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

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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 \( \kappa \), this holds for all Coulomb coupling constants \( c \) for which \( H_0 \) has a distinguished self-adjoint realisation. For positive \( \kappa \), 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.

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 \( (1 + a) \mu_B \) (\( \mu_B = e \hbar / 2mc \), the Bohr magneton) in an electric field \(-\nabla \Phi \) and a magnetic field \( B = \text{curl} A \) by means of the operator

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

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 \( \kappa \in \mathbb{Z} \setminus \{0\} \) is the angular momentum quantum number.

The first mathematical treatment of the operators \( H \) and \( H_a \) is due to Behncke [2, 3, 4]. He showed that \( H_a \) has a unique self-adjoint realisation if

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\( a \neq 0 \) 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] and [11]). 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 \((\frac{Ze^2}{\hbar c})^2 \leq \kappa^2 - \frac{1}{4}\). 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 \( H_0 \) \([2, 3, 4]\).

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) \( c^2 \leq \kappa^2 - \frac{1}{4} \), \( H_a \) converges to \( H_0 \) in the strong resolvent sense as \( a \to 0 \) (\[11\] Thm 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 \( c, \kappa \). 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 \( \kappa^2 > c^2 + \left(\frac{3}{2}\right)^2 \) 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 \( \kappa \). Indeed, for negative \( \kappa \), the eigenvalues of \( H_0 \) are exactly the limits of eigenvalues of \( H_a \) for all values of \( c \). For positive \( \kappa \), however, there are (finitely or infinitely many) exceptional values \( c_0 > c_1 > \ldots \) 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 \( \kappa \).

More precisely, we have the following results.
Theorem 1.1 (Spectral convergence and stability for negative $\kappa$)

Let $\kappa < 0$, $c \in (\kappa, 0)$, and let $\lambda_0$ [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 $0 < \varepsilon < \text{dist}(\lambda_0, \sigma(H_0) \setminus \{\lambda_0\})/2$. 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 $\lambda_a$ in $(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$.

Theorem 1.2 (Spectral convergence and stability for positive $\kappa$)

Let $\kappa > 0$; then there are at least $[(\kappa \log 4)/\pi - 1]$ values $0 > c_0 > c_1 > \ldots > -\kappa$, which can only accumulate at $-\kappa$, such that the following holds.

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

Here $[x] := \sup\{m \in \mathbb{Z} \mid m \leq x\}$ ($x \in \mathbb{R}$) 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 equation (2) below) as $a$ tends to 0. After rescaling $\tau = r/|a|$, 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 equation (1) (where $k = |\kappa|$ and $\alpha = -\text{sgn}(\kappa)$), and hence the qualitative behaviour of its solutions, shows a fundamental difference depending on the sign of $\alpha$.

For negative $\kappa$ ($\alpha = 1$), the $(\varrho, \vartheta)$ 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 $\vartheta_0$ which corresponds to an $L^2(0, \cdot)$ solution of the eigenvalue equation for $H_a$ cannot change by more than $\pi$, and eventually tends towards an asymptotic value $\vartheta_+(c)$ (Prop. 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, Prop. 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 $\infty$. 

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A curious phenomenon occurs, however, in the case of positive $\kappa$ ($\alpha = -1$). For $\varrho$ close to 0 and for large $\varrho$, one again has $\vartheta$-regions of opposite sign of the right-hand side of (1), and hence of essential confinement of the solutions, and for large $\varrho$, the distinguished angle $\vartheta_0$ generically tends to the limit $\vartheta_+ (c) \bmod \pi$. In contrast to the previous situation, there is now a $\varrho$-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 $\vartheta_0$ changes by several multiples of $\pi$ in this interval if $-c$ is large enough (Prop. 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 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, Prop. 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 $\vartheta_0$ 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.
Figure 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.

(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

$$\rho^2 = c + (k + \alpha/\rho) \sin 2\theta$$

(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 $H_\alpha$ by omitting the $O(1)$ ($\rho \to \infty$) terms after rescaling $r = |a|\rho$, which eliminates $|a|$.

The asymptotic zeros $\theta_\pm(c)$ of the right-hand side of equation (1) satisfy

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

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

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

We first show that (1) has a stable and an unstable asymptotic critical point at both singular end-points 0 and $\infty$ (Lemma 2.1, 2.2). The distinguished (unstable) solution at 0, $\theta_0$, converges to the stable limit at $\infty$ for all $c$ if $\alpha = 1$;
if \( \alpha = -1 \), one has the convergence with a shift by an integer multiple of \( \pi \) unless \( c \) is one of a sequence of exceptional values (Prop. 2.3).

