Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
J. Differential Equations 205 (2004) 408–423
Journal of Differential Equations
http://www.elsevier.com/locate/jde

Spectral stability of the Coulomb–Dirac Hamiltonian with anomalous magnetic moment

Hubert Kalf[a] and Karl Michael Schmidt[b,*]

[a] *Mathematisches Institut der Universität, Theresienstr. 39, D-80333 München, Germany*
[b] *School of Mathematics, Cardiff University, 23 Senghennydd Road, Cardiff CF24 4YH, UK*

Received November 28, 2003

Available online 21 July 2004

Dedicated to A. Schneider on the occasion of his 70th birthday

Abstract

We show that the point spectrum of the standard Coulomb–Dirac operator H_0 is the limit of the point spectrum of the Dirac operator with anomalous magnetic moment H_a as the anomaly parameter tends to 0. For negative angular momentum quantum number κ, this holds for all Coulomb coupling constants c for which H_0 has a distinguished self-adjoint realisation. For positive κ, however, there are some exceptional values for c, and in general an index shift between the eigenvalues of H_0 and the limits of eigenvalues of H_a appears, accompanied with additional oscillations of the eigenfunctions of H_a very close to the origin.

Keywords: Dirac operator; Anomalous magnetic moment; Eigenvalue stability; Singular perturbation

1. Introduction

In a 1930 letter to O. Klein [9, letter 261] and in a survey to be given at the 8th Solvay Congress, planned for October 1939, Pauli suggested to describe the motion of a particle with rest mass $m>0$, charge e, spin $\hbar/2$ and magnetic moment $(1+a)\mu_B$ ($\mu_B=\frac{e\hbar}{2mc}$ the Bohr magneton) in an electric field $-\nabla\Phi$ and a magnetic field

*Corresponding author.
E-mail address: karl.m.schmidt@cs.cardiff.ac.uk (K.M. Schmidt).

0022-0396/$ - see front matter © 2004 Elsevier Inc. All rights reserved.
doi:10.1016/j.jde.2004.04.009

$B = \operatorname{curl} A$ by means of the operator

$$H = c\alpha \cdot \left(p - \frac{e}{c} A\right) + mc^2\beta + e\Phi - a\mu_B(i\alpha \cdot \nabla\Phi + \sigma \cdot B).$$

A revised version of this review appeared in [8] (the relevant equation is (91)); the original manuscript was not published until 1993 in [10, pp. 827–901].

If $\Phi(x) = V(|x|)$ and $A = 0$, self-adjoint realisations of H in $L^2(\mathbb{R}^3)^4$ are unitarily equivalent to the orthogonal sum of self-adjoint realisations of

$$H_a = \sigma_2 p + \frac{mc}{\hbar}\sigma_3 + \left(\frac{\kappa}{r} + \frac{a\mu_B}{\hbar c} V'(r)\right)\sigma_1 + \frac{e}{\hbar c} V(r)$$

in $L^2((0,\infty))^2$, where $\kappa \in \mathbb{Z}\backslash\{0\}$ is the angular momentum quantum number.

The first mathematical treatment of the operators H and H_a is due to Behncke [2–4]. He showed that H_a has a unique self-adjoint realisation if $a \neq 0$ for a very large class of potentials V, including the Coulomb potential $V(r) = -\frac{Ze}{r}$ for all values of the coupling constant Ze (for alternative proofs see [5,1]). This is in marked contrast to the case $a = 0$ where it is well known that H_0 is essentially self-adjoint on its minimal domain if and only if $(\frac{Ze^2}{\hbar c})^2 \leqslant \kappa^2 - \frac{1}{4}$. For larger values of Z the singular end-point 0 is in the limit-circle case; but as long as $(\frac{Ze^2}{\hbar c})^2 < \kappa^2$ one still has a distinguished self-adjoint realisation of H_0 defined by the requirement that functions in the domain behave like the principal solution of the eigenvalue equation of H_0 at 0.

The location of the essential spectrum of H_a is comparatively easy to determine and for a wide range of potentials, notably the Coulomb potential, coincides with that of H_0 [2–4].

In the following, we normalise constants and write the Coulomb Hamiltonian as

$$H_a = -i\sigma_2 \frac{d}{dr} + \sigma_3 + \left(\frac{\kappa}{r} + \frac{a}{r^2}\right)\sigma_1 + \frac{c}{r}$$

assuming $a, c < 0$. (The cases of positive c and/or a can be reduced to this situation by means of suitable unitary transformations.) The discrete spectrum of H_0 accumulates at the right end-point of the gap $(-1, 1)$ in the essential spectrum. Since $C_0^\infty((0,\infty))^2$ is a common core for H_0 and H_a if (and only if) $c^2 \leqslant \kappa^2 - \frac{1}{4}$, H_a converges to H_0 in the strong resolvent sense as $a \to 0$ [11, Theorem VIII.25(a)], and as a consequence, the spectrum of H_a cannot expand in the limit $a \to 0$ for this range of the parameters c, κ. However, it is reasonable to expect (and has been used as a basis for a perturbative calculation of the eigenvalues of H_a) that the point spectrum is stable in the limit $a \to 0$ in the sense that the eigenvalues of H_a converge to those of H_0, and each eigenvalue of H_0 is the limit of exactly one eigenvalue branch of H_a. Decoupling the eigenvalue equation of H_a and using a comparison theorem for principal and non-principal solutions of second-order equations, Behncke [4] proved this stability for $\kappa^2 > c^2 + (\frac{3}{2})^2$ if $\kappa < 0$, and $\kappa > c^2 + \frac{5}{2}$ if $\kappa > 0$. He conjectured that $\kappa^2 > c^2 + \frac{5}{2}$ might be sufficient in the latter case. (Farther-reaching conjectures are to be found in [12, p. 218 seq.])

In the present paper, we study the convergence of the point spectrum of H_a as a tends to 0, for the whole parameter range for which a distinguished realisation of H_0 exists, i.e. for $\kappa^2 - c^2 > 0$. We find a surprising qualitative difference in the limiting behaviour depending on the sign of κ. Indeed, for negative κ, the eigenvalues of H_0 are exactly the limits of eigenvalues of H_a for all values of c. For positive κ, however, there are (finitely or infinitely many) exceptional values $c_0 > c_1 > \cdots$ in $(-\kappa, 0)$; for $c \in (c_m, c_{m-1})$, the eigenvalues of H_0 are still the limits of the eigenvalues of H_a, but with a shift of size m in the eigenvalue numbers. This shift is reflected in the appearance of m additional oscillations of the corresponding eigenfunction of H_a, compared to that of H_0, very close to the origin. It seems a delicate question to decide whether the number of exceptional values c_m is finite or infinite; in any case it grows beyond all bounds with increasing κ.

