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On the nonrelativistic limit of the Dirac hamiltonian

by

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ABSTRACT. — In this paper, by a systematic use of the reduction scheme for the analytic perturbation of pseudoresolvents, the nonrelativistic limit of the Dirac Hamiltonian is reconsidered. The main results are: the $1/c^4$ — correction to the bound states energies in the degenerate case and the $1/c^2$ — correction to the scattering amplitude. The relation of the Foldy-Wouthuysen transformation with the reduction scheme, and with the relativistic corrections that we derived is discussed.

RÉSUMÉ. — Dans ce travail on reconsidère le problème de la limite non relativiste de l'hamiltonien de Dirac, en utilisant des pseudo-resolvantes. Les résultats principaux qu'on obtient sont: la correction en $1/c^4$ pour les énergies des états stationnaires dans le cas dégénéré et la correction en $1/c^2$ pour l'amplitude de diffusion. On discute aussi la relation de la transformée de Foldy-Wouthuysen avec le schema de réduction et les corrections calculées.

I. INTRODUCTION

In this paper, the nonrelativistic limit problem for the Dirac operator is once more considered. It was one of the earliest successes of the Dirac equation, that in the nonrelativistic limit it goes into the Pauli equation, but the calculation of the relativistic corrections met a lot of difficulties whose origins were understood only recently. The original elimination method of Pauli [20] had some nonhermiticity problems that were cured (at the formal level) by Berestetky [1]. The first systematic expansion in $1/c$ has been derived by Foldy and Wouthuysen [9] in 1951. Although the terms appearing in the F-W expansions have nice physical interpretation, they are so singular with respect to the leading Pauli-hamiltonian that, at a first sight, a bona fide perturbation theory around the Pauli-limit does not exist. Thus, in spite of its wide use, the status of the F-W method remained unclear [6]. On the other hand, as early as 1948, Titchmarch proved that for certain spherically symmetric potentials the bound-state energies are analytic in $1/c$. The way to the solution of the problem has been opened by Veselić [25] who realised that the resolvent of the Dirac operator is analytic at $1/c=0$, although the limit is a pseudoresolvent and not a resolvent. This allowed the use of the analytic perturbation theory for the bound states: Veselić [25] treated the case with zero magnetic field, Hunziker [12] treated the general case and in [10] Gesztezy, Grosse and Thaller have obtained explicit formulae for the corrections up to $(1/c)^4$, for the nondegenerate case. Concerning the bound states problem, our paper, aside from a further simplification, adds the following results: explicit formulae for the relativistic corrections up to order $(1/c)^4$ in the general degenerate case and the proof of the fact stated in [12] but not recovered in [10] that in general degenerate case, the eigenvalues depend only in $(1/c)^2$.

Section IV contains the main results of the paper concerning the scattering theory. Although it was clear [12] that for analytic dilation or exponentially decaying potentials the boundary values of the (pseudo) resolvent is still analytic in $1/c$ in some appropriate weighted spaces, and that the scattering amplitude is analytic in $1/c$ at a fixed energy, only the leading term has been identified [26]. Our main result here is the fact that the existence of an asymptotic (analytic) expansion of the scattering amplitude depends on the derivability (analyticity) of the boundary value of the Pauli resolvent with respect to the energy. In the case of pure magnetic field, it turns out that the scattering amplitude of the Dirac hamiltonian equals the scattering amplitude of the corresponding Pauli hamiltonian at some shifted energy, multiplied by a correction factor depending on the energy (*see* Theorem IV. 3). Explicit formulae of the relativistic corrections to the scattering amplitude, up to $(1/c)^2$, are given (we think for the first time).

Finally in the last section, various problems concerning the Foldy-Wouthuysen transformation are clarified and its relation with the results of Sections II-IV is discussed. For completitude, the equality of the corrections given by the Foldy-Wouthuysen transformation and by the analytic perturbation method is discussed in the Appendix.

In the rest of this section we shall fix the notations, discuss the various types of conditions on the potentials that will appear further, and recall the main facts about pseudoresolvent families and the reduction scheme that we shall use.

Let us briefly recall the description of a quantum relativistic particle of nonzero mass and spin $\frac{1}{2}$. The Hilbert space is taken to be:

$$\mathscr{H} = \mathbb{C}^2 \otimes L^2(\mathbb{R}^3; \mathbb{C}^2). \tag{I.1}$$

We define:

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{I.2}$$

and the Pauli matrices σ_1, σ_2, σ_3 as operators on $\mathbb{C}^2$, and $D_j = -i\partial_j$ the self-adjoint extension in $L^2(\mathbb{R}^3; \mathbb{C}^2)$ of the formal differential operator (∂_j being the derivative with respect to x_j, for $j=1, 2, 3$) and the vector-valued operator $D=(D_1, D_2, D_3)$. We denote $\sigma . D$ the self-adjoint operator on $L^2(\mathbb{R}^3; \mathbb{C}^2)$ defined by: $\sigma_1 D_1 + \sigma_2 D_2 + \sigma_3 D_3$. We still define two orthogonal projections giving an orthogonal decomposition of $\mathscr{H}$:

$$\begin{aligned} N &= \frac{1}{2}(\beta + 1) = \nu \otimes 1 \\ M &= \frac{1}{2}(1 - \beta) = \mu \otimes 1. \end{aligned} \tag{I.3}$$

Then, the evolution of a free relativistic particle of mass $m > 0$ and spin $\frac{1}{2}$ is generated by the *free Dirac hamiltonian*:

$$H_0 = c\,\alpha \otimes \sigma . D + m c^2 (\beta - 1) \tag{I.4}$$

where c is the velocity of light. We remark that, being interested only in the nonrelativistic limit, we have substracted from the usual free Dirac hamiltonian, a constant term, the rest energy $m c^2$. We shall use this convention through all our paper. We shall also frequently use "matrix notation" for operators on $\mathbb{C}^2 \otimes L^2(\mathbb{R}^3; \mathbb{C}^2)$. Thus we shall write:

$$H_0 = \begin{pmatrix} 0 & c\,\sigma . D \\ c\,\sigma . D & -2 m c^2 \end{pmatrix} \tag{I.5}$$

We shall consider that the particle may interact with an external magnetic field and with an external potential, both being supposed stationary. The interaction with the magnetic field is described by replacing the derivatives

D_j with covariant derivatives:

$$D_A = (D_1 - A_1, D_2 - A_2, D_3 - A_3) \equiv D - A \tag{I.6}$$

where (A_1, A_2, A_3) is the vector potential of the magnetic field $B = (B_1, B_2, B_3)$, *i. e.* $B = \text{rot } A$. Following Hunziker [12] we have scaled the magnetic potential so as to cancel the $\frac{1}{c}$ factor which appears in front of A in the usual definition of the covariant derivative. This is done in order to separate the relativistic corrections due to the dynamics of the particle from those coming from the relativistic behaviour of the electromagnetic field, and to preserve the interaction with the magnetic field also in the "nonrelativistic limit". The interaction with the external electric potential is described by adding to H_0 the operator:

$$V = \nu \otimes V_+ + \mu \otimes V_- = \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix} \tag{I.7}$$

where V_+ and V_- are self-adjoint operators on $L^2(\mathbb{R}^3; \mathbb{C}^2)$ given by multiplication with the real functions (which we shall denote by the same symbol) $V_\pm : \mathbb{R}^3 \to \mathbb{R}$. Thus by denoting $\sigma . D_A$ the self adjoint operator on $L^2(\mathbb{R}^3; \mathbb{C}^2)$ defined by: $\sigma_1 . (D_1 - A_1) + \sigma_2 . (D_2 - A_2) + \sigma_3 . (D_3 - A_3)$ we have that the evolution with interaction is given by *the total Dirac hamiltonian*:

$$H = c\,\alpha \otimes \sigma . D_A + mc^2(\beta - 1) + V = \begin{pmatrix} V_+ & c\,\sigma . D_A \\ c\,\sigma . D_A & -2mc^2 + V_- \end{pmatrix} \tag{I.8}$$

We use the following notations:

$$\begin{aligned} \mathscr{D}_0 &= \alpha \otimes \sigma . D \\ \mathscr{D} &= \alpha \otimes \sigma . D_A \\ \mathscr{A} &= \alpha \otimes \sigma . A = \alpha \otimes (\sigma_1 A_1 + \sigma_2 A_2 + \sigma_3 A_3) \end{aligned} \tag{I.9}$$

Then we may write:

$$\begin{aligned} H_0 &= c\,D_0 - 2mc^2 M \\ H &= c\,\mathscr{D} - 2mc^2 M + V = H_0 + \mathscr{V} \end{aligned} \tag{I.10}$$

where $\mathscr{V}$ represents the perturbation due to the interaction, given by:

$$\mathscr{V} = V - c\,\mathscr{A} \tag{I.11}$$

We shall now briefly recall the Pauli description of a quantum nonrelativistic particle of mass $m > 0$ and spin 1/2. The Hilbert space is taken to be:

$$h = L^2(\mathbb{R}^3; \mathbb{C}^2) \tag{I.12}$$

The free evolution group is generated by the *free Pauli hamiltonian*:

$$h_0=\frac{1}{2m}(\sigma.\mathrm{D})^2=-\frac{1}{2m}\Delta \tag{I.13}$$

and the total evolution group is generated by the *total Pauli hamiltonian*:

$$h=\frac{1}{2m}(\sigma.\mathrm{D_A})^2+\mathrm{V}_+. \tag{I.14}$$

We observe that

$$\begin{aligned}(\sigma.\mathrm{D_A})^2&=(\sigma.\mathrm{D})^2-\mathrm{A}.\mathrm{D}-\mathrm{D}.\mathrm{A}+\mathrm{A}^2-\sigma.(\mathrm{rot}\,\mathrm{A})\\ &=-\Delta-2\mathrm{A}.\mathrm{D}+(\mathrm{div}.\mathrm{A})+\mathrm{A}^2-\sigma.\mathrm{B}\end{aligned} \tag{I.15}$$

and the total perturbation representing the interaction is:

$$\begin{aligned}\mathrm{v}&=\frac{1}{2m}[(\sigma.\mathrm{D_A})^2-(\sigma.\mathrm{D})^2]+\mathrm{V}_+\\ &=-\frac{1}{2m}[2\mathrm{A}.\mathrm{D}-(\mathrm{div}.\mathrm{A})-\mathrm{A}^2+\sigma.\mathrm{B}]+\mathrm{V}_+.\end{aligned} \tag{I.16}$$

In order to give a meaning to the operator sums defining H and h some conditions have to the imposed to the functions V_+, V_-, A_j, $j=1, 2, 3$.

DEFINITION I.1. — *We shall say that a function $f: \mathbb{R}^3 \to \mathbb{R}$ satisfies condition S_4 if:*

$$\sup_{x\in\mathbb{R}^3}\left\{(1+|x|^2)^s\int_{|x-y|\leq 1}|\mathrm{f}(y)|^2|x-y|^{\mu-3}\right\}<\infty \tag{I.17}$$

for some positive $\mu<4$ and $s>0$. We shall say that f *satisfies condition S_2 if* (I.17) *is true with some positive $\mu<2$ and $s>0$.*

Remark: One can easily verify that condition S_2 is verified if f is locally L^p with $p>3$ and S_4 if $p>\frac{3}{2}$.

One can prove now the following results:

THEOREM I.1. — *Suppose H_0 is given by* (I.4) *and V_+, V_-, A_1, A_2, A_3 are real functions on $\mathbb{R}^3$ satisfying condition S_2. Then $\mathscr{V}$ is H_0-relatively compact so that* H *given by* (I.8) *admits a unique self-adjoint extension (which we shall denote by* H *too) having the same domain as H_0 and the same essential spectrum*

$$\sigma_{\mathrm{ess}}(\mathrm{H})=\sigma(\mathrm{H}_0)=(-\infty, -2mc^2]\cup[0, \infty).$$

In the complement in $\mathbb{R}$ of $\sigma_{\mathrm{ess}}(\mathrm{H})$, there can be only finitely degenerated eigenvalues accumulating only at $-2mc^2$ or 0.

