and

$$\nu_0 = \left[(2S_3^z - S_3^x - S_3^y) / 18p_2 c_3 \right]^{\frac{1}{2}}.$$
 (50)

For $I=\frac{3}{2}$, Eq. (49) is indeterminate but c_3 can be determined by eliminating ν_0 between Eqs. (37) and (47).

Experimental data recently obtained from Al²⁷ and Be⁹ resonances in beryl¹⁰ have been reviewed in terms of the above procedure. The resulting coupling constants were found to be essentially identical with those calculated previously on the basis of expressions for individual energy levels.

The third special case involves determining S_2 and S_3 at two different magnitudes of the magnetic field, say *H* and λH . From the resulting two sets of equations for $S_2(H), S_2(\lambda H), S_3(H), S_3(\lambda H)$ it follows that

$$\nu_0 = \{ [S_2(\lambda H) - S_2(H)] / p_1(\lambda^2 - 1) \}^{\frac{1}{2}}$$
(51)

$$c_{3}^{2}(1+\eta^{2}/3) = [\lambda^{2}S_{2}(H) - S_{2}(\lambda H)]/p_{2}(\lambda^{2}-1)$$

$$c_{3}^{3}(1-\eta^{2}) = [\lambda^{2}S_{3}(H) - S_{3}(\lambda H)]/p_{3}(\lambda^{2}-1),$$
(52)

(53) I≠<u>3</u>.

The values of η and c_3 follow from Eqs. (52) and (53) in

a manner similar to that given by Eqs. (45) and (46). It should be noted that, for $\eta=0$, the quantities S_2

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"Contact Interaction" in the Relativistic Energy of Two-Electron Atoms

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It is shown that the "contact interaction" recently pointed out by Sessler, Sucher, and Foley for the relativistic two-electron atoms can be very simply and unambiguously obtained from the field-theoretical form of the theory of Breit and Møller, whereas the original "reduction" procedure (reducing the equation for the 16-component wave function to one for the four big components by successive approximation) does not lead to this contact term. The effect of the singular behavior of relativistic wave function at the origin gives rise to a correction of order α^4 in the energy.

I. INTRODUCTION¹

HE problem of finding the relativistic energy of a two-electron atom (He-like atoms) was first treated by Breit.² Many calculations have been made

Our result is essentially the same as that of Berestetskii and Landau, reference 5. Our method differs from theirs in that we use the wave functions in (15) thereby obtaining the relativistic correction very simply by one simple integration in (18), whereas the other authors express the small components in terms of the big components and obtain the various operators in (11) and (12) in separate forms in a longer calculation.
 ² G. Breit, Phys. Rev. 34, 553 (1929); 39, 616 (1932).

subsequently. Recently, Sessler and Foley³ gave on classical arguments an additional term of order $(v/c)^2$ in the energy of the ground state of helium, and in a more recent paper. Sucher and Folev⁴ obtained this additional term from the original method of Breit. This term, of the nature of a contact potential and previously found also by Berestetskii and Landau⁵ in connection with the positronium problem, has in fact been found much earlier and included in their work by Breit and his co-workers,6 although not explicitly in connection with the ground state of helium. The purpose of the present work is to point out that by

and S_3 determined at two values of H_0 are sufficient to determine the angle θ between the field and the unique axis of ∇E .

III. CONCLUSIONS

The procedure of relating experimental data to theory through the coefficients of secular polynomials can be used advantageously in those cases in which the mathematically equivalent method of relating their roots, the individual energy levels, presents computational difficulties.

Application of the procedure to nuclear resonances in crystals results in relatively simple general expressions for the coupling constants in terms of the resonant frequencies.

Energy relations for the asymmetric rotator, similar to those for the pure quadrupole case, can be developed by a corresponding procedure.

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¹After the above work was finished, our attention has been called by Dr. S. Shanmugadhasan, to whom we wish to express our thanks, to a paper by A. I. Andreev, Vestnik Moskov. Univ. Ser. Fiz.-Mat. i Estestven. Nauk 3, No. 5, 65–9 (1954), in which the author employs simultaneously the reduction procedure to the big components and the matrix element of H in (1) with respect to the 16-component wave function, thereby obtaining the contact term H_c of (12), but also the B'^2 term in (10) [or the $H^{(7)}$ in (11)] as well. The procedure given in Sec. III in the present note gives H_c but not $H^{(7)}$.