More precisely, we have the following results.

Theorem 1.1 (Spectral convergence and stability for negative κ). *Let $\kappa < 0$, $c \in (\kappa, 0)$, and let λ_0 [not] be an eigenvalue of the Coulomb–Dirac Hamiltonian*

$$H_0 = -i\sigma_2 \frac{d}{dr} + \sigma_3 + \frac{\kappa}{r}\sigma_1 + \frac{c}{r}.$$

Let $0 < \varepsilon < \operatorname{dist}(\lambda_0, \sigma(H_0)\backslash\{\lambda_0\})/2$. Then for $a < 0$ with sufficiently small $|a|$ the Hamiltonian with anomalous magnetic moment

$$H_a = -i\sigma_2 \frac{d}{dr} + \sigma_3 + \left(\frac{\kappa}{r} + \frac{a}{r^2}\right)\sigma_1 + \frac{c}{r}$$

has exactly one [no] eigenvalue λ_a in $(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$.

Theorem 1.2 (Spectral convergence and stability for positive κ). *Let $\kappa > 0$; then there are at least $[(\kappa \log 4)/\pi - 1]$ values $0 > c_0 > c_1 > \cdots > -\kappa$, which can only accumulate at $-\kappa$, such that the following holds.*

Let $c \in (-\kappa, 0)\backslash\{c_0, c_1, \ldots\}$, and let λ_0 [not] be an eigenvalue of H_0. Let $0 < \varepsilon < \operatorname{dist}(\lambda_0, \sigma(H_0)\backslash\{\lambda_0\})/2$. Then for $a < 0$ with sufficiently small $|a|$, H_a has exactly one [no] eigenvalue λ_a in $(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$.

Here $[x] := \sup\{m \in \mathbb{Z} \mid m \leqslant x\}$ $(x \in \mathbb{R})$ denotes the Gauß bracket.

The proof of these theorems is based on oscillation theory, in particular on an asymptotic study of the behaviour of the Prüfer angle of solutions of the eigenvalue equation for H_a (i.e. the solutions of Eq. (2) below) as a tends to 0. After rescaling $\varrho = r/|a|$, the mass term and spectral parameter are lower-order terms in the limit and can be omitted in order to obtain an overview of solutions in the asymptotic regime near the origin.

The direction field of the resulting simplified Eq. (1) (where $k = |\kappa|$ and $\alpha = -\operatorname{sgn}\kappa$), and hence the qualitative behaviour of its solutions, shows a fundamental difference depending on the sign of α.

For negative κ ($\alpha = 1$), the (ϱ, ϑ) plane is divided into essentially horizontal strips in which the right-hand side of (1) is alternatingly positive and negative (cf. Fig. 1); as a consequence, the distinguished angle ϑ_0 which corresponds to an $L^2(0,\cdot)$ solution of the eigenvalue equation for H_a, cannot change by more than π, and eventually tends towards an asymptotic value $\vartheta_+(c)$ (Proposition 2.3(a)) which turns out to be the limiting angle at 0 of the principal solution of the eigenvalue equation for H_0 as well (Lemma 3.1(b)). On the original r scale, the convergence becomes faster as $a \to 0$.

A stability argument (Lemma 3.2, Proposition 3.3) then shows that for a certain point $R > 0$ the influence of the previously neglected mass and spectral parameter terms can be controlled on $(0, R)$, and that the solution of the full Prüfer equation (2) converges at that point to the Prüfer angle of the principal solution of the equation for $a = 0$.

Theorem 1.1 follows in view of the uniformity of this convergence with respect to the spectral parameter, and the fact that the presence of the anomalous magnetic moment does not significantly affect the behaviour of the solutions at ∞.

A curious phenomenon occurs, however, in the case of positive κ ($\alpha = -1$). For ϱ close to 0 and for large ϱ, one again has ϑ-regions of opposite sign of the right-hand side of (1), and hence of essential confinement of the solutions, and for large ϱ, the distinguished angle ϑ_0 generically tends to the limit $\vartheta_+(c) \bmod \pi$. In contrast to the previous situation, there is now a ϱ-interval $(\varrho_-(c), \varrho_+(c))$ on which the right-hand side of (1) has no zeros and is strictly negative (cf. Fig. 2).

Depending on c, the size of this gap increases, vanishing as $c \to 0$ and becoming infinite as $c \to -\kappa$. Moreover, one can show that the angle ϑ_0 changes by several multiples of π in this interval if $-c$ is large enough (Proposition 2.3(b)), and hence will eventually converge to $\vartheta_+(c) - m\pi$ for some $m \in \mathbb{N}_0$. Thus the corresponding $L^2(0,\cdot)$ solution of the eigenvalue equation for H_a will perform m oscillations which

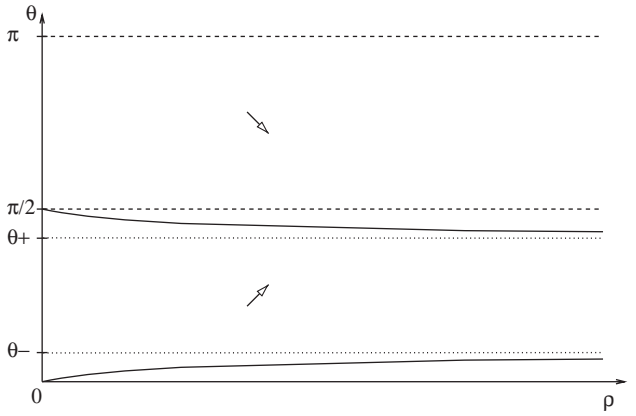

Fig. 1. Zones in the directional field of the simplified equation for $\alpha = 1$. The arrows indicate the sign of the right-hand side of (1), the solid lines represent its zeros.

