\mu} = S_1 \Psi_S; \quad H_{\text{sym}} \Psi_S = E_N \Psi_S, \quad (44)$$

$$(\Psi_S, \Psi_S) = (\Psi_{N\kappa\mu}, S_1^{-2} \Psi_{N\kappa\mu}) = 1, \quad (45)$$

$$(\Psi_S, H_{\text{sym}} \Psi_S) = (\Psi_{N\kappa\mu}, \tilde{H} \Psi_{N\kappa\mu}) = E_N. \quad (46)$$

We thus have a situation similar to the Pauli adjoint in the Dirac theory. For expanding an arbitrary vector in this complete orthonormal set we use the projection operator

$$\mathcal{P}_{N\kappa\mu} = \Psi_{N\kappa\mu} (\Psi_{N\kappa\mu}, S_1^{-2}), \quad (47)$$

and

$$\Psi = \sum_{N\kappa\mu} \mathcal{P}_{N\kappa\mu} \Psi. \quad (48)$$

Introducing the dimensionless functions

$$\epsilon_N = [1 + (\alpha Z/N)^2]^{1/2}, \quad (49)$$

$$\zeta(\kappa^2) = \epsilon_N [1 + (\alpha Z/\kappa)^2]^{1/2}, \quad (50)$$

the normalized eigenfunctions are

$$\Psi_{N-\kappa\mu} = \begin{pmatrix} \left\{ \frac{[\zeta(\kappa^2) - 1] \epsilon_N}{2(2\zeta^2 - 1)} \right\}^{1/2} |N-\kappa\mu\rangle \\ - \left\{ \frac{[\zeta(\kappa^2) + 1] \epsilon_N}{2(2\zeta^2 - 1)} \right\} |N\kappa\mu\rangle \end{pmatrix}. \quad (51)$$

Let us next consider the second-order differential equation satisfied by the solutions of \tilde{H} . It is easiest to work in the frame S wherein, after iterating SO_S^{-1} , we get

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{2\alpha Z E}{r} + (E^2 - m_0^2) - \frac{\Gamma(\Gamma - 1)}{r^2} \right] \Phi = 0. \quad (52)$$

¹⁴ H. A. Bethe and L. C. Maximon, Phys. Rev. **93**, 768 (1953).

¹⁵ In discussing the inaccuracy in the S-M-M-F functions Bethe and Maximon initially asserted that the error was of the order of $(\alpha Z/l)^2$. A note added in proof (p. 773) corrects this to $(\alpha Z)^2/l$ —although one may be misled by the fact that the abstract and introductory discussion of their paper have not been corrected accordingly.

Transforming this into the frame of the symmetric Hamiltonian we have

$$\Gamma \rightarrow \rho_3 K \rightarrow \kappa, \quad \Gamma^2 \rightarrow \kappa^2. \quad (53)$$

Using the relation

$$\kappa(\kappa+1) = l(l+1), \quad (54)$$

this gives

$$[\nabla^2 + (2\alpha ZE/r) + E^2 - m_0^2]\Phi = 0. \quad (55)$$

This second-order differential operator is precisely the Klein-Gordon operator for the Coulomb field with the single exception that the term $(\alpha Z/r)^2$ has been discarded. \tilde{H} is thus an exact factorization of the Klein-Gordon equation given in Eq. (55).

VI. BOUND STATES

The energies of the bound states, the wave functions for which have already been given in Eq. (51), are given by

$$E_N = m_0 c^2 / [1 + (\alpha Z/N)^2]^{1/2}. \quad (56)$$

In contrast to the usual Dirac equation it is here seen that the energy is dependent only on the "principal quantum number N " just as in the nonrelativistic case. The system is therefore again degenerate, or, as stated earlier, the fine structure is "turned off." From the usual boundary condition on the wave function we see that the radial part of the wave function satisfies the requirement that $N-l-1$ is 0 or a positive integer. We have, however,

$$\kappa = l \quad \text{if } \kappa = +(j + \frac{1}{2}), \quad \text{or} \quad l = |\kappa|, \quad (57)$$

$$= -(l+1) \quad \text{if } \kappa = -(j + \frac{1}{2}), \quad \text{or} \quad l+1 = |\kappa|. \quad (58)$$

