The Nonrelativistic Limit

B.Thaller

Institute f. Mathematics
Universität Graz
Heinrichstrasse 36
A-8010 Graz

In this article[1] we analyze the behavior of the Dirac equation in the nonrelativistic limit and derive the explicit form of the first order relativistic correction. There are two main reasons for this investigation. The first is purely conceptual: It is important to see how the relativistic theory contains the successful nonrelativistic theory as a limiting case. The second reason is a practical one: In some cases it is useful to replace the Dirac theory by the much simpler Schrödinger theory together with some relativistic corrections. The first order corrections can sometimes be calculated explicitly, but it is not always necessary and is often impossible to calculate higher order corrections or the exact solution of the Dirac equation. Besides, for a higher accuracy we expect quantum electrodynamical effects to play a certain role (e.g., the Lamb shift). These effects cannot be described by the Dirac equation alone.

We achieve the nonrelativistic limit by letting c, the relativistic bound for the propagation speed of signals, tend to infinity. Unfortunately, the Dirac operator $H(c)$ itself, even after subtracting the rest mass, makes no sense for $c = \infty$. The correct way to analyze the parameter dependence of unbounded operators is to look at its resolvent. We shall prove norm-convergence as $c \to \infty$ of $(H(c) - mc^2 - z)^{-1}$ for one (and hence all) z with $\operatorname{Im} z \neq 0$. The nonrelativistic limit of the Dirac resolvent is the resolvent of a Schrödinger or Pauli operator times a projection to the upper components of the Dirac wavefunction. The Dirac resolvent is even analytic in $1/c$ (Sect. 1).

From the explicit expansion of the resolvent in powers of $1/c$ we obtain complete information about the behavior of the relativistic energy spectrum in a neighborhood of $c = \infty$ (Sect. 2). The necessary background from perturbation theory is quickly reviewed in Sect. 2.1. The Rayleigh-Schrödinger perturbation series for the eigenvalue $\lambda(c)$ of the resolvent determines its expansion into powers of $1/c$. The corresponding expansion of the eigenvalue $E(c)$ of the Dirac operator is easily obtained from $\lambda(c) = (E(c) - mc^2 - z)^{-1}$. It turns out that the eigenvalues of the Dirac operator are analytic in the parameter $1/c^2$. We determine explicit formulas for the relativistic corrections to the nonrelativistic binding energies. For the corrections of order $1/c^2$ only the knowledge of the corresponding nonrelativistic solutions (Schrödinger or Pauli equation) is required. The result can be written as a sum of expectation values which have a nice physical interpretation (spin-orbit coupling, etc.).

We formulate the theory in terms of abstract Dirac operators in a "supersymmetric" framework. In this way the calculations can be performed with the least amount of writing and the results are applicable to the widest range of concrete situations.

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[1] This article is a version of Chapter 6 of the book by the author: "The Dirac Equation", Texts and Monographs in Physics, Springer 1992

1 c-Dependence of Dirac Operators

1.1 General Setup

In nonrelativistic physics it is assumed that there is no principal bound for the propagation speed of signals. In the theory of relativity the constant parameter c (the velocity of light) represents such a bound. Nevertheless we expect that the relativistic theory is similar to the nonrelativistic one, if c is very large compared to all velocities of the system under consideration. In the nonrelativistic limit, c should be "infinitely large" compared to the other velocities. The only way to achieve this without restricting the consideration to motionless systems is to allow c to be a variable parameter. The nonrelativistic limit can then be mathematically described by letting c tend to infinity.

In this chapter we describe the dependence of the Dirac operator on c, especially in the region near $c = \infty$. The parameter c appears in various places in the Dirac equation. For example, in an electromagnetic field the Dirac operator reads

$$H(c) = c\boldsymbol{\alpha} \cdot \Big(-\mathrm{i}\,\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\Big) + \beta mc^2 + e\,\phi_{\mathrm{el}}(\boldsymbol{x}). \tag{1}$$

Before defining a c-dependent abstract Dirac operator we want to make the following two remarks:

Remark 1. The Dirac operator describes the energy of the electron including its rest energy mc^2 ($-mc^2$ in the positron subspace). The rest energy is a purely relativistic object (it has no nonrelativistic limit) and has to be subtracted before letting c tend to infinity. Otherwise there is no possibility to get a nonrelativistic limit for the expression (1).

Remark 2. The factor $1/c$ in front of $\boldsymbol{A}(\boldsymbol{x})$ has nothing to do with relativistic quantum mechanics. It's origin is the replacement $\boldsymbol{p} \to \boldsymbol{p} - (e/c)\boldsymbol{A}$ (i.e., the "minimal coupling principle") hence it would also appear in the Schrödinger equation with an external magnetic field. So if we don't want to "turn the light off", we have to keep this factor constant in the nonrelativistic limit. For simplicity, we absorb the factor $1/c$ and the coupling constant e into $\boldsymbol{A}$ and write henceforth $H(c) = c\boldsymbol{\alpha} \cdot (-\mathrm{i}\,\nabla - \boldsymbol{A}) + \beta mc^2 + V$.

Motivated by these considerations we make the following definition of c-dependence for an abstract Dirac operator.

Let $\mathfrak{H}$ be a Hilbert space with a unitary involution τ, in which a supercharge Q and a strictly positive, self-adjoint operator M commuting with Q are defined as in Sect. 5.4.1 of "The Dirac Equation[1]". Define

$$H(c) \equiv cQ + Mc^2\tau + V, \qquad c > 0, \tag{2}$$

where V is symmetric on $\mathfrak{D}(Q)$ and bounded relative to Q, i.e.,

$$\|Vf\| < a\,\|Qf\| + b\,\|f\|, \qquad 0 < a, b < \infty. \tag{3}$$

Thus, if $c > a$, then $H(c)$ is self-adjoint on $\mathfrak{D}(Q)$ by the Kato-Rellich theorem. Moreover, we assume, that V is an even operator, i.e.,

$$\tau V = V\tau \quad \text{on } \mathfrak{D}(Q). \tag{4}$$

Hence we may conclude that $H(c)$ with $c > a$ is an abstract Dirac operator. In the standard representation we may write

$$H(c) = \begin{pmatrix} M_+ c^2 + V_+ & cD^* \\ cD & -M_- c^2 + V_- \end{pmatrix}. \tag{5}$$

Our assumptions include in particular the Coulomb potential with an arbitrarily large coupling constant.

1.2 Supersymmetric Dirac Operators

The operator

$$H_0(c) \equiv cQ + \tau M c^2, \qquad c > 0, \tag{6}$$

is a Dirac operator with supersymmetry. According to Remark 1 above we subtract the "rest energy" Mc^2 and investigate the convergence of $H_0(c) - Mc^2$ in the limit $c \to \infty$. It will turn out that only the positive energy part of this expression survives in the limit. Alternatively, in order to obtain a nontrivial limit in the negative energy subspace, we can *add* the term Mc^2 and consider the nonrelativistic limit of the operator $H_0(c) + Mc^2$.

The main mathematical tool for investigating the parameter dependence of unbounded operators (which need not have a common domain of definition for all values of the parameter) is the resolvent[2]. For any self-adjoint operator A and z with $\mathrm{Im}(z) \neq 0$, the resolvent is defined as the bounded operator $(A - z)^{-1}$. The next theorem gives an expression for the resolvent of the operator (6) from which the nonrelativistic limit can be read off immediately.