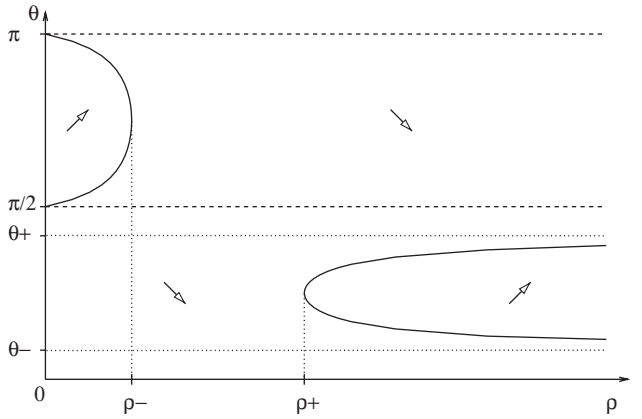

Fig. 2. Zones in the directional field of the simplified equation for $\alpha = -1$. The arrows indicate the sign of the right-hand side of (1), the solid lines represent its zeros.

are absent in the principal solution of the eigenvalue equation for H_0, to which it however converges in phase at the point $R>0$.

Theorem 1.2 then follows by way of the same stability argument as before (Lemma 3.2, Proposition 3.3).

As c crosses the exceptional value, a transition of the asymptotic limit from $\vartheta_+(c) - m\pi$ to $\vartheta_+(c) - (m+1)\pi$ takes place. At $c = c_m$, the distinguished solution ϑ_0 of the simplified equation (1) approaches an unstable limit as $\varrho \to \infty$. The asymptotics of the solutions of the full Prüfer equation (2) appear to be a rather delicate matter in these cases, and the limiting behaviour of H_a with $c = c_m$ remains an interesting open question.

The basic analytical tool of the present paper is the study of the direction field of Prüfer and Riccati type ordinary differential equations near a singularity (for related earlier but simpler results see [7] and the references therein). The underlying comparison techniques are outlined in the appendix.

2. The simplified equation

In this section, we consider the scaled and simplified equation

$$\varrho\vartheta' = c + (k + \alpha/\varrho)\sin 2\vartheta \tag{1}$$

(with $k>0$, $c\in(-k,0)$ and $\alpha\in\{-1,1\}$) which arises from the Prüfer equation (2) equivalent to the eigenvalue equation for H_a by omitting the $O(1)$ ($\varrho\to\infty$) terms after rescaling $r = |a|\varrho$, which eliminates $|a|$.

The asymptotic zeros $\vartheta_\pm(c)$ of the right-hand side of Eq. (1) satisfy

$$0<\vartheta_-(c)<\pi/4<\vartheta_+(c)<\pi/2,$$

$$\sin 2\vartheta_\pm(c) = -c/k, \quad \tan\vartheta_\pm(c) = \frac{k\pm\sqrt{k^2-c^2}}{-c}.$$

Moreover, in case $\alpha=-1$ there are the exceptional points $\varrho_\pm(c)=1/(k\pm c)$, between which the right-hand side of (1) is strictly negative; for later convenience we define $\varrho_+(c)=0$ if $\alpha=1$.

We first show that (1) has a stable and an unstable asymptotic critical point at both singular end-points 0 and ∞ (Lemmas 2.1 and 2.2). The distinguished (unstable) solution at 0, ϑ_0, converges to the stable limit at ∞ for all c if $\alpha=1$; if $\alpha=-1$, one has the convergence with a shift by an integer multiple of π unless c is one of a sequence of exceptional values (Proposition 2.3).

Lemma 2.1 (The existence of a distinguished solution at ∞). *For each $c\in(-k,0)$, (1) has a unique solution $\vartheta_\infty(\cdot,c)$ such that*

$$\lim_{\varrho\to\infty}\ \vartheta_\infty(\varrho,c)=\vartheta_-(c).$$

All other solutions $\vartheta(\cdot,c)$ satisfy either $\vartheta(\varrho,c)=\vartheta_\infty(\varrho,c)+m\pi(\varrho>0)$ for some $m\in\mathbb{Z}$, or else $\lim_{\varrho\to\infty}\vartheta(\varrho,c)=\vartheta_+(c)\bmod\pi$. Furthermore, for each $\varrho>0$, $\vartheta_\infty(\varrho,\cdot)$ is continuous and strictly decreasing.

The *proof* of this lemma, based on an asymptotic study of the direction field of (1), can be found in the appendix. Similarly, one can prove

Lemma 2.2 (The existence of a distinguished solution at 0). *For each $c\in(-k,0)$ there is a unique solution $\vartheta_0(\cdot,c)$ such that*

$$\lim_{\varrho\to0}\ \vartheta_0(\varrho,c)=\begin{cases}\pi & \text{if } \alpha=-1,\\ \pi/2 & \text{if } \alpha=1.\end{cases}$$

All other solutions are either shifts of ϑ_0 by an integer multiple of π, or have

$$\lim_{\varrho\to0}\ \vartheta(\varrho,c)=\begin{cases}\pi/2\bmod\pi & \text{if } \alpha=-1,\\ 0\bmod\pi & \text{if } \alpha=1.\end{cases}$$

For fixed $\hat\varrho>0$, $\vartheta_0(\hat\varrho,\cdot)$ is continuous non-decreasing.

Proposition 2.3.

(a) *If $\alpha=1$, we have $\lim_{\varrho\to\infty}\vartheta_0(\varrho,c)=\vartheta_+(c)$ $(c\in(-k,0))$.*

(b) *If* $\alpha=-1$, *there are at least* $[(k\log 4)/\pi-1]$ *values* $0>c_0>c_1>c_2>\cdots>-k$ (*accumulating at* $-k$ *if infinitely many*) *such that*

$$\lim_{\varrho\to\infty}\ \vartheta_0(\varrho,c)=\vartheta_+(c)-m\pi\quad(c\in\mathscr{C}_m)$$

and $\lim_{\varrho\to\infty}\vartheta_0(\varrho,c_m)=\vartheta_-(c_m)-m\pi$.

Here $\mathscr{C}_m:=(c_m,c_{m-1})$ (*where* $c_{-1}:=0$) *for all* $m\in\mathbb{N}_0$ *for which* c_m *exists*; *if there is a minimal* $c_{m_{\max}}>-k$, *define* $\mathscr{C}_{m_{\max}+1}:=(-k,c_{m_{\max}})$.

Remark. For later convenience, we also define $\mathscr{C}_0:=(-k,0)$ in the case $\alpha=1$.

Proof. (a) The interval $[\pi/4,\pi]$ is stable for (1) by Lemma A.2 (cf. the appendix), so $\vartheta_0(\cdot,c)$ (which by Lemma 2.2 is close to $\pi/2$ for small ϱ) cannot tend to $\vartheta_-(c)$ mod π. The assertion follows by Lemma 2.1.