 ³ A. M. Sessler and H. M. Foley, Phys. Rev. 92, 1321 (1953).
 ⁴ J. Sucher and H. M. Foley, Phys. Rev. 95, 966 (1954).
 ⁵ V. Berestetskii and L. Landau, J. Exptl. Theoret. Phys. (U.S.S.R.) 19, 673 (1949).
 ⁶ G. Breit, Phys. Rev. 72, 1023 (1947); G. Breit and G. E. Brown, Phys. Rev. 74, 1278 (1948); Breit, Brown, and Arfken, Phys. Rev. 76, 1299 (1949).

following the original procedure (reduction of 16component wave equation to one for the 4 big components), one does not obtain the contact term, whereas a calculation of the interaction between the two electrons in the manner of Breit and of Møller⁷ does lead very simply and unambiguously to this contact term.

II. "REDUCTION" PROCEDURE

The theory of Breit² in the earlier form is as follows. The Hamiltonian of a two-electron atom is taken to be

$$H(1,2) = H_0(1) + H_0(2) + \frac{e^2}{r_{12}} + B, \qquad (1)$$

where H_0 is the Dirac Hamiltonian for one electron:

$$H_0(1) = -c(\boldsymbol{\alpha}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) - \beta_{\mathrm{I}} m c^2 - Z e^2 / r_1, \qquad (2)$$

$$B = -\frac{e^2}{2r_{12}} \left[(\boldsymbol{\alpha}_{\mathrm{I}} \cdot \boldsymbol{\alpha}_{\mathrm{II}}) + \frac{1}{r_{12}^2} (\boldsymbol{\alpha}_{\mathrm{I}} \cdot \mathbf{r}_{12}) (\boldsymbol{\alpha}_{\mathrm{II}} \cdot \mathbf{r}_{12}) \right], \quad (3)$$

$$\mathbf{\Pi}_{\mathbf{I}x} = p_{\mathbf{I}x} + (e/c)A_{\mathbf{I}x}.$$

Here and in the following, the subscripts I, II refer to electron 1 and 2 respectively. On writing

$$\mathbf{\Pi}_{0} = -\frac{\hbar}{i} \frac{\partial}{\partial t} + \frac{Ze^{2}}{c} \left(\frac{1}{r_{1}} + \frac{1}{r_{2}}\right) - \frac{e^{2}}{cr_{12}}, \qquad (4)$$

and on denoting the 16-component wave function ψ by four 4-component wave functions

ψ

$$= \begin{pmatrix} \phi & u \\ v & \Psi \end{pmatrix}, \tag{5}$$

and writing

$$B' = \frac{e^2}{2r_{12}} \bigg[(\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\sigma}_{\mathrm{II}}) + \frac{1}{r_{12}^2} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{r}_{12}) (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{r}_{12}) \bigg], \qquad (6)$$

where σ_{I} , σ_{II} are the Pauli matrices for the two electrons, the wave equation can be put in the form

$$(\Pi_0 - 2mc)\Psi + (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})u + (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}})v + (B'/c)\phi = 0, (7a)$$

$$(\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})\Psi + \boldsymbol{\Pi}_{0}\boldsymbol{u} + (B'/c)\boldsymbol{v} + (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}})\boldsymbol{\phi} = 0, (7\mathrm{b})$$

$$(\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}})\Psi + (B'/c)u + \Pi_0 v + (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})\phi = 0, \ (7c)$$

$$(B'/c)\Psi + (\boldsymbol{\sigma}_{II} \cdot \boldsymbol{\Pi}_{II})u + (\boldsymbol{\sigma}_{I} \cdot \boldsymbol{\Pi}_{I})v + (\Pi_{0} + 2mc)\phi = 0.$$
 (7d)

The 12 small components ϕ , u, v are expressed in terms of the 4 big components Ψ by solving (7b), (7c), (7d) by successive approximation,⁸

$$\phi \cong \frac{1}{4m^2c^2} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi - \frac{B'}{4mc^2} \Psi, \qquad (8)$$

$$u \cong - \Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \Psi + \underbrace{2mc^2}_{2mc^2} B' \Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi - \Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \phi,$$
(9)

$$v \cong -\Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi + \frac{1}{2mc^2} B' \Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \Psi - \Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \phi,$$