THEOREM I.2. — *Suppose h_0 is given by* (I.13) *and* V_+, V_-, A_1, A_2, A_3 *satisfy condition* S_2. *Then h given by* (I.14) *admits a unique self-adjoint extension (which we shall denote by h too) having the same domain as h_0 and the same essential spectrum $\sigma_{ess}(h)=\sigma(h_0)=[0, \infty)$. In the complement in $\mathbb{R}$ of $\sigma_{ess}(h)$, there can be only finitely degenerated eigenvalues accumulating only at* 0.

The proof of theorem I.1 is an immediate consequence of the results of [11, 21, 22]. The theorem I.2. is also an easy consequence of [12, 22]. We would like to make some comments concerning the conditions imposed to the potential functions. First it is evident that the condition at infinity may be weakened [12], but we prefer to use conditions S_2 and S_4, being general enough for physical applications and allowing a complete treatment of the scattering theory. Now concerning the local behaviour, condition S_2 excludes the Coulomb-type singularities. Some more general treatment, including local Coulomb-type singularities, is given in [18]. In the following we shall not work in this framework in order to avoid to complicate the formalism but our results can be extended to this case too. Some comments in this respect will be made after the main results. We would also like to stress that in dealing with the corrections to the scattering amplitude some strengthening of the condition at infinity will be necessary.

Our problem in this paper is to study the limit $c \to \infty$ for H and compare it to the Pauli hamiltonian *h*. We shall systematically use the notation:

$$\kappa = \frac{1}{c} \tag{I.18}$$

In order to point out the difficulties, we shall consider H_0 (*i. e.* the case $A=V=0$) and we shall proceed formally. As it is well known [23] one can define a unitary operator U on $\mathscr{H}$ (the so called *free Foldy-Wouthuysen transformation*), such that:

$$UH_0U^{-1} = \beta \otimes \sqrt{m^2c^4 + c^2D^2} - mc^2 = \begin{pmatrix} h_+(c) & 0 \\ 0 & h_-(c) \end{pmatrix} \tag{I.19}$$

More precisely U is of the form $U = e^{is}$ where:

$$S = -i(\beta\alpha \otimes \sigma . D)\frac{1}{2|D|}\operatorname{arctg}\frac{|D|}{mc} \tag{I.20}$$

Hence, we see that formally:

$$h_+(c) = \frac{1}{2m}D^2 + \mathcal{O}\left(\frac{1}{c^2}\right) = h_0 + \mathcal{O}(\kappa^2) \tag{I.21}$$

But the problems are first that in fact $h_-(c)$ diverges for $c \to \infty$, and secondly that the formal power expansion in $1/c$ of $h_+(c)$ contains operators which are more and more singular (being higher powers of $D^2 = -\Delta$). In order to handle with these difficulties, Veselić [25] proposes to look at the resolvent of H, and observe that although in the limit $c \to \infty$ it will no longer be injective [in connection with the divergence of $h_-(c)$], one can construct a family of pseudoresolvents which is analytic near $\kappa = 0$. In this paper we shall prove that this is enough in order to control the limit $c \to \infty$ for all interesting physical quantities (bound states and scattering amplitude) and we shall use this method in order to do explicit calculations of the limit and the first corrections. First, let us remind for completness, some results concerning pseudoresolvents.

DEFINITION I.2. — *Let $\Delta \subset \mathbb{C}$ be a symmetric domain* (i.e. $\Delta = \bar{\Delta}$). *A function $\mathscr{R} : \Delta \to \mathscr{B}(\mathscr{H})$ defined on Δ with values bounded operators on the Hilbert space $\mathscr{H}$, is said to be a pseudoresolvent if it satisfies the first resolvent equation.*

(i) $\mathscr{R}(\lambda) - \mathscr{R}(\mu) = (\lambda - \mu)\, \mathscr{R}(\lambda)\, \mathscr{R}(\mu)$ *for any* $\lambda, \mu \in \Delta$,

and the symmetry condition:

(ii) $\mathscr{R}(\lambda)^* = \mathscr{R}(\bar{\lambda})$.

In [25] such a function is called a symmetric pseudoresolvent, but because we shall not use more general pseudoresolvents we prefer to shorten the terminology. The structure of a pseudoresolvent is described by the following result:

THEOREM I.3. — *If $\mathscr{R}$ is a pseudoresolvent, then there exist an orthogonal projection Q and a selfadjoint operator A in $Q\mathscr{H}$ such that:*

$$\mathscr{R}(\lambda) = Q(A - \lambda)^{-1} Q \qquad \textit{for any} \quad \lambda \in \Delta.$$

It follows that $\mathscr{R}$ is analytic in Δ (with respect to the norm-topology in $\mathscr{B}(\mathscr{H})$ and has an analytic continuation to the resolvent set $\rho(A)$ of A. In what follows we shall (improperly) call $\rho(A)$ the resolvent set of $\mathscr{R}$ and $\sigma(A) = \mathbb{C} \setminus \rho(A)$ the spectrum of $\mathscr{R}$. If $Q = 1$, then $\mathscr{R}$ is the resolvent of a selfadjoint operator in $\mathscr{H}$. The necessary and sufficient condition for a pseudoresolvent $\mathscr{R}$ to be a resolvent is injectivity. The point in considering pseudoresolvents instead of resolvents is that the norm limit (which does not preserve injectivity) of pseudoresolvents is still a pseudoresolvent. Moreover we have the following result concerning the "continuity of the spectrum":

THEOREM I.4. — *Let $\{\mathscr{R}_n\}_{n \in \mathbb{N}}$ be a family of pseudoresolvents. Suppose $z_0 \in \mathbb{C}$ with $\operatorname{Im} z_0 \neq 0$ is such that $\mathscr{R}_n(z_0)$ is a norm-convergent sequence of operators. Then $\mathscr{R}_n(z)$ is a norm convergent sequence of operators for any* *non-real z, and:*

$$\mathscr{R}_\infty(z) \overset{d}{=} \lim_{n\to\infty} \mathscr{R}_n(z)$$

is a pseudoresolvent. Moreover:

$$\lim_{n\to\infty} dist(\sigma(\mathscr{R}_n), \sigma(\mathscr{R}_\infty)) = 0.$$

As is usual in regular perturbation theory, we shall deal with analytic families of pseudoresolvents:

DEFINITION I.3. — *The family $\{\mathscr{R}_\varkappa\}_{\varkappa\in\mathbb{C}}$ of pseudoresolvents is said to be analytic at zero if there exist $r>0$ and $z_0 \in \rho(\mathscr{R}_\varkappa)$ for $|\kappa|<r$ such that $\mathscr{R}_\varkappa(z_0)$ is analytic in κ for $|\kappa|<r$.*

THEOREM I.5. — *Suppose $\{\mathscr{R}_\varkappa\}_{\varkappa\in\mathbb{C}}$ is analytic at zero. Then if $z\in\rho(\mathscr{R}_0)$ there exists $r(z)>0$ such that $\mathscr{R}_0(z)$ is analytic in κ for $|\kappa|<r(z)$. Moreover if $K \subset \rho(\mathscr{R}_0)$ is a compact set, then $\inf_{z\in K} r(z) \equiv r_K > 0$.*

These results make it possible to define an analytic functional calculus for pseudoresolvents, and in this way, to reduce some singular perturbation problems to the scheme of analytic perturbations described in [14].

Let us now consider the hamiltonian (I.8) as a family of hamiltonians $\{H(c)\}_{c>0}$. We define the family of pseudoresolvents:

$$\mathscr{R}_\varkappa(z) \overset{d}{=} (H(c) - z\,1)^{-1}. \tag{I.22}$$

We shall prove that it is analytic at $\kappa=0$ and we shall see that one can write:

$$\mathscr{R}_\varkappa(z) = Q(\kappa)(H(c) - z\,1)^{-1} Q(\kappa) \tag{I.23}$$

where: $Q(\kappa)=1$ for $\kappa>0$ and $Q(0) \lneqq 1$. Thus $Q(\kappa)$ is surely not norm-analytic. Let us define $H(\infty)$ as the selfadjoint operator on $Q(0)\mathscr{H}$, defined by theorem I.3, and let σ_0 be *a bounded* isolated part of $\sigma(H(\infty))$. We define the orthogonal projection corresponding to σ_0:

$$P_0 \overset{d}{=} \frac{1}{2\pi i}\int_{\Gamma_0} \mathscr{R}_0(z)\,dz \tag{I.24}$$

where Γ_0 is a closed differentiable curve in $\mathbb{C}$ isolating σ_0 from the rest of $\sigma(H(\infty))$. One can see that the function:

$$\kappa \to \frac{1}{2\pi i}\int_{\Gamma_0} \mathscr{R}_\varkappa(z)\,dz \overset{d}{=} P_\varkappa \tag{I.25}$$

is analytic and defines an analytic family of orthogonal projections corresponding to the part $\sigma_0(\kappa)$ of the spectrum of $H(c)$ which lies inside Γ_0.

From the projections $P_\varkappa$ which commute with $H(c)$, one can construct an analytic family of hamiltonians:

$$\mathring{H}_\varkappa \stackrel{d}{=} P_\varkappa H(c) P_\varkappa = \frac{1}{2\pi i}\int_{\Gamma_0} z\,\mathscr{R}_\varkappa(z)\,dz. \tag{I.26}$$

Each $P_\varkappa$ having generally a different image subspace, each $\mathring{H}_\varkappa$ will generally act in a different subspace of $\mathscr{H}$. Now, $P_\varkappa$ being analytic in κ, for $|\kappa|$ small enough one has that $\|P_\varkappa - P_0\| < 1$ so that one can use the Nagy formula [14] in order to construct an unitary operator $U_\varkappa$ intertwining between $P_\varkappa \mathscr{H}$ and $P_0 \mathscr{H}$:

$$\begin{gathered} U_\varkappa = [1-(P_\varkappa - P_0)^2]^{-1/2}[(1-P_\varkappa)(1-P_0)+P_\varkappa P_0] \\ U_\varkappa P_0 = P_\varkappa U_\varkappa \end{gathered} \tag{I.27}$$

Thus, the reduced hamiltonians, defined by:

$$\begin{aligned} \tilde{H}_\varkappa \stackrel{d}{=} U_\varkappa^{-1} P_\varkappa H(c) P_\varkappa U_\varkappa &= P_0 U_\varkappa^{-1} \mathring{H}(c) U_\varkappa P_0 \\ &= \frac{1}{2\pi i} P_0 U_\varkappa^{-1} \int_{\Gamma_0} z\,\mathscr{R}_\varkappa(z)\,dz\, U_\varkappa P_0 \end{aligned} \tag{I.28}$$

form an analytic family of bounded hamiltonians in $P_0 \mathscr{H}$.

Note that in the above construction the condition that σ_0 is bounded is essential. The troubles with the Foldy-Wouthuysen transformation came from the fact that the corresponding part of the spectrum is unbounded.