(b) In the limit $c\to 0$, we have, using $\vartheta'(\varrho)\geqslant(1/\varrho)(c-|k-1/\varrho|)$,

$$\begin{aligned}
&\vartheta_0(\varrho_+(c),c)-\vartheta_0(\varrho_-(c),c)\\
&\geqslant\int_{\varrho_-(c)}^{1/k}\frac{1}{\varrho}\left(c-\frac{1}{\varrho}+k\right)d\varrho+\int_{1/k}^{\varrho_+(c)}\frac{1}{\varrho}\left(c+\frac{1}{\varrho}-k\right)d\varrho\\
&=k-\frac{1}{\varrho_-(c)}-(c+k)\log(k\varrho_-(c))-\frac{1}{\varrho_+(c)}+k+(c-k)\log(k\varrho_+(c))\\
&=(c-k)\log\frac{k}{k+c}-(c+k)\log\frac{k}{k-c}\to 0.
\end{aligned}$$

As a consequence, $\lim_{\varrho\to 0}\vartheta_0(\varrho,c)=\vartheta_+(c)$ for $c<0$ sufficiently close to 0.

On the other hand, noting that $\vartheta'(\varrho)\leqslant(1/\varrho)(c+|k-1/\varrho|)$ and $\vartheta_\infty(\varrho_+(c),c)\in[0,\pi/4]$, we have

$$\begin{aligned}
\vartheta_0(1/k,c)-\vartheta_\infty(1/k,c)&\leqslant\vartheta_0(\varrho_-(c),c)+\int_{\varrho_-(c)}^{1/k}\frac{1}{\varrho}\left(c+\frac{1}{\varrho}-k\right)d\varrho\\
&\quad-\vartheta_\infty(\varrho_+(c),c)+\int_{1/k}^{\varrho_+(c)}\frac{1}{\varrho}\left(c-\frac{1}{\varrho}+k\right)d\varrho\\
&\leqslant\pi-k+\frac{1}{\varrho_-(c)}+(k-c)\log(k\varrho_-(c))+\frac{1}{\varrho_+(c)}-k\\
&\quad+(k+c)\log(k\varrho_+(c))\to\pi-k\log 4\quad(c\to-k).
\end{aligned}$$

The assertion follows, as $\vartheta_0(1/k,\cdot)$ and $\vartheta_\infty(1/k,\cdot)$ are continuous and monotone non-decreasing and decreasing, resp. □

Remark. The first part of the proof of Proposition 2.3(b) yields a quantitative estimate for the first exceptional value c_0. Indeed, using Lemma A.1 one can see that

$\vartheta_0(\varrho_-(c_0), c_0) \geqslant \frac{3\pi}{4}$ and $\vartheta_0(\varrho_+(c_0), c_0) \leqslant \frac{\pi}{4}$, so

$$\frac{\pi}{2} \leqslant (c_0 - k)\log\frac{k + c_0}{k} - (c_0 + k)\log\frac{k - c_0}{k}.$$

Setting $x := -c_0/k \in (0,1)$ and observing that

$$\begin{aligned} x\log\frac{1+x}{1-x} - \log(1-x^2) &= \sum_{j=1}^{\infty} x^{2j}\left(\frac{1}{j} + \frac{1}{j-\frac{1}{2}}\right) \\ &= x^2\left(3 + x^2\sum_{j=0}^{\infty} x^{2j}\left(\frac{1}{j+2} + \frac{1}{j+\frac{3}{2}}\right)\right) \\ &\leqslant x^2\left(3 + \frac{x^2}{1-x^2}\frac{7}{6}\right) = \frac{x^2(18-11x^2)}{6(1-x^2)}, \end{aligned}$$

we find $11x^4 - (18 + 3\pi/k)x^2 + 3\pi/k \leqslant 0$, and thus

$$c_0^2 \geqslant \frac{1}{22}\left(18k^2 + 3\pi k - \sqrt{(18k^2 + 3\pi k)^2 - 132\pi k^3}\right).$$

For $k = 1$, this gives the bound $c_0 \leqslant -0.64157$.

Hence, one has convergence and stability of the eigenvalues by Theorem 1.2 for all $\kappa \in \mathbb{Z}\backslash\{0\}$ at least for nuclear charge number $Z \leqslant 87$.

3. The convergence of the original equation for $a \to 0$, $c \in \mathscr{C}_m$

Throughout this section, we fix $\alpha, \mu \in \{-1, 1\}$ and $k > 0$, and assume that $c \in \mathscr{C}_m$ for some admissible $m \in \mathbb{N}_0$.

Consider the Prüfer equation

$$\Theta' = \frac{c}{r} + \left(\frac{k}{r} + \frac{\alpha|a|}{r^2}\right)\sin 2\Theta + \mu\cos 2\Theta - \lambda \tag{2}$$

and the corresponding equation for $a = 0$,

$$X' = \frac{c}{r} + \frac{k}{r}\sin 2X + \mu\cos 2X - \lambda. \tag{3}$$

We shall study the following distinguished solutions, whose existence and properties can be proved in analogy to Lemma 2.1.

Lemma 3.1.

(a) *There is exactly one solution* Θ_0 *of* (2) *with*

$$\lim_{r\to 0} \Theta_0(r,c,a,\lambda) = \begin{cases} \pi & \text{if } \alpha = -1, \\ \pi/2 & \text{if } \alpha = 1, \end{cases}$$

all other solutions either being shifts of Θ_0 *by an integer multiple of* π, *or having*

$$\lim_{r\to 0} \Theta(r,c,a,\lambda) = \begin{cases} \pi/2 \bmod \pi & \text{if } \alpha = -1, \\ 0 \bmod \pi & \text{if } \alpha = 1. \end{cases}$$

For fixed r, c *and* a, $\Theta_0(r,c,a,\cdot)$ *is continuous decreasing.*

(b) *There is exactly one solution* X_0 *of* (3) *with*

$$\lim_{r\to 0} X_0(r,c,\lambda) = \vartheta_+(c),$$

all other solutions either being shifts of X_0 *by an integer multiple of* π, *or having*

$$\lim_{r\to 0} X(r,c,\lambda) = \vartheta_-(c) \bmod \pi.$$

For fixed r *and* c, $X_0(r,c,\cdot)$ *is continuous decreasing.*

Now we show that the solutions X_0 and Θ_0 become asymptotically close $\bmod \pi$ at some point for small a; this is a consequence of the convergence of the solution ϑ_0 (which is close to Θ_0) of the simplified equation (Proposition 2.3).

