where the Green's function, $G(\mathbf{r}_1\mathbf{r}_2; \mathbf{r}_1'\mathbf{r}_2')$ is obtained for the operator on the left-hand side of Eq. (18) under the condition that it represents outgoing waves.

If λ is set equal to zero, (19) reduces to a homogeneous integral equation which has the solution zero under the given initial conditions. For from (15), if the interaction vanishes, so must the function ϕ. This property has the further consequence that exchange terms cannot appear when the interaction between the electrons is not taken into account.

The inhomogeneous term in (19) vanishes with the interaction between incident and bound electrons. Therefore, this equation is in a suitable form for carrying out an iterative procedure.

Using the parameter λ to indicate orders of magnitude, the desirability of carrying out a partial integration of the second integral in (19) becomes apparent. In this way, the contribution of the $1/r_1$ term, of the same order of magnitude as the inhomogeneous term, can be obtained.

In the course of the derivation of Eq. (19), we have verified most of the statements listed in the summary of the text. The others are consequences which readily follow from our definitions and equations.

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Reduction of Relativistic Wave Equations and the "Contact Interaction"

FRANCIS N. GLOVER* AND ZENO V. CHRAPLYVY
Saint Louis University, Saint Louis, Missouri

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A new formulation of the large-component reduction method for one- and two-particle relativistic wave equations is presented and compared with the reduction procedure by the method of successive canonical transformations. Sufficient conditions are given for the identity, to the order $(1/c)^2$, of the energy spectra obtained by the two methods. The "contact interaction" term resulting from the latter procedure is shown to arise in the former as well, contrary to a statement by Wu and Tauber.

INTRODUCTION

TO reduce the number of components of a relativistic wave equation, two methods are in general use: one method is based on the fact that some of the components of Ψ are larger than others[1]; and the other applies successive canonical transformations (also known as the Foldy-Wouthuysen method).[2] The latter has some distinct advantages. Moreover, as Becker[3] has shown, it is the method to which one is led when one attempts consistently to meet the basic requirements that the reduced wave equation have (to within an approximation) an energy spectrum identical with that of the full equation. Since in the past the older large-component method has enjoyed wide use, the question may be raised whether its application does not in some way impair the results. This question has become of interest recently, as Wu and Tauber have stated[4] that it was impossible to obtain the so-called "contact interaction" term in a two-particle problem by means of the large-component method. This is our motivation for presenting in this note some considerations, hitherto unpublished,[5] on the two methods.

We first formulate the large-component method in a way that will facilitate a comparison with the method of successive canonical transformations, both for the one-particle and the two-particle case. Then we establish sufficient conditions for their equivalence, and finally we show that the term in question is obtained by either method.

ONE-PARTICLE CASE

A one-particle relativistic wave equation of the Dirac type may be written as

$$\mathcal{H}\Psi \equiv \{\beta mc^2 + \mathcal{E} + \mathcal{O}\}\Psi = i\hbar \frac{\partial}{\partial t}\Psi. \tag{1}$$

The even[6] part $\mathcal{E}$ and the odd part $\mathcal{O}$ of the Hamiltonian can be written as follows:

$$\mathcal{E} = \begin{pmatrix} \mathcal{E}' & 0 \\ 0 & \mathcal{E}'' \end{pmatrix}; \quad \mathcal{O} = \begin{pmatrix} 0 & \mathcal{O}' \\ \mathcal{O}'' & 0 \end{pmatrix}, \tag{2}$$

where $\mathcal{E}'$, $\mathcal{E}''$, $\mathcal{O}'$, $\mathcal{O}''$ are 2×2 matrix operators. We shall assume that $\mathcal{O}$ (and $\mathcal{O}'$, $\mathcal{O}''$) is of the order of c, and $\mathcal{E}$ (with $\mathcal{E}'$, $\mathcal{E}''$) of order c^0. We consider here only the case of a time-independent $\mathcal{H}$. The usual substitution

$$\Psi = \exp\left\{\frac{W+mc^2}{i\hbar}t\right\}\begin{vmatrix} \psi \\ \psi'' \end{vmatrix}, \tag{3}$$

* Now at Woodstock College, Woodstock, Maryland.