We use the following notation.

$$P_\pm \equiv \frac{1}{2}(1 \pm \tau). \tag{7}$$

M and M^{-1} are bounded and commute with Q Hence the operator

$$H_{0,\infty} \equiv \frac{1}{2M} Q^2 \tag{8}$$

is defined and self-adjoint on $\mathfrak{D}(Q^2)$. Moreover, $H_{0,\infty}$ is a Hamiltonian with supersymmetry (see Sect. 5.1.2 "The Dirac Equation[1]"). In typical applications $H_{0,\infty}$ is a nonrelativistic Schrödinger or Pauli operator (a perturbation of the Laplacian).

Theorem 1. Let $H_0(c) = cQ + Mc^2\tau$ be a Dirac operator with supersymmetry. Then for each $z \in \mathbb{C} \setminus \mathbb{R}$

[2] see, e.g., [Ka 80] or [RS 72]

$$\bigl(H_0(c) \mp Mc^2 - z\bigr)^{-1} =$$

$$\Bigl(P_\pm \pm \frac{1}{c^2}\,\frac{cQ \pm z}{2M}\Bigr)\Bigl(\mathbf{1} \mp \frac{1}{c^2}\,\frac{z^2}{2M}\,(\pm H_{0,\infty} - z)^{-1}\Bigr)^{-1}(\pm H_{0,\infty} - z)^{-1}. \tag{9}$$

Proof. Denoting

$$A_\pm = H_0(c) \pm Mc^2 \pm z = cQ \pm 2Mc^2 P_\pm \pm z, \tag{10}$$

we find

$$A_+ A_- = A_- A_+ = c^2 Q^2 - 2Mc^2 z - z^2, \tag{11}$$

from which we obtain

$$A_\pm^{-1} = \frac{A_\mp}{2Mc^2}\left(\frac{Q^2}{2M} - z - \frac{z^2}{2Mc^2}\right)^{-1}. \tag{12}$$

Using

$$(A + B)^{-1} = (\mathbf{1} + A^{-1}B)^{-1}A^{-1} \tag{13}$$

with

$$A \equiv \frac{Q^2}{2M} - z, \qquad B \equiv -\frac{z^2}{2Mc^2} \tag{14}$$

the result (9) follows immediately. □

The operators

$$T_\pm(c) \equiv \frac{1}{c^2}\,\frac{z^2}{2M}\,(\pm H_{0,\infty} - z)^{-1} \tag{15}$$

which occur in Eq. (9) are bounded with norm less than 1 for c sufficiently large (depending on z). In this case we can expand

$$\bigl(\mathbf{1} \mp T_\pm(c)\bigr)^{-1} = \sum_{n=0}^{\infty}\bigl(\pm T_\pm(c)\bigr)^n, \quad \text{if } \|T_\pm(c)\| < 1, \tag{16}$$

where the sum is convergent in the operator norm. As $c \to \infty$, $\|T_\pm(c)\| \to 0$, and we obtain from (9) the following corollary.

Corollary 2. Let $H_0(c) = cQ + Mc^2\tau$ be a supersymmetric Dirac operator. Then

$$\lim_{c\to\infty}\bigl(H_0(c) \mp Mc^2 - z\bigr)^{-1} = P_\pm\,(\pm H_{0,\infty} - z)^{-1}. \tag{17}$$

The limit in (17) is a norm-limit of bounded operators. In the standard representation (17) can be written in the form

$$\lim_{c\to\infty}\begin{pmatrix} -z & cD^* \\ cD & -2M_-c^2 - z \end{pmatrix}^{-1} = \begin{pmatrix} \left((2M_+)^{-1}D^*D - z\right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{18}$$

resp.

$$\lim_{c\to\infty}\begin{pmatrix} 2M_+c^2 - z & cD^* \\ cD & -z \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(-(2M_-)^{-1}DD^* - z\right)^{-1} \end{pmatrix}. \tag{19}$$

Inserting (16) into (9) gives an expansion of the resolvent of the operator $H_0(c) \mp Mc^2$ into powers of $1/c$. Thus the resolvent is holomorphic in $1/c$ in a z-dependent neighborhood of $1/c = 0$. We extend this result to arbitrary Dirac operators of the form (5) in the next section. We finally mention the following corollary, which is immediate from Eq. (12).

Corollary 3. Let $M = m\mathbf{1}$, $m > 0$. Then $z \in \mathbb{C}$ is in the resolvent set of the Dirac operator $H_0(c) - mc^2$ if and only if $z(1 + z/2mc^2)$ is in the resolvent set of $H_{0,\infty} = Q^2/2m$.

1.3 Analyticity of the Resolvent

From now on we consider only the Dirac operator with rest energy subtracted. The calculations are similar in the other case.

Theorem 4. Let $H(c) = H_0(c) + V$ be defined as in (2)-(5). Then, for $\mathrm{Im}\,(z) \neq 0$,

$$(H(c) - Mc^2 - z)^{-1} =$$

$$= \left(P_+ + \frac{1}{c^2}\,\frac{cQ+z}{2M}\right) K(c^{-2}) \left(\mathbf{1} + \frac{1}{c^2}\,V\,\frac{cQ+z}{2M}K(c^{-2})\right)^{-1}, \tag{20}$$

where

$$K(c^{-2}) = \left(H_\infty - z - \frac{1}{c^2}\,\frac{z^2}{2M}\right)^{-1} = \left(\mathbf{1} - \frac{1}{c^2}\,\frac{z^2}{2M}R_\infty\right)^{-1} R_\infty, \tag{21}$$

$$R_\infty \equiv (H_\infty - z)^{-1}, \qquad H_\infty = \frac{Q^2}{2M} + VP_+. \tag{22}$$

and where P_+ is defined as in (7).

Proof. We denote

$$K_0 = \left(\frac{Q^2}{2M} - z - \frac{1}{c^2}\,\frac{z}{2M}\right)^{-1}, \tag{23}$$

and A_- as in Eq. (10). Hence we obtain from (12)

$$\big(H(c) - Mc^2 - z\big)^{-1} = (A_- + V)^{-1} = A_-^{-1}(1 + VA_-^{-1})^{-1}$$
$$= \left(P_+ + \frac{1}{c^2}\,\frac{cQ+z}{2M}\right) K_0 \left(\mathbf{1} + VP_+K_0 + \frac{1}{c^2}\,V\,\frac{cQ+z}{2M}\,K_0\right)^{-1}. \tag{24}$$

The last factor $(\ldots)^{-1}$ can be written as

$$(1 + VP_+K_0)^{-1}\left(\mathbf{1} + \frac{1}{c^2}\,V\,\frac{cQ+z}{2M}\,K_0\,(1+VP_+K_0)^{-1}\right)^{-1}. \tag{25}$$

Finally, we arrive at the result (20), by using the relation

$$K(c^{-2}) = K_0(\mathbf{1} + VP_+K_0)^{-1}. \tag{26}$$

□

Corollary 5. Let $H(c) = H_0(c) + V$ be as above. Then $(H(c) - Mc^2 - z)^{-1}$, $\mathrm{Im}\,(z) \neq 0$, is holomorphic in $1/c$ in a z-dependent neighborhood of $1/c = 0$,

$$(H(c) - Mc^2 - z)^{-1} = \sum_{n=0}^{\infty} \frac{1}{c^n}\,R_n(z). \tag{27}$$

The sum converges in the operator norm. We have

$$R_0(z) = R_\infty P_+ = (H_\infty - z)^{-1}P_+, \tag{28}$$
$$R_1(z) = P_+R_\infty\,\frac{Q}{2M} + \frac{Q}{2M}\,R_\infty P_+, \tag{29}$$
$$R_2(z) = R_\infty\,\frac{Q}{2M}\left(z - \left(\frac{Q^2}{2M} - z\right)R_\infty V\right)\frac{Q}{2M}\,R_\infty, \tag{30}$$

etc.

