Commun. math. Phys. 40, 215—222 (1975)

On the Nonrelativistic Limit of the Dirac Theory

W. Hunziker

Institut für Theoretische Physik der ETH, Zürich, Switzerland

Received October 15, 1974

Abstract. The relation between a "nonrelativistic" Hamiltonian of the form $H^\infty = (A+B)^2 + C$ and a corresponding family of "Dirac-Hamiltonians" $H(c)$ in the limit $c \to \infty$ is investigated. It is shown that the resolvent $(z - H(c))^{-1}$ and the relativistic perturbation of isolated eigenvalues of H^∞ are analytic in $1/c$ for sufficiently large $|c|$.

1. Introduction

The Hamiltonian of a Dirac-electron of charge $e = 1$ and mass $m = 1/2$ may be written as

$$H(c) = c\boldsymbol{\alpha}(\boldsymbol{p} - \boldsymbol{A}(\boldsymbol{x})) + \tfrac{1}{2}\beta c^2 + \varphi(\boldsymbol{x}), \tag{1}$$

where $\boldsymbol{p} = -id/d\boldsymbol{x}$ and with the 4×4-matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix},$$

whose elements are the 2×2-matrices $\mathbb{1}$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3) =$ set of Pauli spin-matrices. $\boldsymbol{A}(\boldsymbol{x})$ and $\varphi(\boldsymbol{x})$ are the potentials of the static electromagnetic field. The usual factor $1/c$ in front of $\boldsymbol{A}(\boldsymbol{x})$ is omitted on purpose since it must be kept fixed in the nonrelativistic limit $c \to \infty$. $H(c)$ acts on the Hilbertspace $C^4 \otimes L^2(R^3)$ of square-integrable 4-component wave functions.

On a formal level, it is well understood that the nonrelativistic limit $c \to \infty$ is described by the Pauli-Hamiltonian

$$H^\infty = (\boldsymbol{\sigma}(\boldsymbol{p} - \boldsymbol{A}(\boldsymbol{x}))^2) + \varphi(\boldsymbol{x}) \tag{2}$$

on the smaller Hilbertspace $C^2 \otimes L^2(R^3)$, and there exists a sytematic scheme for obtaining corrections to H^∞ in the form of a power series in $1/c$ [1]. However, these "relativistic perturbations" of H^∞ are given by more and more singular operators which are by no means small with respect to H^∞. One might therefore suspect that perturbation expansions in powers of $1/c$ are at best asymptotic.

Nevertheless, Titchmarsh [2] has proved analyticity in $1/c$ of eigenvalues and eigenfunctions for the spherically symmetric case without magnetic field: $\varphi = \varphi(r)$, $\boldsymbol{A} = 0$; and Veselić [3] has extended this result to the case without spherical symmetry: $\varphi = \varphi(\boldsymbol{x})$, $\boldsymbol{A} = 0$.

In this note we investigate the general case $\boldsymbol{A} \neq 0$ which poses essentially new problems-already in the nonrelativistic limit. One of the points we wish to make is that it is profitable to treat a general Hamiltonian of type $H^\infty = (A+B)^2 + \mathrm{C}$ as a nonrelativistic limit of a corresponding Dirac-Hamiltonian $H(c)$.

In order to keep the conditions on A and φ fairly general, we here restrict ourselves to the discrete spectrum of H. The analyticity properties of the resolvent in $1/c$ will of course also be needed in the discussion of the continuum. However, additional assumptions for the electromagnetic field (like dilatation-analyticity or sufficiently rapid fall-off at infinity) are then necessary and the arguments become more technical [4].

2. The Hamiltonian and Its Spectrum

We summarize some (but not all!) known results on the selfadjointness and on the spectrum of $H(c)$. This is intended only as a background for the more general set-up introduced in Section 3.