⁷ C. Møller, Z. Physik **70**, 786 (1931). ⁸ From (7b) and (7c), one obtains u, v up to (v/c). Putting these into (7d), one obtains ϕ up to $(v/c)^2$ in (8). Putting this back in (7b) and (7c) one obtains u, v in (9).

such that when they are substituted in Eq. (7a), all quantities of order $(v/c)^4$ are included. On using (8) and (9), Eq. (7a) gives the original equation of Breit for the 4 big components

$$\frac{1}{2mc} - 1 - \frac{1}{2mc} \{ (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \boldsymbol{\Pi}_{0}^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \\
+ (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \boldsymbol{\Pi}_{0}^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \} - \frac{1}{8m^{4}c^{4}} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})^{2} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}})^{2} \\
+ \frac{1}{8m^{3}c^{4}} \{ (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) B' (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) + (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) B' (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \\
+ B' (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) + (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) B' \} \\
- \frac{1}{8m^{2}c^{4}} B'^{2} \Psi = 0. \quad (10)$$

This equation can be put in the form⁹

⁹ The various operators are given in reference 2 and in the notation of (11) by H. A. Bethe, *Handbuch der Physik* (J. Springer, Berlin, 1933), Vol. 24, Part 1. Concerning the operators $H^{(1)}$, $H^{(3a)}$, $H^{(4)}$ [see H. A. S. Ericksson, Z. Physik 109, 762 (1938), and reference 3], the following remarks may be useful. The above operators come from the terms operators come from the terms

$(\sigma_{\mathrm{I}}\!\cdot\!\Pi_{\mathrm{I}})\Pi_{\mathrm{0}}^{-1}(\sigma_{\mathrm{I}}\!\cdot\!\Pi_{\mathrm{I}})\!+\!(\sigma_{\mathrm{II}}\!\cdot\!\Pi_{\mathrm{II}})\Pi_{\mathrm{0}}^{-1}(\sigma_{\mathrm{II}}\!\cdot\!\Pi_{\mathrm{II}})$

in (10). In the following it is sufficient to refer to the first of these two terms and to consider the case with no external field $(\mathbf{\Pi} = \mathbf{p})$. On omitting the subscript I, one has

$$c(\mathbf{\sigma} \cdot \mathbf{p}) \Pi_0^{-1} (\mathbf{\sigma} \cdot \mathbf{p}) = \frac{1}{2m} (\mathbf{\sigma} \cdot \mathbf{p}) \frac{1}{U} (\mathbf{\sigma} \cdot \mathbf{p})$$
$$= \frac{1}{2mU} (\mathbf{\sigma} \cdot \mathbf{p})^2 + \frac{1}{2m} (\mathbf{\sigma} \cdot \mathbf{p}) U^{-1} \cdot (\mathbf{\sigma} \cdot \mathbf{p}), \quad (A)$$

where

$$U = 1 + \frac{1}{2mc^2} (E - 2mc^2 + eV) \equiv 1 + \mathfrak{v}$$

$$\cong 1 + O(v^2/c^2), \text{ except at } r_1, r_2, r_{12} = 0,$$

$$\to \infty \text{ as } \frac{1}{r_1}, \frac{1}{r_2}, \frac{1}{r_{12}} \text{ as } r_1, r_2, r_{12} \to 0 \text{ respectively.}$$

The dot behind U^{-1} indicates that the operator in the front does not extend beyond U^{-1} . On carrying out the calculation, one obtains

$$c(\boldsymbol{\sigma} \cdot \mathbf{p}) \boldsymbol{\Pi}_0^{-1} (\boldsymbol{\sigma} \cdot \mathbf{p}) = \frac{1}{2mU} p^2 + \frac{1}{U^2} (H^{(3a)} + H^{(4)}), \qquad (C)$$

(B)

where

$$H^{(3a)} = \frac{e\hbar}{4m^2c^2} (\llbracket \mathbf{\mathcal{E}} \times \mathbf{p} \rrbracket \cdot \mathbf{\sigma}),$$

$$H^{(4)} = -i\frac{e\hbar}{4m^2c^2} (\mathbf{\mathcal{E}} \cdot \mathbf{p}).$$

$$\mathbf{\mathcal{E}} = -\mathbf{\nabla} V = -(2mc^2/e)\mathbf{\nabla} U.$$

The usual procedure is to expand $1/U \cong 1 - v$ in the first term in The usual procedure is to expand $1/U \cong 1-\mathfrak{v}$ in the first term in (C) and replace U^2 by 1 in the second and third term in (C). This procedure is not correct, it leading to the indeterminate value $\infty \cdot 0$ for the matrix element of $H^{(30)}$. Only working with the exact operator $(1/U^2)H^{(30)}$ gives the value 0 to the spin-orbit interaction for the S-state. [See E. U. Condon and G. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, London, 1935) p. 130] 1935), p. 130.]