If we set $\kappa = -j - \frac{1}{2}$ or $\kappa = -l - 1$, we see that κ can take all possible values $\kappa = -N, -N+1, \dots, +N$. On the other hand, when $\kappa = j + \frac{1}{2}$ or $l = \kappa$, we see that $\kappa = +N$ does not give an acceptable wave function as $N > \kappa + 1$. Thus each $|\kappa|$ occurs twice, except for $\kappa = +N$, and there are $2|\kappa|$ eigenfunctions for each value of κ corresponding to $\mu = -(|\kappa| - \frac{1}{2}), \dots, +(|\kappa| - \frac{1}{2})$. The total number of eigenfunctions belonging to a given value of N is therefore

$$\sum_{\kappa=-N}^N 2\{2|\kappa| - N\} = 2N^2, \quad (59)$$

corresponding to the N^2 eigenstates, each having the energy $E_{NR}/m = \frac{1}{2}(\alpha Z/N)^2$ in the nonrelativistic theory.

While we have noted that for $\kappa = N$ there is no solution, it is important also to note that for $\kappa = -N$, Ψ has but a single component in ρ space. An interesting way of interpreting these results is provided by a relativistic Coulomb helicity operator $\tilde{\Lambda}$ (to be presently introduced in the next section) which anticommutes with the Dirac operator K . These two operators cannot be simultaneously sharp, *unless one operator has the eigenvalue zero.*

This, in fact, occurs since for $\kappa = -N$, both $\tilde{\Lambda}$ and K are simultaneously sharp and, therefore, $\tilde{\Lambda} \rightarrow 0$. Since $\tilde{\Lambda}$ expresses the degeneracy with respect to the direction of rotation of an ellipse (about a perpendicular axis) one sees that for $\kappa = -N$ the lack of degeneracy ($\tilde{\Lambda} \rightarrow 0$) expresses the fact that the ellipse degenerates to a circular orbit and the rotation of the "major" axis has, therefore, no meaning.

VI. SYMMETRY AND INVARIANT OPERATORS

We have already mentioned that the angular momentum \mathbf{J} and the Dirac operator K commute with the symmetric Hamiltonian. A Hermitean operator which also commutes with this Hamiltonian is the "relativistic Coulomb helicity operator" defined as follows:

$$\tilde{\Lambda} = [m_0^2 - \tilde{H}^2]^{-1/2} \{ \rho_3 \alpha Z \boldsymbol{\sigma} \cdot \hat{r} \tilde{H} - i K \boldsymbol{\sigma} \cdot \mathbf{p} \}. \quad (60)$$

This can be conceived of as the nonrelativistic operator $\boldsymbol{\sigma} \cdot \mathbf{A}$ generalized by ρ_3 doubling to the four-component form and m (i.e., mc^2) replaced by the relativistic energy operator \tilde{H} . $\tilde{\Lambda}$ obeys the commutation relations

$$[\tilde{H}, \tilde{\Lambda}] = 0, \quad (61)$$

$$[\mathbf{J}, \tilde{\Lambda}] = 0, \quad (62)$$

$$[K, \tilde{\Lambda}]_+ = 0. \quad (63)$$

The following operator relations are used in establishing the vanishing of the commutator $[\tilde{\Lambda}, \tilde{H}]$:

$$[K, \rho_2 \boldsymbol{\sigma} \cdot \mathbf{p}] = 0, \quad (64)$$

$$\rho_2 [\boldsymbol{\sigma} \cdot \hat{r}, \boldsymbol{\sigma} \cdot \mathbf{p}]_+ S_1^2 = S_1^{-2} \rho_2 [\boldsymbol{\sigma} \cdot \hat{r}, \boldsymbol{\sigma} \cdot \mathbf{p}]_+, \quad (65)$$

$$[\rho_3 \boldsymbol{\sigma} \cdot \hat{r}, \tilde{H}] = i S_1^2 \rho_2 [\boldsymbol{\sigma} \cdot \hat{r}, \boldsymbol{\sigma} \cdot \mathbf{p}]_+, \quad (66)$$

$$[\boldsymbol{\sigma} \cdot \mathbf{p}, \tilde{H}] = \alpha Z K^{-1} \rho_2 [\boldsymbol{\sigma} \cdot \mathbf{p}, \boldsymbol{\sigma} \cdot \hat{r}]_+ H_p. \quad (67)$$