H is of the form $H_0 + V$ with $H_0 = c\boldsymbol{\alpha p} + \frac{1}{2}c^2\beta$, $V(\boldsymbol{x}) = \varphi(\boldsymbol{x}) - c\boldsymbol{\alpha A}(\boldsymbol{x})$. $V(\boldsymbol{x})$ is a 4×4-matrixvalued function on $R^3 \cdot L^p$-norms of V may be defined with respect to any matrix-norm.

Theorem 1. *Let $V \in L^p + L^\infty$ for some $p > 3$. Then V is H_0-bounded with arbitrarily small relative bound. Therefore, $H = H_0 + V$ is selfadjoint with domain $D(H_0)$.*

Theorem 2. *Suppose that $V \in L^p + \varepsilon L^\infty$ $(p > 3)$, i.e. that the L^∞-part of V can be chosen arbitrarily small in L^∞-norm. Then the spectrum $\sigma(H)$ of H consists of the continuum $\sigma(H_0) = \{z \in R : |z| \geqq \frac{1}{2}c^2\}$ and, in the complement of $\sigma(H_0)$, of isolated eigenvalues with finite multiplicities with can accumulate only at $+\frac{1}{2}c^2$.*

Remarks. Theorem 1 is proved in [5] and follows from the fact that an operator of the form

$$f(\boldsymbol{x})(1 + \boldsymbol{p}^2)^{-1/2} \tag{3}$$

on $L^2(R^3)$ is bounded if $f \in L^p$, $p > 3$. The condition $p > 3$ excludes Coulomb-like singularities. However, $f(\boldsymbol{x}) = |\boldsymbol{x}|^{-1}$ is still relatively bounded with respect to $|\boldsymbol{p}|$ [6].

Theorem 2 can be proved like its analogue for Schrödinger Hamiltonians [7]. The main point is that (3) is a compact operator if $f \in L^p + \varepsilon L^\infty$, i.e. V is relatively compact with respect to H_0.

3. The Nonrelativistic Limit

We now pose the problem in a generalized form. Let A, B, C be symmetric operators on a Hilbertspace $\mathscr{H}$. On $C^2 \otimes \mathscr{H}$ we define the "Dirac-Hamiltonian"

$$H(c) = c\alpha \otimes (A + B) + \frac{c^2}{2}\beta \otimes \mathbb{1} + \mathbb{1} \otimes C,$$

where

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We want to show that the limit $c \to \infty$ is described by the "Pauli-Hamiltonian"

$$H^\infty = (A + B)^2 + C \quad \text{on} \quad \mathscr{H}.$$

Corresponding to the hypothesis of Theorem 1 we assume:

$$A = A^*;\ B \text{ and } C \text{ are } A\text{-bounded, in particular}$$
$$B \text{ has relative bound } < 1 \text{ with respect to } A\,. \tag{4}$$

It follows easily that $H(c)$ is selfadjoint with domain $D(A)$ for c real and sufficiently large. For H^∞ we have

Lemma 1. *H^∞ is selfadjoint with domain $D((A+B)^2)$ and bounded below.*

Proof. By (4), $A+B$ is selfadjoint with domain $D(A)$ and A is $(A+B)$-bounded. Hence C is $(A+B)$-bounded and has therefore arbitrarily small relative bound with respect to $(A+B)^2$.

Remark. For H^∞, the splitting

$$H^\infty = A^2 + (AB + BA + B^2 + C)$$

into unperturbed part plus perturbation is artificial and raises unneccessary domain questions. These will be avoided automatically by treating H^∞ as a limit of $H(c)$.