On forming the matrix element of

$$\frac{1}{2mU}p^2 + \frac{1}{U^2}H^{(4)} = \frac{\hbar^2}{2m} \left[-\frac{1}{U}\nabla^2 + \frac{1}{U^2}(\boldsymbol{\nabla} U \cdot \boldsymbol{\nabla}) \right], \tag{D}$$

$$\begin{bmatrix} H_{NR} + H_r + H^{(6)} + H_B \end{bmatrix} \Psi = E\Psi, H_r = H^{(1)} + H^{(3a)} + H^{(4)},$$
(11)
$$H_R = H^{(2)} + H^{(3b)} + H^{(5)} + H^{(7)}.$$

 H_{NR} is the nonrelativistic Hamiltonian, $H^{(1)}$ the quantum mechanical analog of the classical Sommerfeld correction, $H^{(3a)}$ the spin-orbit interaction, $H^{(4)}$ the "S-state" correction, $H^{(6)}$ the interaction with external fields. The term $H^{(3b)}$ representing some sort of "spinother orbit" interaction and the term $H^{(5)}$ representing the spin-spin interaction, arise from the magnetic interaction $(\alpha_{I} \cdot \alpha_{II})$ in the operator B, the term $H^{(2)}$ arises from the retardation term in B, and the term $H^{(7)}$ from both in B. (10) and (11) are the original result of Breit. It is to be emphasized here that according to this procedure of reduction, the additional contact term,³⁻⁶

$$H_{c} = -\frac{8\pi}{3} \left(\frac{e\hbar}{2mc}\right)^{2} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\sigma}_{\mathrm{II}}) \delta(r_{12}), \qquad (12)$$

does not appear.10

and integrating the first term by parts, one obtains

$$\int \psi \left(\frac{p^2}{2mU} + \frac{1}{U^2} H^{(4)} \right) \psi d\tau = \frac{\hbar^2}{2m} \int \frac{1}{U} (\nabla \psi)^2 d\tau.$$
(E)

On expanding $1/U \cong 1 - v$ and integrating the above integral by parts, one has

$$\frac{\hbar^2}{2m} \int' (1-\mathfrak{v}) (\nabla \psi)^2 d\tau = \frac{\hbar^2}{2m} (\psi \nabla \psi)_S + \frac{1}{2m} \int' \psi p^2 \psi d\tau - \frac{\hbar^2}{2m} (\mathfrak{v} \psi \nabla \psi)_S \\ - \frac{1}{2m} \int' \mathfrak{v} \psi p^2 \psi d\tau - \frac{\hbar}{2mi} \int' \psi (\nabla \mathfrak{v} \cdot \mathbf{p} \psi) d\tau,$$

where the prime on the integrals indicate that a small spherical volume of radius R around each of the poles $r_1, r_2, r_{12}=0$ of U in (B) is to be excluded so that the expansion $1/U=1-\mathfrak{v}$ does not introduce any singularity at these points at which 1/U=0. The two surface integrals denoted by the subscript S vanish in the limit $R \rightarrow 0$. One finally obtains for (E) the usual result

$$\begin{split} \int \psi^* \bigg[\frac{1}{2m} p^2 + H^{(1)} + H^{(4)} \bigg] \psi d\tau \\ &= \frac{1}{2m} \int \psi^* p^2 \psi d\tau - \frac{1}{8m^3 c^2} \int (p^2 \psi^*) (p^2 \psi) d\tau + \int \psi^* H^{(4)} \psi d\tau \end{split}$$

in which the prime has been removed by allowing R to approach

zero. ¹⁰ In the second paper in reference 2, Breit employed a different procedure from the "reduction" procedure outlined in (8), (9), (10) and treated the operator B' as a perturbation in Eqs. (7). From (7) and the approximation

$$u = -\Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \Psi, \quad v = -\Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi,$$
$$\phi = \frac{1}{(2mc)^2} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi, \quad (\mathrm{F})$$

the perturbation energy due to B' comes out to be

$$-\frac{1}{4m^2c^2}\int \{[(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})\Psi]^{\dagger}B'(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})+[(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})\Psi]^{\dagger}B'(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})$$

$$+\Psi^{\dagger}B'(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})+[(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})\Psi]^{\dagger}B'\}\Psi d\tau.$$
 (G)

A correct evaluation of the last term by Sucher and Foley⁴ yields the contact term (12).