[1] See, for example, W. Pauli, *Die Allgemeinen Prinzipien der Wellenmechanik* (Edwards Brothers, Inc., Ann Arbor, 1950), p. 237.

[2] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78**, 29 (1950).

[3] R. Becker, Göttinger Nachr., p. 39 (1945).

[4] Ta-You Wu and G. E. Tauber, Phys. Rev. **100**, 1767 (1955).

[5] Technical report issued Aug. 16, 1955, under a U. S. Air Force contract (unpublished).

[6] We follow the terminology and notation of Z. V. Chraplyvy, Phys. Rev. **91**, 388 (1953); **92**, 1310 (1953), referred to as I and II.

where ψ and ψ'' are two-element columns independent of time, changes Eq. (1) into

$$\begin{aligned}(\mathcal{E}'-W)\psi+\mathcal{O}'\psi''=0,\\(\mathcal{E}''-2mc^2-W)\psi''+\mathcal{O}''\psi=0.\end{aligned}\tag{4}$$

Eliminating the "small" component ψ'' by means of successive approximations, valid to $(1/c)^2$, we obtain the two-component (reduced) equation

$$\mathcal{H}_{\text{red}}\psi=(W+mc^2)\psi,\tag{5}$$

with

$$\mathcal{H}_{\text{red}}\equiv mc^2+\mathcal{E}'+\frac{\mathcal{O}'\mathcal{O}''}{2mc^2}+\frac{1}{4m^2c^4}(\mathcal{O}'\mathcal{E}''\mathcal{O}''-\mathcal{O}'\mathcal{O}''\mathcal{E}')-\frac{(\mathcal{O}'\mathcal{O}'')^2}{8m^3c^6}.\tag{5a}$$

This is, of course, a 2×2 matrix operator, but with the help of the multiplier $b_+=\frac{1}{2}(1+\beta)$, may be expressed in terms of 4×4 matrices:

$$\mathcal{H}_{\text{red}}=b_+\left\{\beta mc^2+\mathcal{E}+\frac{\beta\mathcal{O}^2}{2mc^2}+\frac{1}{4m^2c^4}[\mathcal{O}\mathcal{E},\mathcal{O}]-\frac{\beta\mathcal{O}^4}{8m^3c^6}\right\},\tag{6}$$

which is a form suitable for our purposes of comparison.

As is known, in the Foldy-Wouthuysen procedure the Hamiltonian $\mathcal{H}$ is converted by successive canonical transformations into $\mathcal{H}_{\text{tr}}$, an even operator, so that in the transformed equation

$$\mathcal{H}_{\text{tr}}\psi_{\text{tr}}=E\psi_{\text{tr}}\tag{7}$$

the upper components ψ_u are no longer coupled with the lower components ψ_l. Hence to obtain a reduced equation, the third and fourth line of (7) are simply omitted, which may be symbolized by the application of the b_+ multiplier:

$$\mathcal{H}_{\text{red}}\psi_u\equiv b_+\{\mathcal{H}_{\text{tr}}\psi_{\text{tr}}\}=E\psi_u.\tag{8}$$

To the order $(1/c)^2$, the reduced Hamiltonian[7] is

$$\mathcal{H}_{\text{red}}\equiv b_+\left\{\beta mc^2+\mathcal{E}+\frac{\beta\mathcal{O}^2}{2mc^2}+\frac{1}{8m^2c^4}[[\mathcal{O},\mathcal{E}],\mathcal{O}]-\frac{\beta\mathcal{O}^4}{8m^3c^6}\right\}.\tag{9}$$