We first discuss the unperturbed resolvent $(z - H_0(c))^{-1}$ for

$$H_0(c) = c\alpha A + \tfrac{1}{2}c^2\beta\,,$$

where we have dropped the tensor-product notation. From $\alpha^2 = \beta^2 = 1$ and $\alpha\beta + \beta\alpha = 0$ it follows that

$$H_0^2(c) = c^2 A^2 + \tfrac{1}{4}c^4\,,$$

which shows that $\sigma(H_0)$ has at least the gap $(-\tfrac{1}{2}c^2, +\tfrac{1}{2}c^2)$. For $z \notin \sigma(H_0)$ we have

$$\begin{aligned}(z = H_0)^{-1} &= (z + H_0)(z^2 - H_0^2)^{-1}\\ &= (z + c\alpha A + \tfrac{1}{2}c^2\beta)(z^2 - \tfrac{1}{4}c^4 - c^2A^2)^{-1}\,.\end{aligned}$$

Before taking the nonrelativistic limit $c \to \infty$ we must subtract from $H_0(c)$ or $H(c)$ the rest energy $\tfrac{1}{2}c^2$ or, equivalently, replace in the resolvents z by $z + \tfrac{1}{2}c^2$. This will always be assumed in the following. It is also convenient to use 2-component notation: $u = \begin{pmatrix} u^1 \\ u_2 \end{pmatrix}$, $u_k \in \mathscr{H}$, for vectors $u \in C^2 \otimes \mathscr{H}$ and the corresponding 2×2-matrix notation for operators on $C^2 \otimes \mathscr{H}$. The unperturbed resolvent then takes the form

$$\begin{aligned}G_0(z,c) &= (z - H_0(c))^{-1}\\ &= \begin{pmatrix} 1 + \dfrac{z}{c^2} & \dfrac{A}{c} \\ \dfrac{A}{c} & \dfrac{z}{c^2} \end{pmatrix} \left(z + \frac{z^2}{c^2} - A^2\right)^{-1},\end{aligned}$$

which shows explicitly that, for $z \notin \sigma(A^2)$, $G_0(z,c)$ is analytic in $1/c$ in a z-dependent neighbourhood of $1/c = 0$. To construct the full resolvent $G(z,c) = (z - H(c))^{-1}$ we start from the resolvent equation

$$G(z, c) = G_0(z, c) + K(z, c)\, G(z, c)\,,$$

where

$$K(z, c) = G_0(z, c)\,(H(c) - H_0(c))$$

$$= \left(z + \frac{z^2}{c^2} - A^2\right)^{-1} \begin{pmatrix} \left(1 + \frac{z}{c^2}\right) C + AB & \left(1 + \frac{z}{c^2}\right) cB + \frac{AC}{c} \\ \frac{1}{c}(AC + zB) & AB + \frac{zC}{c^2} \end{pmatrix}.$$

This expression for K must be understood in the following sense: a term like $\left(z + \frac{z^2}{c^2} - A^2\right)^{-1} AB$ is defined on $D(B)$ as the product of the bounded operator $A\left(z + \frac{z^2}{c^2} - A^2\right)^{-1}$ with B. As a consequence of (4), K is therefore defined on $D(A)$ and bounded. In the following we denote with K the unique bounded extension of this operator to all of $C^2 \otimes \mathscr{H}$. For $B \neq 0$ we see that K diverges as $c \to \infty$. To control this divergence we set

$$S(c) = \begin{pmatrix} 1 & 0 \\ 0 & c \end{pmatrix}$$

and introduce

$$\tilde{G}_0(z, c) = S G_0 S^{-1} = \left(z + \frac{z^2}{c^2} - A^2\right)^{-1} \begin{pmatrix} 1 + \frac{z}{c^2} & \frac{A}{c^2} \\ A & \frac{z}{c^2} \end{pmatrix}$$

$$= (z - A^2)^{-1} \begin{pmatrix} 1 & 0 \\ A & 0 \end{pmatrix} \quad \text{for} \quad c = \infty\,. \tag{5}$$

$$\tilde{K}(z, c) = S K S^{-1} = \left(z + \frac{z^2}{c^2} - A^2\right)^{-1} \begin{pmatrix} \left(1 + \frac{z}{c^2}\right) C + AB & \left(1 + \frac{z}{c^2}\right) B + \frac{AC}{c^2} \\ AC + zB & AB + \frac{zC}{c^2} \end{pmatrix}$$

$$= (z - A^2)^{-1} \begin{pmatrix} C + AB & B \\ AC + zB & AB \end{pmatrix} \quad \text{for} \quad c = \infty\,. \tag{6}$$