The procedure employed in the foregoing in arriving at (G), while in agreement with the field-theoretical point of view in treating the Breit operator B' as a perturbation, seems to have involved the multiplication of (7a), (7b), (7c), (7d) by ψ^{\dagger} , u^{\dagger} , v^{\dagger} , ϕ^{\dagger} , respectively, the use of (F), and the addition of the four resulting equations. On writing out these four equations separately before

This "reduction" procedure leads to the term $B^{\prime 2}$ in (10), or $H^{(7)}$ in (11), which Breit² has immediately given some arguments for discarding and which has later been shown by Bethe⁹ to come from the second order perturbation when the Breit operator B is taken to be a perturbation. Even before the development of the field theory, Breit² already cautioned against treating (1) as the exact Hamiltonian. In the later developments, it became clear that there is ground for treating separately the interactions between two electrons through the longitudinal fields which give rise to the Coulomb term e^2/r_{12} , and the interactions through the transverse fields of which the first term in the series in powers of $e^2/\hbar c = \alpha$ is the Breit operator B. In the field-theoretical form of the theory of Breit and of Møller, one does not regard H in (1) as the exact Hamiltonian, but treats B as a perturbation. In the following, we shall show that a simple calculation of the diagonal matrix element of B with respect to the 16-component wave function gives unambiguously H_c in the case of the ground state of two-electron atoms (for which $H^{(2)}$, $H^{(3b)}$, $H^{(5)}$ vanish).

III. CONTACT TERM IN THE THEORY OF BREIT AND MØLLER

Let us consider the case of two electrons in the central field of a charge Ze and let us assume that Z

them, one finds

$$\Psi^{\dagger} \left[\frac{\Pi_{0}}{2mc} - 1 - \frac{1}{2mc} \{ (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \Pi_{0}^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) + (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Pi_{0}^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \} + \frac{B'}{8m^{3}c^{4}} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \right] \Psi = 0, \quad (\mathrm{Ha})$$

$$-\left[\Pi_{0}^{-1}(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})\Psi\right]^{\dagger}\left[\frac{1}{(2mc)^{3}}(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})^{2}-\frac{1}{2mc^{2}}B'\Pi_{0}^{-1}(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})\right]\Psi=0,\quad(\mathrm{Hb})$$

$$- \left[\Pi_0^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi\right]^{\dagger} \left[\frac{1}{(2mc)^3} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})^2 (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \right]$$

$$-\frac{1}{2mc^2}B'\Pi_0^{-1}(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}}) \bigg]\Psi = 0, \quad (\mathrm{Hc})$$

$$[(\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})(\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}})\Psi]^{\dagger} \frac{D}{8m^{3}c^{4}}\Psi = 0. \quad (\mathrm{Hd})$$

While adding these equations leads to с т**г**

$$\Psi^{\dagger} \left[\frac{\Pi_{0}}{2mc} - 1 - \frac{1}{2mc} \{ (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \Pi_{0}^{-1} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) + (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Pi_{0}^{-1} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \} - \frac{1}{8m^{4}c^{4}} (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}})^{2} (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}})^{2} \right] \Psi \\ + \frac{1}{8m^{3}c^{4}} \{ [(\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{I}}) \Psi]^{\dagger} B' (\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) + [(\boldsymbol{\sigma}_{\mathrm{II}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \Psi]^{\dagger} B' (\boldsymbol{\sigma}_{\mathrm{I}} \cdot \boldsymbol{\Pi}_{\mathrm{II}}) \}$$

