Universität Osnabrück

Doctoral Thesis

Relativistic Energy Correction Of The Hydrogen Atom With An Anomalous Magnetic Moment

By

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Dissertation

zur Erlangung des Grades Doktors der Naturwissenschaften

-Dr. rer. nat.-

des Fachbereichs Mathematik

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July 2015

"A mathematical theory is not to be considered complete until you have made it so clear that you can explain it to the first man whom you meet on the street."

David Hilbert, 1862-1943.

Abstract

The electron is known to possess an anomalous magnetic moment, which interacts with the gradient of the electric field. This makes it necessary to compute its effects on the energy spectrum. Even though the Coulomb Dirac equation can be solved in closed form [12, 16, 47], this is no longer possible when the anomalous magnetic moment is included. In fact the interaction due to this term is so strong that it changes the domain of the Hamiltonian. From a differential equation point of view, the anomalous magnetic moment term is strongly singular near the origin. As usual, one has to resort to perturbation theory. This, however, only makes sense if the eigenvalues are stable. To prove stability is therefore a challenge one has to face before actually computing the energy shifts. The first stability results in this line were shown by Behncke [3] for angular momenta $\kappa \geq 3$, because the eigenfunctions of the unperturbed Hamiltonian decay fast enough near the origin. He achieved this by decoupling the system and then using the techniques available for second order differential equations. Later, Kalf and Schmidt [37] extended Behncke's results basing their analysis on the Prüfer angle technique and a comparison result for first order differential equations. The Prüfer angle method is particularly useful because it shows a better stability and because it obeys a first order differential equation. Nonetheless, Kalf and Schmidt had to exclude some coupling constants for $\kappa > 0$. This I believe is an artefact of their method. In this study, I make increasing use of asymptotic integration, a method which is rather well adapted to perturbation theory and is known to give stability results to any level of accuracy. Together with the Prüfer angle technique, this lead to a more general stability result and even allows for an energy shifts estimate.

Hamiltonians traditionally treated in physics to describe the spin-orbit effect are not self adjoint i.e. they are not proper observables in quantum mechanics. Nonetheless, naive perturbation theory gives correct results regarding the spectrum. To solve this mystery, one has to study the nonrelativistic limit of the Dirac operator. In the second part of this study, I have not only given the higher order correction to the Dirac operator but also shown the effects of the spin-orbit term.

Acknowledgements

I wish to express sincere gratitude to my supervisor, Prof. H. Behncke, for his vision and direction, his valuable comments and constructive criticism to the work and also for always being there for consultation.

Am equally grateful to the Kenyan Govt/DAAD-Germany for financing this research and to Osnabrück university for hosting me during this study. To all the staff members of the department of Mathematics, Osnabrück University, I say thank you for your hospitality.

I am also grateful to Maseno University, Kenya and the entire staff members of the school of Mathematics for the role they have played in shaping my academic life. Special thanks goes to Dr. Nyamwala Fredrick for his constant encouragement and support.

I remain emotionally indebted to my family especially my wife Lilian, son Brandly and daughter Dahlia as well as my friends for their emotional comfort and words of encouragement.

Am very grateful to any other person not mentioned here and might have contributed to the successful completion of this research.

Finally, I give thanks to the Almighty God for His gift of life and boundless love.

Contents

To my wife Lilian Jebitok, son Brandly David, daughter Dahlia Rose, late father Henry Ambogo and late mum Dorine Auma

Chapter 1

INTRODUCTION

In order to explain the spectra of atoms in magnetic fields, Uhlenbeck and Goudsmit [49] postulated that an electron has an intrinsic angular momentum $\mathbf{S}$, called spin $\frac{\hbar}{2}$ and a magnetic dipole moment $\frac{e\hbar}{2mc}$, the Bohr magneton. The spin and the magnetic moment were later found to be a consequence of the relativistic invariance of the Dirac equation [21]. This equation has unified the theories of quantum mechanics and special relativity since it is Lorentz invariant [47].

The Dirac theory predicts a gyromagnetic factor of $g = 2$ for the electron spin, which agrees well with measurements though with small deviations because the Dirac theory neglects the coupling of the electron due to radiation fields. Consequently, it led to small deviations in the experimental values which gave $g = 2.00232$ [39]. This difference was later discovered by Kusch et.al [39] in 1947 to be due to the electron's anomalous magnetic moment. These deviations , if included in the Dirac equation, are known to remove degeneracy in its energy levels ([47], Chapter 7).