We notice that for $z \notin \sigma(A^2)$, $\tilde{G}_0(z, c)$ and $\tilde{K}(z, c)$ are analytic in $(1/c)^2$ in a neighbourhood of zero. The resolvent equation transforms into

$$\tilde{G}(z, c) = \tilde{G}_0(z, c) + \tilde{K}(z, c)\, \tilde{G}(z, c) \tag{7}$$

for $\tilde{G} = SGS^{-1}$. Our next task is to connect this equation for $c = \infty$ with the Pauli Hamiltonian H^∞.

Theorem 3. *Let* A, B, C *satisfy* (4) *and let* $z \notin \sigma(A^2)$. *Then the two equations*

$$(z - H^\infty)u = v \tag{8}$$

and

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} (z-A^2)^{-1}v \\ A(z-A^2)^{-1}v \end{pmatrix} + \tilde{K}(z,\infty)\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{9}$$

are equivalent in the following sense: (8) *implies* (9) *for* $\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} u \\ (A+B)u \end{pmatrix}$, (9) *implies* $u_1 \in D((A+B)^2)$, $u_2 = (A+B)u_1$ *and* (8) *for* $u = u_1$.

The straightforward but somewhat lengthy proof is given in Section 5. As a corollary we note that for $z \notin \sigma(A^2)$, $z \notin \sigma(H^\infty)$, $G^\infty(z) = (z - H^\infty)^{-1}$ satisfies

$$\begin{pmatrix} G^\infty(z) & 0 \\ (A+B)G^\infty(z) & 0 \end{pmatrix} = \begin{pmatrix} (z-A^2)^{-1} & 0 \\ A(z-A^2)^{-1} & 0 \end{pmatrix} + \tilde{K}(z,\infty)\begin{pmatrix} G^\infty(z) & 0 \\ (A+B)G^\infty(z) & 0 \end{pmatrix}. \tag{10}$$

Conversely, if $z \notin \sigma(A^2)$ and if $(1 - \tilde{K}(z,\infty))^{-1}$ exists and is bounded, it follows that $z \notin \sigma(H^\infty)$ and that

$$\begin{pmatrix} G^\infty(z) & 0 \\ (A+B)G^\infty(z) & 0 \end{pmatrix}$$

is the unique solution of (10) in $L(C^2 \otimes \mathscr{H})$. Therefore, (10) is a suitable resolvent equation for H^∞ which may also be used, incidentally, as a starting point for time-independent scattering theory [4]. Corresponding to the hypothesis of theorem 2 we now assume in addition to (4) that

$$B \text{ and } C \text{ are relatively compact with respect to } A. \tag{11}$$

As in Theorem 2 it then follows that $H(c)$ can only have isolated eigenvalues of finite multiplicities in the complement of $\sigma(H_0(c))$, in particular in the gap $(-c^2, 0)$ (rest energy subtracted). Since $\tilde{K}(z,\infty)$ is compact for $z \notin \sigma(A^2)$ we obtain a similar result for H^∞:

Lemma 2. *In the complement of* $\sigma(A^2)$, $\sigma(H^\infty)$ *consists only of isolated eigenvalues of finite multiplicities which are bounded below.*

Proof. Suppose that for some $z \notin \sigma(A^2)$, the homogeneous equation

$$\tilde{K}(z,\infty)u = u \tag{12}$$

has a nontrivial solution. Then $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ satisfies (9) with $v = 0$. By Theorem 3, it follows that $u_1 \in D((A+B)^2)$, $u_2 = (A+B)u_1$ and

$$(z - H^\infty)u_1 = 0. \tag{13}$$

We conclude that $u_1 \neq 0$ and that $z \in \sigma(H^\infty)$. By the Fredholm alternative, therefore, $(1 - \tilde{K}(z,\infty))^{-1}$ exists for $z \notin \sigma(H^\infty)$. Since $\tilde{K}(z,\infty)$ is analytic in $z \notin \sigma(A^2)$,

$(1-\tilde{K}(z,\infty))^{-1}$ and therefore $G^\infty(z)$ are meromorphic in $z \notin \sigma(A^2)$. Conversely, (13) implies (12) for $u = \begin{pmatrix} u_1 \\ (A+B)u_1 \end{pmatrix}$, hence the eigenvalues of H^∞ in the complement of $\sigma(A^2)$ are of finite multiplicity. Boundedness below is obvious from Lemma 1. This concludes the proof.