It is to be noted that even if $\mathcal{O}$ and $\mathcal{E}$ are Hermitian, the reduced Hamiltonian of (6) is not seen to be Hermitian due to its fourth term $[\mathcal{O}\mathcal{E},\mathcal{O}]$. On the other hand, the corresponding term of (9), $\frac{1}{2}[[\mathcal{O},\mathcal{E}],\mathcal{O}]$, is Hermitian. This is one of the advantages of the Foldy-Wouthuysen method because of which it will be preferred in all applied work; the more so as our comparison shows that the amount of computational work is about the same in both methods. As the Hamiltonians of (6) and (9) differ only in their fourth term, it follows that if the condition

$$[\mathcal{O}^2,\mathcal{E}]\leq O(c)\tag{10}$$

is satisfied, then, to the order $(1/c)^2$, the energy spectrum will be identical. Thus for the case of a predominantly Coulomb force we have

$$\begin{aligned}\mathcal{O}&=c\boldsymbol{\alpha}\cdot\mathbf{p}+O(c^0),\\\mathcal{E}&=k/r+O(1/c),\end{aligned}$$

and

$$[\mathcal{O}^2,\mathcal{E}]=k\hbar^2c^2[\operatorname{div}(r^{-3}\mathbf{r})+2r^{-3}\mathbf{r}\cdot\boldsymbol{\nabla}]+O(c).\tag{11}$$

The contributions of the two terms in the square brackets just cancel each other so that the condition (10) is satisfied, and the two reduction procedures yield identical energy spectra to the order $(1/c)^2$ for this rather important case.

TWO-PARTICLE CASE

We write a two-particle wave equation of the Breit type as

$$\mathcal{H}\Psi\equiv\{\beta^{\text{I}}m_{\text{I}}c^2+\beta^{\text{II}}m_{\text{II}}c^2+(\mathcal{E}\mathcal{E})+(\mathcal{E}\mathcal{O})+(\mathcal{O}\mathcal{E})+(\mathcal{O}\mathcal{O})\}\Psi=i\hbar\frac{\partial}{\partial t}\Psi.\tag{12}$$

The spinor Ψ consists now of sixteen components, and we may in general eliminate twelve of them as significantly smaller than the four components retained. The procedure will be similar to that in the one-particle case. However, while formerly the two large components were adjacent elements in the spinor, here this is not the case. Hence we first have to rearrange the sixteen equations of (12) so that the four components which will eventually turn out to be the large ones come together to form a subspinor. We introduce the unitary and Hermitian matrix

$$\mathfrak{M}=\mathfrak{M}^{-1}\equiv\begin{pmatrix}1&0&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&0&1&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&1\end{pmatrix}$$

(where each 1 stands for a 2×2 unit matrix) and, with its help, we rewrite (12) as

$$(\mathfrak{M}\mathcal{H}\mathfrak{M}^{-1})\mathfrak{M}\Psi=i\hbar\frac{\partial}{\partial t}\mathfrak{M}\Psi.\tag{13}$$

The effect of $\mathfrak{M}$ on the matrix operators appearing in (12) is as follows: in an even-even (even-odd, etc.) matrix, at least three-fourths of the 256 elements must be zero, while the elements different from zero are found in 2×2 squares, arranged in a regular, chessboard-like pattern, shown in Fig. 2 of II. Applica-

[7] Given in Eq. (4) of I. Note there a mistake in the sign of the fourth term.

tion of the $\mathfrak{M}$-matrix consolidates these 2×2 squares into 4×4 squares. Thus we have

$$\mathfrak{M}(\mathcal{E}\mathcal{E})\mathfrak{M}^{-1}=\begin{pmatrix}(\mathcal{E}\mathcal{E})' & & & \\ & (\mathcal{E}\mathcal{E})'' & & \\ & & (\mathcal{E}\mathcal{E})''' & \\ & & & (\mathcal{E}\mathcal{E})^{iv}\end{pmatrix},\quad \mathfrak{M}(\mathcal{E}\mathcal{O})\mathfrak{M}^{-1}=\begin{pmatrix} & & (\mathcal{E}\mathcal{O})' & \\ & & & (\mathcal{E}\mathcal{O})'' \\ (\mathcal{E}\mathcal{O})''' & & & \\ & (\mathcal{E}\mathcal{O})^{iv} & & \end{pmatrix},$$