Proof. Since R_∞ is bounded for z with $\mathrm{Im}\,z \neq 0$ the operator $K(1/c^2)$ is analytic in $1/c^2$ for c sufficiently large. For any fixed $z \in \mathbb{C}\setminus\mathbb{R}$ the norm of the operator

$$\frac{1}{c^2}\,T(c) \equiv \frac{1}{c^2}\,V\,\frac{cQ+z}{2M}\,K(c^{-2}) \tag{31}$$

is less than 1 for c sufficiently large. In this case the operator $1 + T(c)/c^2$ occurring in the last factor of (20) is invertible and hence (20) is analytic in $1/c$ around $1/c = 0$. From (21) we obtain as in (16) explicitly the series expansion of the operator $K(1/c^2)$

$$K(c^{-2}) = R_\infty + \frac{1}{c^2}\,\frac{z^2}{2M}\,R_\infty^2 + \frac{1}{c^4}\,\frac{z^4}{4M^2}\,R_\infty^3 + \ldots \tag{32}$$

Inserting this in the Neumann series of the operator $(1 + T(c)/c^2)^{-1}$ we obtain finally the series expansion of the Dirac resolvent. We have used the relation

$$\mathbf{1} - R_\infty P_+ V = R_\infty \left(\frac{Q^2}{2M} - z \right) \tag{33}$$

in order to obtain the above expressions for R_1 and R_2. □

Remark. The operators R_0 and R_2 are even (they commute with the unitary involution τ), whereas R_1 is odd (i.e., anticommutes with τ). More generally, in the expansion (27) all operators R_{2n} are even operators, and all R_{2n+1} are odd. This can be seen as follows. The only odd operator occurring (20) is $Q/2Mc$. It is also the only operator coming with $1/c$, all other terms in (20) either contain a factor $1/c^2$, or they do not at all depend on c. Therefore the only odd terms in the expansion (27) are those terms which contain an odd number of factors $Q/2Mc$, and these are precisely the terms containing an odd power of $1/c$.

1.4 Nonrelativistic Limit with Anomalous Moments

As an example we consider the Dirac operator with an anomalous electric and magnetic moment. (Sects. 4.2.3 and 4.2.4 of "The Dirac Equation[1]"). The potential terms describing the interaction due to the anomalous moments are given by Eqs. (4.21) and (4.25). In these expressions we substitute $\mu_a = \mu e/2mc$ and $\delta_a = \delta e/2mc$ (where μ and δ are real numbers) and absorb the constant e into $\phi_{\rm el}$ and $\boldsymbol{E} = -\nabla\phi_{\rm el}$. As explained in Remark 2 of Sect. 1.1, we also substitute A for $(e/c)\boldsymbol{A}$ and correspondingly B for $(e/c)\boldsymbol{B}$. With these conventions, the Dirac operator becomes

$$H = \begin{pmatrix} mc^2 + V_+(c) & cD^*(c) \\ cD(c) & -mc^2 + V_-(c) \end{pmatrix}, \tag{34}$$

$$D(c) = \boldsymbol{\sigma} \cdot (\boldsymbol{p} - \boldsymbol{A}) - \mathrm{i}\,\tfrac{1}{2mc}\boldsymbol{\sigma} \cdot (\tfrac{\mu}{c}\boldsymbol{E} + \delta\boldsymbol{B}), \tag{35}$$

$$V_\pm(c) = \phi_{\rm el} \pm \tfrac{1}{2m}\boldsymbol{\sigma} \cdot (\tfrac{\delta}{c}\boldsymbol{E} - \mu\boldsymbol{B}). \tag{36}$$

Although the operators D and $V_\pm$ (and hence Q and V) now depend on c, we can repeat the calculation in the previous section without changes. The leading term R_∞ of the Dirac resolvent now also depends on c. We obtain the expression

$$R_\infty(c) = \begin{pmatrix} (H_{\rm P}(c) - z)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{37}$$

$$H_{\rm P}(c) = \tfrac{1}{2m} D^*(c) D(c) + V_+(c). \tag{38}$$

A calculation similar to Eq. (5.79) gives

$$\begin{aligned} H_{\rm P}(c) = {}& \tfrac{1}{2m}[(\boldsymbol{p} - \boldsymbol{A})^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B}] + \tfrac{1}{2mc^2} X^2 \\ & - \tfrac{1}{2mc}[\,\mathrm{i}\boldsymbol{\sigma} \cdot \operatorname{rot} \boldsymbol{X} + 2\boldsymbol{\sigma} \cdot \boldsymbol{X} \wedge (\boldsymbol{p} - \boldsymbol{A}) + \operatorname{div} \boldsymbol{X}] \\ & + \tfrac{1}{2m}\boldsymbol{\sigma} \cdot (\tfrac{\delta}{c}\boldsymbol{E} - \mu\boldsymbol{B}) + \phi_{\rm el}, \end{aligned} \tag{39}$$

where $\boldsymbol{X} = \frac{1}{2m}(\frac{\mu}{c}\boldsymbol{E} + \delta\boldsymbol{B})$. Assume that the c-dependent terms are bounded with respect to

$$H_{\mathrm{P}}(\infty) \equiv \tfrac{1}{2m}(\boldsymbol{p} - \boldsymbol{A})^2 - \tfrac{1+\mu}{2m}\boldsymbol{\sigma} \cdot \boldsymbol{B} + \phi_{\mathrm{el}}. \tag{40}$$

Then the resolvent equation shows convergence in the operator norm of

$$(H_{\mathrm{P}}(c) - z)^{-1} \to (H_{\mathrm{P}}(\infty) - z)^{-1}, \quad \text{as } c \to \infty. \tag{41}$$

Hence we consider (40) as the nonrelativistic limit of the Dirac operator with anomalous moments (34). Finally, we may reintroduce the factor e/c and obtain the "Pauli operator"

$$H_{\mathrm{P}} \equiv \tfrac{1}{2m}(\boldsymbol{p} - \tfrac{e}{c}\boldsymbol{A})^2 - (1+\mu)\tfrac{e}{2mc}\boldsymbol{\sigma} \cdot \boldsymbol{B} + e\phi_{\mathrm{el}}. \tag{42}$$

The operator H_{P} describes nonrelativistic particles interacting with an electromagnetic field $(\phi_{\mathrm{el}}, \boldsymbol{A})$. A term of the form $\boldsymbol{\mu} \cdot \boldsymbol{B}$ describes the interaction energy of a magnetic moment μ in a magnetic field. The magnetic moment μ, which is measured in units of Bohr magnetons $e/2mc$, is proportional to the spin $\frac{1}{2}\boldsymbol{\sigma}$ of the particle,

$$\boldsymbol{\mu} = g\tfrac{e}{2mc}\tfrac{1}{2}\boldsymbol{\sigma}. \tag{43}$$

The constant in Eq. (43) is called g-factor of the particle. For particles with small anomalous moments like electrons the g-factor is approximately two. This has been observed experimentally before the invention of the Dirac equation. A comparison of (43) with (42) shows that the Dirac equation gives the right prediction: The ordinary Dirac operator (4.15) describes particles with g-factor exactly equal to 2. If there is an additional interaction of the form (4.21) we obtain $g = 2(1+\mu)$. An anomalous electric moment gives no contribution in the nonrelativistic limit.