II. POWER SERIES EXPANSION FOR THE RESOLVENT

We shall derive an explicit formula for $\mathscr{R}_\varkappa(z) = (H(c) - z\,1)^{-1}$ which will be systematically used in the following calculations. Let us observe that:

$$\begin{gathered} \alpha^2 = \beta^2 = \sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1 \\ \alpha\beta + \beta\alpha = 0 \end{gathered} \tag{II.1}$$

so that

$$(H_0 - z\,1)^{-1} = \left(N + \frac{\kappa}{2m}\mathscr{D}_0 + \frac{\kappa^2 z}{2m} 1\right)(K_0 - tz)^{-1} \tag{II.2}$$

where:

$$\begin{gathered} K_0 \stackrel{d}{=} \frac{1}{2m}\mathscr{D}_0^2 = \nu \otimes h_0 + \mu \otimes h_0 \\ t \stackrel{d}{=} 1 + \frac{z}{2m}\kappa^2. \end{gathered} \tag{II.3}$$

Similarly, by denoting:

$$\begin{aligned} K_A &\stackrel{d}{=} \frac{1}{2m}\mathscr{D}^2 \\ H_A &\stackrel{d}{=} H_0 + c\mathscr{A} = c\mathscr{D} - 2mc^2 M \end{aligned} \tag{II.4}$$

we see that:

$$(H_A - z\,1)^{-1} = \left(N + \frac{\kappa}{2m}\mathscr{D} + \frac{\kappa^2 z}{2m}1\right)(K_A - tz)^{-1}, \tag{II.5}$$

and after some calculations, denoting:

$$K \stackrel{d}{=} K_A + NVN = K_A + NV_+ N \tag{II.6}$$

and observing that:

$$(K_A - tz)^{-1}[1 + NV(K_A - tz)^{-1}]^{-1} = (K - tz)^{-1}$$

we obtain:

$$\begin{aligned}(H - z\,1)^{-1} \equiv \mathscr{R}_\varkappa(z) = &\left(N + \frac{\kappa}{2m}\mathscr{D} + \frac{\kappa^2 z}{2m}1\right)(K - tz)^{-1} \\ &\times\left\{1 + \kappa V\left(\frac{1}{2m}\mathscr{D} + \frac{\kappa z}{2m}\right)(K - tz)^{-1}\right\}^{-1}. \end{aligned} \tag{II.7}$$

In this form, one easily sees that $\mathscr{R}_\varkappa(z)$ is a family of pseudoresolvents analytic at $\kappa = 0$, and:

$$\lim_{\varkappa \to 0} \mathscr{R}_\varkappa(z) = \lim_{\varkappa \to 0} (K - tz)^{-1} = \nu \otimes (h - z\,1)^{-1}, \tag{II.8}$$

so that the limit $\kappa \to 0$ of $\mathscr{R}_\varkappa(z)$ is no longer the resolvent of a selfadjoint operator in $\mathscr{H}$, but its restriction to $N\mathscr{H}$ is just the resolvent of the hamiltonian h. In this sense we say that h is the limit of $H(c)$ for $c \to \infty$, and for c large we may consider $H(c)$ as a perturbation of $\nu \otimes h$, and use the scheme presented in section I in order to develop the usual analytic perturbation theory. We shall do this in section III by taking for σ_0 an isolated eigenvalue of h, and we shall calculate the first two relativistic corrections to the eigenvalue. In section IV we shall use the power series of the total resolvent in order to calculate the first relativistic correction to the scattering amplitude. In section V we shall deal with a more subtle question, the Foldy-Wouthuysen transformation, where it is no more possible to work in a bounded domain of energies so that analyticity of some quantities with respect to κ will no longer be true. However we shall prove the norm-continuity with respect to κ. We shall finish this section by explicitly calculating the first four terms of the power expansion in κ of $\mathscr{R}_\varkappa(z)$, which will be needed in the next sections. First let us introduce some more notations in order to have more compact formulas:

$$\begin{aligned} \mathrm{r}(z) &\overset{d}{=} (h - z\,1)^{-1} \\ \mathscr{E}(z) &\overset{d}{=} \mu \otimes (z - \mathrm{V}_-) \end{aligned} \tag{II.9}$$

THEOREM II.1. — *Let* H *be the selfadjoint operator given by* (I.8) *and suppose* $\mathrm{V}_\pm$, A_j, $\partial_j \mathrm{A}_k$ *satisfy* S_2. *Then* $\mathscr{R}_\varkappa(z) = (\mathrm{H}(c) - z\,1)^{-1})$ *is norm analytic at* $\kappa = 0$ *for* $\operatorname{Im} z \neq 0$, *and we have*

$$\mathscr{R}_\varkappa(z) = \sum_{k=0}^{4} \kappa^k \mathrm{R}_k(z) + \mathscr{O}(\kappa^5)$$

where

$$\mathrm{R}_0(z) = \nu \otimes \mathrm{r}(z)$$

$$\mathrm{R}_1(z) = \frac{1}{2m}[\mathrm{R}_0(z)\mathscr{D} + \mathscr{D}\mathrm{R}_0(z)]$$

$$\mathrm{R}_2(z) = \mathrm{R}_1(z)\mathscr{E}(z)\mathrm{R}_1(z) - \frac{1}{2m}\left[\mathrm{M} - \frac{1}{2m}\mathscr{D}\mathrm{R}_0(z)\mathscr{D}\right]$$

$$\begin{aligned} \mathrm{R}_3(z) = \frac{1}{(2m)^2}\Bigg[&\mathrm{R}_1(z)\mathscr{E}(z)\left(\frac{1}{2m}\mathscr{D}\mathrm{R}_0(z)\mathscr{D} - \mathrm{M}\right) \\ &+ \left(\frac{1}{2m}\mathscr{D}\mathrm{R}_0(z)\mathscr{D} - \mathrm{M}\right)\mathscr{E}(z)\mathrm{R}_1(z)\Bigg] \end{aligned}$$

$$\begin{aligned} \mathrm{R}_4(z) = -\frac{1}{2m}\Bigg[&\mathrm{R}_1(z)\mathscr{E}^2(z)\mathrm{R}_1(z) \\ &- \frac{1}{2m}\mathrm{R}_1(z)\mathscr{E}(z)\mathscr{D}\mathrm{R}_0(z)\mathscr{D}\mathscr{E}(z)\mathrm{R}_1(z)\Bigg] \\ + \frac{1}{(2m)^2}\Bigg[&\mathscr{E}(z) - \frac{1}{2m}(\mathscr{D}\mathrm{R}_0(z)\mathscr{D}\mathscr{E}(z) + \mathscr{E}(z)\mathscr{D}\mathrm{R}_0(z)\mathscr{D}) \\ &+ \frac{1}{(2m)^2}\mathscr{D}\mathrm{R}_0(z)\mathscr{D}\mathscr{E}(z)\mathscr{D}\mathrm{R}_0(z)\mathscr{D}\Bigg]. \end{aligned}$$

Proof: Let us start from formula (II.6) for the resolvent of H(c):

$$\begin{aligned} \mathscr{R}_\varkappa(z) = \Bigg\{ &\mathrm{N}(\mathrm{K} - tz)^{-1} \\ &+ \frac{\kappa}{2m}\mathscr{D}(\mathrm{K} - tz)^{-1} + \kappa^2 \frac{z}{2m}(\mathrm{K} - tz)^{-1}\Bigg\} \\ \times \Bigg\{ &1 + \kappa \frac{1}{2m}\mathrm{V}\mathscr{D}(\mathrm{K} - tz)^{-1} + \kappa^2 \frac{z}{2m}\mathrm{V}(\mathrm{K} - tz)^{-1}\Bigg\}^{-1}. \end{aligned} \tag{II.10}$$

If V_+, V_- satisfy condition S_2 (*see* Definition I.1) then V and $V\mathscr{D}$ are K-relatively bounded so that all the terms in the above formula belong to $\mathscr{B}(\mathscr{H})$ and are analytic in κ. Moreover for any $R<\infty$, if κ is sufficiently small we have that:

$$1+\kappa V\left(\frac{1}{2m}\mathscr{D}+\kappa\frac{z}{2m}\right)(K-tz)^{-1}$$

is invertible for any nonpositive z such that $|z|\leqq R$. Thus for a given z with $\operatorname{Im} z\neq 0$, $\mathscr{R}_\varkappa(z)$ is analytic in κ at $\kappa=0$, so that:

$$\mathscr{R}_\varkappa(z)=\sum_{k=0}^{\infty}\kappa^k\mathscr{R}_k(z)$$

Now we have that:

$$\begin{aligned}(K-tz)^{-1}&=\left[K-z\left(1+\frac{z}{2m}\kappa^2\right)\right]^{-1}\\&=(K-z)^{-1}\left\{1-\kappa^2\frac{z^2}{2m}(K-z)^{-1}\right\}^{-1}\\&=(K-z)^{-1}\left\{1+\kappa^2\frac{z^2}{2m}(K-z)^{-1}\right.\\&\qquad\left.+\kappa^4\frac{z^4}{(2m)^2}(K-z)^{-2}\right\}+\mathscr{O}(\kappa^5).\end{aligned}\qquad\text{(II.11)}$$

Then by multiplying the series we get the desired formulas for $R_k(z)$ $(k=0, 1, 2, 3, 4)$.

Q.E.D.

We would like to remark that the only condition needed in the proof was the K-relative boundedness of V and $V\mathscr{D}$.

III. RELATIVISTIC CORRECTIONS TO THE BOUND-STATES

In this section, we shall apply the reduction scheme presented in section I, taking for σ_0 an isolated eigenvalue e of h. From theorem I.2 it follows that e is negative and of finite multiplicity. Let p_0 be the eigenprojection of h corresponding to the eigenvalue e; *i.e.*:

$$p_0\overset{d}{=}\frac{1}{2\pi i}\int_\Gamma r(z)\,dz \qquad\text{(III.1)}$$

where Γ is a differentiable curve in $\mathbb{C}$ separating e from the rest of $\sigma(h)$. Thus we have

$$h_{|\,p_0\mathrm{h}}=ep_0$$

and $p_0 h$ is finite dimensional. Now, taking into account that $\mathscr{R}_0(z) = R_0(z) = \nu \otimes r(z)$, we define:

$$P_0 \stackrel{d}{=} \nu \otimes p_0 = \frac{1}{2\pi i}\int_\Gamma \mathscr{R}_0(z)\,dz \tag{III.2}$$

and more generally:

$$P_\varkappa \stackrel{d}{=} \frac{1}{2\pi i}\int_\Gamma \mathscr{R}_\varkappa(z)\,dz, \tag{III.3}$$

so that $P_0 \subset N$ and $P_\varkappa$ is norm-analytic in κ at $\kappa=0$, following that:

$$\lim_{\varkappa \to 0} P_\varkappa = P_0,$$

We can now apply the reduction scheme, and we define the unitary intertwining operator:

$$U_\varkappa \stackrel{d}{=} [1-(P_\varkappa - P_0)^2]^{-1/2}[(1-P_\varkappa)(1-P_0)+P_\varkappa P_0], \tag{III.4}$$

which satisfies

$$U_\varkappa P_0 = P_\varkappa U_\varkappa \tag{III.4}$$

and is evidently analytic in κ for sufficiently small κ. Now starting from the series expansion in κ for $\mathscr{R}_\varkappa(z)$ given in theorem II.1 we obtain the series expansions in κ for $P_\varkappa$ and $U_\varkappa$ and

$$\tilde{H}_\varkappa = P_0 U_\varkappa^{-1} \frac{1}{2\pi i}\int_\Gamma z\,\mathscr{R}_\varkappa(z)\,dz\, U_\varkappa P_0. \tag{III.6}$$

In this section we shall prove that in fact $\tilde{H}_\varkappa$ is analytic in κ^2 (a fact first noticed by Hunziker [12]) and we shall use this fact in order to prove some properties of the series expansion for the eigenvalues and eigenvectors of H at $\kappa=0$. We shall finally explicitly calculate the first (κ^2) and second (κ^4) corrections to $\tilde{H}_\varkappa$. We like to insist that the calculus is made for a degenerate eigenvalue as well, the correction in κ^4 for this case being not yet calculated in the literature.

Let us denote by $\mathscr{I}$ the ring of bounded linear operators on h and by $A_\varkappa$ the norm-closed subalgebra of bounded linear operators on $\mathscr{H} = \mathbb{C}^2 \otimes h$ generated by the ring $\mathscr{I}$ over the four generators:

$$\begin{aligned} X_1 &= \nu \otimes 1; \qquad & X_2 &= \mu \otimes 1.\\ Y_1 &= \kappa E_{12} \otimes 1; \qquad & Y_2 &= \kappa E_{21} \otimes 1 \end{aligned} \tag{III.7}$$

where

$$E_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \qquad E_{21} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{III.8}$$

Then we have the following algebraic properties:

$$X_j^k = X_j \quad \text{for} \quad j=1,2 \quad \text{and} \quad k \geqq 1.$$
$$Y_j^k = 0 \quad \text{for} \quad j=1,2 \quad \text{and} \quad k \geqq 2$$
$$X_1 X_2 = X_2 X_1 = 0$$
$$Y_1 Y_2 = \kappa^2 X_1, \qquad Y_2 Y_1 = \kappa^2 X_2.$$

Thus any element $A_\varkappa \in A_\varkappa$ may be considered as a norm-convergent series in κ, of the form:

$$A_\varkappa = \sum_{k=0}^{\infty} \kappa^{2k} (\nu \otimes a_k + \mu \otimes b_k) + \sum_{k=0}^{\infty} \kappa^{2k+1} (E_{12} \otimes c_k + E_{21} \otimes d_k) \quad \text{(III.9)}$$

where: a_k, b_k, c_k, $d_k \in \mathscr{I}$. Now observing that $N = \nu \otimes 1$, we immediately get the following result:

PROPOSITION. — *If* $A_\varkappa \in \mathscr{A}_\varkappa$, *then* $NA_\varkappa N$ *is given by a norm-convergent series expansion in* κ^2 *of the form:*

$$NA_\varkappa N = \sum_{k=0}^{\infty} \kappa^{2k} (\nu \otimes a_k)$$

with $a_k \in \mathscr{I}$ *such that* $A_\varkappa$ *is of the form* (III.9) *with the same coefficients* a_k.