**Lemma 2.1 (The existence of a distinguished solution at \( \infty \))**

For each \( c \in (-k, 0) \), \( \vartheta \) has a unique solution \( \vartheta_\infty(\cdot, c) \) such that

\[
\lim_{\vartheta \to \infty} \vartheta_\infty(\vartheta, c) = \vartheta_-(c).
\]

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

The proof of this lemma, based on an asymptotic study of the direction field of \( \vartheta \), 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

\[
\lim_{\vartheta \to 0} \vartheta_0(\vartheta, c) = \begin{cases} 
\pi & \text{if } \alpha = -1, \\
\pi/2 & \text{if } \alpha = 1.
\end{cases}
\]

All other solutions are either shifts of \( \vartheta_0 \) by an integer multiple of \( \pi \), or have

\[
\lim_{\vartheta \to 0} \vartheta(\vartheta, c) = \begin{cases} 
\pi/2 \mod \pi & \text{if } \alpha = -1, \\
0 \mod \pi & \text{if } \alpha = 1.
\end{cases}
\]

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

**Proposition 2.3**

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

b) If \( \alpha = -1 \), there are at least \( \lfloor (k \log 4)/\pi - 1 \rfloor \) values \( 0 > c_0 > c_1 > c_2 > \ldots > -k \) (accumulating at \( -k \) if infinitely many) such that

\[
\lim_{\vartheta \to \infty} \vartheta_0(\vartheta, c_m) = \vartheta_+(c_m) \mod \pi \quad (c \in \mathcal{C}_m),
\]

and \( \lim_{\vartheta \to \infty} \vartheta_0(\vartheta, c_m) = \vartheta_-(c_m) \mod \pi \).

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

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

**Proof.**

a) The interval \( [\pi/4, \pi] \) is stable for \( \vartheta \) by Lemma 4.2 (cf. the Appendix), so \( \vartheta_0(\cdot, c) \) (which by Lemma 2.2 is close to \( \pi/2 \) for small \( \vartheta \)) cannot tend to \( \vartheta_-(c) \mod \pi \). The assertion follows by Lemma 2.1.

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

\[
\vartheta_0(\vartheta_+(c), c) - \vartheta_0(\vartheta_-(c), c) \geq \int_{\vartheta_-(c)}^{\vartheta_+(c)} \left( c - \frac{1}{\vartheta} + k \right) d\vartheta + \int_{\vartheta_-(c)}^{\vartheta_+(c)} \left( c + \frac{1}{\vartheta} - k \right) d\vartheta \\
= k - \frac{1}{\vartheta_-(c)} - (c + k) \log(k \vartheta_-(c)) - \frac{1}{\vartheta_+(c)} + k + (c - k) \log(k \vartheta_+(c)) \\
= (c - k) \log \frac{k}{k - c} - (c + k) \log \frac{k}{k - c} \to 0.
\]
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 \( \vartheta'(\varrho) \leq (1/\varrho)(c+1-|1+1/\varrho|) \) and \( \vartheta_\infty(\vartheta_+(c), c) \in [0, \pi/4] \), we have

\[
\begin{align*}
\vartheta_0(1/k, c) - \vartheta_\infty(1/k, c) &\leq \vartheta_0(\vartheta_-(c), c) + \int_{1/k}^{\vartheta_-} \frac{1}{\varrho} (c + 1/\varrho - k) \, d\varrho \\
&\leq \pi - k + \frac{1}{\vartheta_-(c)} + (k - c) \log(\varrho_-(-c)) + \frac{1}{\vartheta_+(c)} - k + (k + c) \log(\varrho_+(c)) \\
&\to \pi - k \log 4 \quad (c \to -k).
\end{align*}
\]

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 4.1 one can see that \( \vartheta_0(\vartheta_-(c_0), c_0) \geq \pi/2 \) and \( \vartheta_\infty(\vartheta_+(c_0), c_0) \leq \pi/4 \), so

\[
\frac{\pi}{2} \leq (c_0 - k) \log \frac{k + c_0}{k} - (c_0 + k) \log \frac{k - c_0}{k}.
\]

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

\[
\begin{align*}
x \log \frac{1+x}{1-x} - \log(1-x^2) &= \sum_{j=1}^{\infty} x^{2j} \left( \frac{1}{j} + \frac{1}{j+1} \right) \\
&= x^2 \left( 3 + x^2 \sum_{j=0}^{\infty} x^{2j} \left( \frac{1}{j+2} + \frac{1}{j+3} \right) \right) \\
&\leq x^2 \left( 3 + \frac{x^2}{1-x^2} \right) = \frac{x^2(18-11x^2)}{6(1-x^2),}
\end{align*}
\]

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

\[
c_0^2 \geq \frac{1}{22} (16k^2 + 3\pi k - \sqrt{(16k^2 + 3\pi k)^2 - 108\pi^2 k^3}).
\]

For \( k = 1 \), this gives the bound \( c_0 \leq -0.64157 \).