$$\mathfrak{M}(\mathcal{O}\mathcal{E})\mathfrak{M}^{-1}=\begin{pmatrix} & (\mathcal{O}\mathcal{E})' & & \\ (\mathcal{O}\mathcal{E})'' & & & \\ & & & (\mathcal{O}\mathcal{E})''' \\ & & (\mathcal{O}\mathcal{E})^{iv} & \end{pmatrix},\quad \mathfrak{M}(\mathcal{O}\mathcal{O})\mathfrak{M}^{-1}=\begin{pmatrix} & & & (\mathcal{O}\mathcal{O})' \\ & & (\mathcal{O}\mathcal{O})'' & \\ & (\mathcal{O}\mathcal{O})''' & & \\ (\mathcal{O}\mathcal{O})^{iv} & & & \end{pmatrix}, \tag{14}$$

$$\mathfrak{M}\beta^{\mathrm{I}}\mathfrak{M}^{-1}=\begin{pmatrix}\delta & & & \\ & -\delta & & \\ & & \delta & \\ & & & -\delta\end{pmatrix},\quad \mathfrak{M}\beta^{\mathrm{II}}\mathfrak{M}^{-1}=\begin{pmatrix}\delta & & & \\ & \delta & & \\ & & -\delta & \\ & & & -\delta\end{pmatrix},$$

where δ is the 4×4 unit matrix. From (13) by means of the substitution

$$\mathfrak{M}\Psi=\exp\left\{\frac{W+m_{\mathrm{I}}c^2+m_{\mathrm{II}}c^2}{i\hbar}t\right\}\begin{vmatrix}\psi' \\ \psi'' \\ \psi''' \\ \psi^{iv}\end{vmatrix}, \tag{15}$$

the following set of equations is obtained, each involving 4×4 matrices and four-component spinors:

$$\begin{aligned}
&\{(\mathcal{E}\mathcal{E})'-W\}\psi'+(\mathcal{E}\mathcal{O})'\psi'''+(\mathcal{O}\mathcal{E})'\psi''+(\mathcal{O}\mathcal{O})'\psi^{iv}=0,\\
&\{(\mathcal{E}\mathcal{E})''-W-2m_{\mathrm{I}}c^2\}\psi''\\
&\qquad+(\mathcal{E}\mathcal{O})''\psi^{iv}+(\mathcal{O}\mathcal{E})''\psi'+(\mathcal{O}\mathcal{O})''\psi'''=0,\\
&\{(\mathcal{E}\mathcal{E})'''-W-2m_{\mathrm{II}}c^2\}\psi'''+(\mathcal{E}\mathcal{O})'''\psi'\\
&\qquad+(\mathcal{O}\mathcal{E})'''\psi^{iv}+(\mathcal{O}\mathcal{O})'''\psi''=0,\\
&\{(\mathcal{E}\mathcal{E})^{iv}-W-2(m_{\mathrm{I}}+m_{\mathrm{II}})c^2\}\psi^{iv}+(\mathcal{E}\mathcal{O})^{iv}\psi''\\
&\qquad+(\mathcal{O}\mathcal{E})^{iv}\psi'''+(\mathcal{O}\mathcal{O})^{iv}\psi'=0.
\end{aligned} \tag{16}$$

By assuming $(\mathcal{E}\mathcal{O})$ and $(\mathcal{O}\mathcal{E})$ (i.e., all their nonzero elements) to be of order c, and $(\mathcal{E}\mathcal{E})$ and $(\mathcal{O}\mathcal{O})$ to be of order c^0, we have the following order of magnitude relationship between the components

$$\psi'\approx c\psi''\approx c\psi'''\gtrsim c^2\psi^{iv}.$$

Thus the four elements of ψ' are clearly the large components. In successive approximations [valid to $(1/c)^2$] the ψ'', ψ''', ψ^{iv} may be eliminated, yielding

$$\mathfrak{H}'\psi'=E\psi', \tag{17}$$

with

$$E=W+m_{\mathrm{I}}c^2+m_{\mathrm{II}}c^2.$$

This is the result of the reduction: ψ' consists of four components, and correspondingly, $\mathfrak{H}'$ is a 4×4 matrix operator. However for our present purposes, we prefer to replace formally ψ' by a column consisting of sixteen components, of which twelve are zero, and likewise to amplify $\mathfrak{H}'$, by the addition of zero elements, into an equivalent 16×16 matrix. This will be done by the aid of a 16×16 multiplier b_{++} (the direct product of b_+ with itself) in the following way:

$$\begin{aligned}\psi'&=\mathfrak{M}b_{++}\psi,\\ \mathfrak{H}'&=\mathfrak{M}b_{++}\mathfrak{H}^*\mathfrak{M}.\end{aligned} \tag{18}$$