We can now prove our result concerning $\tilde{H}_\varkappa$:

THEOREM III.1. — *If e is an isolated eigenvalue of h, and if* $V_\pm$, A_j, $\partial_j A_k$ *satisfy* S_2 *then the corresponding reduced hamiltonian* H (see III.6) *is a finite rank selfadjoint operator which depends norm-analytically in* κ^2 *at* $\kappa = 0$. *Thus its eigenvalues and eigenprojections depend analytically in* κ^2. *Moreover we have*

$$\tilde{H}_\varkappa = e P_0 + \kappa^2 \tilde{H}_1 + \kappa^4 \tilde{H}_2 + \mathcal{O}(\kappa^6)$$

where:

$$\tilde{H}_1 = \frac{1}{(2m)^2} P_0 \mathscr{D}\mathscr{E}(e) \mathscr{D} P_0$$

$$\tilde{H}_2 = -\frac{1}{(2m)^3} P_0 \mathscr{D}\mathscr{E}^2(e) \mathscr{D} P_0 + \frac{1}{(2m)^4} (P_0 \mathscr{D}\mathscr{E}(e) \mathscr{D} (\nu \otimes \bar{h}(e)) \mathscr{D}\mathscr{E}(e) \mathscr{D} P_0 - \frac{1}{2} [P_0 \mathscr{D}^2 P_0 \mathscr{D}\mathscr{E}(e) \mathscr{D} P_0 + P_0 \mathscr{D}\mathscr{E}(e) \mathscr{D} P_0 \mathscr{D}^2 P_0] \}$$

using the notations (II.9) *and* $\bar{h}(e)$ *being the reduced resolvent of h at e defined by*

$$\bar{h}(z)=(h-z)^{-1}-\frac{1}{e-z}p_0$$

and continued at $z=e$ *by continuity.*

Proof: The first part of the theorem is a direct consequence of the last Proposition if we prove that $\tilde{\mathrm{H}}_\varkappa \in A_\varkappa$. In order to do that we observe:

$$(\mathrm{K}-z)^{-1}=\nu\otimes\left(\frac{1}{2m}(\sigma.\mathrm{D_A})^2+\mathrm{V}_+-z\right)^{-1}+\mu\otimes\left(\frac{1}{2m}(\sigma.\mathrm{D_A})^2-z\right)^{-1}$$
$$\kappa\mathscr{D}=\kappa\mathrm{E}_{12}\otimes\sigma.\mathrm{D}+\kappa\mathrm{E}_{21}\otimes\sigma.\mathrm{D}$$

so that using (II.11) and (II.10) we get that $\mathscr{R}_\varkappa(z)\in A_\varkappa$ for $\mathrm{Im}\,z\neq 0$, or for $z\in\Gamma$. Now, $A_\varkappa$ being a norm-closed subalgebra of $\mathscr{B}(\mathscr{H})$, from (III.3), (III.4) and (III.6) we get the desired result.

In order to do the calculations for $\tilde{\mathrm{H}}_1$, $\tilde{\mathrm{H}}_2$ we remark that:

$$\begin{aligned}\tilde{\mathrm{H}}_\varkappa&=\mathrm{P}_0\mathrm{U}_\varkappa^{-1}\frac{1}{2\pi i}\int_\Gamma z\,\mathscr{R}_\varkappa(z)\,dz\,\mathrm{U}_\varkappa\mathrm{P}_0\\&=e\,\mathrm{P}_0+\mathrm{P}_0\mathrm{U}_\varkappa^{-1}\frac{1}{2\pi i}\int_\Gamma(z-\mathrm{E})\,\mathscr{R}_\varkappa(z)\,dz\,\mathrm{U}_\varkappa\mathrm{P}_0.\qquad\text{(III.10)}\end{aligned}$$

First, let us remark that *a priori*, in order to compute $\tilde{\mathrm{H}}_2$ one would have to know explicitly $\mathrm{R}_6(z)$, because H(c) contains terms of order $\kappa^{-2}=c^2$. It is only due to formula (III.10) that only the terms up to $\mathrm{R}_4(z)$ are necessary in order to compute $\tilde{\mathrm{H}}_2$. Now by computing the contour integrals one gets the formulas for $\tilde{\mathrm{H}}_1$ and $\tilde{\mathrm{H}}_2$.

Q.E.D.

COROLLARY. – *Let* H(c) *be the hamiltonian defined by* (I.8) *and let e be an isolated eigenvalue of h* [*as defined by* (I.14)], *of finite multiplicity m. Then for* κ *sufficiently small there are k isolated eigenvalues of* H(c), *given by the functions*: $\mathrm{E}_1(\kappa),\ldots,\mathrm{E}_k(\kappa)$ *which are analytic in* κ^2 *on a neighbourhood of* $\kappa=0$, *have multiplicities* $m_1,\ldots,m_k$ *such that* $m_1+\ldots+m_k=m$ *and satisfy*: $\lim_{\varkappa\to 0}\mathrm{E}_j(\kappa)=e$ for $j=1,\ldots,k$. *The corresponding eigenvectors may be choosen to depend analytically in* κ (*for* κ *small*) *and to have the form:*

$$\Psi_j(\kappa)=\xi_j(\kappa)+\kappa.\eta_j(\kappa)$$

with: $\xi_j(\kappa)\in\mathrm{N}\mathscr{H}$, $\eta_j(\kappa)\in\mathrm{M}\mathscr{H}$, ξ_j *and* η_j *analytic in* κ^2 (*for* κ *small*) *and* $\lim_{\varkappa\to 0}\xi_j(\kappa)\in\mathrm{P}_0\mathscr{H}$.

Proof: We only have to use theorem III.1 and observe that any eigenvector $\Psi_j(\kappa)$ of H(c) corresponding to one of the eigenvalues $\mathrm{E}_j(\kappa)$, is of the form:

$$\Psi_j(\kappa) = U_\varkappa \Psi_j$$

with $\Psi_j \in P_0 \mathscr{H} \subset N\mathscr{H}$. But $U_\varkappa \in A_\varkappa$ and the Proposition gives the stated result concerning the structure of $\Psi_j(\kappa)$.

Q.E.D.

We would like to remark that all the results of this chapter remain true under weaker conditions on V_+, V_-, A_1, A_2, A_3. All that we need is that $\mathscr{V}$ should be H_0-relatively bounded with bound less than 1. More than that, a similar argument can be given with a symmetric decomposition of the potential.

IV. THE SCATTERING AMPLITUDE

In this section we study the nonrelativistic limit of the scattering amplitude and derive an explicit formula for the first relativistic correction. This problem is more subtle than the study of bound states due to the fact that one deals with the boundary value of the resolvent along the positive semiaxis which is no longer a bounded operator in the original Hilbert space of the system and is certainly no more an analytic function of the energy. We don't want to insist here on problems related to the Limiting Absorption Principle for Dirac hamiltonians or to the differentiability with respect to the energy of the boundary value of their resolvents. Our method will be to use the algebraic structure of the Dirac hamiltonian and formulas (III.2) and (III.7) in order to deal with Schrödinger-type hamiltonians, and to take advantage of the fact that being interested only in the limit $\kappa \to 0$ we can suppose κ as small as we need. We would like to remark that we deal with Schrödinger type operators acting on $\mathbb{C}^4 \otimes L^2(\mathbb{R}^3)$, but all the usual theorems can be easily generalized to this case and we shall no more instist upon this point. Now, let us present the results on Schroedinger operators that we shall need:

THEOREM IV.1. — *Suppose h is the Pauli hamiltonian given by* (I.14) *and suppose* v *is a compact operator in* $\mathscr{B}(\mathscr{H}^2_{-s}; \mathscr{H}^0_s)$ *for some* $s > \frac{1}{2}$. *Then* $(h-z)^{-1}$ *considered as an analytic function from* $\Pi_\pm = \{ z \in \mathbb{C} \mid \operatorname{Im} z \gtrless 0 \}$ *into* $\mathscr{B}(\mathscr{H}^0_s; \mathscr{H}^2_{-s})$ *has a continuous extension to* $\Pi_\pm \cup \{(0, \infty) \setminus \Lambda\}$ (Λ *being the discrete set of positive eigenvalues of h*). *Moreover these extensions are locally Hoelder—continuous of exponent* $s - \frac{1}{2}$.

The assertions of this theorem are proved in [2, 15, 16].

THEOREM IV.2. — *Suppose h is the Pauli hamiltonian given by* (I.14) *and* ν *is a compact operator in* $\mathscr{B}(\mathscr{H}^2_{-s}; \mathscr{H}^0_s)$ *for* $s > \frac{1}{2} + k$ with $k \in \mathbb{N}$. *Then* $(h-z)^{-1}$ *considered as an analytic function from* $\Pi_\pm$ *into* $\mathscr{B}(H^0_{+s}; \mathscr{H}^2_{-s})$ *has a* C^k *extension to* $\Pi_\pm \cup \{(0, \infty) \setminus \Lambda\}$.

This theorem is a consequence of the analysis done in [5, 13].

Remark: We stress that ν is a compact operator in $\mathscr{B}(\mathscr{H}^2_{-s}, \mathscr{H}^0_s)$ if the following condition is satisfied:

$$\begin{gathered}\text{(i) } A_1, A_2, A_3 \text{ satisfy condition } S_2 \text{ for a given } s > \frac{1}{2}.\\ \text{(ii) } V_+, V_-, A^2 = A_1^2 + A_2^2 + A_3^2 \text{ and } \partial_j A_k (\text{for } j, k = 1, 2, 3), \\ \text{satisfy condition } S_4 \text{ for a given } s > \frac{1}{2}.\end{gathered} \tag{IV.1}$$

Now let us consider the resolvent of the total Dirac hamiltonian, as given by (II.7). First we remark that:

$$\begin{gathered}K = \nu \otimes h + \mu \otimes h_A\\ h = h_0 + \nu\\ h_A = h_0 + \nu_A\\ \nu_A = \nu - V_+\end{gathered}$$

so that

$$K = 1 \otimes h_0 + (\nu \otimes \nu + \mu \otimes \nu_A). \tag{IV.2}$$

Secondly, we observe that the function:

$$z \mapsto z\,.\,t(z) = z\left(1 + \frac{\kappa^2}{2m} z\right) \tag{IV.3}$$

is a C^∞ function on $\mathbb{C}$ which restricts to a C^∞ bijection of $(0, \infty)$ on itself. Moreover we have $\lim_{\kappa \to 0} z\,.\,t(z) = z$ uniformly on compact subsets of $\mathbb{C}$. Now let us suppose that the potentials V and A satisfy hypothesis (IV.1). Now let us consider the Schroedinger type operator K and make use of theorem IV.1. Suppose Λ is the discrete set of positive eigenvalues of K and let Λ_κ denote the inverse image of Λ for the application $(0, \infty) \ni E \mapsto E\,.\,t(E) \in (0, \infty)$. Thus $(K - tz)^{-1}$ has a continuous extension to $\Pi_\pm \cup \{(0, \infty) \setminus \Lambda_\kappa\}$ with values in $\mathscr{B}(\mathscr{H}^0_s, \mathscr{H}^2_{-s})$ which is uniformly continuous in κ for κ in any compact subset of $[0, \infty)$. Now, under hypothesis (IV.1), it is evident that for any compact subset $C \subset (0, \infty) \setminus \Lambda$

there is some $\kappa_C < \infty$ such that for any $\kappa \leqq \kappa_C$, and $E \in C$ we have:

$$C \subset (0, \infty) \setminus \Lambda_\varkappa$$

$$\left\| \kappa V \left(\frac{1}{2m} \mathcal{D} + \kappa \frac{E}{2m} \right) (K - E\, t(E))^{-1} \right\|_{\mathcal{B}(\mathcal{H}_s^0, \mathcal{H}_s^0)} < 1.$$

Thus for any compact $C \subset (0, \infty) \setminus \Lambda$ one has a $\kappa_C < \infty$ such that formula (II.7) holds for $z = E \in C$.