Lemma 3.2. *For each* $\varepsilon > 0$ *there are* $r_0(\varepsilon) \in (0,\varepsilon]$ *and* $a_0 > 0$ *such that for all* $\lambda \in [-1,1]$ *and* $-a_0 < a < 0$

$$\begin{aligned} |\Theta_0(r_0(\varepsilon),c,a,\lambda) + m\pi - \vartheta_+(c)| &< \frac{2\varepsilon}{3}, \\ |X_0(r_0(\varepsilon),c,\lambda) - \vartheta_+(c)| &< \frac{\varepsilon}{3}, \end{aligned}$$

and consequently $|\Theta_0(r_0(\varepsilon),c,a,\lambda) + m\pi - X_0(r_0(\varepsilon),c,\lambda)| < \varepsilon$.

Proof. Let $\gamma > 0$ be so small that $[c-\gamma, c+\gamma] \subset \mathscr{C}_m$. Then there is $\delta \in (0,\gamma)$ such that $|\vartheta_+(c \pm \delta) - \vartheta_+(c)| < \varepsilon/3$. By Proposition 2.3 there is $\varrho_0 > 0$ such that $|\vartheta_0(\varrho, c \pm \delta) - \vartheta_+(c \pm \delta) + m\pi| < \varepsilon/3$ $(\varrho \geqslant \varrho_0)$, so the function $r \mapsto \vartheta_0(r/|a|, c)$ (which is a solution of the simplified equation

$$\tilde{\Theta}'(r) = \frac{c}{r} + \left(\frac{k}{r} + \frac{\alpha|a|}{r^2}\right) \sin 2\tilde{\Theta})$$

satisfies $|\vartheta_0(r/|a|, c\pm\delta) - \vartheta_+(c) + m\pi| < 2\varepsilon/3$ $(|a| \leqslant \frac{r}{\varrho_0}, r>0)$. Now let $r_0(\varepsilon) \coloneqq \min\{\delta/2, \varepsilon\}$. Estimating in (3) and (2)

$$|\mu\cos 2X - \lambda|, \quad |\mu\cos 2\Theta - \lambda| \leqslant 2 \leqslant \frac{\delta}{r} \quad (r \leqslant r_0(\varepsilon)),$$

Lemma A.1 yields the bounds

$$\vartheta_0(r/|a|, c-\delta) \leqslant \Theta_0(r, c, a) \leqslant \vartheta_0(r/|a|, c+\delta) \quad (0<r\leqslant r_0(\varepsilon))$$

and

$$\vartheta_+(c-\delta) \leqslant X_0(r, c) \leqslant \vartheta_+(c+\delta) \quad (0<r\leqslant r_0(\varepsilon))$$

and the assertion follows. □

The preceding lemma shows that the solutions converge to each other; however, the point of comparison $r_0(\varepsilon)$ depends on ε and tends to 0 rather rapidly. We now show that the convergence remains stable, and hence also holds at a certain fixed point R.

Proposition 3.3. *There is* $R>0$ *such that* $\lim_{a\to 0} \Theta_0(R, c, a, \lambda) = X_0(R, c, \lambda)$ *uniformly w.r.t.* $\lambda \in [-1, 1]$.

Proof. Consider the Riccati equations for $z(r) \coloneqq \tan X_0(r, c)$ and $y(r, a) \coloneqq \Theta_0(r, c, a)$,

$$rz' = (c - (\lambda+1)r)z^2 + 2kz + c - (\lambda-1)r \tag{4}$$

and

$$ry' = (c - (\lambda+1)r)z^2 + 2(k + \alpha|a|/r)z + c - (\lambda-1)r. \tag{5}$$

Let $y_+(c) \coloneqq \tan\vartheta_+(c) = \frac{k+\sqrt{k^2-c^2}}{-c}$. Choose $0<d<\sqrt{k^2-c^2}/(3|c|)$ and $0<R\leqslant d$ so small that

$$\frac{3}{d}|\,|\lambda+1|(y_+(c)+d)^2 + |\lambda-1|\,|R, 6|\lambda+1|(y_+(c)+d)R < \sqrt{k^2-c^2}$$

for all $\lambda\in[-1, 1]$. For any $\hat{r}\in(0, R)$, set

$$a_1(\hat{r}) \coloneqq \frac{\sqrt{k^2-c^2}}{6(\frac{y_+(c)}{d}+1)}\hat{r}.$$

Now let $\varepsilon>0$, $\varepsilon<R\leqslant d$. By Lemma 3.2, there is $r_0(\varepsilon)<\varepsilon$ and $a_0>0$ such that

$$|z(r_0(\varepsilon)) - y_+(c)| < \varepsilon/2, \quad |y(r_0(\varepsilon), a) - y_+(c)| < \varepsilon/2 \quad (0<|a|<a_0).$$

On $[r_0(\varepsilon), R]$, the interval $[y_+(c)-d, y_+(c)+d]$ is stable for (4) and (5) by Lemma A.2 if $|a|<a_1(r_0(\varepsilon))$, since the right-hand side for $y_+(c)\pm d$ takes the value

$$\begin{aligned}&(c-(\lambda+1)r)(y_+(c)\pm d)^2+2(k+\alpha|a|/r)(y_+(c)\pm d)+c-(\lambda-1)r\\&\quad=cd^2\pm 2(k+y_+(c)c)d+2\frac{\alpha|a|}{r}(y_+(c)\pm d)-(\lambda+1)r(y_+(c)\pm d)^2-(\lambda-1)r\\&\quad\mp d\left[2\sqrt{k^2-c^2}\pm cd\pm 2\frac{\alpha|a|}{r}\left(\frac{y_+(c)}{d}\pm 1\right)\mp((\lambda+1)(y_+(c)\pm d)^2-\lambda-1)\frac{r}{d}\right],\end{aligned}$$

and the factor in square brackets is not less than $\sqrt{k^2-c^2}$.

Hence $|y(r,a)-y_+(c)|, |z(r)-y_+(c)|\leqslant d$ for all $r\in[r_0(\varepsilon), R]$ if $0<|a|<\min\{a_0, a_1(r_0(\varepsilon))\}$.