2 c-Dependence of Eigenvalues

2.1 Browsing Analytic Perturbation Theory

In this section we state some mathematical results which are needed later. The reader is referred to the literature for the proofs of the various results[3].

Let H be a self-adjoint operator in a Hilbert space $\mathfrak{H}$. The resolvent set $\rho(H)$ is given by those complex numbers z for which the resolvent $R(z) = (H-z)^{-1}$ exists and is a bounded operator. The complement $\sigma(H) = \mathbb{C} \setminus \rho(H)$ (the spectrum of H) is a closed subset of the real axis. The singularities of $R(z)$ are just the eigenvalues of H. Let E be an isolated eigenvalue of H and let Γ be a closed positively oriented curve which encloses λ but no other part of $\sigma(H)$. Then

[3] [Ka 80], [RS 78]

$$P \equiv -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma R(z)\, dz \tag{44}$$

is an orthogonal projector onto the eigenspace belonging to the eigenvalue E. The multiplicity $m \equiv \dim P\mathfrak{H}$ of the eigenvalue is assumed to be finite. Then we have the following representation[4], of H in $P\mathfrak{H}$

$$PHP = EP = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma z\, R(z)\, dz. \tag{45}$$

An eigenvalue E is called nondegenerate, if $m = 1$.

Now, let $H(\kappa)$ be an operator valued function of a (possibly complex) variable κ, such that the resolvent $R(\kappa, z)$ is analytic in κ, i.e.,

$$R(\kappa, z) = \sum_{n=0}^{\infty} \kappa^n R_n(z), \qquad z \in \mathbb{C} \setminus \mathbb{R}, \tag{46}$$

where all $R_n(z)$ are bounded operators and the sum converges in the operator norm, uniformly on compact subsets of $\rho(H(0))$. Assume that E_0 is an isolated eigenvalue of $H(0)$, and define the closed curve Γ as in (44). Then

$$P(\kappa) = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma R(\kappa, z)\, dz \tag{47}$$

is (for sufficiently small $|\kappa|$) a projection onto an m-dimensionsal subset of $\mathcal{H}$ (the orthogonal direct sum of the eigenspaces of all the eigenvalues of $H(\kappa)$ lying inside Γ). Obviously, $P(\kappa)$ is analytic around $\kappa = 0$,

$$P(\kappa) = \sum_{n=0}^{\infty} \kappa^n P_n, \qquad P_n = -\frac{1}{2\pi \mathrm{i}} \oint_\Gamma R_n\, dz. \tag{48}$$

With the help of the projection operators $P(\kappa)$ and $P_0 = P(0)$ we define the unitary operator[5]

$$U(\kappa) = \big(\mathbf{1} - (P(\kappa) - P_0)^2\big)^{-1/2} \big(P(\kappa)P_0 + (\mathbf{1} - P(\kappa))(\mathbf{1} - P_0)\big) \tag{49}$$

Note that $A \equiv (P(\kappa) - P_0)^2$ commutes with $P(\kappa)$ and P_0. We can define the inverse square root in Eq. (49) as

$$(\mathbf{1} - A)^{-1/2} = \sum_{n=0}^{\infty} \binom{-\frac{1}{2}}{n} (-A)^n = \mathbf{1} + \tfrac{1}{2}\, A + \tfrac{3}{8}\, A^2 + \dots, \tag{50}$$

if $\|A\| < 1$ which is the case for sufficiently small $|\kappa|$, because $\lim_{\kappa\to 0} P(\kappa) = P_0$ in the operator norm.

The operator valued function $U(\kappa)$ is called transformation function for $P(\kappa)$, because

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4 [Ka 80], Sect. I.5

5 [Ka 80], Sects. I.4.6 and I.6.8.

$$U(\kappa)\,P_0 = P(\kappa)\,U(\kappa), \tag{51}$$

i.e., $U(\kappa)$ intertwines between the projections $P(\kappa)$ and P_0. Clearly, $U(\kappa)$ is analytic in κ around $\kappa = 0$, from the expansion of $P(\kappa)$ and Eq. (50), we obtain

$$U(\kappa)\,P_0 = P_0 + \kappa P_1 P_0 + \kappa^2 (P_2 P_0 + \tfrac{1}{2}\, P_1^2 P_0) + \dots \tag{52}$$

Similarly as in Eq. (45) we can define an analytic family of bounded self-adjoint operators

$$P(\kappa)H(\kappa)P(\kappa) = -\frac{1}{2\pi\mathrm{i}} \oint_\Gamma z\, R(\kappa, z)\, dz. \tag{53}$$

The range of the projection $P(\kappa)$ is generally different for each κ. But with the help of the transformation function we can define an analytic family of bounded self-adjoint operators which is unitarily equivalent to (53) and which acts on one fixed subspace $P_0\mathfrak{H}$.

$$\begin{aligned}\tilde{H}(\kappa) &= U(\kappa)^{-1} P(\kappa) H(\kappa) P(\kappa) U(\kappa) \\ &= -\frac{1}{2\pi\mathrm{i}}\, P_0 U(\kappa)^{-1} \oint_\Gamma z\, R(\kappa, z)\, dz\, U(\kappa) P_0 \\ &= E_0 P_0 - \frac{1}{2\pi\mathrm{i}}\, P_0 U(\kappa)^{-1} \oint_\Gamma (z - E_0)\, R(\kappa, z)\, dz\, U(\kappa) P_0. \end{aligned} \tag{54}$$

Hence the problem of finding the eigenvalues of $H(\kappa)$ near the eigenvalue E_0 of $H(0)$ is completely reduced to the diagonalization of a self-adjoint operator in a finite dimensional Hilbert space. Hence we can apply the following theorem of Rellich.

Theorem 6. Let $\tilde{H}(\kappa)$ be a family of operators in a finite dimensional Hilbert space, such that $\tilde{H}(\kappa)$ is analytic in a neighborhood of $\kappa = 0$. Suppose that $\tilde{H}(\kappa)$ is self-adjoint for real κ and let E_0 be an eigenvalue of $\tilde{H}(0)$ with multiplicity m. Then there are $k < m$ distinct functions, $E^1(\kappa), \dots, E^k(\kappa)$, which are analytic in κ in a neighborhood of $\kappa = 0$, and which are all eigenvalues of $\tilde{H}(\kappa)$ with multiplicities m^j, such that $\sum_{j=1}^k m_j = m$.