Suppose now that hypothesis (IV.1) is satisfied for some $s > \frac{1}{2} + k$ with $k \in \mathbb{N}$. Then, using theorem IV.2 we conclude that the limit: $(K - E\, t(E))^{-1}$ is locally of class C^k (as a function with values in $\mathcal{B}(\mathcal{H}_s^0, \mathcal{H}_{-s}^2)$) and moreover that:

$$\frac{\partial^k}{\partial E^k} (K - E\, t(E))^{-1} = \lim_{\varepsilon \to 0+} \frac{\partial^k}{\partial E^k} (K - (E + i\varepsilon)\, t(E + i\varepsilon))^{-1} \quad \text{(IV.4)}$$

From formula (II.7) one immediately observes that the only problem in differentiating $\mathcal{R}_\varkappa(E)$ with respect to κ is the differentiability of $(K - E\, t(E))^{-1}$. But:

$$\frac{\partial}{\partial \kappa} (K - E\, t(E))^{-1} = \frac{E^2 \kappa}{m} \frac{\partial}{\partial E} (K - E\, t(E))^{-1} \quad \text{(IV.5)}$$

so that if the potentials satisfy hypothesis (IV.1) with $s > \frac{1}{2} + k$, we have that $\mathcal{R}_\varkappa(E)$ is of class C^k with respect to κ (as a function with values in $\mathcal{B}(\mathcal{H}_s^0, \mathcal{H}_{-s}^1)$ and:

$$\frac{\partial^k}{\partial \kappa^k} \mathcal{R}_\varkappa(E) = \lim_{\varepsilon \to 0+} \frac{\partial^k}{\partial \kappa^k} \mathcal{R}_\varkappa(E + i\varepsilon). \quad \text{(IV.6)}$$

Thus we may use the development of theorem II.1 for $z = E \in (0, \infty) \setminus \Lambda$ for κ sufficiently small, as an asymptotic development up to order k, for functions with values in $\mathcal{B}(\mathcal{H}_s^0, \mathcal{H}_{-s}^1)$, $\left(s > \frac{1}{2} + k \right)$. We would like to stress that the explicit formulas for R_1, R_2, R_3, R_4 may not have a meaning as operators in $\mathcal{B}(\mathcal{H}_s^0, \mathcal{H}_{-s}^1)$, because in deriving them some operations have been done, which are meaningful only in $\mathcal{B}(\mathcal{H})$ which is an algebra. If one wants to compute $R_1(E)$, $R_2(E)$, $R_3(E)$, $R_4(E)$, one has just to multiply term by term the series in (II.10) and (II.11). However, the formulas of theorem II.1 will be useful in studying the scattering cross-section.

Let us now discuss the limit of the scattering amplitude for the pair (H_0, H) at a given energy E where it is well defined. First let us denote by

E the relativistic energy and by

$$e=\mathrm{E}\,t(\mathrm{E})=\mathrm{E}\left(1+\frac{\kappa^2}{2m}\mathrm{E}\right) \tag{IV.7}$$

the nonrelativistic energy, corresponding to the same momentum:

$$e=\frac{p^2}{2m}$$
$$\mathrm{E}=\sqrt{m^2 c^4+p^2 c^2}-mc^2$$

Let Ψ_0 be a generalized eigenfunction of H_0 with positive energy E:

$$\mathrm{H}_0\Psi_0=\mathrm{E}\Psi_0. \tag{IV.8}$$

Then one can easily see that Ψ_0 may be written as:

$$\begin{aligned}\Psi_0(\mathrm{E};x)&=\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\Phi_0(e;x)\\ \Phi_0(e:x)&=\begin{pmatrix}\varphi_0(e;x)\\ 0\end{pmatrix}\end{aligned} \tag{IV.9}$$

where $\varphi_0(e;x)\in\mathbb{C}^2$ and defines a solution of the equation:

$$h_0\varphi_0=e\varphi_0. \tag{IV.10}$$

Now let us consider some arbitrary vectors:

$$\omega\in \mathrm{S}^1_{\mathbb{R}^3}=\{y\in\mathbb{R}^3\,|\,|y|=1\}$$
$$\xi\in \mathrm{S}^1_{\mathbb{C}^2}=\{z\in\mathbb{C}^2\,|\,|z|=1\}$$

and let us denote:

$$\begin{aligned}\varphi_0(e;\omega,\xi;x)&\overset{d}{=}(2\pi)^{-3/2}e^{i\sqrt{2me}\,\omega.x}\xi\\ \Psi_0(\mathrm{E};\omega,\xi;x)&\overset{d}{=}\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\Phi_0(e;\omega,\xi;x)\end{aligned} \tag{IV.11}$$

and by $\Psi(\mathrm{E};\omega,\xi;x)$ the generalized solution of the total Dirac hamiltonian given by:

$$\Psi(\mathrm{E})=[1+(\mathrm{H}_0-\mathrm{E})^{-1}\mathscr{V}]^{-1}\Psi_0(\mathrm{E})=[1-\mathscr{R}_\kappa(\mathrm{E})\mathscr{V}]\Psi_0(\mathrm{E}) \tag{IV.12}$$

where:

$$\mathscr{V}=\mathrm{V}+c\alpha\otimes\sigma.\mathscr{A} \tag{IV.13}$$

Then the scattering amplitude associated with the pair $(\mathrm{H}_0,\mathrm{H})$ is given by

$$\begin{aligned}\mathscr{T}_{\xi\eta}(\mathrm{E};\omega',\omega)&=\int_{\mathbb{R}^3}\langle\Psi_0(\mathrm{E};\omega',\xi;x),\mathscr{V}(x)\Psi(\mathrm{E};\omega,\eta;x)\rangle d^3x\\ &=\int_{\mathbb{R}^3}\langle\Phi_0(e;\omega',\xi;x),\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\mathscr{V}(x)\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\end{aligned}$$

$$\times \Phi_0(e;\omega,\eta;x)\rangle\, d^3x$$
$$-\int_{\mathbb{R}^3}\langle \Phi_0(e;\omega',\xi;x),\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\mathscr{V}(x)\mathscr{R}_\varkappa(\mathrm{E})\mathscr{V}(x)$$
$$\times\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\Phi_0(e;\omega,\eta;x)\rangle\, d^3x \quad \text{(IV.14)}$$

where $\langle .,. \rangle$ is the usual scalar product in $\mathbb{C}^2\otimes\mathbb{C}^2$.

Remark: If we strenghthen hypothesis (IV.1) and suppose:

$$\mathscr{V}=\mathrm{V}+c\,\alpha\otimes\sigma.\mathrm{A} \quad \text{(IV.15)}$$

has matrix elements of class L_s^2 with $s>\frac{1}{2}$, then the first integral in (IV.14) may be interpreted by the same procedure as the Fourier transform of a L^2 function and the second as the duality map between L_s^2 and L_{-s}^2, taking into account that $\varphi_0\in\mathrm{C}^\infty\cap\mathrm{L}^\infty$ and $\mathrm{D}\varphi_0=-\sqrt{e}\,\omega\varphi_0$. We shall still need the following condition:

$$\mathrm{A}_j \text{ is of class } \mathscr{H}_s^1 \text{ for some } s>\frac{1}{2}. \quad \text{(IV.16)}$$

We may give now the main result of this chapter:

THEOREM IV.3. — *Suppose the real functions* V_+, V_-, A_1, A_2, A_3 *are given on* $\mathbb{R}^3$ *verifying hypothesis* IV.1, IV.15 *and* IV.16 *for some* $s>\frac{1}{2}$, *and let the hamiltonians* H_0, H, h_0, h, K *be given respectively by the formulas*: I.4; I.8; I.13; I.14; II.6. *Then the scattering amplitude for the pair* $(\mathrm{H}_0,\mathrm{H})$ *is well defined by the formula* (IV.14) *and if we denote by* $t_{\xi\eta}(e)$ *the scattering amplitude for the pair* (h_0, h) *defined by a formula similar to* (IV.14), *this is well defined and we have:*

1. $\lim_{\varkappa\to 0}\mathscr{T}_{\xi\eta}(\mathrm{E})=t_{\xi\eta}(\mathrm{E})$ *for any* $e\in(0,\infty)\setminus\Lambda$.
2. *If* $s>\frac{1}{2}+k$, then $\mathscr{T}_{\xi\eta}(\mathrm{E})$ *is of class* C^k *in* κ^2 *at* $\kappa=0$ *locally in* E.
3. *If* $\mathscr{T}_{\xi\eta}(\mathrm{E})$ *is of class* C^1 *in* κ^2 *at* $\kappa=0$, *we have*:

$$\mathscr{T}_{\xi\eta}(\mathrm{E})=t_{\xi\eta}(e)+\kappa^2\int_{\mathbb{R}^3}\overline{\Phi_0(e;\omega',\xi;x)}$$
$$\times\mathrm{T}(\mathrm{E};x)\Phi_0(e;\omega,\eta;x)\,dx^3+\mathscr{O}(\kappa^4)$$

where:

$$e=\mathrm{E}\left(1+\frac{\mathrm{E}\kappa^2}{2m}\right)$$

$$\mathrm{T}(\mathrm{E}; x) = -\mathrm{v}\mathrm{r}(\mathrm{E})\,\mathrm{u} - \mathrm{u}\mathrm{r}(\mathrm{E})\,\mathrm{v} + \mathrm{u} - \frac{1}{2m}\mathrm{v}\mathrm{r}(\mathrm{E})\,\mathscr{D}(\mathrm{E}-\mathrm{V}_-)\,\mathscr{D}\mathrm{r}(\mathrm{E})\,\mathrm{V}$$

$$\mathrm{u} = \frac{1}{(2m)^2}\mathscr{D}\mathrm{V}_-\mathscr{D} + \frac{\mathrm{E}}{(2m)^2}(\mathscr{D}_0^2 - \mathscr{D}^2).$$

4. *If* $\mathrm{V}=0$, *we have*:

$$\mathscr{T}_{\xi\eta}(\mathrm{E}) = \frac{\mathrm{E}}{e}\, t_{\xi\eta}(e).$$

Proof: The existence of the scattering amplitude is a direct consequence of the hypothesis on the potentials and the previous remark. Conclusion 1 has evidently been proved once we have shown the limiting absorption principle for $(\mathrm{K}-zt)^{-1}$ (theorem IV.1), the other contributions to $\mathscr{R}_\varkappa(z)$ in formula (II.7) being evidently of class C^∞ in κ for κ small. Now let us prove conclusion 2. First let us observe that for $z=\mathrm{E}+i\varepsilon$, $\varepsilon>0$:

$$\mathscr{T}_{\xi\eta}(\mathrm{E}) = \lim_{\varepsilon\to 0} \mathscr{T}_{\xi\eta}(\mathrm{E}; \varepsilon)$$

$$\begin{aligned}\mathscr{T}_{\xi\eta}&(\mathrm{E}; \varepsilon)\\ &= \int_{\mathbb{R}^3} \langle \Phi_0(e), \left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right](\mathrm{V}-\mathrm{c}\mathscr{A})\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\Phi_0(e)\rangle\, d^3x\\ &\quad - \int_{\mathbb{R}^3} \langle \Phi_0(e), \left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right](\mathrm{V}-\mathrm{c}\mathscr{A})\,\mathscr{R}_\varkappa(\mathrm{E}+i\varepsilon)(\mathrm{V}-\mathrm{c}\mathscr{A})\\ &\qquad\qquad \times\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\Phi_0(e)\rangle\, d^3x.\end{aligned} \qquad \text{(IV.18)}$$