Since then, an electron has been known to posses an anomalous magnetic moment which interacts with the gradient of the electric potential. For spherically symmetric potentials, the anomalous magnetic moment term is known to induce very strong repulsive force at extremely small distances. This has profound effects on the spectrum as well as the domain of the underlying operator. In fact, near the origin, the anomalous magnetic moment term is so singular that the regular perturbation methods of Kato and Rellich [38] cannot be applied. For the Coulomb problem, it leads to an irregular singularity of r^{-2}. Thus, one has to resort to other perturbation theories in order to analyse its effects.

The anomalous magnetic moment potential generally has the form $V_a = -\mu_a V_e'$,

see ([47], equation 5.46) where $\mu_a = 0.00058$ is the anomalous magnetic moment for an electron. This term μ_a will henceforth be denoted by a and the anomalous magnetic moment potential by aV_a. If $a = 0$, then one has the Coulomb-Dirac problem, the solutions of which are known and a formula for its eigenvalues exists [12, 16]. The eigenfunctions in this case are products of $r^{\gamma}e^{-\beta r}$ and confluent hypergeometric functions which degenerate to polynomials. The case when the anomalous magnetic moment term aV_a' is included does not allow closed form solutions and even the eigenvalues are hard to compute by analytical means.

The mathematical investigation of the Dirac operator with anomalous magnetic moment, here denoted by H_a, was initiated by Behncke [1, 2]. He showed that this operator is essentially self-adjoint for a very large class of potentials including the Coulomb potential $V_e(r) = \frac{c}{r}, \quad c = -Ze^2, \ r = |\mathbf{x}|$, by decoupling the eigenvalue equation for H_a and using the already developed self-adjoint techniques for second order differential equations. This is in marked contrast to the case when the anomalous magnetic moment term is absent i.e. $a = 0$, where it is well known that, the Coulomb-Dirac operator H_0, is essentially self-adjoint on its minimal domain $C_0^{\infty}(\mathbb{R}^3_+)^4$ if and only if $c^2 \leq \kappa^2 - \frac{1}{4}$ [47, 54]. Gesztesy, Simon and Thaller [28] later confirmed Behncke's results using operator theoretic methods.

The essential spectrum of H_a is given by $(-\infty, -m] \cup [m, \infty)$ which is similar to that of the unperturbed operator H_0 [2]. H_0 is known to have infinitely many eigenvalues in the spectral gap $(-m, m)$, which at most accumulate at the end points $\pm m$ depending on the sign of the perturbing potential $V_e(r)$. 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, at least for $c^2 \leq \kappa^2 - \frac{1}{4}$, which means the spectrum cannot suddenly expand in the limit though it could contract, see ([41], Theorem VIII. 24(a), 25(a)), ([38], Chapter VIII, cor.1.6).

Any valid perturbation theory should not induce large changes in the eigenvalues. Stability of these eigenvalues, which in this study are the eigenvalues of H_0 is therefore very crucial if one has to employ perturbation theory in the study of the perturbed operator H_a.

The first stability results in this direction were obtained by Behncke [3] where he proved stability for at least angular momenta $\kappa \geq 3$. He showed also that for $\kappa \geq 3$ the corrections to the eigenvalues are linear in a. He achieved this by

decoupling the Dirac equation to second order and applying the already developed tools for second order differential equations. Later, Kalf and Schmidt [37], using the Prüfer transformation techniques and a comparison result for first order differential equations, extended Behncke's results for almost all κ, though, they had to exempt some exceptional values for $\kappa > 0$, which I believe is due to their technique. Both results in [3] and [37] did not give precise estimates on the energy shifts of the electron and did not even settle the stability problem for all κ.

The aim of this study is to extend the stability results in [3, 37] using the method of asymptotic integration, in conjunction with the Prüfer angle techniques. This stability problem forms the bulk of this study.

Asymptotic integration is well adapted to perturbation theory and is also known to give stability results to any level of accuracy. Thus, making increasing use of this method, together with the Prüfer angle techniques, I have extended the stability results in [3, 37] for all κ. A general stability result has also been obtained for a larger class of interactions. As a consequence, I have obtained estimates on the eigenvalue shifts for the hydogen-like atoms.

