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

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Abstract

By use of asymptotic integration and Prüfer angles, we show that the point spectrum of the Coulomb-Dirac operator H_0 is the limit of the point spectrum of the Dirac operator with anomalous magnetic moment H_a as $a \to 0$. For negative angular momentum quantum number κ, this holds for all coupling constants c for which H_0 has self-adjoint realisation. For positive κ, there is a region near the origin where the eigenfunctions of H_a experience oscillations.

Introduction

By separation of variables in spherical coordinates, the Dirac operator with a Coulomb potential

$$H_0 = -i\vec{\alpha}\cdot\nabla + \beta m - \frac{Ze}{|x|}, \text{ taking } \hbar = c = 1 \qquad (1)$$

with $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β symmetric 4×4 matrices satisfying the anticommutation relations

$$\begin{aligned} \alpha_i\alpha_j + \alpha_j\alpha_i &= 2\delta_{ij} I \;\; \forall\, i,j = 1,2,3 \\ \alpha_i\beta + \beta\alpha_i &= 0 \\ \alpha^2 = \beta^2 &= I, \end{aligned}$$

is unitarily equivalent to a direct sum of one-dimensional Dirac operators on the half line

$$H_0 = -i\sigma_2\frac{d}{dr} + m\sigma_3 + \frac{\kappa}{r}\sigma_1 - \frac{Ze}{r} \quad r \in (0,\infty) \qquad (2)$$

defined on $L^2(0,\infty)^2$ with domain $D = C_0^\infty(0,\infty)^2$. The σ_i are the Pauli matrices and $\kappa \in \mathbb{Z}\setminus 0$ is the angular momentum quantum number. Z is the atomic number.
Pauli suggested a modification of (1) to include the anomalous magnetic moment term and equation (2) with this term becomes

$$H_a = -i\sigma_2\frac{d}{dr} + m\sigma_3 + (\frac{\kappa}{r} + \frac{a}{r^2})\sigma_1 + \frac{c}{r} \quad r \in (0,\infty) \qquad (3)$$

defined on $L^2(0,\infty)^2$ with $c = -Ze$. The mathematical investigation of (3) was initiated by Behncke [1], [2] and [3]. He has shown that H_a is essentially self-adjoint for a very large class of potentials including the Coulomb potential. This is in marked contrast to the case of H_0 [5] which is essentially self-adjoint on its minimal domain if and only if $c^2 < \kappa^2 - \frac{1}{4}$. $C_0^\infty(0,\infty)^2$ is a common core for both H_0 and H_a at least for $c^2 < \kappa^2 - \frac{1}{4}$ and hence $H_a \overset{srs}{\to} H_0$ as $a \to 0$, meaning the spectrum cannot expand suddenly in the limit though it can contract. The essential spectrum $\sigma_{ess}(H_a)$ of H_a is similar that of H_0 and is $(-\infty,-m] \cup [m,\infty)$. H_0 is known to have infinitely many eigenvalues in the spectral gap $[-m,m]$, which accumulate at right end point m. One would therefore expect that the eigenvalues of H_a will be perturbations of those of H_0 such that each eigenvalue of H_0 will be the limit of exactly one eigenvalue branch of H_a as $a \to 0$. This expectation is partly influenced by the strong resolvent convergence of H_a to H_0. Behncke [3] by decoupling equation (3) has shown stability of the point spectra at least for $\kappa \geq 3$. Kalf and Schmidt [4] extended Behncke's results to hold for all κ by using asymptotic analysis of Pruefer and Riccati equations equivalent to the eigenvalue equation of H_a. In our study we use the asymptotic integration in conjunction with the Pruefer angle to obtain similar results as those of Kalf and Schmidt.