Since (as will be seen below) $\mathfrak{H}^*$ is even-even, and therefore commutes with b_{++}, and since $(b_{++})^2=b_{++}$ and $\mathfrak{M}^2=1$, we obtain

$$b_{++}\mathfrak{H}^*\psi=b_{++}E\psi, \tag{19}$$

an equation equivalent to (17), provided we choose

$$b_{++}\mathfrak{H}^*=b_{++}\Big\{\beta^{\mathrm{I}}m_{\mathrm{I}}c^2+\beta^{\mathrm{II}}m_{\mathrm{II}}c^2+(\mathcal{E}\mathcal{E}) \tag{20a}$$

$$+\frac{\beta^{\mathrm{I}}(\mathcal{O}\mathcal{E})^2}{2m_{\mathrm{I}}c^2}+\frac{\beta^{\mathrm{II}}(\mathcal{E}\mathcal{O})^2}{2m_{\mathrm{II}}c^2}-\frac{\beta^{\mathrm{I}}(\mathcal{O}\mathcal{E})^4}{8m_{\mathrm{I}}{}^3c^6}-\frac{\beta^{\mathrm{II}}(\mathcal{E}\mathcal{O})^4}{8m_{\mathrm{II}}{}^3c^6} \tag{20b}$$

$$+\frac{1}{4m_{\mathrm{I}}{}^2c^4}[(\mathcal{O}\mathcal{E})(\mathcal{E}\mathcal{E}),(\mathcal{O}\mathcal{E})]+\frac{1}{4m_{\mathrm{II}}{}^2c^4}\times[(\mathcal{E}\mathcal{O})(\mathcal{E}\mathcal{E}),(\mathcal{E}\mathcal{O})] \tag{20c}$$

$$+\frac{\beta^{\mathrm{I}}\beta^{\mathrm{II}}}{4m_{\mathrm{I}}m_{\mathrm{II}}c^4}[[(\mathcal{O}\mathcal{E}),(\mathcal{O}\mathcal{O})]_+,(\mathcal{E}\mathcal{O})]_+ \tag{20d}$$

$$+\frac{\beta^{\mathrm{I}}m_{\mathrm{I}}-\beta^{\mathrm{II}}m_{\mathrm{II}}}{2(m_{\mathrm{I}}{}^2-m_{\mathrm{II}}{}^2)c^2}(\mathcal{O}\mathcal{O})^2\Big\}. \tag{20e}$$

For the sake of brevity in this last expression certain terms are not shown, which are negligible if

$$[(\mathcal{O}\mathcal{E}),(\mathcal{E}\mathcal{O})]\leq O(c), \tag{21a}$$

as is usually the case. The foregoing Hamiltonian, although obtained by the large-component method, shows much similarity with that obtained according to I as the result of the application of successive canonical transformations, namely

$$\mathcal{H}_{\rm red}=b_{++}\mathcal{H}_{\rm tr}=b_{++}\Big\{\cdots \tag{22a, b}$$

$$+\frac{1}{8m_{\rm I}^2c^4}[[(\mathcal{O}\mathcal{E}),(\mathcal{E}\mathcal{E})],(\mathcal{O}\mathcal{E})]+\frac{1}{8m_{\rm II}^2c^4}$$

$$\times[[[(\mathcal{E}\mathcal{O}),(\mathcal{E}\mathcal{E})],(\mathcal{E}\mathcal{O})] \tag{22c}$$

$$+\cdots\Big\}. \tag{22d, e}$$

(The dots are used to indicate terms identical in both expressions.) A sufficient condition for the identity of the energy spectra yielded by the two procedures is

$$[(\mathcal{E}\mathcal{O}),(\mathcal{O}\mathcal{E})]\leq O(c), \tag{21a}$$

$$[(\mathcal{O}\mathcal{E})^2,(\mathcal{E}\mathcal{E})]\leq O(c), \tag{21b}$$

$$[(\mathcal{E}\mathcal{O})^2,(\mathcal{E}\mathcal{E})]\leq O(c). \tag{21c}$$

"CONTACT INTERACTION" TERM

The "contact interaction" or δ term, important for the calculation of ionization potentials,[8] arises from the expressions (20d) or (22d), that is, it can be obtained equally well by the application of either the large-component or the successive-transformations method. Actually it had been obtained[9] in I, Eq. (8e), by a straightforward calculation, paying due attention to expressions which yield the δ function.