The strategy to achieve this is to decompose the interval $(0, \infty)$ by making a cut off at a fixed point $x = R > 0$ to give intervals $(0, R]$ and $[R, \infty)$. This consequently leads to the decomposition of the operator H_a as direct sum of operators $H_{a-} \oplus H_{a+}$, where $H_{a-} = H_a|_{L^2((0,R])^2}$ and $H_{a+} = H_a|_{L^2([R,\infty))^2}$, with the domain restricted by the boundary conditions at R. Asymptotic integration is then applied to each of these intervals. Details on the decomposition method and asymptotic integration theory as applied in spectral theory can be found in [6–8, 10, 23] and references there in.

In addition, I have also obtained further relativistic corrections to the Dirac operator. In the nonrelativistic limit, this operator reproduces the Pauli-Schrödinger operator to first order. The resultant expansion can then be used to compute further relativistic corrections to the eigenvalues of the Dirac operator.

I hope that my attempt on this problem has yielded better estimates for the energy shifts and have also settled the stability problem so that physicists can be able to calculate the energy levels of various atoms with high precision.

This thesis is ordered as follows: Chapter 1 gives the basic background on our study. Chapter 2 and chapter 3 deals with stability problem while in chapter 4, we give further relativistic approximation to the Dirac operator.

1.1 The Dirac Equation

It is well known that the Dirac equation that is mostly treated in the quantum mechanics books is just the minimal coupling equation, which treats the electromagnetic field as a classical field. A more general covariant equation which models quantum electrodynamics effects and is linear in the external field is given in [1] in the standard physicists notation as

$$\begin{aligned}[\gamma^\mu p_\mu - m_0 - \Sigma_{n=0}^{\infty} e_n \Box^n \gamma^\mu A_\mu + \\ \frac{i}{4}\Sigma_{n=0}^{\infty} f_n \Box^n (\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu)(\partial_\nu A_\mu - \partial_\mu A_\nu)\Big]\psi = 0\end{aligned} \tag{1.1}$$

Of these we only consider the lowest order correction, because higher order terms are better treated in quantum electrodynamics. The anomalous electrical moment will not be considered in this study since it is parity violating. The equation above is more general than we need in this study but for completeness purposes its inclusion is necessary. The higher order terms $e_1, e_2, \ldots, f_1, f_2, \ldots$ in (1.1) give rise to contributions, which are of the same size as other field theoretic corrections and will be neglected. Written out more fully with $e_1 = e_2 = f_1 = f_2 \ldots = 0$ and $e_0 = e,\ f_0 = f$ equation (1.1) for static electromagnetic fields becomes

$$\begin{aligned}i\partial_t\psi = \big\{\Sigma_{k=1}^{3}\gamma^0\gamma^k(-i\partial_k - eA^k) + eA^0 + m_0\gamma^0 + \\ if\Sigma_{k,l=1,k\neq l}^{3}\gamma^0\gamma^k\gamma^l\partial_l A^k - \gamma^k\partial_k A^0\big\}\,\psi\end{aligned} \tag{1.2}$$

Here $\partial_k = \frac{\partial}{\partial x_k}, k = 1, 2, 3$, the γ^j are the well known Dirac gamma matrices and A is the magnetic vector potential. For more details on these gamma matrices we refer to the book of Bethe and Jackiw [13]. The Dirac equation, in the form we will use, is derived in the sections that will follow but is essentially of the form (1.2).

1.1.1 Derivation of the Dirac Equation

The general interpretation of non-relativity quantum mechanics is made possible by the wave equation being of the form

$$(H - E)\psi = 0$$

i.e. being linear in $E = \frac{\partial}{\partial t}$, so that the wave function at any time determines the wave function at any later time. The wave equation of the relativity quantum mechanics must also be linear in E if a general interpretation is to be possible. Such a wave equation had been obtained by Klein and Gordon separately, however, their equation did not satisfy the requirement for a quantum evolution equation that time and space must be treated on the same footing and that the wave equation must be invariant under a Lorentz transformation.
To overcome these difficulties, Dirac [21] derived the famous Dirac equation by linearization using the relativistic relation

$$E^2 = c^2p^2 + m^2c^4. \tag{1.3}$$

Here, E is the energy, $m-$ mass of the electron, $\mathbf{p}-$ momentum and c, henceforth assumed to be unity is the velocity of light. Consequently, this led to the famous Dirac equation

$$E = \alpha \cdot \mathbf{p} + \beta m \tag{1.4}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and $\alpha_4 = \beta$ are Hermitian 4×4 matrices satisfying the commutation relations

$$\alpha_j\alpha_k + \alpha_k\alpha_j = 2\delta_{jk}I_4, \quad j,k = 1,2,3,4 \tag{1.5}$$

and

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \quad \forall\, j = 1,2,3,.$$