$\tilde{\Lambda}$ reverses the sign of κ in $\Psi_{N\kappa\mu}$ and the analog of Eq. (21) is obtained by straightforward computation,

$$\tilde{\Lambda}' \Psi_{N\kappa\mu} \equiv i S(-\kappa) [N^2 - K^2]^{-1/2} \tilde{\Lambda} \Psi_{N\kappa\mu} = \Psi_{N-\kappa\mu}. \quad (68)$$

Defining an operator $\tilde{\xi} = \tilde{H} [1 + (\alpha Z/K)^2]^{1/2}$, if we rewrite $\tilde{\Lambda}$ as

$$\tilde{\Lambda} = [m_0^2 - \tilde{H}^2]^{-1/2} \{ \rho_2 K m_0 + i \rho_1 K \tilde{\xi} \} \quad (69)$$

and square both sides we get

$$[m_0^2 - \tilde{H}^2] \tilde{\Lambda}^2 = -K^2 \{ i m_0 [\rho_2, \rho_1 \tilde{\xi}]_+ - (\rho_1 \tilde{\xi})^2 + m_0^2 \}. \quad (70)$$

Using the following relation

$$[\rho_1 \tilde{H}, \rho_2]_+ = -2i \rho_3 [1 + (\alpha Z/K)^2]^{1/2} S_1^{-2} \tilde{H}, \quad (71)$$

Eq. (70) reduces to

$$\tilde{\Lambda}^2 + K^2 = (\alpha Z)^2 \tilde{H}^2 [m_0^2 - \tilde{H}^2]^{-1} = \tilde{N}^2. \quad (72)$$

One can also define an operator

$$\tilde{N} = \tilde{\Lambda} + K = \{ (\alpha Z)^2 \tilde{H}^2 [m_0^2 - \tilde{H}^2]^{-1} \}^{1/2},$$

which has the eigenfunction

$$\begin{aligned} \Phi_{Nj\mu} &= [(N+\kappa)/2N]^{1/2} \Psi_{N-\kappa\mu} \\ &+ [1/2N(N+\kappa)]^{1/2} \tilde{\Lambda} \Psi_{N-\kappa\mu} \\ &\equiv \begin{pmatrix} a | -Nj\mu \rangle \\ b | +Nj\mu \rangle \end{pmatrix}, \quad (73a) \end{aligned}$$

a and b being the functions multiplying the spinors in Eq. (51). The eigenvalues of \tilde{N} are $\pm N$, for all $j \neq N - \frac{1}{2}$, while for $j = N - \frac{1}{2}$ only $-N$ occurs. The $\Phi_{Nj\mu}$ are "helicity" eigenstates and do not have a sharp parity except for $j = N - \frac{1}{2}$.

While the operator that reverses the sign of κ is easily obtained from a generalization of the corresponding operator in the NRS system, it is unfortunate that the "raising" and "lowering" operators are not so simply obtained. The basic structure of the operator is given below:

$$\begin{aligned} \rho_1 S_1^{-2} \left[\left(\frac{\boldsymbol{\sigma} \times \mathbf{L}}{2} \right)_q \left(\frac{1 + \rho_3}{2} \right), \tilde{H} \right] \Psi_{N\kappa\mu} &\equiv (\boldsymbol{\Omega})_q \Psi_{N\kappa\mu} \\ &= \omega_- C(j(\kappa), 1, j(\kappa-1); \mu, q, \mu+q) \Psi_{N-\kappa-1, \mu+q}, \quad (73) \end{aligned}$$

where ω_- is a function of κ^2 and N . Making use of the operators

$$\alpha Z \tilde{H} [m_0^2 - \tilde{H}^2]^{-1/2} = \tilde{N} \rightarrow N, \quad (74)$$

$$\tilde{D} = \tilde{N} - \frac{1}{2} \rightarrow D = N - \frac{1}{2}, \quad (75)$$

we build the following three parts of a vector operator and indicate what they do to an eigenfunction of the symmetric Hamiltonian \tilde{H} .