In the differential equation for the difference $x(r,a) := y(r,a)-z(r)$,

$$rx' = (c-(\lambda+1)r)(y+z)+2k)\,x-\frac{2\alpha|a|}{r}y, \tag{6}$$

the factor of x on the right-hand side can be estimated

$$\begin{aligned}&c(y(r,a)+z(r))+2k-(\lambda+1)r(y+z)\\&\quad\leqslant -2\left(\sqrt{k^2-c^2}+cd\right)+2R|\lambda+1|(y_+(c)+d)\\&\quad\leqslant -\sqrt{k^2-c^2}.\end{aligned}$$

Hence, if a additionally satisfies

$$|a|<\frac{\sqrt{k^2-c^2}\,r_0(\varepsilon)}{2(y_+(c)+d)}\varepsilon,$$

then the interval $[-\varepsilon,\varepsilon]$ is stable for (6) on $[r_0(\varepsilon), R]$ by Lemma A.2, and because of $|x(r_0(\varepsilon),a)|<\varepsilon$ we find $|y(R,a)-z(R)|<\varepsilon$. □

For the proof of the main theorems, we need the following distinguished solution of (3) at infinity, whose existence and properties can be proven along the lines of Lemma 2.1. Let $X_\pm(\lambda)\in[0,\pi]$ such that $\cos 2X_\pm(\lambda)=\mu\lambda$ and $\sin 2X_\pm(\lambda)=\pm\mu\sqrt{1-\lambda^2}$ $(\lambda\in[-1,1])$.

Lemma 3.4. *For $\lambda\in[-1,1]$, there is exactly one solution X_∞ of (3) with*

$$\lim_{r\to\infty} X_\infty(r,c,\lambda)=X_-(\lambda),$$

all other solutions either being shifts of X_0 by an integer multiple of π, or having

$$\lim_{r\to\infty} X(r,c,\lambda) = X_+(\lambda) \bmod \pi.$$

For fixed r and c, $X_\infty(r,c,\cdot)$ is continuous increasing.

Now we are in a position to prove the main results.

Proof of Theorem 1.1. Let $\alpha = 1$, $\mu = -1$, $k = |\kappa| = -\kappa$, and $R>0$ as in Proposition 3.3. It is sufficient to prove the assertion for the auxiliary Hamiltonian

$$\tilde{H}_a = -i\sigma_2 \frac{d}{dr} + \sigma_3 + \left(\frac{\kappa}{r} + \frac{a}{r^2}\chi_{(0,R)}(r)\right)\sigma_1 + \frac{c}{r}$$

instead of H_a, since the eigenvalues of H_a are within $|a|/R$ of those of $\tilde{H}_a$.

Introducing the Prüfer transformation

$$u = |u| \begin{pmatrix} \sin\vartheta \\ -\cos\vartheta \end{pmatrix}$$

in the eigenvalue equation $(\tilde{H}_a - \lambda)\, u = 0$, we find the Prüfer equation for ϑ

$$\vartheta' = -\cos 2\vartheta - \left(\frac{\kappa}{r} + \frac{a}{r^2}\chi_{(0,R)}(r)\right)\sin 2\vartheta + \frac{c}{r} - \lambda,$$

which in view of the above choices for α, μ and k coincides with (2) on $(0, R)$ and with (3) on (R, ∞).

For the Prüfer radius $|u|$ we have

$$(\log|u|)'(r) = -\sin 2\vartheta + \left(\frac{\kappa}{r} + \frac{a}{r^2}\chi_{(0,R)}(r)\right)\cos 2\vartheta.$$

Hence, if $\vartheta = \Theta_0$ on $(0, R)$, where Θ_0 is the distinguished solution from Lemma 3.1(a) (with $\alpha = 1$), we find $(\log|u|)'(r) \sim |a|/r^2$ $(r\to 0)$, and hence

$$\int_0 |u|^2(r)\, dr \sim \text{const} \int_0 e^{-2|a|/r}\, dr < \infty.$$

Thus Θ_0 is the Prüfer angle of an $L_2(0,\cdot)$ solution of the eigenvalue equation for $\tilde{H}_a$.

Similarly, for $a = 0$ we find for a solution u with Prüfer angle $\vartheta = X_0$, where X_0 is the distinguished solution from Lemma 3.1(b),

$$(\log|u|)'(r) \sim \frac{\sqrt{k^2 - c^2}}{r},$$

so $|u|(r) \sim \text{const}\, r^{\sqrt{k^2-c^2}}$ $(r \to 0)$, whereas for all other solutions v

$$(\log|v|)'(r) \sim \frac{-\sqrt{k^2-c^2}}{r}$$

and hence $|v|(r) \sim \text{const}\, r^{-\sqrt{k^2-c^2}}$ $(r \to 0)$. Thus X_0 is the Prüfer angle of the principal solution of the eigenvalue equation for H_0.

Analogously, if (for either $a<0$ or $a=0$) $\vartheta = X_\infty$ on (R, ∞), where X_∞ is the distinguished solution from Lemma 3, we have

$$(\log|u|)'(r) = -\sin 2X_\infty - \frac{k}{r}\cos 2X_\infty \sim -\sqrt{1-\lambda^2} \quad (r \to \infty),$$

so

$$\int^\infty |u|^2(r)\, dr \sim \text{const} \int^\infty e^{-2\sqrt{1-\lambda^2}r}\, dr < \infty.$$

Thus X_∞ is the Prüfer angle of an $L^2(\cdot, \infty)$ solution of the eigenvalue equations for H_0 and $\tilde{H}_a$.

As a consequence, the eigenvalues of $\tilde{H}_a$ are the (isolated) values of λ at which the monotone decreasing continuous function $\Theta_0(R, a, c, \cdot)$ and the monotone increasing continuous function $X_\infty(R, c, \cdot)$ take the same value $\bmod \pi$. Similarly, the eigenvalues of H_0 are the intersection points $\bmod \pi$ of $X_0(R, c, \cdot)$ and $X_\infty(R, c, \cdot)$. Hence the assertion follows in view of the uniform convergence of $\Theta_0(R, a, c, \cdot)$ to $X_0(R, c, \cdot)$ as $a \to 0$ (Proposition 3.3). □

Proof of Theorem 1.2. Let $\alpha = -1$, $\mu = 1$, $k = |\kappa| = \kappa$, and $R>0$ as in Proposition 3.3. As in the preceding proof, it is sufficient to show the assertion for the auxiliary Hamiltonian $\tilde{H}_a$. We now use the Prüfer transformation

$$u = |u| \begin{pmatrix} \cos\vartheta \\ \sin\vartheta \end{pmatrix},$$

which leads to the Prüfer equation

$$\vartheta' = \cos 2\vartheta + \left(\frac{\kappa}{r} + \frac{a}{r^2}\chi_{(0,R)}(r)\right)\sin 2\vartheta + \frac{c}{r} - \lambda,$$

which in view of the above choices for α, μ and k coincides with (2) on $(0, R)$ and with (3) on (R, ∞). By studying the asymptotics of $|u|$ as above, we again find that Θ_0 from Lemma 3.1(a) corresponds to an $L^2(0, \cdot)$ solution of the eigenvalue equation for $\tilde{H}_a$, X_0 from Lemma 3.1(b) corresponds to the principal solution of the eigenvalue equation for H_0, and X_∞ corresponds to an $L^2(\cdot, \infty)$ solution of either eigenvalue equation.