σ_j are the standard 2×2 Pauli matrices. I_2 denotes the 2×2 unit matrix which will be identified with the unit operator on $\mathcal{H}$, the configuration space. Equation (1.4) can be transformed to quantum mechanics by taking $E = i\frac{\partial}{\partial t}$ and $\mathbf{p} = -i\nabla$ leading to [47]

$$i\frac{\partial}{\partial t}\Psi(t,x) = (-i\alpha \cdot \nabla + \beta m)\Psi(t,x) = H_{00}\Psi(t,x). \tag{1.6}$$

Here, H_{00} is the free Dirac Hamiltonian defined by the matrix-valued differential expression

$$H_{00} = -i\alpha \cdot \nabla + \beta m = \begin{pmatrix} mI_2 & -i\sigma \cdot \nabla \\ -i\sigma \cdot \nabla & -mI_2 \end{pmatrix} \tag{1.7}$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ and H_{00} acts on a four-component wave function $\Psi(t,x) \in \mathbb{C}^4$. Equation (1.6) describes the relativistic motion of a free electron and H_{00}

gives the total energy of the quantum system.
The commutation relations in (1.5) implies

$$H_{00}^2 = (-\Delta + m^2)I_4.$$

For a detailed account on the Dirac equation and its derivation, we refer to [12, 13, 21, 40]

From the mathematical formulation of quantum mechanics, any quantum system is described on a Hilbert space $\mathcal{H}$. In that case any measurable quantity (observable) like energy, momentum e.t.c. is identified (described) by a self-adjoint operator on that Hilbert space and the normalized vectors in this configuration space describe the state of the system at any time t. Thus, only self-adjoint operators are physically important in the quantum mechanics realm.
One must therefore always check the self-adjointness property of any operator describing a quantum system. This is not always easy because of the domain issues and most researchers resort to checking instead the essential self-adjointness of the operator which essentially guarantees existence of a unique self-adjoint extension. A suitable state space for the Dirac equation must consists of vector-valued functions with four components, in order to match the dimension of the Dirac matrices. If one assumes that each of the four components is a square integrable (in the sense of Lebesgue) function of position $\mathbf{x}$, then we obtain the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)^4$. Its elements Ψ are called 4-spinors. The choice of such a function space is warranted by the particular representation of the Heisenberg commutation relations and the algebraic structure of this operator. $\mathbb{R}^3$ here is the coordinate space. Note that the most important operator for the quantum system (1.4) is H_{00}, the energy operator, because H_{00} is the infinitesimal generator of time translation [38, 47]. Written out explicitly, the Hilbert space $\mathcal{H}$ is given by

$$\mathcal{H} = L^2(\mathbb{R}^3)^4 = \left\{ \Psi | \Psi(\mathbf{x}) = \begin{pmatrix} \Psi_1(\mathbf{x}) \\ \Psi_2(\mathbf{x}) \\ \Psi_3(\mathbf{x}) \\ \Psi_4(\mathbf{x}) \end{pmatrix} : \mathbb{R}^3 \to \mathbb{C}^4, \int_{\mathbb{R}3} |\Psi_i(\mathbf{x})|^2 d^3x < \infty \right\} \tag{1.8}$$

with scalar product

$$\langle \Psi, \Phi \rangle = \int_{\mathbb{R}^3} \sum_{i=1}^{4} \overline{\Psi_i(\mathbf{x})} \Phi_i(\mathbf{x}) d^3x, \quad \Psi,\ \Phi \in L^2(\mathbb{R}^3)^4 \tag{1.9}$$

The bar denotes complex conjugation.
The quantity $|\Psi(t,x)|^2$ is interpreted as the probability density of the particle at the time t. Therefore, the wave function $\Psi(t,x)$ must be normalized according to

$$\int_{\mathbb{R}^3} |\Psi(t,\mathbf{x})|^2 d^3x = 1, \quad t \in \mathbb{R}. \tag{1.10}$$

The free Dirac operator H_{00} is therefore defined on this Hilbert space on a suitable domain $\mathcal{D}(H_{00})$.
The following theorem characterizes the free Dirac operator H_{00}.