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APPENDIX

The following result will be of use in computing the energy contribution from (20d) and (22d).

For $\mathbf{A}$ and $\mathbf{B}$ arbitrary vectors and ψ^*, ψ arbitrary functions uniformly continuous at and in the vicinity of $r=0$, we have

$$\int_\tau\psi^*\{\mathbf{A}\cdot\operatorname{curl}(\mathbf{B}\times\mathbf{r}/r^3)\}\psi d\tau$$

$$=\int_\tau\psi^*\Big\{\frac{3(\mathbf{A}\cdot\mathbf{r})(\mathbf{B}\cdot\mathbf{r})}{r^5}-\frac{\mathbf{A}\cdot\mathbf{B}}{r^3}$$

$$+\frac{8\pi}{3}(\mathbf{A}\cdot\mathbf{B})\delta(\mathbf{r})\Big\}\psi d\tau, \tag{A}$$

where the integration may be taken over any region where ψ^* and ψ are uniformly continuous. We indicate a proof.

If τ includes the singular point $r=0$, we decompose τ into a sphere S of vanishing radius centered at the singularity, and the remainder τ'. Then as the radius of the small sphere S approaches zero, we have in the limit (using Gauss's theorem and the theorem of mean value for integrals),

$$\int_S\psi^*\{\mathbf{A}\cdot\operatorname{curl}(\mathbf{B}\times\mathbf{r}/r^3)\}\psi d\tau$$

$$=\psi^*(0)\psi(0)\int_S\nabla\cdot\{(\mathbf{B}\times\mathbf{r})\times\mathbf{A}/r^3\}d\tau$$

$$=\psi^*(0)\psi(0)\Big\{(\mathbf{A}\cdot\mathbf{B})\int_S\frac{dS}{r^2}-\int_S\frac{(\mathbf{A}\cdot\mathbf{r})(\mathbf{B}\cdot\mathbf{r})}{r^4}dS\Big\}$$

$$=\psi^*(0)\psi(0)\Big\{4\pi(\mathbf{A}\cdot\mathbf{B})-\frac{4\pi}{3}(\mathbf{A}\cdot\mathbf{B})\Big\},$$

which may be written as

$$\int_S\psi^*\{(8\pi/3)(\mathbf{A}\cdot\mathbf{B})\delta(\mathbf{r})\}\psi d\tau.$$

By adding an integral which due to symmetry is zero we obtain

$$\int_S\psi^*\{\mathbf{A}\cdot\operatorname{curl}(\mathbf{B}\times\mathbf{r}/r^3)\}\psi d\tau$$

$$=\int_S\psi^*\Big\{\frac{3(\mathbf{A}\cdot\mathbf{r})(\mathbf{B}\cdot\mathbf{r})}{r^5}-\frac{(\mathbf{A}\cdot\mathbf{B})}{r^3}\Big\}\psi d\tau$$

$$+\int_S\psi^*\{(8\pi/3)(\mathbf{A}\cdot\mathbf{B})\delta(\mathbf{r})\}\psi d\tau. \tag{B}$$

But (B) holds as well for the singularity-free region τ', since by vector analytical formulas the left-hand integrand is identical with the first integrand on the right while the last integral vanishes. Thus (B) holds for the total region, and (A) is verified.

[8] J. Sucher and H. M. Foley, Phys. Rev. **95**, 966 (1954).

[9] Unfortunately the numerical factor given there is erroneous, as has since been stated. [Phys. Rev. **99**, 324 (1955)]. It should be $8\pi/3$ rather than 4π.