Hence the assertion follows as in the preceding proof. □

Acknowledgments

H.K. wishes to thank E.B. Davies for his hospitality at King's College London during the summer of 2002 when the present work was begun.

Appendix A

In the proofs of this paper we frequently use the following fundamental observations about first-order ordinary differential equations. The first lemma (cf. [6, p. 27]) is sometimes called Čaplygin's inequality, but actually goes back to Peano [6, p. 44].

Lemma A.1. *Let $I\subset\mathbb{R}$ be an interval, $x_0\in I$ and $f_j : I\times\mathbb{R}\to\mathbb{R}$ locally integrable in the first, and locally Lipschitz continuous in the second argument, $j\in\{1,2\}$, with $f_1(x,y)\leqslant f_2(x,y)$ $(x\in I, y\in\mathbb{R})$. Furthermore, let $y_1^0\leqslant y_2^0$, and y_j be the solution of the initial value problem*

$$y'(x)=f_j(x,y),\quad y(x_0)=y_j^0\quad (j\in\{1,2\}).$$

Then $y_1(x)\leqslant y_2(x)$ $(x\in I, x\geqslant x_0)$.

An immediate consequence is the following stability criterion.

Lemma A.2. *Let $I\subset\mathbb{R}$ be an interval, $f : I\times\mathbb{R}\to\mathbb{R}$ locally integrable in the first, and locally Lipschitz continuous in the second argument. The interval $[y_1,y_2]$ is stable for the differential equation*

$$y'(x)=f(x,y) \tag{A.1}$$

on I if $f(x,y_1)>0, f(x,y_2)<0$ $(x\in I)$.

Here an interval J is called *stable* on I for (A.1) if $y(x_0)\in J\Rightarrow y(x)\in J$ $(x\in I, x\geqslant x_0)$ for all $x_0\in I$.

We now use these observations to prove Lemma 2.1.

Proof of Lemma 2.1. (a) Let $c\in(-k,0)$. Define $J_\pm := \{\vartheta\in\mathbb{R}\mid \pm(c+k\sin 2\vartheta)>0\}$, and $j_\pm^{(\varepsilon)} := \{\vartheta\in J_\pm\mid |\vartheta-\vartheta_\pm(c)+j\pi|>\varepsilon (j\in\mathbb{Z})\}$ $(\varepsilon>0)$.

Then for each $\varepsilon>0$ there are $\gamma>0$, $P_0>\varrho_+(c)$ such that for $\varrho\geqslant P_0$

$$\pm(c+(k+\alpha/\varrho)\sin\vartheta)>\gamma\quad (\vartheta\in J_\pm^{(\varepsilon)}).$$

Now consider a solution $\vartheta(\cdot,c)$ of (1). If for all $\varepsilon>0$ there is $P>0$ and $j\in\mathbb{Z}$ such that

$$|\vartheta(\varrho,c)-\varrho_-(c)|\leqslant\varepsilon\quad (\varrho>P),$$

this means that $\lim_{\varrho\to\infty}\vartheta(\varrho,c)=\varrho_-(c)-j\pi$ for some $j\in\mathbb{Z}$.

Otherwise, let ε be already so small that this is not true, and $\gamma, P_0 > 0$ as above. Then there is $\varrho_0 > P_0$ such that $|\vartheta(\varrho_0, c) - \vartheta_-(c) + j\pi| > \varepsilon$ $(j \in \mathbb{Z})$, and hence

$$\vartheta(\varrho_0, c) \in J_+^{(\varepsilon)} \cup J_-^{(\varepsilon)} \cup \bigcup_{j\in\mathbb{Z}} [\vartheta_+(c) - j\pi - \varepsilon, \vartheta_+(c) - j\pi + \varepsilon].$$

In $J_\pm^{(\varepsilon)}$ we have $\pm\vartheta'(\varrho, c) > \gamma/\varrho$, so if $\vartheta(\varrho_0, c) \in J_\pm^{(\varepsilon)}$, then

$$\pm\vartheta(\varrho, c) \geqslant \pm\vartheta(\varrho_0, c) - \gamma \log \varrho/\varrho_0$$

as long as $\vartheta(\varrho, c)$ remains in $J_\pm^{(\varepsilon)}$; consequently there is ϱ_1 and $j \in \mathbb{Z}$ such that $\vartheta(\varrho_1, c) \in [\vartheta_+(c) - j\pi - \varepsilon, \vartheta_+(c) - j\pi + \varepsilon]$.

The latter interval is stable by Lemma A.2. As $\varepsilon > 0$ was arbitrary, it follows that $\lim_{\varrho\to\infty} \vartheta(\varrho, c) = \vartheta_+(c) \bmod \pi$.

(b) Let Γ be an open interval with $\bar{\Gamma} \subset (-k, 0)$, and $\hat{\varrho} > \varrho_+(c)$ $(c \in \Gamma)$. For $\hat{\vartheta} \in \mathbb{R}$ and $c \in \Gamma$, denote by $\vartheta(\varrho, c, \hat{\vartheta})$ the solution of (1) with initial value $\vartheta(\hat{\varrho}, c, \hat{\vartheta}) = \hat{\vartheta}$, and consider the sets

$$S_j := \left\{ (c, \hat{\vartheta}) \in (-k, 0) \times \mathbb{R} \,|\, \lim_{\varrho\to\infty} \vartheta(\varrho, c, \hat{\vartheta}) = \vartheta_+(c) - j\pi \right\},$$

$j \in \mathbb{Z}$. S_j is open. Indeed, let $(c_0, \vartheta_0) \in S_j$, $\delta := (\vartheta_+(c_0 - \pi/4)/2$. Since $\vartheta_+(c)$ depends continuously on c, there is $\varepsilon > 0$ such that

$$[\vartheta_+(c) - \delta, \vartheta_+(c) + \delta] \subset (\pi/4, \pi) \quad (c \in [c_0 - \varepsilon, c_0 + \varepsilon]).$$