Now, from theorem (II.1) we conclude that for $\varepsilon>0$, $\mathscr{R}_\varkappa(\mathrm{E}+i\varepsilon)$ is analytic in κ, belongs to the algebra $A_\varkappa$ (section III), and we have:

$$\mathscr{R}_\varkappa(\mathrm{E}+i\varepsilon) = \sum_{j=0}^{\infty} \kappa^j \mathrm{R}_j(\mathrm{E}+i\varepsilon)$$

In order to study the behaviour of $\mathscr{T}_{\xi\eta}(\mathrm{E}; \varepsilon)$ (which apparently contains positive powers of c) we remark that due to (IV.9):

$$\langle \Phi_0, \mathrm{X}\Phi_0\rangle = \langle \Phi_0, \mathrm{v}\mathrm{X}\mathrm{v}\Phi_0\rangle. \qquad \text{(IV.19)}$$

Now let us compute the different contributions to (IV.18):

$$\begin{aligned}\mathrm{N}&\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right](\mathrm{V}-\mathrm{c}\mathscr{A})\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]\mathrm{N}\\ &= \mathrm{N}\mathrm{V}_+\mathrm{N} - \frac{1}{2mt}\mathrm{N}[\mathscr{D}_0\mathscr{A}+\mathscr{A}\mathscr{D}_0]\mathrm{N} + \frac{\kappa^2}{2mt}\mathrm{N}\mathscr{D}_0\mathrm{V}_-\mathscr{D}_0\mathrm{N}.\end{aligned} \qquad \text{(IV.20)}$$

$$\mathrm{N}\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right](\mathrm{V}-\mathrm{c}\mathscr{A})\,\mathscr{R}_\varkappa(\mathrm{E}+i\varepsilon)(\mathrm{V}-\mathrm{c}\mathscr{A})\left[1+\frac{\kappa}{2mt}\mathscr{D}_0\right]$$

$$= \mathrm{N}\left(\mathrm{V} - \frac{1}{2mt}\mathscr{D}_0\mathscr{A}\right)\mathrm{N}\sum_{k=0}^{\infty}\kappa^{2k}\mathrm{R}_{2k}(z)\mathrm{N}\left(\mathrm{V} - \frac{1}{2mt}\mathscr{A}\mathscr{D}_0\right)\mathrm{N}$$
$$+\mathrm{N}\left(\frac{\kappa^2}{2mt}\mathscr{D}_0\mathrm{V} - \mathscr{A}\right)\mathrm{M}\sum_{k=0}^{\infty}c^2\kappa^{2k}\mathrm{R}_{2k}(z)\mathrm{M}\left(\frac{\kappa^2}{2mt}\mathrm{V}\mathscr{D}_0 - \mathscr{A}\right)\mathrm{N}$$
$$+\mathrm{N}\left(\frac{\kappa^2}{2mt}\mathscr{D}_0\mathrm{V} - \mathscr{A}\right)\mathrm{M}\sum_{k=0}^{\infty}c\kappa^{2k+1}\mathrm{R}_{2k+1}(z)\mathrm{N}\left(\mathrm{V} - \frac{1}{2mt}\mathscr{A}\mathscr{D}_0\right)\mathrm{N}$$
$$+\mathrm{N}\left(\mathrm{V} - \frac{1}{2mt}\mathscr{D}_0\mathscr{A}\right)\mathrm{N}$$
$$\times\sum_{k=0}^{\infty}c\kappa^{2k+1}\mathrm{R}_{2k+1}(z)\mathrm{M}\left(\frac{\kappa^2}{2mt}\mathrm{V}\mathscr{D}_0 - \mathscr{A}\right)\mathrm{N}. \quad \text{(IV.21)}$$

One can observe that $c\kappa^{2k+1} = \kappa^{2k}$ and $\mathrm{MR}_0(z)\mathrm{M} = 0$ so that both expressions (IV.20) and (IV.21) define analytic functions of κ^2 for κ small and $\varepsilon \gtrless 0$, $\left(\text{one sees that } t(\kappa) = 1 + \frac{z}{2m}\kappa^2 \text{ is analytic in } \kappa^2\right)$. Let us denote by $\mathrm{T}_\varkappa(\mathrm{E}, \varepsilon)$ the sum of the two operators given by the expressions (IV.20) and (IV.21) so that:

$$\mathrm{T}_{\xi\eta}(\mathrm{E}; \varepsilon) = \int_{\mathbb{R}^3}\langle \Phi_0(e), \mathrm{T}_\varkappa(\mathrm{E}, \varepsilon)\Phi_0(e)\rangle d^3x. \quad \text{(IV.22)}$$

Then $\mathrm{T}_\varkappa(\mathrm{E}; \varepsilon)$ is analytic in κ^2 for $\varepsilon \gtrless 0$. In order to study the limit $\varepsilon \to 0$ let us remark that the only problems arise from the behaviour of $(\mathrm{K} - zt(z))^{-1}$ appearing in the expression (II.7) of $\mathscr{R}_\varkappa(z)$, all the other contributions to $\mathrm{T}_\varkappa(\mathrm{E}, \varepsilon)$ being analytic in κ^2, uniformly for $\varepsilon \in [0, \varepsilon_0)$. But one can easily see that:

$$\frac{\partial^k}{\partial(\kappa^2)^k}(\mathrm{K} - \mathrm{E}t(\mathrm{E}))^{-1} = \left(\frac{\mathrm{E}^2}{2m}\right)^k\frac{\partial^k}{\partial\mathrm{E}^k}(\mathrm{K} - \mathrm{E}t(\mathrm{E}))^{-1}$$
$$= \left(\frac{\mathrm{E}^2}{2m}\right)^k\lim_{\varepsilon\to 0}\frac{\partial^k}{\partial\mathrm{E}^k}(\mathrm{K} - zt(z))^{-1}. \quad \text{(IV.23)}$$

Now using theorem IV.2 one gets conclusion 2. For conclusion 3 one has to use the development of $\mathscr{R}_\varkappa(\mathrm{E} + i\varepsilon)$ given in theorem II.1 and remark that all the integrals make sense when interpreted as duality between L^2_s and L^2_{-s}. Now in order to prove conclusion 4 we just consider $\mathrm{V} = 0$ in (II.7) and (IV.18) obtaining:

$$\mathscr{R}_\varkappa(z) = t(z)\nu\otimes(h_\mathrm{A} - z)^{-1} + \frac{\kappa^2 z}{2m}\mu\otimes(h_\mathrm{A} - z)^{-1} + \frac{\kappa}{2m}\mathscr{D}(k_\mathrm{A} - z)^{-1}$$

$$\begin{aligned}
&\mathcal{T}_{\xi\eta}(\mathrm{E}, \varepsilon)\\
&\quad = -\mathrm{c}\int_{\mathbb{R}^3}\left\langle \Phi_0(e), \left[1+\frac{\kappa}{2mt}\mathcal{D}_0\right]\mathcal{A}\left[1+\frac{\kappa}{2mt}\mathcal{D}_0\right]\Phi_0(e)\right\rangle d^3x\\
&\quad -\mathrm{c}^2\int_{\mathbb{R}^3}\left\langle \Phi_0(e), \left[1+\frac{\kappa}{2mt}\mathcal{D}_0\right]\mathcal{A}\mathcal{R}_\kappa(z)\mathcal{A}\left[1+\frac{\kappa}{2mt}\mathcal{D}_0\right]\Phi_0(e)\right\rangle d^3x
\end{aligned}$$

and observe that for $e\in(0, \infty)\setminus\Lambda$:

$$\mathrm{E}t(\mathrm{E}) = e = -(h_\mathrm{A}-e)+\frac{1}{2m}\mathcal{D}^2.$$

Q.E.D.

In ending this section we would like to remark, that in order to have differentiability of $\mathcal{T}_{\xi\eta}(\mathrm{E})$ with respect to κ^2, what is really needed is the differentiability of $(h-e)^{-1}$ with respect to the energy (the nonrelativistic energy), condition (IV.1) being just a sufficient condition to have this differentiability. Thus some improvement along this line could probably permit also local Coulomb-like singularities.

V. THE FOLDY-WOUTHUYSEN TRANSFORMATION

In this section we shall deal with some problems related to the Foldy-Wouthuysen (F−W) transformation. For a review and extensive bibliography about this subject see [6]. We shall be interested mainly in two questions:

1. the existence of an one-electron relativistic equation;
2. the connection of the F−W transformation with the nonrelativistic limit discussed in the previous sections.

At the abstract level the F−W transformation is an unitary operator U:

$$\mathrm{U}:\quad \mathcal{H}\to(\mathrm{L}^2(\mathbb{R}^3))^2\oplus(\mathrm{L}^2(\mathbb{R}^3))^2\equiv \mathrm{N}\mathcal{H}\oplus\mathrm{M}\mathcal{H} \tag{V.1}$$

such that:

$$\mathrm{UHU}^* = \mathrm{H}_{e^-}\oplus\mathrm{H}_{e^+}. \tag{V.2}$$

In other words U is an unitary transformation which brings H into a block-diagonal form with respect to the orthogonal decomposition given by the orthogonal projection N [*see* formula (I.3)]. From the very beginning one can observe that H_{e^-} is the analog of $\tilde{\mathrm{H}}$ of Sections I and II, with the difference that instead of an isolated eigenvalue we consider now the entire "electron spectrum". In this setting, the F−W transformation is thus just a particular (albeit singular) case of the well-known reduction process used in perturbation theory. The first problem is to decide what part of the spectrum of H is the "electron spectrum". For H_0 this is a simple question, the answer being: the "electron spectrum" is the positive continuum: $[0, +\infty)$. For the interacting case ($\mathscr{V} \neq 0$), we shall adopt the adiabatic point of view ([17], ch. IV § 32) the electron spectrum is the part of the spectrum of H, emerging from the positive continuum of H_0 as the interaction is switched on. More precisely, consider

$$H_\lambda = H_0 + \lambda \mathscr{V} \tag{V.3}$$

for $\lambda \in [0, \infty)$ and c considered fixed. Under the conditions imposed on $\mathscr{V}$ [*see* Definition I.1 and hypothesis (IV.1)], H_λ has in the interval $(-2mc^2, 0)$ only finitely degenerated eigenvalues emerging from the continua and depending analytically on λ.

DEFINITION V.1. — *We define the critical coupling constant as the positive number* $\lambda_{cr}(c)$ *(depending on the velocity of light* c*) such that for* $\lambda \in [0, \lambda_{cr}(c))$, *no eigenvalue of* $H_\lambda(c)$ *emerging from the positive (respectively negative) continuum touches the negative (respectively the positive) one.*

We shall prove now that one can construct a F–W transformation as far as $\lambda \in [0, \lambda_{cr}(c))$. The result is optimal in the sense that for $\lambda > \lambda_{cr}$ the spontaneous pair creation makes the one particle Dirac theory meaningless (*see* the discussion in [19] and references therein). Before giving this construction let us remind that the F–W transformation is not unique. More precisely if the unitary operator W commutes with N and U is a F–W transformation, then WU is also a F–W transformation.

Let $P_{(\lambda)}$ be the spectral projection of H_λ corresponding to the "electron spectrum". We need the following technical information about $P_{(\lambda)}$:

LEMMA V.1. — *We shall suppose that* A *and* V *satisfy hypothesis* IV.1. *and moreover that it exists* $\alpha \in (0, 1)$ *such that* $\mathscr{V}$ *is* $|H_0|^\alpha$ *relatively bounded.*

1°. *For* $\lambda \in (0, \lambda_{cr}(c))$, $P_{(\lambda)}$ *depends analytically on* λ. *In particular* $P_{(\lambda)}$ *and* $d/d\lambda\, P_{(\lambda)}$ *are norm continuous in* λ.

2° $P_{(\lambda)} - P_{(0)}$ *is compact and for* λ *fixed we have:*

$$\lim_{c \to \infty} \| P_{(\lambda)} - P_{(0)} \| = 0$$

3° $\| P_{(0)} - N \| = \dfrac{1}{\sqrt{2}}$.