 $+\Psi^{\dagger}B'(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})+[(\boldsymbol{\sigma}_{\mathrm{I}}\cdot\boldsymbol{\Pi}_{\mathrm{I}})(\boldsymbol{\sigma}_{\mathrm{II}}\cdot\boldsymbol{\Pi}_{\mathrm{II}})\Psi]^{\dagger}B'\}\Psi=0, (\mathrm{I})$ adding and hence to (G) with the contact term, the four equations (H) are obviously incorrect. There is thus an ambiguity in the result depending on whether one first adds up the four equations $\Psi^{\dagger} \times (7a), u^{\dagger} \times (7b),$ etc., and then puts in (F), or whether one first uses (F) as above to get the equations (H) and then adds them. That the equations (H) are incorrect arises from the fact that the approximation (F) does not satisfy Eqs. (7) up to $(v/c)^4$ [the lowest order term being $(v/c)^2$ in (7a)].

is large so that the electron-electron interactions, up so that to α^2 ,

$$\frac{e^{2}}{r_{12}} - \frac{e^{2}}{2r_{12}} \left\{ (\alpha_{\mathrm{I}} \cdot \alpha_{\mathrm{II}}) + \frac{1}{r_{12}^{2}} (\alpha_{\mathrm{I}} \cdot \mathbf{r}_{12}) (\alpha_{\mathrm{II}} \cdot \mathbf{r}_{12}) \right\}, \quad (13)$$

are small compared with the electron-nucleus interactions. In this case one may calculate the interaction energy between the electrons through their fields by calculating the diagonal matrix element of (13) with respect to the 16-component wave function of the two hydrogenic electrons. The work of Breit,² Møller⁷ and Bethe and Fermi¹¹ shows that taking the diagonal matrix element of (13) is equivalent to calculating the integral

$$\int \int \frac{1}{r_{12}} \exp\left(\frac{2\pi i \nu_{if} r_{12}}{c}\right) \\ \times \left[\rho(1)\rho'(2) - \mathbf{j}(1) \cdot \mathbf{j}'(2)\right] d\tau_1 d\tau_2.$$
(14)

For the ground state of He-like atoms,

 $v_{if} = 0.$

To take account of the Pauli principle, one has

$$\begin{split} \rho(1)\rho'(2) &= \frac{e^2}{2} \begin{vmatrix} \psi_{\frac{1}{2}}^{\dagger}(1) & \psi_{-\frac{1}{2}}^{\dagger}(1) \\ \psi_{\frac{1}{2}}^{\dagger}(2) & \psi_{-\frac{1}{2}}^{\dagger}(2) \end{vmatrix} \begin{vmatrix} \psi_{\frac{1}{2}}(1) & \psi_{\frac{1}{2}}(2) \\ \psi_{-\frac{1}{2}}(1) & \psi_{-\frac{1}{2}}(2) \end{vmatrix} \\ &= \frac{1}{2} \left[\rho_{\frac{1}{2},\frac{1}{2}}(1)\rho_{-\frac{1}{2},-\frac{1}{2}}(2) + \rho_{-\frac{1}{2},-\frac{1}{2}}(1)\rho_{\frac{1}{2},\frac{1}{2}}(2) \\ &- \rho_{\frac{1}{2},-\frac{1}{2}}(1)\rho_{-\frac{1}{2},\frac{1}{2}}(2) - \rho_{-\frac{1}{2},\frac{1}{2}}(1)\rho_{\frac{1}{2},-\frac{1}{2}}(2) \right], \\ \rho_{\frac{1}{2},-\frac{1}{2}}(1) &= -e\psi_{\frac{1}{2}}^{\dagger}(1)\psi_{-\frac{1}{2}}(1), \quad \text{etc.}, \end{split}$$

 $\psi_{\frac{1}{2}}$ being a four-component column matrix corresponding to $M = \frac{1}{2}, \psi_{1}^{\dagger}$ a row matrix, etc. Similarly,