Now let $\varrho_0 \geqslant \hat{\varrho}$ be so large that $|\vartheta(\varrho_0, c_0, \vartheta_0) - \vartheta_+(c_0) + j\pi| < \delta/2$. As $\vartheta(\varrho_0, c, \hat{\vartheta})$ depends continuously on $(c, \hat{\vartheta})$, there is positive $\tilde{\varepsilon} < \varepsilon$ with

$$|\vartheta(\varrho_0, c, \hat{\vartheta}) - \vartheta_+(c_0) + j\pi| < \delta \quad (c \in [c_0 - \tilde{\varepsilon}, c_0 + \tilde{\varepsilon}], \hat{\vartheta} \in [\vartheta_0 - \tilde{\varepsilon}, \vartheta_0 + \tilde{\varepsilon}])$$

and therefore $\vartheta(\varrho_0, c, \hat{\vartheta}) + j\pi$ lies in the stable interval $(\pi/4, \pi)$.

By (a) $\lim_{\varrho\to\infty} \vartheta(\varrho, c, \hat{\vartheta}) = \vartheta_+(c) - j\pi$, i.e.

$$(c, \hat{\vartheta}) \in S_j \quad (c \in [c_0 - \tilde{\varepsilon}, c_0 + \tilde{\varepsilon}], \hat{\vartheta} \in [\vartheta_0 - \tilde{\varepsilon}, \vartheta_0 + \tilde{\varepsilon}]).$$

(c) For each $c \in (-k, 0)$, there is exactly one solution $\vartheta_\infty(\cdot, c)$ such that $\lim_{\varrho\to\infty} \vartheta_\infty(\varrho, c) = \vartheta_-(c)$. Indeed, there is at least one, as c is in some suitable set Γ and the corresponding sets

$$\Sigma_j(c) = \{\hat{\vartheta} \in (0, \pi/4) | (c, \hat{\vartheta}) \in S_j\},$$

$j \in \{0, 1\}$, are nonempty by (a) and open by (b).

Assume there are two solutions $\vartheta_1 < \vartheta_2$ with $\lim_{\varrho\to\infty} \vartheta_i(\varrho) = \vartheta_-(c)$, $i \in \{1,2\}$. Then $\varphi := 2(\vartheta_2 - \vartheta_1) > 0$ satisfies

$$\begin{aligned}\varrho\,\varphi'(\varrho) &= 2(k + \alpha/\varrho)(\sin 2\vartheta_2 - \sin 2\vartheta_1)\\ &= 2(k+\alpha/\varrho)\left(\sin 2\vartheta_1 \frac{\cos\varphi - 1}{\varphi} + \cos 2\vartheta_1 \frac{\sin\varphi}{\varphi}\right)\varphi\\ &\sim 2\sqrt{k^2 - c^2}\,\varphi > 0 \quad (\varrho\to\infty),\end{aligned}$$

contradicting $\varphi(\varrho)\to 0$.

(d) Finally, for fixed $\hat\varrho > 0$, $\vartheta_\infty(\hat\varrho, c)$ is strictly monotone decreasing: if $c_1 < c_2$ and $\vartheta_\infty(\hat\varrho, c_1) \leqslant \vartheta_\infty(\hat\varrho, c_2)$, then by Lemma A.1

$$\vartheta_-(c_1) = \lim_{\varrho\to\infty} \vartheta_\infty(\varrho, c_1) \leqslant \lim_{\varrho\to\infty} \vartheta_\infty(\varrho, c_2) = \vartheta_-(c_2),$$

which is not true.

Also, $\vartheta_\infty(\hat\varrho, \cdot)$ is continuous. Indeed, if $c_n \nearrow \hat c$ $(n\to\infty)$, then $\vartheta_\infty(\hat\varrho, c_n) > \vartheta_\infty(\hat\varrho, \hat c)$ because of the monotonicity, so $\lim_{n\to\infty} \vartheta_\infty(\hat\varrho, c_n) \geqslant \vartheta_\infty(\hat\varrho, \hat c)$. However, '$>$' would imply $(\hat c, \lim_{n\to\infty} \vartheta_\infty(\hat\varrho, c_n)) \in S_0$ in contradiction to the facts that S_0 is open and $(c_n, \vartheta_\infty(\hat\varrho, c_n)) \notin S_0$ $(n\in\mathbb{N})$. The right continuity follows in the same way.

References

[1] V. Arnold, H. Kalf, A. Schneider, Separated Dirac operators and asymptotically constant linear systems, Math. Proc. Cambridge Philos. Soc. 121 (1) (1997) 141–146.

[2] H. Behncke, The Dirac equation with an anomalous magnetic moment, Math. Z. 174 (1980) 213–225.

[3] H. Behncke, The Dirac equation with an anomalous magnetic moment II, in: Proceedings of the 7th Conference on Ordinary and Partial Differential Equations, Lecture Notes in Mathematics, Vol. 964, Springer, Berlin, 1982.

[4] H. Behncke, Spectral properties of the Dirac equation with anomalous magnetic moment, J. Math. Phys. 26 (10) (1985) 2556–2559.

[5] F. Gesztesy, B. Simon, B. Thaller, On the self-adjointness of Dirac operators with anomalous magnetic moment, Proc. AMS 94 (1985) 115–118.

[6] Ph. Hartman, Ordinary Differential Equations, Wiley, New York, 1964.

[7] H. Kalf, A limit-point criterion for separated Dirac operators and a little known result on Riccati's equation, Math. Z. 129 (1972) 75–82.

[8] W. Pauli, Relativistic field theories of elementary particles, Rev. Mod. Phys. 13 (1941) 203–232.

[9] W. Pauli, in: K. von Meyenn (Ed.), Wiss. Briefwechsel mit Bohr, Einstein, Heisenberg u.a. Bd.II, 1930–1939, Springer, Berlin, 1985.

[10] W. Pauli, in: K. von Meyenn (Ed.), Wiss. Briefwechsel mit Bohr, Einstein, Heisenberg u.a. Bd.III, 1940–1949, Springer, Berlin, 1993.

[11] M. Reed, B. Simon, Methods of Modern Mathematical Physics I: Functional Analysis, Academic Press, New York, 1980.

[12] B. Thaller, The Dirac Equation, Springer, Berlin, 1992.