We are now prepared to discuss the analyticity properties in $1/c$ of $G(z,c)$. Let $z \notin \sigma(A^2) \cup \sigma(H^\infty)$. Then $(1-\tilde{K}(z,\infty))^{-1}$ exists. Since $\tilde{K}(z,c)$ is analytic in $(1/c)^2$ it follows that $(1-\tilde{K}(z,c))^{-1}$ exists and is analytic in $(1/c)^2$ for $|c|$ sufficiently large. The same is true for $\tilde{G}_0(z,c)$ and therefore, by (7), for $\tilde{G}(z,c)$. From (5) and (10) we see that the power series of $\tilde{G}(z,c)$ in $(1/c)^2$ begins with

$$\tilde{G}(z,c) = \begin{pmatrix} G^\infty(z) & 0 \\ (A+B)G^\infty(z) & 0 \end{pmatrix} + 0\left(\frac{1}{c^2}\right).$$

Due to the particular form of the leading term, $G(z,c) = S^{-1}(c)\tilde{G}(z,c)S(c)$ is still analytic in $1/c$ with an expansion

$$G(z,c) = \begin{pmatrix} G^\infty(z) & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{c}\begin{pmatrix} 0 & (A+B)G^\infty(z) \\ (A+B)G^\infty(z) & 0 \end{pmatrix} + 0\left(\frac{1}{c^2}\right).$$

In general, the diagonal elements of $G(z,c)$ are even in $1/c$, the off-diagonal elements are odd. These analyticity properties of the resolvent are the basis from which the analyticity properties of eigenvalues and eigenfunctions follow in the usual way [6]. As has been remarked by Veselić, the fact that $G(z,\infty)$ is a pseudo-resolvent rather than a resolvent is thereby no obstacle. We only give the final result:

Theorem 4. *Let A, B, C satisfy* (4) *and* (11). *Let z be an eigenvalue of H^∞ in the complement of $\sigma(A^2)$ and m its (finite) multiplicity. Then z is the limit for $c \to \infty$ of eigenvalues $z_k(c)$ of $H(c)$ (with rest-energy subtracted) of total multiplicity m. The functions $z_k(c)$ are analytic in $(1/c)^2$ for $|c|$ sufficiently large. An orthonormal set of corresponding eigenvectors of $H(c)$ can be chosen such that each eigenvector is of the form $\begin{pmatrix} u_1(c) \\ u_2(c) \end{pmatrix}$ where $u_1(c)$ and $c^{-1}u_2(c)$ are analytic in $(1/c)^2$ and where $u_1(\infty)$ is an eigenvector of H^∞ with eigenvalue z.*

Remark. In general there will be other eigenvalues of $H(c)$ which for $c \to \infty$ will not converge to an eigenvalue of H^∞ in the complement of $\sigma(A^2)$. However, these eigenvalues will leave any compact not intersecting $\sigma(A^2)$, i.e. they will either join $\sigma(A^2)$ or disappear to $\pm\infty$. In fact it is equally possible to study the limit $c \to \infty$ of $-H(c) - \frac{1}{2}c^2$ which leads to a Pauli Hamiltonian $(A+B)^2 - C$.