We also note that the eigenvectors of $\tilde{H}(\kappa)$ are simply given by

$$\phi^l(\kappa) = U(\kappa)\phi_0^l, \quad l = 1, \dots, m, \tag{55}$$

where the vectors ϕ_0^l, form a basis of the eigenspace of H_0 belonging to the eigenvalue E_0. This result follows immediately from the fact that the unitary operator $U(\kappa)$ maps $P_0\mathfrak{H}$ onto $P(\kappa)\mathfrak{H}$. Analyticity of $\tilde{H}$ and its eigenvalues implies that there is an expansion of the form

$$\tilde{H}(\kappa) = \sum_{n=0}^\infty \tilde{H}_n, \qquad E^j(\kappa) = \sum_{n=0}^\infty E_n^j. \tag{56}$$

If E_0 is nondegenerate, then the first order term in the expansion of $E(\kappa)$, is given by

$$E_1 = (\phi_0, \tilde{H}_1 \phi_0). \tag{57}$$

If E_0 has multiplicity m, then $E^j(\kappa)$, $j = 1, \ldots, k$, are the eigenvalues of the self-adjoint $m \times m$ matrix

$$A_{jk} = (\phi_0^j, \tilde{H}_1 \phi_0^k). \tag{58}$$

2.2 The Reduced Dirac Operator

We apply the general results of the previous section to the Dirac operator $H(c) - Mc^2$. From Sect. 1.3 we know that the resolvent of this operator is analytic in $1/c$, and

$$\lim_{c\to\infty} (H(c) - Mc^2 - z)^{-1} = (H_\infty - z)^{-1} P_+. \tag{59}$$

We assume that E_0 is an isolated eigenvalue with multiplicity m of the operator $H_\infty P_+$. The corresponding eigenspace $P_0\mathfrak{H}$ is contained in $P_+\mathfrak{H}$. Let Γ be a circle in $\mathbb{C}$ which separates E_0 from the rest of $\sigma(H_0)$. The projection operator

$$P(\tfrac{1}{c}) = -\frac{1}{2\pi\mathrm{i}} \oint_\Gamma (H(c) - Mc^2 - z)^{-1}\, dz \tag{60}$$

is analytic in $1/c$. We can define the transformation operator

$$U(\tfrac{1}{c}) = \bigl(\mathbf{1} - (P(\tfrac{1}{c}) - P_0)^2\bigr)^{-1/2} \bigl(P(\tfrac{1}{c})P_0 + (\mathbf{1} - P(\tfrac{1}{c}))(\mathbf{1} - P_0)\bigr), \tag{61}$$

which is analytic in $1/c$. We shall need the first term in the series expansion of $U(1/c)P_0$. From Eq. (52) it is clear that

$$\lim_{c\to\infty} U(\tfrac{1}{c})P_0 = P_0 = \lim_{c\to\infty} P_0 U(\tfrac{1}{c}). \tag{62}$$

We are interested in the reduced Dirac operator

$$\begin{aligned} \tilde{H}(\tfrac{1}{c}) &= U(\tfrac{1}{c})^{-1} P(\tfrac{1}{c})(H(c) - Mc^2)P(\tfrac{1}{c})U(\tfrac{1}{c}) \\ &= E_0 P_0 - \frac{1}{2\pi\mathrm{i}}\, P_0 U(\tfrac{1}{c})^{-1} \oint_\Gamma (z - E_0)\,(H(c) - Mc^2 - z)^{-1}\, dz\, U(\tfrac{1}{c})P_0 \end{aligned} \tag{63}$$

which is bounded and self-adjoint and analytic in $1/c$ for sufficiently large c. In order to obtain the series expansion of $\tilde{H}$ in powers of $1/c$, we note that

$$\oint_\Gamma (z - E_0)\, R_0(z)\, dz = 0, \qquad \oint_\Gamma (z - E_0)\, R_1(z)\, dz = 0. \tag{64}$$

This can be seen from the explicit forms of R_0, R_1 given in Eqs. (28), (29) and Cauchy's integral formula, because

$$-\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} (z - E_0)\, R_\infty(z)\, P_0 \, dz = -\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} \frac{z - E_0}{E_0 - z} \, dz = 0. \tag{65}$$

Therefore the first nontrivial term in the $1/c$-expansion of Eq. (63) is given by

$$-\frac{1}{2\pi \mathrm{i}} P_0 \oint_{\Gamma} (z - E_0)\, \tfrac{1}{c^2}\, R_2(z) \, dz \, P_0. \tag{66}$$

But from Eq. (30) we find

$$P_0 R_2(z) P_0 = P_0 \, \frac{Q}{2M} \, \frac{z - V}{(E_0 - z)^2} \, \frac{Q}{2M} \, P_0. \tag{67}$$

Hence, with Cauchy's integral formula we obtain immediately

$$\tilde{H}(\tfrac{1}{c}) = E_0 P_0 + \frac{1}{c^2} \, P_0 \, \frac{Q}{2M} \, (V - E_0) \, \frac{Q}{2M} \, P_0 + \dots \tag{68}$$

Remark. It is easy to see that the expansion (68) contains only even powers of $1/c$. As we know from the remark at the end of Sect. 1.3, the $1/c^{2n+1}$-terms in the expansion of the resolvent are all odd operators. Hence the same is true for the expansions of $P(1/c)$ and hence for the series of $U(1/c)P_0$ and $P_0U(1/c)^*$. Therefore, also in the series expansion of $\tilde{H}(1/c)$ the odd powers of $1/c$ can only occur with odd operators. But $\tilde{H}(1/c) = P_+\tilde{H}(1/c)P_+$ is an even operator and hence it is anlaytic in $1/c^2$. It follows immediately from this observation and from Theorem 6 that the eigenvalues of $\tilde{H}(1/c)$ are analytic in $1/c^2$. Using first order perturbation theory we obtain the following results.

2.3 Analyticity of Eigenvalues and Eigenfunctions

Theorem 7. Let $H(c) = cQ + \tau Mc^2 + V$ be a Dirac operator defined as in Eqs. (2)–(5). Let E_0 be an isolated eigenvalue with finite multiplicity m of the operator $H_\infty P_+$, which is the nonrelativistic limit of $H(c) - Mc^2$ (cf. Theorem 4). Then $H(c)-Mc^2$ has $k \le m$ distinct eigenvalues $E^j(1/c^2)$, $j = 1, \dots, k$, with multiplicities m_j (with $\sum_j m_j = m$), such that each E^j is analytic in $1/c^2$ in a neighborhood of $c = \infty$. The corresponding eigenvectors ψ^{j,r_j}, $r_j = 1, \dots m_j$ can be chosen in the form

$$\psi^{j,r_j}(c) = \phi_+^{j,r_j}(\tfrac{1}{c^2}) + \tfrac{1}{c}\, \phi_-^{j,r_j}(\tfrac{1}{c^2}), \qquad \phi_\pm^{j,r_j}(\tfrac{1}{c^2}) \in P_\pm \mathfrak{H}, \tag{69}$$

where $\phi_\pm^{j,r_j}(\tfrac{1}{c^2})$ are analytic in $1/c^2$.

Proof. The result follows immediately from the analyticity of $\tilde{H}(\tfrac{1}{c})$ and Theorem 6. By the remark at the end of the preceding section, the series expansion of $U(\tfrac{1}{c})$ is of the form

$$U(\tfrac{1}{c}) = U_{\mathrm{even}}(\tfrac{1}{c^2}) + \tfrac{1}{c} U_{\mathrm{odd}}(\tfrac{1}{c^2}) \tag{70}$$

Eq. (69) follows, because the eigenvectors of $H_\infty P_+$ belonging to isolated (i.e., nonzero) eigenvalues are in $P_+\mathfrak{H}$. □

2.4 First Order Corrections of Nonrelativistic Eigenvalues

Theorem 8. Under the assumptions of Theorem 7, the eigenvalues E^j of the Dirac operator $H(c) - Mc^2$ have the expansion

$$E^j(\tfrac{1}{c^2}) = E_0 + \tfrac{1}{c^2}\, E_1^j + O(\tfrac{1}{c^4}), \tag{71}$$

where the E_1^j, $j = 1, \dots, k$, are the eigenvalues of the self-adjoint matrix

$$A_{ik} = \Big(\frac{Q}{2M}\, \phi_0^i \,,\, (V - E_0)\, \frac{Q}{2M}\, \phi_0^k \Big). \tag{72}$$

The vectors $\phi_0^1, \dots, \phi_0^m$ form an orthonormal system of eigenvectors of $H_\infty P_+$ belonging to the eigenvalue E_0.