Theorem 1.1. *The free Dirac operator H_{00} is essentially self-adjoint on the dense domain $C_0^\infty(\mathbb{R}^3_+)^4$ $\left(\mathbb{R}^3_+ = \mathbb{R}^3 \setminus \{0\}\right)$ and self-adjoint on the first Sobolev space $D(H_{00}) = H^1(\mathbb{R}^3)^4$ (the space for first order differential equations). Its spectrum is purely absolutely continuous and given by $\sigma(H_{00}) = (-\infty, -m] \cup [m, \infty)$.*

Proof. See ([47], Theorem 1.1) for the proof. □

1.1.2 Dirac Equation in External Fields

In reality, electrons do not move freely. They interact with external forces. These forces are called the electromagnetic fields. Let $\mathbf{A}$, V_e denote magnetic vector and electrostatic potentials respectively. The electric field $\mathbf{E}$ is then given by

$$\mathbf{E} = -\nabla V_e - \frac{\partial \mathbf{A}}{\partial t} \tag{1.11}$$

Taking $\mathbf{p} \to \mathbf{p} - e\mathbf{A}$, and $E \to E - V_e$ in equation (1.6) we obtain

$$i\frac{\partial \Psi}{\partial t} = \left(\alpha \cdot (\mathbf{p} - e\mathbf{A}) + \beta m + V_e\right) \Psi = H_0 \Psi \tag{1.12}$$

with e, as the electron charge. Equation (1.12) is the Dirac equation in an external electromagnetic field. Here, V_e may be taken as the Coulomb potential or any other suitable potential.

1.1.2.1 Separated Dirac Equation

The bulk of this thesis is devoted to spherically symmetric potentials $V(r)$, of which only the radial part of the operator will be useful. A potential is said to be spherically symmetric if it is invariant under rotations.
For these potentials, the Dirac Hamiltonian commutes with the angular momentum $\mathbf{J}$ and the spin-orbit operator $\sigma \cdot \mathbf{L}$.
The total angular momentum $\mathbf{J}$ is defined by $\mathbf{J} = \mathbf{L} + \mathbf{S}$ where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital angular momentum and $\mathbf{S}$ is the spin angular momentum matrix defined as $\mathbf{S} = \frac{1}{2}\begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$. $\mathbf{J}$ commutes with the Dirac Hamiltonian H_0 provided the potentials are real-valued. One may, therefore, classify the eigenstates of H_0 according to the eigenvalues of $\mathbf{J}^2$ and J_z, the $z-$component of $\mathbf{J}$. These eigenstates are called spherical spinors in the Clifford algebra terms. It is known that these spherical spinors are also eigenfunctions of $\sigma \cdot \mathbf{L}$, the spin-orbit operator and therefore, also of the operator $K = -1 - \sigma \cdot \mathbf{L}$. The operator K has eigenvalues $\kappa = \pm 1, \pm 2, \ldots$, which actually characterizes the radial Dirac Hamiltonian. These values of κ can be summarized in terms of the eigenvalues of $\mathbf{J}^2$ as

$$\kappa = \pm(j + \frac{1}{2}) = \begin{cases} -(l+1), \text{ for } j = l + \frac{1}{2} \\ \quad l, \text{ for } j = l - \frac{1}{2} \end{cases}, \qquad l = 0, 1, 2, \ldots$$

The underlying Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)^4$ and the Hamiltonian can be decomposed, see ([47], pp. 126-130). The Hilbert space $\mathcal{H}$ is thus decomposed into its radial and angular parts, i.e. $\mathcal{H} = L^2(\mathbb{R}^3)^4 \cong L^2((0,\infty), dr) \otimes L^2(S^2)^4$, where S^2 is a unit sphere. Each Hilbert space $L^2(S^2)^4$ is the orthogonal direct sum of two dimensional Hilbert spaces $\mathfrak{h}_{m_i,\kappa_j}$, which are spanned by the simultaneous eigenfunctions $\Phi^{\pm}_{m_j,\kappa_j}$ of $\mathbf{J}^2$, $\mathbf{J}_z$ and $\mathbf{K}$, see ([47], equation 4.119).
Each partial wave subspace $L^2(\mathbb{R}_+, dr) \otimes \mathfrak{h}_{m_i,\kappa_j}$ is isomorphic to $L^2(\mathbb{R}_+, dr)^2$ if we choose the basis $\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\}$ in $\mathfrak{h}_{m_i,\kappa_j}$. Thus, the Dirac operator of interest has the following representation