$$\begin{aligned} (\mathbf{K}^-)_q \Psi_{N-\kappa\mu} &= [\tilde{D}^2 - (K + \frac{1}{2})^2]^{1/2} \left(\frac{1}{2K+1} \right) \left(\frac{K}{K+1} \right)^{1/2} (\boldsymbol{\Omega})_q \\ &\times \{ 2(2\tilde{\xi}^2 - 1)(\tilde{\xi} - 1)^{-1} \tilde{H}^{-1} \}^{1/2} \Psi \quad (76) \\ &= D [2 - (\kappa - \frac{1}{2})^2]^{1/2} C(\kappa - \frac{1}{2}, 1, \kappa - \frac{3}{2}; \frac{1}{2}, 0, \frac{1}{2}) \\ &\times C(j(\kappa), 1, j(\kappa-1); \mu, q, \mu+q) \\ &\times \Psi_{N-(\kappa-1), \mu+q}. \quad (77) \end{aligned}$$

$$\begin{aligned} (\mathbf{K}^+)_q &= [\tilde{D}^2 - (K - \frac{1}{2})^2]^{1/2} \\ &\times \left(\frac{1}{2K-1} \right) \left(\frac{K}{K-1} \right)^{1/2} \tilde{\Lambda}' (\boldsymbol{\Omega})_q \\ &\times \tilde{\Lambda}' \{ 2(2\tilde{\xi}^2 - 1)(\tilde{\xi} - 1)^{-1} \tilde{H}^{-1} \}^{1/2}. \quad (78) \end{aligned}$$

$$\begin{aligned} (\mathbf{K}^+)_q \Psi_{N-\kappa\mu} &= [D^2 - (\kappa + \frac{1}{2})^2]^{1/2} \\ &\times C(\kappa - \frac{1}{2}, 1, \kappa + \frac{1}{2}; \frac{1}{2}, 0, \frac{1}{2}) \\ &\times C(j, 1, j(\kappa+1); \mu, q, \mu+q) \\ &\times \Psi_{N-(\kappa+1), \mu+q}. \quad (79) \end{aligned}$$

$$(\mathbf{K} \parallel)_q = \frac{1}{2} D [(K - \frac{1}{2})(K + \frac{1}{2})]^{-1/2} (\mathbf{J})_q. \quad (80)$$

$$\begin{aligned} (\mathbf{K} \parallel)_q \Psi_{N-\kappa\mu} &= D C(\kappa - \frac{1}{2}, 1, \kappa - \frac{1}{2}; \frac{1}{2}, 0, \frac{1}{2}) \\ &\times C(j, 1, j; \mu, q, \mu+q) \Psi_{N-\kappa, \mu+q}. \quad (81) \end{aligned}$$

In other words, the three parts commute with the symmetric Hamiltonian and, therefore, the vector operator $\mathbf{K} = \mathbf{K}^+ + \mathbf{K}^- + \mathbf{K} \parallel$ is an invariant. In spite of the occurrence of operators in the denominators of \mathbf{K} it is important to note that the circumstances are such that the operators are always well defined. ζ for instance cannot assume the value 1, and by restriction of the values which κ can take relative to a given N , ζ^2 can never assume the value $\frac{1}{2}$. By construction ζ is positive and hence $\zeta + 1$ cannot be singular. The operators $K \pm 1$ do not operate before the commutator $[\boldsymbol{\sigma} \times \mathbf{L}, \tilde{H}]$ and this ensures that they do not contribute any singularity. The factor $[(K - \frac{1}{2})(K + \frac{1}{2})]^{1/2}$ is just $[j(j+1)]^{1/2}$. Thus, though very complicated in structure, \mathbf{K} is always well defined. The following relations are easily established by direct computation:

$$[K_i, K_j] \Psi_{N\kappa\mu} = i \epsilon_{ijk} J_k \Psi_{N\kappa\mu}, \quad (82)$$

$$2\mathbf{J} \cdot \mathbf{K} \Psi_{N\kappa\mu} = (\tilde{N} - \frac{1}{2}) \Psi_{N\kappa\mu}, \quad (83)$$

$$\{ (\mathbf{J} + \mathbf{K})^2 + 1 \} \Psi_{N\kappa\mu} = \tilde{N}^2 \Psi_{N\kappa\mu}. \quad (84)$$