Proof. See the discussion after Theorem 6. □

Remark 1. Note that all eigenvectors ϕ_0^j are in $P_+\mathfrak{H}$. The commutation relation $(Q/2M)P_+ = P_-(Q/2M)$ shows that only the part V_- of V in $P_-\mathfrak{H}$ is relevant for the calculation of the $1/c^2$-correction to the nonrelativistic eigenvalue.

Remark 2. For a nondegenerate eigenvalue E_0, i.e., $H_\infty \phi_0 = E_0 \phi_0$, with $\|\phi_0\| = 1$, there is only one eigenvalue $E(1/c^2) = E_0 + E_1/c^2 + \dots$ of $H(c) - Mc^2$, and Eq. (72) simplifies to

$$E_1 = \Big(\frac{Q}{2M}\, \phi_0 \,,\, (V - E_0)\, \frac{Q}{2M}\, \phi_0 \Big). \tag{73}$$

2.5 Interpretation of the First Order Correction

In the standard representation, we denote the component of $\psi_0 \in P_+\mathfrak{H}$ by ψ_0^+. Let E_0 be a nondegenerate eigenvalue of $H_\infty P_+$ with corresponding eigenvector ψ_0, i.e.,

$$\Big(\frac{1}{2M_+} D^* D + V_+ \Big) \psi_0^+ = E_0 \psi_0^+. \tag{74}$$

According to Eq. (73) the first relativistic correction E_1 can be written in the form

$$E_1 = \Big(\frac{1}{2M_-}\, D\psi_0^+ \,,\, (V_- - E_0)\, \frac{1}{2M_-}\, D\psi_0^+ \Big). \tag{75}$$

The scalar product in (75) is the scalar product in $P_-\mathfrak{H}$.

Let us now consider a special case, namely the electron in an electrostatic potential. We have $\mathfrak{H} = L^2(\mathbb{R}^3)^4$, $\tau = \beta$,

$$V_+(\boldsymbol{x}) = V_-(\boldsymbol{x}) = \phi_{\mathrm{el}}(\boldsymbol{x}) \mathbf{1}_2, \qquad \boldsymbol{x} \in \mathbb{R}^3, \tag{76}$$

$$D = D^* = \boldsymbol{\sigma} \cdot \boldsymbol{p} = -\mathrm{i}\,\boldsymbol{\sigma} \cdot \nabla, \qquad M_+ = M_- = m. \tag{77}$$

The nonrelativistic limit of the Dirac operator $H(c) - mc^2$ is given in $L^2(\mathbb{R}^3)^2$ by the following "Schrödinger operator with spin"

$$H_\infty = \Big(-\frac{1}{2m}\Delta + \phi_{\mathrm{el}}(\boldsymbol{x})\Big)\,\mathbf{1}_2. \tag{78}$$

Thus the Schrödinger operator H_∞ describes particles with spin (i.e., two-component wavefunctions) but the spin does not interact with the electrostatic field.

Theorem 9. Assume $\phi_{\mathrm{el}}(\boldsymbol{x})$ is a twice continuously differentiable function of $\boldsymbol{x}$. Let ψ_0^+ be a nondegenerate bound state of H_∞, i.e., $H_\infty \psi_0^+ = E_0 \psi_0^+$, and $\|\psi_0\| = 1$. Then a first approximation to the corresponding eigenvalue of the Dirac operator $c\boldsymbol{\alpha} \cdot \boldsymbol{p} + (\beta - \mathbf{1})mc^2 + \phi_{\mathrm{el}}\mathbf{1}$ is given by $E_0 + E_1/c^2$, where

$$\begin{aligned} E_1 &= \frac{1}{4m^2}\,(\boldsymbol{\sigma} \cdot \boldsymbol{p}\,\psi_0^+, (\phi_{\mathrm{el}} - E_0)\boldsymbol{\sigma} \cdot \boldsymbol{p}\,\psi_0^+) \\ &= \frac{1}{4m^2}\,\Big(\psi_0^+\,,\,\{-\frac{1}{2m}\boldsymbol{p}^4 + \boldsymbol{\sigma} \cdot (\nabla\phi_{\mathrm{el}}) \wedge \boldsymbol{p} + \frac{1}{2}\,(\Delta\phi_{\mathrm{el}})\,\}\,\psi_0^+\Big). \end{aligned} \tag{79}$$

Proof. Inserting (77) into (75) gives

$$\begin{aligned} E_1 &= \frac{1}{4m^2}\,(\psi_0^+, \boldsymbol{\sigma} \cdot \boldsymbol{p}\,(\phi_{\mathrm{el}} - E_0)\,\boldsymbol{\sigma} \cdot \boldsymbol{p}\,\psi_0^+) \\ &= \frac{1}{4m^2}\,(\psi_0^+, \{\boldsymbol{\sigma} \cdot \boldsymbol{p}\,\phi_{\mathrm{el}}\,\boldsymbol{\sigma} \cdot \boldsymbol{p} - E_0(\boldsymbol{\sigma} \cdot \boldsymbol{p})^2\}\,\psi_0^+) \\ = \quad &= \frac{1}{4m^2}\,\big(\psi_0^+, \{\boldsymbol{\sigma} \cdot \boldsymbol{p}\,\phi_{\mathrm{el}}\,\boldsymbol{\sigma} \cdot \boldsymbol{p} - \big(\frac{1}{2m}\boldsymbol{p}^2 + \phi_{\mathrm{el}}\big)(\boldsymbol{\sigma} \cdot \boldsymbol{p})^2\}\psi_0^+\big) \\ &= \frac{1}{4m^2}(\psi_0^+, \{-\frac{1}{2m}\boldsymbol{p}^4 + [\boldsymbol{\sigma} \cdot \boldsymbol{p}, \phi_{\mathrm{el}}]\boldsymbol{\sigma} \cdot \boldsymbol{p}\}\,\psi_0^+). \end{aligned} \tag{80}$$

Using $\boldsymbol{p} = -\mathrm{i}\,\nabla$ we obtain

$$[\boldsymbol{\sigma} \cdot \boldsymbol{p}, \phi_{\mathrm{el}}]\,\boldsymbol{\sigma} \cdot \boldsymbol{p} = -\mathrm{i}\,(\boldsymbol{\sigma} \cdot \nabla\phi_{\mathrm{el}})\,\boldsymbol{\sigma} \cdot \boldsymbol{p}. \tag{81}$$

From the relation (1.212) we get

$$[\boldsymbol{\sigma} \cdot \boldsymbol{p}, \phi_{\mathrm{el}}]\boldsymbol{\sigma} \cdot \boldsymbol{p} = -(\nabla\phi_{\mathrm{el}}) \cdot \nabla + \boldsymbol{\sigma} \cdot (\nabla\phi_{\mathrm{el}}) \wedge \boldsymbol{p}. \tag{82}$$