Proof: First let us remark that

$$P_{(0)} = \frac{1}{2}(1 + H_0 |H_0|^{-1}). \tag{V.4}$$

In order to define $P_{(\lambda)}$ we shall take advantage of the fact that H_λ has only finitely degenerated eigenvalues in the interval $(-2mc^2, 0)$ which can accumulate only at 0 and $-2mc^2$. Let us choose $\delta > 0$ such that in $(-\delta, 0)$,

H_λ has no eigenvalue emerging from the negative continuum (λ is supposed less than λ_{cr}), and let us suppose there are N eigenvalues $(E_1, \ldots, E_N)$ in the interval $(-2mc^2, -\delta)$ that have emerged from the positive continuum, with the associated eigenprojections (of finite rank) $P^{(1)}, \ldots, P^{(N)}$. Then if we denote $H_{\lambda,\delta} \stackrel{d}{=} H_\lambda + \delta 1$ we have that

$$P_{(\lambda)} = \sum_{j=1}^{N} P^{(j)} + \frac{1}{2}(1 + H_{\lambda,\delta} | H_{\lambda,\delta} |^{-1}). \tag{V.5}$$

Now, in order to prove the assertions of the lemma, we need an explicit formula for $P_{(\lambda)} - P_0$ in terms of the resolvents:

$$P_{(\lambda)} - P_0 = \frac{1}{2\pi i} \int_\Gamma (\mathscr{R}_\varkappa(z; \lambda) - \mathscr{R}_\varkappa(z; 0))\, dz \tag{V.6}$$

First let us precisely define the contour Γ. It is formed by the axis $L_\delta = \{ -\delta + iy \mid y \in \mathbb{R} \}$ to which we add N loops surrounding the N isolated eigenvalues contained in $(-2mc^2, -\delta)$ and coming from the positive continuum. Let us observe that L_δ may be obtained by continuously deforming a contour Γ_0 passing through $-\delta$ and surrounding the positive continuum. It is well known that the integral of the resolvent along Γ_0 (defined in the strong-convergence topology) represents precisely the spectral projection corresponding to the positive continuum and to the eigenvalues contained in the interior of Γ_0. The important observation is that using the second resolvent equation and the $|H_0|^\alpha$-boundedness of $\mathscr{V}$ (for $0 < \alpha < 1$) one obtains that:

$$\begin{aligned} &\| \mathscr{R}_\varkappa(x+iy; \lambda) - \mathscr{R}_\varkappa(x+iy; 0) \| \\ &\qquad \leq |\lambda| . \| \mathscr{R}_\varkappa(x+iy; 0) \mathscr{V} \mathscr{R}_\varkappa(x+iy; \lambda) \| \\ &\quad \leq |\lambda| \| \mathscr{R}_\varkappa(x+iy; 0) \| \| \mathscr{V} | H_0 |^{-\alpha} \| \| | H_0 |^\alpha \mathscr{R}_\varkappa(x+iy; 0) \| \\ &\quad \times \| [1 + \lambda \mathscr{V} \mathscr{R}]^{-1} \| \leq C |\lambda| \sup_t \frac{1}{\sqrt{(x-t)^2 + y^2}} \sup_u \frac{u^\alpha}{\sqrt{(x-u)^2 + y^2}}. \end{aligned} \tag{V.7}$$

Using the estimation (V.7) one gets that the integral along Γ in (V.6) converges in the uniform topology and the integral along a curve joining L_δ to Γ_0 tends to 0. By explicitly differentiating with respect to λ we get conclsuion 1° of the theorem.

Now, $\mathscr{V}$ being H_0-compact, from the second resolvent equation and formula (V.6) one gets the compacity of $P_{(\lambda)} - P_{(0)}$. It is also easy to observe that for $c \to \infty$ one can choose $\delta \to 0$ so that using formula (V.6) and the estimation (V.7) conclusion 2° follows immediately. In order to prove conclusion 3° we shall compute the eigenvalues of $P_{(0)} - N$ and estimate their upper bound.

$$P_{(0)} = \frac{1}{2}\left(1 + \frac{H_0}{|H_0|}\right)$$

$$N=\frac{1}{2}(1+\beta)$$

First let us observe that in computing $P_{(0)}$ we may replace H_0 by

$$\tilde{H}_0=c\,\alpha\otimes\sigma.p+mc^2\beta=H_0+mc^2.1$$

both having the same subspace of positive spectrum. Thus:

$$P_{(0)}-N=\frac{1}{2}\left(\frac{\tilde{H}_0}{|\tilde{H}_0|}-\beta\right)=\frac{1}{2|\tilde{H}_0|}(\tilde{H}_0-|\tilde{H}_0|.\beta).$$

Now it is easy to see that

$$|\tilde{H}_0|=c\sqrt{p^2+m^2c^2}.1$$

and the eigenvalues of $P_{(0)}-N$ are $\pm\sqrt{\frac{1}{2}\left(1-\frac{mc}{\sqrt{p^2+m^2c^2}}\right)}$ so that:

$$\|P_{(0)}-N\|=\frac{1}{\sqrt{2}}.$$

Q.E.D.

Now let us describe the construction of the F−W transformation using the Nagy-formula (as in section II). It is worth mentioning from the beginning that Eriksen's method [6, 7, 8] of constructing the F−W transformation is indeed just an utilisation of the Nagy formula. Indeed, with our notations Eriksen's formula in [6] is:

$$\begin{aligned}U_E=&(1+(2N-1)(2P_{(\lambda)}-1))\\&\times[2+(2N-1)(2P_{(\lambda)}-1)+(2P_{(\lambda)}-1)(2N-1)]^{-1/2}\\&=[2+(2N-1)(2P_{(\lambda)}-1)\\&+(2P_{(\lambda)}-1)(2N-1)]^{-1/2}(1+(2N-1)(2P_{(\lambda)}-1)\end{aligned}$$

and it is easy to verify that:

$$1+(2N-1)(2P_{(\lambda)}-1)=2[NP_\lambda+(1-N)(1-P_{(\lambda)})]$$
$$2+(2N-1)(2P_{(\lambda)}-1)+(2P_{(\lambda)}-1)(2N-1)=4[1-(P_{(\lambda)}-N)^2]$$

proving the equivalence. This remark, clarifies the question of the range of valability of the Eriksen's method: it works as far as $(N-P_{(\lambda)})^2<1$.

In order to construct a F−W transformation at a fixed c and $\lambda\in[0,\lambda_{cr})$ let us choose a family $\{\lambda_i\}_{i=0,\ldots,N}$ such that:

$$\left.\begin{aligned}&\lambda_i\in[0,\lambda],\qquad \lambda_0=0,\qquad \lambda_N=\lambda\\&\|P_{(\lambda_i)}-P_{(\lambda_{i-1})}\|<1.\end{aligned}\right\}\tag{V.8}$$

Then let us define the Foldy-Wouthuysen transformation by the unitary operator:

$$U_\lambda\overset{d}{=}U_N U_{N-1}\ldots U_1 U_0\tag{V.9}$$

where $\{U_i\}_{i=0,\ldots,N}$ are the unitary operators given by the Nagy formula:

$$U_i=[1-(P_{(\lambda_i)}-P_{(\lambda_{i-1})})^2]^{-1/2}[P_{(\lambda_i)}P_{(\lambda_{i-1})} +(1-P_{(\lambda_i)})(1-P_{(\lambda_{i-1})})] \quad (V.10)$$

and intertwining between the pair $(P_{(\lambda_i)}, P_{(\lambda_{i-1})})$ for $i=1,\ldots,N$ and between $P_{(0)}$ and N for $i=0$.

At this point we would like to remind that for some particular types of potentials $\mathscr{V}$, due to their algebraic structure, one can construct a F−W transformation directly, without the need of the above method, by giving an explicit form for U. One example known for a long time is the pure magnetic field case [4]. A large class of such $\mathscr{V}$ has been treated recently in an interesting paper by B. Thaller [24], using the methods of supersymmetric quantum mechanics. Note however that the electric field, which is the most interesting perturbation from the physical point of view, cannot be treated by the "supersymmetric" methods.

We have to discuss now to what extent the operator:

$$\tilde{H}_{e^-}(\lambda)=N\,U_\lambda\,H(\lambda)\,U_\lambda^*\,N \quad (V.11)$$

is the desired relativistic one-electron operator, *i. e.*: gives the same physics as the original Dirac operator. Clearly the spectra are the same. Concerning the scattering matrix the things are less clear. Indeed let us consider the two one-electron operators in $N\mathscr{H}$, the free one: $\tilde{H}_{e^-}(0)$ and the total one: $\tilde{H}_{e^-}(\lambda)$. The problem we shall analyse is which is the relation between the scattering operator $S_{e^-}(\lambda)$ associated to the pair: $(\tilde{H}_{e^-}(0), \tilde{H}_{e^-}(\lambda))$ and $S(\lambda)$ the one associated to the pair: (H_0, H_λ). As it is well known, the interaction $\mathscr{V}$ being time independent, with respect to the decomposition: $1=P_{(0)}\oplus P_{(0)}^\perp$ corresponding to the positive and to the negative continuum spectra of H_0, the scattering matrix has the block-diagonal form:

$$S(\lambda)=S_+(\lambda)+S_-(\lambda) \quad (V.12)$$

where:

$$\left.\begin{aligned} S_+(\lambda)&=P_{(0)}\,S(\lambda)\,P_{(0)} \\ S_-(\lambda)&=P_{(0)}^\perp\,S(\lambda)\,P_{(0)}^\perp. \end{aligned}\right\} \quad (V.13)$$

Let us introduce some more notations:

$$\begin{aligned} \tilde{U}_\lambda&=U_\lambda\,U_0^{-1} \\ \tilde{H}(0)&=U_0\,H_0\,U_0^{-1} \\ \tilde{H}(\lambda)&=U_\lambda\,H_\lambda\,U_\lambda^{-1} \\ \tilde{H}_\lambda&=\tilde{U}_\lambda\,H_\lambda\,\tilde{U}_\lambda^{-1} \end{aligned} \quad (V.14)$$

The physical information about the scattering of electrons is contained in $S_+(\lambda)$, and the fact that $\tilde{H}_{e^-}(\lambda)$ may be interpreted as the relativistic one-electron hamiltonian is supported by the following result showing that the

F − W transformed hamiltonian which is block-diagonal for the decomposition $1 = N \oplus M$ gives the same S matrix as the real Dirac hamiltonian (block-diagonal for the λ-dependent decomposition $1 = P_{(\lambda)} \oplus P_{(\lambda)}^{\perp}$).

THEOREM V.1. — *With the above notations and with the conditions of Lemma V.1 we have:* $S_{e^-}(\lambda) = U_0 S_+(\lambda) U_0^{-1}$.

Proof: In fact we shall prove that:

$$\tilde{S}(\lambda) = U S(\lambda) U_0^{-1} \tag{V.15}$$

where $\tilde{S}(\lambda)$ is the scattering matrix for the pair $(\tilde{H}(0), \tilde{H}(\lambda))$. In fact once we have proved (V.15), by multiplying it to the left and to the right with N and by taking into account that $NU_0 = U_0 P_{(0)}$ and that $\tilde{H}(0)$ and $\tilde{H}(\lambda)$ are block-diagonal for the decomposition $1 = N \oplus M$, one gets immediatley the desired conclusion.

Now, in order to prove (V.15) we observe that if we denote by $\tilde{S}_\lambda$ the scattering matrix for the pair $(H_0, \tilde{H}_\lambda)$ one has the evident equality:

$$\tilde{S}(\lambda) = U_0 \tilde{S}_\lambda U_0^{-1} \tag{V.16}$$

so that all we have to prove is that:

$$\tilde{S}_\lambda = S(\lambda). \tag{V.17}$$

But:

$$\left.\begin{aligned} \tilde{S}_\lambda &= \tilde{\Omega}_{\lambda,-}^* \tilde{\Omega}_{\lambda,+} \\ S(\lambda) &= \Omega_{\lambda,-}^* \Omega_{\lambda,+} \end{aligned}\right\} \tag{V.18}$$

and

$$\begin{aligned} \tilde{\Omega}_{\lambda,\pm} = s\text{-}\lim_{t \to \mp\infty} & e^{-i\tilde{H}_\lambda t} e^{iH_0 t} \\ &= s-\lim_{t \to \mp\infty} \tilde{U}_\lambda e^{-iH_\lambda t} \tilde{U}_\lambda^{-1} e^{iH_0 t} \\ &= \tilde{U}_\lambda \Omega_{\lambda,\mp} + \tilde{U}_\lambda s\text{-}\lim_{t \to \mp\infty} e^{-iH_\lambda t} (\tilde{U}_\lambda^{-1} - 1) e^{iH_0 t}. \end{aligned} \tag{V.19}$$

In the following we shall prove that the second term in the last equality is zero so that:

$$\tilde{\Omega}_{\lambda,\mp} = \tilde{U}_\lambda \Omega_{\lambda,\mp} \tag{V.20}$$

this finishing the proof of (V.17).