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

3 The convergence of the original equation for \( a \to 0, \ c \in C_m \)

Throughout this section, we fix \( \alpha, \mu \in \{-1, 1\} \) and \( k > 0 \), and assume that \( c \in C_m \) for some admissible \( m \in \mathbb{N}_0 \).
Consider the Prüfer equation

\[ \Theta' = \frac{c}{r} + \left( \frac{k}{r} + \frac{\alpha a}{r^2} \right) \sin 2\Theta + \mu \cos 2\Theta - \lambda \]  \hspace{1cm} (2)

and the corresponding equation for \( a = 0, \)

\[ X' = \frac{c}{r} + \frac{k}{r} \sin 2X + \mu \cos 2X - \lambda. \]  \hspace{1cm} (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 \( \Theta_0 \) 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 \( \Theta_0 \) by an integer multiple of \( \pi, \) or having

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

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 \( \pi, \) or having

\[ \lim_{r \to 0} X(r, c, \lambda) = \vartheta_-(c) \mod \pi. \]

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

Now we show that the solutions \( X_0 \) and \( \Theta_0 \) become asymptotically close \( \mod \pi \) at some point for small \( a; \) this is a consequence of the convergence of the solution \( \vartheta_0 \) (which is close to \( \Theta_0 \)) of the simplified equation (Prop. 2.3).

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

\[ |\Theta_0(r_0(\epsilon), c, a, \lambda) + m\pi - \vartheta_+(c)| < \frac{2\epsilon}{3}, \]

\[ |X_0(r_0(\epsilon), c, \lambda) - \vartheta_+(c)| < \frac{\epsilon}{3}, \]

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

Proof. Let \( \gamma > 0 \) be so small that \( [c - \gamma, c + \gamma] \subset \mathcal{C}_m. \) Then there is \( \delta \in (0, \gamma) \) such that \( |\vartheta_+(c \pm \delta) - \vartheta_+(c)| < \epsilon/3. \) By Proposition 2.3 there is \( \vartheta_0 > 0 \) such that
Proposition 3.3 There is a fixed point \( r \) of the point of comparison. The preceding lemma shows that the solutions converge to each other; however, and the assertion follows. □

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

satisfies \( |\Theta_0(r/|a|, c - \theta) - \Theta_0(r/|a|, c + \theta) + m\pi| < 2\varepsilon/3 \) \((|a| \leq \varepsilon/9, r > 0)\). Now let \( r_0(\varepsilon) := \min\{\delta/2, \varepsilon\} \). Estimating in \( [3], [2] \)

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

Lemma 4.1 yields the bounds

\[ \Theta_0(r/|a|, c - \delta) \leq \Theta_0(r, c, \lambda) \leq \Theta_0(r/|a|, c + \delta) \quad (0 < r \leq r_0(\varepsilon)) \]

and

\[ \theta_+ (c - \delta) \leq \theta_+ (c + \delta) \quad (0 < r \leq r_0(\varepsilon)) \]

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 \( \varepsilon \) 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 \( z(r) := \tan X_0(r, c) \) and \( y(r, a) := \Theta_0(r, c, a) \),

\[ r z' = (c - (\lambda + 1)r)z^2 + 2kz + c - (\lambda - 1)r \quad (4) \]

and

\[ r y' = (c - (\lambda + 1)r)z^2 + 2(k + \alpha|a|/r)z + c - (\lambda - 1)r \quad (5) \]

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

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

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

\[ a_1(\tilde{r}) := \frac{\sqrt{k^2 - c^2}}{6(\frac{y_+(c)}{d} + 1)} \tilde{r}. \]

Now let \( \varepsilon > 0, \varepsilon < R \leq d \). 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 4.2 if \(|a| < a_1(r_0(\varepsilon))\), since the right-hand side for \(y_+(c) \pm d\) takes the value

\[(c - (\lambda + 1)r)(y_+(c) \pm d)^2 + 2(k + |a|/r)(y_+(c) \pm d) + c - (\lambda - 1)r\]

\[= cd^2 + 2(k + y_+(c)cd + 2\frac{|a|}{r}(y_+(c) \pm d) - (\lambda + 1)r(y_+(c) \pm d)^2 - (\lambda - 1)r\]

\[\mp d\left[2\sqrt{k^2 - c^2} \pm cd \pm 2\frac{|a|}{r}(\frac{y_+(c)}{d} \pm 1) \mp ((\lambda + 1)(y_+(c) \pm d)^2 - \lambda - 1)^2\right],\]