Next we calculate

$$\begin{aligned} &(\psi_0^+, \tfrac{1}{2}\,(\Delta\phi_{\mathrm{el}})\,\psi_0^+ + (\nabla\phi_{\mathrm{el}})(\nabla\psi_0^+)\,) \\ &= \tfrac{1}{2}\,(\psi_0^+, [\Delta, \phi_{\mathrm{el}}]\psi_0^+) = \tfrac{1}{2}\,(\psi_0^+, 2m[\phi_{\mathrm{el}} - E_0\,, \phi_{\mathrm{el}}]\psi_0^+) = 0. \end{aligned} \tag{83}$$

This gives finally

$$(\psi_0^+\,,\,[\boldsymbol{\sigma} \cdot \boldsymbol{p}\,,\,\phi_{\mathrm{el}}\,]\,\boldsymbol{\sigma} \cdot \boldsymbol{p}\,\psi_0^+) = (\psi_0^+\,,\,\{\tfrac{1}{2}\,(\Delta\phi_{\mathrm{el}}) + \boldsymbol{\sigma} \cdot (\nabla\phi_{\mathrm{el}}) \wedge \boldsymbol{p}\}\,\psi_0^+). \tag{84}$$

□

Remark. The various terms in Eq. (79) have a nice interpretation. The term $-(2m)^{-3}\,\boldsymbol{p}^4$ is the *kinetic energy correction* of order $1/c^2$ as expected from the correspondence principle: In classical mechanics, the relativistic kinetic energy as a function of the momentum is given by

$$\sqrt{c^2\boldsymbol{p}^2 - m^2c^4} - mc^2 = \frac{1}{2m}\,\boldsymbol{p}^2 - \frac{1}{8m^3c^2}\,\boldsymbol{p}^4 + \mathrm{O}\Big(\frac{1}{c^4}\Big). \tag{85}$$

The second summand in Eq. (79), $(2m)^{-2}\,\boldsymbol{\sigma}\cdot(\nabla\phi_{\mathrm{el}})\wedge\boldsymbol{p}$, is called *spin orbit coupling term*. It can be explained as follows. The electron has a magnetic moment $\boldsymbol{\mu} = -(eg/2mc)\boldsymbol{S} = -(e/2mc)\boldsymbol{\sigma}$ (the Dirac equation without modifications describes electrons with g=2). The magnetic moment interacts with an external magnetic field, the corresponding contribution to the energy is $-\boldsymbol{\mu}\cdot\boldsymbol{B}$. According to the special theory of relativity, an observer moving with velocity $\boldsymbol{v}$ in an electrostatic field of strength $\boldsymbol{E}$ feels a magnetic field of strength $\boldsymbol{B} = -\boldsymbol{E}\wedge\boldsymbol{v}/c$. Hence we expect that the interaction energy of order $1/c^2$ is given by

$$-\frac{e}{2m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{E}\wedge\boldsymbol{p}. \tag{86}$$

This is twice the spin orbit term, if we set $-e\boldsymbol{E} = \nabla\phi_{\mathrm{el}}$. But there is still another contribution coming from the Thomas precession. This is a purely kinematical effect in the special theory of relativity. An accelerated frame of reference performs an additional precession with the frequency

$$\boldsymbol{\omega} = -\frac{1}{2c^2}\dot{\boldsymbol{v}}\wedge\boldsymbol{v}. \tag{87}$$

For the motion in an electric field, the acceleration is given by $\dot{\boldsymbol{v}} = -e\boldsymbol{E}/m$. The precession of the spin axis gives an additional interaction term

$$\boldsymbol{\omega}\cdot\boldsymbol{S} = \frac{e}{4m^2c^2}\,\boldsymbol{\sigma}\cdot\boldsymbol{E}\wedge\boldsymbol{p}, \tag{88}$$

which combines with (86) to give the spin orbit coupling term. The last contribution to Eq. (79), $\frac{1}{8m^2}\,(\Delta\phi_{\mathrm{el}})$, is known as the *Darwin term*. It can be heuristically explained as an effect related to Zitterbewegung.

2.6 Example: Separable Potential

We calculate the first-order relativistic correction for the bound state of the radial Schrödinger equation with a separable potential V. A separable potential is an operator of finite rank. Given some $v \in L^2([0,\infty); dr)$ and $\gamma > 0$ we assume that V is of the form

$$V\phi = -\gamma\,(v,\phi)\,v, \quad \text{all } \phi \in L^2([0,\infty); dr), \tag{89}$$

where $(v,\phi) = \int_0^\infty \overline{v(r)}\,\phi(r)\,dr$ is the scalar product in $L^2([0,\infty);dr)$. The radial Schrödinger equation with orbital angular momentum $l = 0$ and energy $E < 0$ becomes

$$-\phi''(r) - \mu\,(v,\phi)\,v(r) = -\epsilon^2\phi(r), \tag{90}$$

where we have used the abbreviations

$$\mu = \frac{2m\gamma}{\hbar^2} > 0, \qquad \epsilon^2 = -\frac{2mE}{\hbar^2} > 0. \tag{91}$$

A Fourier transformation $\phi \to \hat\phi$, where $\hat\phi(k) = \sqrt{2/\pi}\int_0^\infty \phi(r)\,\sin(kr)\,dr$, converts Eq. (90) into

$$k^2\,\hat\phi(k) - \mu\,(v,\phi)\,\hat v(k) = -\epsilon^2\hat\phi(k). \tag{92}$$

Hence the solution ϕ_ϵ must satisfy

$$\hat\phi_\epsilon(k) = \mu\,(v,\phi_\epsilon)\,\hat u_\epsilon(k), \qquad \text{where} \quad \hat u_\epsilon(k) = \frac{\hat v(k)}{\epsilon^2 + k^2}. \tag{93}$$

From $(v,\phi_\epsilon) = (\hat v,\hat\phi_\epsilon) = \mu\,(v,\phi_\epsilon)\,(\hat v,\hat u_\epsilon)$ we find

$$(\hat v,\hat u_\epsilon) = (v,u_\epsilon) = 1/\mu. \tag{94}$$

This equation can be used to determine an energy ϵ for which a square-integrable u_ϵ exists.

For the explicit calculation we assume that V is a "Yamaguchi potential",

$$v(r) = e^{-ar}, \quad a > 0, \qquad \text{i.e.,} \quad \hat v(k) = \sqrt{\frac{2}{\pi}}\,\frac{k}{a^2+k^2}. \tag{95}$$

Hence we find

$$u_\epsilon(r) = \frac{e^{-ar} - e^{-\epsilon r}}{\epsilon^2 - a^2}, \qquad (v,u_\epsilon) = \frac{1}{2a(\epsilon+a)^2}. \tag{96}$$

Therefore, with Eq. (94) we conclude that

$$\epsilon = (\mu/2a)^{1/2} - a, \tag{97}$$

which is only positive for $\mu > 2a^3$ (otherwise u_ϵ is not square-integrable). In this case the radial Schrödinger equation with the Yamaguchi potential supports precisely one bound state ϕ_0 with energy E_0,

$$\phi_0(r) = \sqrt{2\epsilon a\,(\epsilon+a)^3}\;u_\epsilon(r), \qquad E_0 = -\frac{\hbar^2}{2m}\,\epsilon^2. \tag{98}$$

The normalization factor has been chosen such that $\|\phi_0\| = 1$.