Now, we shall prove that for $\lambda \in [0, \lambda_{cr})$: $\tilde{U}_\lambda - 1$ is compact, and using the fact that for any compact operator K:

$$s\text{-}\lim_{t \to \infty} K e^{iH_0 t} = 0$$

the proof of the theorem will be finished. Indeed if U_λ is given by (V.9) then we have, with the notations introduced above:

$$\begin{aligned} \tilde{U}_\lambda &= U_N . U_{N-1} \dots U_1 \\ \tilde{U}_\lambda - 1 &= (U_N - 1) U_{N-1} \dots U_1 \\ &\quad + (U_{N-1} - 1) U_{N-2} \dots U_1 + \dots + (U_1 - 1). \end{aligned} \tag{V.21}$$

Now using (V.10) one immediately sees that:

$$\begin{aligned} U_j - 1 = \{ [1 - (P_{(\lambda_j)} - P_{(\lambda_{j-1})})^2]^{-1/2} - 1 \} \\ \times [P_{(\lambda_j)} P_{(\lambda_{j-1})} + (1 - P_{(\lambda_j)})(1 - P_{(\lambda_{j-1})})] \\ + P_{(\lambda_j)}(P_{(\lambda_{j-1})}) + (P_{(\lambda_j)} - P_{(\lambda_{j-1})}) P_{(\lambda_{j-1})} \end{aligned} \tag{V.22}$$

and we have that $P_{(\lambda_j)} - P_{(\lambda_{j-1})}$ is compact (by lemma V.1) and $\| P_{(\lambda_j)} - P_{(\lambda_{j-1})} \| < 1$. Now by observing that $f(z) = [1 - z^2]^{-1/2}$ is analytic for $|z| < 1$ and $f(0) = 1$, and by using the fact that the compact operators form a norm-closed ideal in $\mathscr{B}(H)$ one obtains that $\tilde{U}_\lambda - 1$ is compact and evidently the same is true for $\tilde{U}_\lambda^* - 1$.

Q.E.D.

Remark: In fact the content of theorem V.1 is that the pairs (H_λ, H_0) and $(\tilde{U}_\lambda H_\lambda \tilde{U}_\lambda^*, H_0)$ have the same scattering matrix.

Let us discuss now the limit $c \to \infty$ (at fixed λ). From conclusions 2° and 3° of lemma V.1 it follows that for sufficiently large c, we have:

$$\| P_{(\lambda)} - N \| < 1 \tag{5.23}$$

so that we can use the Nagy formula to define a one-step F-W transformation:

$$U(c) = [1 - (P_{(\lambda)} - N)^2]^{-1/2} [N P_{(\lambda)} + (1 - N)(1 - P_{(\lambda)})] \tag{V.24}$$

and

$$\tilde{H}_{e^-}(\lambda; c) = N U(c) H U^*(c) N. \tag{V.25}$$

One can expand the right hand side of (V.25) in powers of $1/c^2$ to obtain the known expressions [6]. The unpleasant thing concerning $\tilde{H}_{e^-}$ is that its resolvent is no more analytic in $1/c^2$ for $c \to \infty$. The reason of that is that:

$$(\tilde{H}_{e^-} - z)^{-1} = N U(c) (H - z)^{-1} U^*(c) N \tag{V.26}$$

and while $(H - z)^{-1}$ is analytic in $\frac{1}{c}$ for $c \to \infty$, $U(c)$ is not, because the radius of convergence of $\mathscr{R}_\varkappa(z)$ goes to zero when $z \to \infty$, and in order to define $P_{(\lambda)}$ one needs to integrate along an unbounded contour. Consequently, if $\tilde{H}_{e^-}$ is expanded in series of $1/c^2$:

$$\tilde{H}_{e^-} = \tilde{H}_0 + \frac{1}{c^2} \tilde{H}_1 + \frac{1}{c^4} \tilde{H}_2 + \dots \tag{V.27}$$

the operators $\tilde{H}_i$ are more and more singular and the theory of perturbations runs into difficulties as it is well known. However these difficulties are spurious since all the nonanalyticity is concentrated in the unitary rotation which does not affect the physical quantities.

Summing up, while both $\tilde{H}_{e^-}$ and H give the same physical results, $\tilde{H}_{e^-}$ is more satisfactory from the conceptual point of view, but in the nonrelativistic limit it is less suitable from the computational point of view since it introduces some spurious nonanalyticity due to the F—W transformation. Moreover, some care should be taken when treating the relativistic corrections for the scattering amplitude in the F—W formalism. Naively one may think for example that the first correction is given by the Born approximation given by $\tilde{H}_1$ [of formula (V.27)] to the Pauli scattering amplitude. This is not so because the scattering amplitude relates $\tilde{H}_{e^-}(\lambda)$ to $\tilde{H}_{e^-}(0)$ and $\tilde{H}_{e^-}(0)$ itself has relativistic corrections. The proper way of dealing with the scattering problem in the F—W approach is given in the Appendix.

APPENDIX

In this appendix we would like to comment upon the relation between the method of computing relativistic corrections that we have described in sections I-IV and the other method that makes use of the Foldy-Wouthuysen transformation and which is generally used by physicists. The idea of this second method is to compare the free hamiltonian H_0 and the total one H, in the free Foldy-Wouthuysen representation (*i. e.* transformed by U of section V) in order to define a kind of effective potential in the Pauli hamiltonian which appears as a series in $1/c^2$ and is treated as a perturbation. First some care should be taken, when one looks at the scattering amplitude, in identifying the relativistic corrections which are due to the free hamiltonian and this will be discussed at point B of this appendix. Secondly, and this is the reason which makes it very difficult to give a meaning to the formal manipulations of this method, the perturbation series is no longer analytic in $1/c$ the perturbation terms being more and more singular, as discussed in section V. In this appendix we shall compare the two methods (the second one being treated formally) up to terms in $\kappa^2 = 1/c^2$. Thus let us consider the two hamiltonians H_0 and H in the free F—W representation [23].

$$
\begin{aligned}
U_0 H_0 U_0^{-1} &= \tilde{H}(0) \\
&= c\sqrt{\mathcal{D}_0^2 + m^2 c^2}\,\beta - m^2 c^4 1 = \tilde{\tilde{H}}_0 + \mathcal{O}(\kappa^4) \\
\tilde{\tilde{H}}_0 &= \left[\frac{\mathcal{D}_0^2}{2m} - \frac{\kappa^2}{(2m)^3}\mathcal{D}_0^4\right]\beta \\
U_0 H U_0^{-1} &= \tilde{\tilde{H}} + \mathcal{O}(\kappa^4) \\
\tilde{\tilde{H}} &= \frac{\mathcal{D}^2}{2m}\beta + V + \frac{\kappa^2}{2m}\left[-\frac{\mathcal{D}^4}{(2m)^2}\beta + \mathcal{D} V \mathcal{D} - \frac{1}{2}(V\mathcal{D}^2 + \mathcal{D}^2 V)\right]
\end{aligned} \tag{A.1}
$$

A. Bound states

In section III we have computed the relativistic corrections to the eigenvalues of the total Pauli hamiltonian by using the reduced Dirac hamiltonian corresponding to a given isolated eigenvalue e of the Pauli hamiltonian (*see* Theorem III.1). Now taking into account that $(v \otimes h) P_0 = e\, P_0$ and the fact that

$$v \otimes h = N \frac{\mathcal{D}^2}{2m} N + V_+$$

after some simple calculations one can see that:

$$P_0 \tilde{\tilde{H}} P_0 = e\, P_0 + \kappa^2 \tilde{H}_1 \tag{A.2}$$

so that on the subspace of bound states the relativistic corrections computed with the reduced hamiltonians (III.6) are formally the same as those computed by the Foldy-Wouthuysen method and corresponding to the effective potential, derived from relations (A.1):

$$w = v + \frac{\kappa^2}{2m}\left[\mathcal{D} V \mathcal{D} - \frac{1}{2}(\mathcal{D}^2 V + V\mathcal{D}^2) + \frac{1}{(2m)^2}(\mathcal{D}_0^4 - \mathcal{D}^4)\right] \tag{A.3}$$

B. Scattering amplitude

We want to show now, that the relativistic correction to the scattering amplitude computed in section IV (Theorem IV.3, point 3) can be obtained formally up to order κ^2 by adding to the free hamiltonian $\tilde{\tilde{H}}_0$ in the free F−W representation, the effective potential (A.3). In fact let us consider in the free F−W representation the two hamiltonians: $\tilde{\tilde{H}}_0$ and $\tilde{\tilde{H}}_0 + w$ with w given by (A.3) and the scattering amplitude corresponding to this pair of hamiltonians:

$$
\begin{aligned}
&\tilde{\mathcal{T}}_{\xi\eta}(e;\omega',\omega) \\
&= \int_{\mathbb{R}^3} \overline{\Psi_0(e;\xi;x)}\,[w - w\,\mathcal{R}(e;x)\,w]\,\Psi_0(e;\omega',\eta;x)\,d^3x
\end{aligned} \tag{A.4}
$$

where:

$$\tilde{\Psi}_0(e;\omega;\xi;x) = U_0\Psi_0(E;\omega;\xi;x)$$
$$= \sqrt{\frac{2(E+mc^2)}{E+2mc^2}}\, N\Psi_0(E;\omega',\xi;x)$$
$$= \left(1+\frac{\kappa^2}{2(2m)^2}\mathcal{D}_0^2\right)N\Psi_0(E;\omega',\xi;x)+\mathcal{O}(\kappa^4)$$
$$\tilde{\mathcal{R}}(e;\kappa) = (\tilde{\tilde{H}}_0+w-E(e)\,1)^{-1} \tag{A.5}$$
$$= v\otimes r(e) - \frac{e^2\kappa^2}{2m} v\otimes r^2(e)+\mathcal{O}(\kappa^4).$$
$$E(e) = c\sqrt{2me+m^2c^2}-m^2c^4 = e-\frac{e^2}{2m}\kappa^2+\mathcal{O}(\kappa^4).$$

Now let us observe that the scattering amplitude computed in Theorem IV.3 point 3, can be recast after some algebraic manipulations exactly in the form (A.4). In doing this one will use the formula: $e\Psi_0(E) = \frac{1}{2m}\mathcal{D}_0^2\Psi_0(E)$ and the first resolvent equation.

Let us remark here that naively one would be tempted to include the term $-\frac{\kappa^2}{(2m)^3}\mathcal{D}_0^4$ of $\tilde{\tilde{H}}_0$ in the effective potential. This term being very singular makes difficult the construction of the S-matrix, but the above analysis shows that in order to proceed coherently one must consider this term as a correction to the free hamiltonian. Also let us point out that the arguments in the proof of Theorem V.1 allows us to perform the same F−W transformation (the free one) on both H and H_0 when computing the S-matrix. One more remark may be of some interest, concerning the fact that one can be tempted to look at the Pauli hamiltonian and its relativistic correction in the Hilbert space *h* and compute the scattering amplitude in this way. Some difficulties arise from the normalisation of the generalised wave-function which depends on c introducing some extra corrections.

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Note added: After finishing this paper, we became aware that a result similar to that of the Proposition before Theorem III.1 was proved in Wiegner, A., Uber den nichtrelativistischen Grenzwert der Eigenwerte der Diracgleichung, Diploma Thesis, Fernuniversitat-Gesamthochschule Hagen, F.R.G., 1984.

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