4. Proof of Theorem 3

(8)→(9):
We define $u_1 = u$ and $u_2 \in D(A)$ by

$$(A+B)u_1 - u_2 = 0. \tag{14}$$

Then (8) takes the form

$$(z-C)u_1-(A+B)u_2-v=0, \tag{15}$$

and the combination $A(z-A^2)^{-1}(14)-(z-A^2)^{-1}(15)$ gives the upper component of (9)

$$u_1=(z-A^2)^{-1}v+A(z-A^2)^{-1}Bu_1+(z-A^2)^{-1}Cu_1+(z-A^2)^{-1}Bu_2. \tag{16}$$

All terms in (16) are in $D(A)$. The combination $A(16)+(14)$ leads to the lower component of (9):

$$u_2=A(z-A^2)^{-1}v+z(z-A^2)^{-1}Bu_1+A(z-A^2)^{-1}Cu_1+A(z-A^2)^{-1}Bu_2. \tag{17}$$

(9)→(8):

(9) is equivalent to the set (16) (17) with two important modifications. First, all operator products must be replaced by their bounded extensions to $\mathscr{H}$. To indicate this extension we write, for example, $[A(z-A^2)^{-1}B]$ for the extension of $A(z-A^2)^{-1}B$. Secondly, we start only with the information that u_1 and u_2 are in $\mathscr{H}$. The combination $A(z-A^2)^{-1}(16)+(z-A^2)^{-1}(17)$ gives

$$[(z-A^2)^{-1}(A+B)]u_1=(z-A^2)^{-1}u_2, \tag{18}$$

where we have used identities like

$$A(z-A^2)^{-1}[(z-A^2)^{-1}C]=(z-A^2)^{-1}[A(z-A^2)^{-1}C],$$

which hold trivially on $D(A)$ and extend by continuity to all of $\mathscr{H}$. We now take the scalar product of (18) with an arbitrary $f\in\mathscr{H}$ and set $g=(\bar{z}-A^2)^{-1}f$. Using $[(z-A^2)^{-1}(A+B)]^*=(A+B)(\bar{z}-A^2)^{-1}$ we find

$$((A+B)g,u_1)=(g,u_2) \tag{19}$$

for all $g\in D(A^2)$. Since A is the closure of its restriction to $D(A^2)$ and since B is A-bounded, this extends by continuity to all $g\in D(A)$. Since $A+B$ is selfadjoint with domain $D(A)$, it follows that

$$u_1\in D(A+B) \quad \text{and} \quad u_2=(A+B)u_1. \tag{20}$$

Writing (20) in the form

$$u_1=z(z-A^2)^{-1}u_1+A(z-A^2)^{-1}Bu_1-A(z-A^2)^{-1}u_2$$

and subtracting this from (16) we get

$$(z-A^2)^{-1}(z-C)u_1=(z-A^2)^{-1}v+[(z-A^2)^{-1}(A+B)]u_2.$$

In the same way as before we conclude that

$$((A+B)g,u_2)=(g,(z-C)u_1-v)$$

for all $g\in D(A)$. It follows that $u_2\in D(A+B)$ and $(A+B)u_2=(z-C)u_1-v$. Combined with (20) this is the desired result:

$$u_1\in D((A+B)^2), \quad u_2=(A+B)u_1 \quad \text{and} \quad (z-H^\infty)u_1=v.$$

References

1. See for instance Bjorken, J. D., Drell, S. D.: Relativistic Quantum Mechanics. New York: Mc Graw Hill Inc. 1964
2. Titchmarsh, E. C.: Proc. Roy. Soc. **266** A, 33 (1962)
3. Veselić, K.: Commun. math. Phys. **22**, 27 (1971)
4. Hunziker, W.: unpublished report, available from the Institute of theoretical physics of the ETH
5. Prosser, R. T.: J. Math. Phys. **4**, 1048 (1964)
6. Kato, T.: Perturbation theory for linear operators. Berlin-Heidelberg-New York: Springer 1966
7. Hunziker, W.: Helv. Phys. Acta **39**, 452 (1966)

Communicated by K. Hepp

W. Hunziker
Institut für Theoretische Physik der E. T. H.
CH-8049 Zürich, Switzerland