Theorem 1.2. *[47] The Dirac operator with the potential*

$$V(x) = \phi_{sc}(r)\beta + \phi_{el}(r)I_4 + i\beta\alpha \cdot e_r\phi_{am}(r)$$

leaves the partial wave subspaces $C_0^\infty(\mathbb{R}_+) \otimes \mathfrak{h}_{m_i,\kappa_j}$ invariant. With respect to the basis $\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\}$, the action of the Dirac operator on each subspace can be

represented by the operator

$$h_{m_j,\kappa_j} = \begin{pmatrix} m + \phi_{sc}(r) + \phi_{el}(r) & -\frac{d}{dr} + \frac{\kappa_j}{r} + \phi_{am}(r) \\ \frac{d}{dr} + \frac{\kappa_j}{r} + \phi_{am}(r) & -m - \phi_{sc}(r) + \phi_{el}(r) \end{pmatrix} \tag{1.13}$$

which is well defined on $C_0^\infty(0,\infty)^2 \subset L^2((0,\infty), dr)^2$.

Proof. For the proof see ([47], Theorem 4.14.) □

The Dirac operator H on $C_0^\infty(\mathbb{R}^3)^4$ is unitarily equivalent to the direct sum of the partial wave Dirac operators h_{m_j,κ_j}, see ([47], equation 4.130). It is known that H is essentially self adjoint if and only if each of the operators h_{m_j,κ_j} is essentially self adjoint. For more details, we refer to [32, 47, 51].

In order to apply the representation (1.13) to our problem, it suffices to analyse only one of the operators h_{m_j,κ_j}. In the sequel we will denote h_{m_j,κ_j} by H_a and refer to it as the radial Dirac operator with the anomalous magnetic moment. The explicit form of H_a for the Coulomb potential will be given later.

The general solutions of the radial Dirac equation for a state with energy λ and angular momentum quantum number (κ, m), where m is the quantum number for the z-component of $\mathbf{J}$, take the form

$$\Psi_{\kappa,m}(r) = \frac{1}{r} \begin{pmatrix} f(r) Y_{\kappa,m}(\theta,\vartheta) \\ ig(r) Y_{-\kappa,m}(\theta,\vartheta) \end{pmatrix} \tag{1.14}$$

where r is the radial variable and f, g are the two-component Dirac radial functions. They are usually referred to as the large and the small components respectively. $Y_{\kappa,m}(\theta,\vartheta)$ are the spherical harmonics. They are defined with the help of the associated Legendre polynomials P_κ^m, see([47], pp.126).

The radial eigenfunctions and their associated eigenvalues ,λ, can be determined analytically for a Coulomb potential. In most cases, however, the eigenvalue problem must be solved numerically.

Putting $\mathbf{A} = 0$ and $e\phi = V(r) = \frac{c}{r}$ where $c = -Z\alpha < 0$ in equation (1.12), we obtain the the Coulomb-Dirac operator. Here $V(r)$, $r = |\mathbf{x}|$ is the Coulomb potential, Z is the atomic number and α, the fine structure constant $\alpha \approx \frac{1}{137}$.

1.1.2.2 Coulomb-Dirac Equation

An electron in the field of a point nucleus is described by the Coulomb potential $V_e(|\mathbf{x}|) = -\frac{Z\alpha}{|\mathbf{x}|} = \frac{c}{r}$. The subscript e refers just to the electric potential. The notation will become useful later when we will study the general Dirac type operators. The Dirac-Coulomb Hamiltonian takes the form

$$H_0(\kappa) = H_{00} + V_e(r) \tag{1.15}$$

with H_{00} representing the radial free Dirac operator and $V_e(r) = \frac{c}{r}$ with $c < 0$.
It is well known [1, 47] that the Dirac operator with Coulomb potential, $H_0(\kappa)$ is unitarily equivalent to a direct sum of one-dimensional Dirac operators on the half-line,

$$H_0(\kappa) = \begin{pmatrix} m + \frac{c}{r} & -\frac{d}{dr} + \frac{\kappa}{r} \\ \frac{d}{dr} + \frac{\kappa}{r} & -m + \frac{c}{r} \end{pmatrix} \tag{1.16}$$