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

Hence \(|y(r, a) - y_+(c)|, |z(r) - y_+(c)| \leq d\) 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 \(x(r, a) := y(r, a) - z(r)\),

\[r x' = (c - (\lambda + 1)r)(y + z) + 2k) x - \frac{2|a|}{r} y,\]

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

\[c(y(r, a) + z(r)) + 2k - (\lambda + 1)r(y + z)\]

\[\leq -2(\sqrt{k^2 - c^2} + cd) + 2R|\lambda + 1|(y_+(c) + d)\]

\[\leq -\sqrt{k^2 - c^2}.\]

Hence, if \(a\) additionally satisfies

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

then the interval \([-\varepsilon, \varepsilon]\) is stable for (4) on \([r_0(\varepsilon), R]\) by Lemma 4.2, and because of \(|x(r_0(\varepsilon), \cdot)| < \varepsilon\) we find \(|y(R, a) - z(R)| < \varepsilon\). \(\Box\)

For the proof of the main theorems, we need the following distinguished solution of (5) 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 \(\sin 2X_\pm(\lambda) = \pm \mu \sqrt{1 - X^2} \lambda \in [-1, 1]\).

**Lemma 3.4** For \(\lambda \in [-1, 1]\), there is exactly one solution \(X_\infty\) of (5) 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 \(\pi\), or having

\[\lim_{r \to \infty} X(r, c, \lambda) = X_+(\lambda) \mod \pi.\]

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

$$u = |u| \left(\begin{array}{c} \sin \vartheta \\ -\cos \vartheta \end{array}\right)$$

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

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

which in view of the above choices for $\alpha, \mu$ and $k$ coincides with (2) on $(0, R)$ and with (3) on $(R, \infty)$.

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 $\Theta_0$ 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

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

Thus $\Theta_0$ is the Prüfer angle of an $L_2(0, \cdot)$ solution of the eigenvalue equation for $H_a$.

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),

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

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

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

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 $(R, \infty)$, where $X_{\infty}$ is the distinguished solution from Lemma 3.1 we have

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

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

Thus \( X_{\infty} \) 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 \( \lambda \) 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 mod \( \pi \). Hence the assertion follows in view of the uniform convergence of \( \Theta_0(R, a, c, \cdot) \) to \( X_0(R, c, \cdot) \) as \( a \to 0 \) (Prop. 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 \( \alpha, \mu \) and \( k \) coincides with \[2\] on \((0, R)\) and with \[4\] on \((R, \infty)\). By studying the asymptotics of \(|u|\) as above, we again find that \( \Theta_0 \) 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 \( X_\infty \) corresponds to an \( L^2(\cdot, \infty) \) solution of either eigenvalue equation.

Hence the assertion follows as in the preceding proof. \( \square \)

### 4 Appendix

In the proofs of this paper we frequently use the following fundamental observations about first-order ordinary differential equations. The first lemma (cf. \[9\] p. 27) is sometimes called Čaplygin’s inequality, but actually goes back to Peano (\[10\] p. 44).

**Lemma 4.1** 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 \( f_1(x, y) \leq f_2(x, y) \) \((x \in I, y \in \mathbb{R})\). Furthermore, let \( y_1^0 \leq y_2^0 \), and \( y_j \) be the solution of the initial value problem

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

Then \( y_1(x) \leq y_2(x) \) \((x \in I, x \geq x_0)\).

An immediate consequence is the following stability criterion.
Lemma 4.2 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

$$y'(x) = f(x, y)$$

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 (7) if $y(x_0) \in J \Rightarrow y(x) \in J$ ($x \in I, x \geq x_0$) 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 $J_+: = \{ \vartheta \in \mathbb{R} \mid \pm(c + k \sin \vartheta) > 0 \}$, and $J_+: = \{ \vartheta \in J_+ \mid |\vartheta - \vartheta_j + j\pi| > \varepsilon (j \in \mathbb{Z}) \}$ ($\varepsilon > 0$).