Asymptotic Integration

Our starting point is the eigenvalue equation $(H_a - \lambda)y = 0$. Written explicitly one obtains

$$y' = Ay \quad A = \begin{pmatrix} -(\frac{a}{x^2} + \frac{\kappa}{x}) & -\frac{c}{x} + m + \lambda \\ \frac{c}{x} + m - \lambda & \frac{a}{x^2} + \frac{\kappa}{x} \end{pmatrix} \qquad (4)$$

The equivalent Pruefer differential equations are

$$\begin{aligned} \theta'(x) &= \frac{c}{x} - \lambda + (\frac{a}{x^2} + \frac{\kappa}{x})\sin 2\theta + m\cos 2\theta \\ (\ln\rho)' &= m\sin 2\theta - (\frac{a}{x^2} + \frac{\kappa}{x})\cos 2\theta \end{aligned}$$

Using asymptotic integration, we study the behaviour of eigenfunctions near the end points 0 and ∞. Clearly, the eigenvalue equation is singular at these points. For spectral convergence and stability, we need the eigenfunctions to be square integrable. Stability here implies that for $\epsilon > 0$ and for some $\lambda_a \in (\lambda_0 - \epsilon, \lambda_0 + \epsilon)$, the λ_a-eigenfunction $y(\lambda, x)$ are ϵ-approximate to those of H_0. If one can show that for sufficiently small a, the equivalent Pruefer angles corresponding to the L^2 solutions of H_a converge to those of H_0, then we are done. To perform asymptotic integration, we need distinct eigenvalues and the corresponding eigenvectors.

Behaviour near infinity

Here m and λ terms are dominant and the eigenvalues are given as

$$\mu_a \approx \pm(m_+m_-)^{\frac{1}{2}}\left(1 + \frac{c\lambda}{m_+m_-x} + \frac{\kappa^2 - c^2}{2m_+m_-x^2} + o(x^{-3})\right) \qquad (5)$$

The corresponding eigenvectors are

$$\begin{pmatrix} 1 \\ b_+ \end{pmatrix} \text{ and } \begin{pmatrix} b_- \\ 1 \end{pmatrix} \text{ for } \mu_a \gtrless 0,$$

respectively with $b_\pm \approx \pm(m_\pm)^{-1}\left\{(m_+m_-)^{\frac{1}{2}} + \frac{c\lambda}{x(m_+m_-)^{\frac{1}{2}}} + \frac{\kappa}{x} \pm (\frac{m_\mp}{m_\pm})^{\frac{1}{2}}\frac{c}{x} + o(x^{-2})\right\}$ The diagonalising matrix T is formed by these vectors as its columns and the transformation $y = Tz$ yields $z' = (\Lambda - T^{-1}T')z$, with $\Lambda = \text{diag}(\mu, -\mu)$. The correction terms can be easily obtained. Further diagonalisation can be carried out, however in our case the first one is sufficient. The eigenfunctions thus have the form $y(\lambda, x) \approx (\vec{b} + r(x))x^{\pm\frac{m\lambda}{m_+m_-}}e^{\pm(m_+m_-)^{\frac{1}{2}}x}$ with $r(x) \approx o(x^{-2})$. The L^2-angle is thus given by $\tan\theta_a \approx b_-^{-1} = -\left(\frac{m_-}{m_+}\right)^{\frac{1}{2}} + \frac{a_1}{x} + \frac{a_2}{x^2} + \frac{a}{m_+x^2}$ where $a_1 = \frac{m}{m_+^{\frac{3}{2}}m_-^{\frac{1}{2}}}\left(\frac{\kappa z}{1+z} - c\right)$ and $\frac{\lambda^2}{m^2} = (1+z)^{-1}$ with $z = \frac{c^2}{(n' + (\kappa^2 - c^2)^{\frac{1}{2}})^2}$, and $a_2 = \left(\frac{m_-}{m_+}\right)^{\frac{1}{2}}\frac{(\kappa^2 - c^2)}{2m_+m_-} + \frac{c^2\lambda}{(m_+m_-)^{\frac{3}{2}}} + \frac{c\kappa}{m_+m_-}$. For $a = 0$, this L^2-angle has the same value as that of H_0. This means that $\theta_a \to \theta_0$ as $a \to 0$, giving exact convergence for all κ.