Since the $\Psi_{N\kappa\mu}$ form a complete orthonormal set, we conclude that the operator relations are themselves valid. From \mathbf{J} and \mathbf{K} we can form the commuting pair of vectors

$$\mathbf{j}_1 = \frac{1}{2} (\mathbf{J} + \mathbf{K}), \quad (85)$$

$$\mathbf{j}_2 = \frac{1}{2} (\mathbf{J} - \mathbf{K}), \quad (86)$$

$$[\mathbf{j}_1, \mathbf{j}_2] = 0, \quad (87)$$

which guide us in the computation of the total number of independent vectors in the subspace of a given N (degree of degeneracy, in the case of bound states). Since $\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2$ we have, by the vector addition theorem,

$$j_1 + j_2 \geq J \geq |j_1 - j_2|.$$

We have the following assignment dictated by the admissible values of κ :

$$\begin{aligned} \kappa = -ve; \quad j_1 + j_2 = N - \frac{1}{2}; \quad |j_1 - j_2| = \frac{1}{2}; \\ j_1 = N/2; \quad j_2 = (N-1)/2, \\ \text{number of states} = N(N+1) \end{aligned}$$

$$\begin{aligned} \kappa = +ve; \quad j_1 + j_2 = N - \frac{3}{2}; \quad |j_1 - j_2| = \frac{1}{2}; \\ j_1 = (N/2) - 1; \quad j_2 = (N-1)/2, \\ \text{number of states} = N(N-1). \end{aligned}$$

Thus the total number of states is $2N^2$, a result which has been established earlier from the wave functions. In view of Eqs. (76)–(87) we conclude that the group of the symmetric Hamiltonian is at least as large as the four dimensional rotation group R_4 .¹⁶

¹⁶ The complete symmetry group is, however, larger and appears to be a factor group of a semidirect product of $(SU_2)^2$.

It is interesting to note in passing that there exists for the plane-wave free-particle Dirac Hamiltonian a vector *invariant* operator which can be obtained by letting $(\alpha Z) \rightarrow 0$ in Eq. (73) and after slight modification, as

$$\mathfrak{R}/i = \rho_2 [H_p, i\sigma \times \mathbf{L}/2] [H_p^2 - m_0^2]^{-1/2}. \quad (88)$$

If we multiply this vector operator by i we see that it obeys the relation

$$\mathfrak{R} \times \mathfrak{R} = -i\mathbf{J}. \quad (89)$$

This is to be contrasted with the generator of the inhomogeneous Lorentz group corresponding to the "Lorentz rotation" discussed by Foldy¹⁷

$$\frac{1}{2} [\mathbf{r}, H_p]_+ - t\mathbf{p}. \quad (90)$$

However, unlike the latter, \mathfrak{R} does not satisfy the requirement

$$[\mathfrak{R}_i, H_p] = ip_i. \quad (91)$$

¹⁷ L. Foldy, Phys. Rev. **102**, 569 (1956).

ACKNOWLEDGMENTS

We would like to thank Professor E. Greuling and Professor F. Tangherlini for several helpful discussions on the contents of this paper.

Note added in proof. We would like to call attention to the work of Egil Hylleraas [Z. Physik **164**, 493 (1961)], which—in addition to the work of P. C. Martin and R. J. Glauber (cited in I)—also obtained earlier some of the results given in I. [Let us note, too, that K. A. Johnson's suggestion of the importance of the operator Γ is, by mistake, cited (in I) wrongly in footnote 3 and not footnote 2 where it belonged!]

The earliest work along these lines is contained in the book of G. Temple [*The General Principles of Quantum Mechanics*, (Methuen, and Company, Ltd., New York, 1948), p. 92 ff]. We are indebted to Professor E. Guth, Professor S. Bludman, and Professor C. Schwartz for calling Temple's work to our attention, too late to be included in paper I, however. Unfortunately Temple's treatment is not wholly correct.