Then for each $\varepsilon > 0$ there are $\gamma > 0$, $P_0 > \vartheta_+(c)$ such that for $\vartheta \geq P_0$

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

Now consider a solution $\vartheta(\cdot, c)$ of (11). If for all $\varepsilon > 0$ there is $P > 0$ and $j \in \mathbb{Z}$ such that

$$|\vartheta(q, c) - q_-(c)| \leq \varepsilon \quad (q > P),$$

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

Otherwise, let $\varepsilon$ be already so small that this is not true, and $\gamma, P_0 > 0$ as above. Then there is $q_0 > P_0$ such that $|\vartheta(q_0, c) - \vartheta_j(c) + j\pi| > \varepsilon (j \in \mathbb{Z})$, and hence

$$\vartheta(q_0, c) \in J_+^{(c)} \cup J_-^{(c)} \cup \bigcup_{j \in \mathbb{Z}} [\vartheta_j(c) - j\pi - \varepsilon, \vartheta_j(c) + j\pi + \varepsilon] .$$

In $J_+^{(c)}$ we have $\vartheta'(q, c) > \gamma/\vartheta$, so if $\vartheta(q_0, c) \in J_+^{(c)}$, then

$$\vartheta(q, c) \geq \vartheta(q_0, c) - \gamma \log q/q_0$$

as long as $\vartheta(q, c)$ remains in $J_+^{(c)}$; consequently there is $q_1$ and $j \in \mathbb{Z}$ such that

$$\vartheta(q_1, c) \in [\vartheta_j(c) - j\pi - \varepsilon, \vartheta_j(c) - j\pi + \varepsilon] .$$

The latter interval is stable by Lemma 4.2. As $\varepsilon > 0$ was arbitrary, it follows that $\lim_{q \to \infty} \vartheta(q, c) = \vartheta_+(c)$ mod $\pi$.

b) Let $\Gamma$ be an open interval with $\Gamma \subset (-k, 0)$, and $\hat{c} > \vartheta_+(c)$ ($c \in \Gamma$). For

$$\hat{c} \in \mathbb{R} \text{ and } c \in \Gamma,$$

denote by $\vartheta(\vartheta, c, \hat{c})$ the solution of (11) with initial value $\vartheta(\hat{c}, c, \hat{c}) = \hat{c}$, and consider the sets

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

$j \in \mathbb{Z}, S_j$ 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

$$[\vartheta_+(c) - \delta, \vartheta_+(c) + \delta] \subset (\pi/4, \pi)$$

$(c \in [c_0 - \varepsilon, c_0 + \varepsilon])$. 

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

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

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

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

\[
(c, \hat{\varrho}) \in S_j \quad (c \in [c_0 - \tilde{\varepsilon}, c_0 + \tilde{\varepsilon}], \hat{\varrho} \in [\varrho_0 - \tilde{\varepsilon}, \varrho_0 + \tilde{\varepsilon}]).
\]

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

\[
\Sigma_j(c) = \{ \hat{\varrho} \in (0, \pi / 4) \mid (c, \hat{\varrho}) \in S_j \},
\]

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

Assume there are two solutions \( \vartheta_1 < \vartheta_2 \) with \( \lim_{\varepsilon \to \infty} \vartheta_i(\varrho) = \vartheta_-(c) \), \( i \in \{1, 2\} \).

Then \( \varphi := 2(\vartheta_2 - \vartheta_1) > 0 \) satisfies

\[
\varrho \varphi'(\varrho) = 2(k + \alpha / \varrho)(\sin 2\varrho_2 - \sin 2\varrho_1)
\]

\[
= 2(k + \alpha / \varrho)(\sin 2\varrho_1 \cos \varphi_{\infty} - \cos 2\varrho_1 \sin \varphi_{\infty}) \varphi
\]

\[
\sim 2\sqrt{\varrho_2 - \varrho_1^2} \varphi > 0 \quad (\varrho \to \infty),
\]

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 \( \vartheta_\infty(\hat{\varrho}, c_1) \leq \vartheta_\infty(\hat{\varrho}, c_2) \), then by Lemma 4.1

\[
\vartheta_-(c_1) = \lim_{\varepsilon \to \infty} \vartheta_\infty(\varrho, c_1) \leq \lim_{\varepsilon \to \infty} \vartheta_\infty(\varrho, c_2) = \vartheta_-(c_2),
\]

which is not true.

Also, \( \vartheta_\infty(\hat{\varrho}, \cdot) \) is continuous. Indeed, if \( c_n \not\to \hat{\varrho} \) \( (n \to \infty) \), then \( \vartheta_\infty(\hat{\varrho}, c_n) > \vartheta_\infty(\hat{\varrho}, \hat{\varrho}) \) because of the monotonicity, so \( \lim_{n \to \infty} \vartheta_\infty(\hat{\varrho}, c_n) \geq \vartheta_\infty(\hat{\varrho}, \hat{\varrho}) \). However, \( '>' \) would imply \( (\hat{\varrho}, \lim_{n \to \infty} \vartheta_\infty(\hat{\varrho}, c_n)) \notin S_0 \) 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.

\[\Box\]

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