Behaviour near zero.

Here we introduce a new variable $t = x^{-1}$, giving a new system

$$y' = Ay, \quad A = \begin{pmatrix} a + \frac{\kappa}{t} & \frac{c}{t} - t^{-2}(m + \lambda) \\ -\frac{c}{t} - t^{-2}(m - \lambda) & -(a + \frac{\kappa}{t}) \end{pmatrix} \qquad (6)$$

Here m and λ terms are small and can be neglected. Thus the eigenvalues are $\mu_a \approx \pm\frac{1}{t}[(at + \kappa)^2 - c^2]^{\frac{1}{2}}$ and the corresponding eigenvectors are

$$\begin{pmatrix} 1 \\ b \end{pmatrix} \text{ and } \begin{pmatrix} b \\ 1 \end{pmatrix} \text{ for } \mu_a \gtrless 0,$$

respectively with $b = -\frac{(\mu_a + a + \frac{\kappa}{t})}{\frac{c}{t}}$. The above diagonalisation procedure can be done again and the eigenfunctions thus takes the form $y(\lambda, x) \approx (\vec{b} + r(x))e^{\int_a^t \mu_a ds}$.
The corresponding L^2-angle is given by

$$\tan\theta_a \approx \frac{[(at + \kappa)^2 - c^2]^{\frac{1}{2}} + at + \kappa}{-c}. \qquad (7)$$

Here we distinguish between two cases: $\kappa < 0$ and $\kappa > 0$.

Case $\kappa < 0, \;\; a < 0$

Close to the origin, the term $at + \kappa$ is dominant. By assumption, $|\kappa| > |c|$ and hence $b \to 0$. This means that $\tan\theta_a \to 0$ as $x \to 0$ and thus $\theta_a \to n\pi, \;\; n = 0, 1, 2, \ldots$. If $a \to 0$, we have $\tan\theta_a \to \frac{(\kappa^2 - c^2)^{\frac{1}{2}} + \kappa}{-c}$ which is equal to the case for H_0. This is in line with the results obtained by Kalf and Schmidt and we have the following stability result.

Proposition 1 *For any $\epsilon > 0$ and λ_0 there exists $a_0 < 0$ and $R(\epsilon)$ so that any normalized $\lambda(a)-$ eigenfunction u of H_a with $\lambda(a) - \lambda_0 \leq \epsilon$ satisfies $||y|| \leq \epsilon$ uniformly in $[\lambda_0 - \epsilon, \lambda_0 + \epsilon]$ and $a_0 < a < 0$*

Case $\kappa > 0, \;\; a < 0$

Here we have three regions to consider. The region where κ is dominant, the region where a term is dominant and the the region where the a term is approximately equal to κ. In the latter case, μ_a changes sign and the eigenfunctions experiences oscillations. This transition takes place in the interval $\frac{\kappa + |c|}{-a} < t < \frac{\kappa - |c|}{-a}$. Thus there are values of c where μ_a is imaginary. Except for these values of c, the eigenfunctions are stable since in the region $\frac{\kappa + |c|}{-a} < t < \frac{\kappa - |c|}{-a}$, the functions are approximately constant. In the region where κ is dominant, $\frac{a}{x^2}$ is integrable and we have a regular perturbation. Near the origin, where the a term is dominant, we can apply asymptotic integration to obtain the behaviour of the eigenfunctions.

Conclusion

In quantum mechanics, the eigenvalues correspond to the energy levels. The eigenfunctions are the states of the system at any time t. Stability therefore of the eigenvalues implies one has a bound on the energy levels and hence also a bound on the states. Our method, asymptotic integration, can be used in obtaining better estimates of the energy levels and thus can provide Physicists with an easier way of obtaining bound states.

References

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