$$\mathbf{j}(1) \cdot \mathbf{j}'(2) = \frac{1}{2} \begin{bmatrix} \mathbf{j}_{\frac{1}{2},\frac{1}{2}}(1) \cdot \mathbf{j}_{-\frac{1}{2},-\frac{1}{2}}(2) + \mathbf{j}_{-\frac{1}{2},-\frac{1}{2}}(1) \cdot \mathbf{j}_{\frac{1}{2},\frac{1}{2}}(2) \\ - \mathbf{j}_{\frac{1}{2},-\frac{1}{2}}(1) \cdot \mathbf{j}_{-\frac{1}{2},\frac{1}{2}}(2) - \mathbf{j}_{-\frac{1}{2},\frac{1}{2}}(1) \cdot \mathbf{j}_{\frac{1}{2},-\frac{1}{2}}(2) \end{bmatrix}$$
where
$$\mathbf{j}_{\frac{1}{2},-\frac{1}{2}}(1) \cdot \mathbf{j}_{-\frac{1}{2},\frac{1}{2}}(2) - \mathbf{j}_{-\frac{1}{2},\frac{1}{2}}(1) \cdot \mathbf{j}_{\frac{1}{2},-\frac{1}{2}}(2) \end{bmatrix}$$

$$j_{\frac{1}{2},-\frac{1}{2}}(1) = e\psi_{\frac{1}{2}}^{\dagger}\alpha_{I}\psi_{-\frac{1}{2}}, \text{ etc}$$

For the hydrogenic electron, we have¹²

$$M = \frac{1}{2}, \qquad \psi_{\frac{1}{2}}^{\dagger} = N(if \cos\vartheta, if \sin\vartheta e^{-i\varphi}, g, 0),$$

$$M = -\frac{1}{2}, \qquad \psi_{-\frac{1}{2}}^{\dagger} = N(-if \sin\vartheta e^{i\varphi}, if \cos\vartheta, 0, -g),$$

$$g = e^{-Zr/a}r^{\gamma}, \qquad \gamma = [1 - (Z\alpha)^{2}]^{\frac{1}{2}} - 1,$$

$$f = \frac{Z\alpha}{1 + [1 - (Z\alpha)^{2}]^{\frac{1}{2}}}g, \qquad \alpha = \frac{e^{2}}{\hbar c},$$
(15)

$$(\rho\rho' - \mathbf{j} \cdot \mathbf{j'}) = N^4 e^2 \{ [f^2(1) + g^2(1)] [f^2(2) + g^2(2)] + 8f(1)g(1)f(2)g(2)\cos\vartheta_{12} \}.$$
(16)

Evaluation of (14) leads to

$$\int \int \frac{1}{r_{12}} \rho \rho' d\tau_1 d\tau_2 = \frac{5}{4} + 0.46 Z^3 \alpha^2$$

in Rydberg units, (17)

$$-\int \int \frac{1}{r_{12}} \mathbf{j} \cdot \mathbf{j}' d\tau_1 d\tau_2 = \frac{1}{2} Z^3 \alpha^2 \quad \text{in Rydberg units.} \quad (18)$$

The matrix element (18) of the Breit operator B is to be compared with the terms $H^{(2)}$, $H^{(3b)}$, $H^{(5)}$ in (11) that arise from the operator B. The matrix elements of $H^{(2)}$, $H^{(3b)}$, $H^{(5)}$ with respect to hydrogenic wave functions are all zero for the ground state of He-like atoms, but the matrix element of the contact interaction H_c in the same approximation is exactly $\frac{1}{2}Z^3\alpha^2$ Rydberg. Thus the matrix element of B with respect to the 16-component wave function does lead to the contact term H_{e} for the relativistic energy of the ground state of two-electron atoms. It is, however, not yet clear why H_c does not appear if one follows the "reduction" procedure, as shown in Sec. II. This might again be traced to a cause related to that mentioned at the end of Sec. II.

Expressions (17) and (18) give the energy from the electron-electron interaction (13); the total relativistic energy of the two-electron atom of course is the sum of (17), (18), and the relativistic energy of the two hydrogenic electrons containing the Sommerfeld, the spin-orbit and the S-state corrections for the two electrons. The first term in (17) is the nonrelativistic energy arising from e^2/r_{12} . The second term, which in this approximation of unscreened relativistic hydrogenic wave function is $0.46Z^3\alpha^2$ Rydberg, has no corresponding term in (10)-(12). It arises from the singular behavior of the wave function (15) at the origin, and is the consequence of treating (13) by the perturbation procedure. A rigorous treatment of the relativistic system

$$\left[H_0(1) + H_0(2) + \frac{e^2}{r_{12}}\right] \psi = E \psi$$
 (19)

is not known; but on plausible considerations, the effect of the singular behavior of the relativistic wave function in (19) at the origin can be expected to contribute a correction of the order α^4 , and must be treated together with the higher order interactions in the field theory.

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