With our previous notation we have

$$D = \hbar\left(\frac{d}{dr} - \frac{1}{r}\right), \qquad H_\infty = \frac{\hbar^2}{2m}\,\frac{d^2}{dr^2} + V, \tag{99}$$

and we can use Eq. (73) to calculate E_1,

$$\begin{aligned} E_1 &= \frac{\hbar^2}{4m^2}\left\{-\gamma\left|(\,v\,,\,\phi_0'-\phi_0/r\,)\right|^2 + E_0\,(\phi_0\,,\phi_0'')\right\} \\ &= -\frac{\hbar^4}{8m^3}\,\epsilon\,a\left\{a\,(\epsilon+a)\left[1-2\,\frac{\epsilon+a}{\epsilon-a}\ln\frac{\epsilon+a}{2a}\right]^2-\epsilon^2\right\}. \end{aligned} \tag{100}$$

The separable potential discussed here can be regarded as a very simple model of the nucleon-nucleon interaction. For a rough estimate we insert for m the reduced mass of the proton-neutron system, $mc^2 = 469,46$ MeV, and choose $a = 1$, $\gamma = 124,3$ MeV fm^{-1}. Then we have $E_0 = -2.08$ MeV and $E_1/c^2 = -0.13$ MeV. The constants have been chosen to fit the bound state energy of the proton-neutron system (the deuteron), $E \approx E_0 + E_1/c^2 = -2.22$ MeV. We see that the relativistic correction gives a contribution of about 6% of the nonrelativistic bound state energy.

Notes

Section 1. Pauli was the first to study the connection between the Dirac theory and its nonrelativistic approximation by separating the "large" and "small" components of the wavefunction [1]. For the early literature on this subject, see [2], or [BS 59]. We mention [3], where Eq. (73) is derived for a special case using formal expansions of wavefunctions. Pauli's method was developed further in [4], still at a formal level, and more rigorously by Schoene [5], who investigated in particular the convergence of the solutions in the nonrelativistic limit. The spherically symmetric case is studied rigorously by Titchmarsh in [6], spherically symmetric scattering problems are treated in [7, 8].

A completely different approach was taken by Foldy and Wouthuysen [9], who developed a formal scheme of applying successively Foldy-Wouthuysen (FW) transformations in order to obtain operator perturbations of the nonrelativistic Pauli operator H_{P} of order $1/c^2$ and higher. In principle, this method gives an expansion of the Dirac operator into powers of $1/c^2$. This method became the most popular one [10] and can be found in most textbooks on relativistic quantum mechanics. However, even the first order perturbation of H_{P} is so singular that it destroys completely all spectral properties of H_{P}. For example, all bound states of H_{P} dissolve into a continuous spectrum [11]. Mathematically, one is actually forced to consider H_{P} as a small perturbation of the $1/c^2$ term. Adding higher order corrections makes the situation even worse. The divergence of the Foldy-Wouthuysen series for a special case is also noted in [12]. Nevertheless, the first order corrections of eigenvalues obtained in this formal way are correct and agree with the expressions obtained in Theorem 9. Therefore it should be clear that the "operator perturbations" cannot not be taken literally. The FW corrections are not meaningful in an operator sense and should only be considered if applied to wavefunctions with energies in a neighborhood of the bound state energy under consideration. We refer to [13] for further clarification. Attempts to understand the status of the FW method are also made in [11, 14-16].

The resolvent approach which is presented here was suggested first by Veselić [17] (see also his earlier paper [18]). He derived the analyticity of the resolvent by perturbation theoretic arguments. A similar approach was used by Hunziker [19] for a larger class of potentials. The explicit expansion of the resolvent into powers of $1/c$ was obtained for the first time in [20] and [21]. The last paper also contains estimates on the convergence radius of the expansion. The convergence of solutions of the Dirac equation in the nonrelativistic limit is also considered in [22, 23].

Section 2. For the complicated systems in atomic and molecular physics the calculation of relativistic corrections is of great practical importance. Many-body analogues of the Dirac equation can be used to deduce formulas for the first-order relativistic corrections. It is perhaps not meaningful to calculate higher-order corrections or the exact solution of the many-particle Dirac equation, because in higher orders one expects contributions from QED which cannot be described by the Dirac equation alone. More on the applications of Dirac-type equations in many-particle systems can be found, e.g., in the books T. P. Das: *Relativistic Quantum Mechanics of Electrons*, Harper and Row, New York 1973, G. L. Malli (ed.): *Relativistic Effects in Atoms, Molecules, and Solids*, Nato ASI Series B: Physics, Vol. 87, Plenum

Press, New York, London 1983, P. Pykkö: *Relativistic Theory of Atoms and Molecules*, Lecture Notes in Chemistry, Vol. 41, Springer Verlag, Berlin, Heidelberg, New York 1986, or in [24]. As a review of the various methods used in the perturbation theory of relativistic corrections we recommend [16, 25].

The problem of finding relativistic corrections to bound state energies was solved rigorously and for a large class of potentials by Gesztesy, Grosse and Thaller [21]. Formula (73) was known before only in some special cases [3, 6]. The result is folklore in the form of Eq. (79), although the derivation of (79) had been based on heuristic and formal arguments [9] (see also the discussion of the Foldy-Wouthuysen method in the notes to Sect. 1). The approach in [21] uses perturbation theory of resolvents and the explicit $1/c^2$ expansion to obtain the result (73), but only in the case of nondegenerate eigenvalues. The analyticity of eigenvalues had already been stated by Hunziker [19] without giving the proof in the degenerate case. Theorem 8 for degenerate eigenvalues was proven first by Wiegner [26]. Some essential simplifications of the method have been obtained by Grigore, Nenciu and Purice [13], who independently gave a proof in the degenerate case. Our presentation here follows closely their elegant exposition.

The method of finding relativistic corrections to nonrelativistic quantities by the resolvent method is extended to the Breit-Fermi Hamiltonian for two-fermion systems in [27]. One dimensional Dirac operators with a periodic potential are considered in [28]. In this case the first order corrections of the energy band edges are again given by Eq. (72).

Relativistic corrections for the scattering matrix are derived in [15]; the scattering amplitude is considered in [13]. For exponentially decaying potentials the holomorphy of the scattering matrix at fixed energy is derived in [15] in the framework of Kuroda's stationary scattering theory. Again, the first order correction to the nonrelativistic S-matrix can be obtained explicitly. Unfortunately the resulting expression is too complicated to be reproduced here. Ref. [13] requires a weaker decay of the potential, which implies only differentiability of the scattering amplitude instead of holomorphy. This is, however, sufficient to obtain first order corrections of the scattering amplitude. The nonrelativistic limit of stationary scattering theory and the analyticity of resonances in $1/c$ is investigated in [29]. Among earlier results on the nonrelativistic limit of Dirac scattering theory we mention the proof of strong convergence of wave operators as $c \to \infty$, in [30] and [31].

The explicit form of the correction terms arising from the FW method and given in Eq. (79) has always been a strong argument in favor of the Dirac equation. A more detailed discussion of their physical interpretation is given, e.g., in the book M. E. Rose: *Relativistic Electron Theory*, Wiley, New York 1961 (Sects. I.7 and IV. 22), which also contains a derivation of the Thomas precession (Appendix B).

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