For simplicity, we shall write H_0 instead of $H_0(\kappa)$ provided confusion does not arise. Each H_0 operates on $L^2((0,\infty))^2$ with the minimal domain $\mathcal{D}(H_0) = C_0^\infty((0,\infty))^2$, $\kappa \in \mathbb{Z} \setminus \{0\}$ denotes the angular momentum quantum number.
H_0 is essentially self-adjoint (see [47, 54]) on its minimal domain $\mathcal{D}$ if and only if $c^2 \leq \kappa^2 - \frac{1}{4}$. If $c^2 > \kappa^2 - \frac{1}{4}$, then the essential self-adjointness breaks down. This corresponds to the atomic number $Z = 118$. Fortunately, this problem arises only for point-like nuclei which do not occur in reality. However, for large c it is still possible to define physically meaningful self adjoint extensions for $|c| < \kappa$ [37, 54]. The closure of H_0 is self-adjoint on $H^1((0,\infty))^2$, the natural domain for first order differential operators.
For the theory of self-adjoint extension of this operator H_0, an excellent review is given by the works of Schmincke [46] and Wuest [55]. This can easily be studied also by the method of deficiency indices originally introduced by Von Neumann and described in details in [42, 53]. The case of strong fields i.e. when $c > 1$, has been studied by Case [17] and by Burnap and et. al [16] and it will not be tackled in this thesis.
The explicit solutions of the Coulomb-Dirac eigenvalue equation $H_0\psi = \lambda\psi$, exist

and are of the form

$$\begin{aligned} f(r) &= (1+\varepsilon)^{\frac{1}{2}} e^{-\frac{\rho}{2}} \rho^{\mu} \left[F(\mu-\varepsilon\delta, 1+2\mu, \rho) + \right. \\ &\quad \left. \frac{\varepsilon\delta-\mu}{\kappa-\delta} F(\mu-\varepsilon\delta+1, 1+2\mu, \rho)\right] \\ g(r) &= (1-\varepsilon)^{\frac{1}{2}} e^{-\frac{\rho}{2}} \rho^{\mu} \left[-F(\mu-\varepsilon\delta, 1+2\mu, \rho) + \right. \\ &\quad \left. \frac{\varepsilon\delta-\mu}{\kappa-\delta} F(\mu-\varepsilon\delta+1, 1+2\mu, \rho)\right] \end{aligned} \tag{1.17}$$

where

$$\varepsilon = \frac{\lambda}{m},\ \rho = 2(1-\varepsilon^2)^{\frac{1}{2}} r,\quad \delta = \frac{-c}{(1-\varepsilon^2)^{\frac{1}{2}}} \text{ and } \mu = (\kappa^2 - c^2)^{\frac{1}{2}}$$

$F(a; b, \rho) = 1 + \frac{a}{b}\rho + \frac{a(a+1)}{2!b(b+1)}\rho^2 + \cdots$ is the confluent hypergeometric function. Important about this is that the terms in square brackets represent a finitely terminating power series. It is this fact which is usually employed to determine the eigenvalues. These are given by the formula

$$\lambda = m\left(1 + \frac{c^2}{(n'+\mu)^2}\right)^{-\frac{1}{2}} \tag{1.18}$$

here n' is the index where the series terminate. We refer to [12] for more details on these solutions .

The following theorem characterizes H_0 and is sufficient for many applications of physical interest including the Coulomb potential. It is based on the Kato-Rellich theorem [38] which gives a condition on the potential $V_e(|\mathbf{x}|),\ |\mathbf{x}| = r$ that guarantee essential self-adjointness.

Theorem 1.3. *[47] Let V be a multiplication operator with a Hermitian 4×4 matrix such that each component V_{ij} is a function satisfying the estimate*

$$|V_{ij}(x)| \leq a\frac{c}{2|x|} + b,\quad \textit{all } x \in \mathbb{R}^3 \setminus \{0\},\ i,j = 1,\ldots,4 \tag{1.19}$$

for some constants $b > 0$ and $a < 1$. Then the operator $H_0 = H_{00} + V$, where H_{00} is the free Dirac operator , is essentially self-adjoint on $C_0^{\infty}(\mathbb{R}^3 \setminus \{0\})^4$ and self-adjoint on $D(H_{00}) = H^1(\mathbb{R}^3)^4$.

Proof. For the proof, see ([47], Theorem 4.2) □

Remark 1.4. Self adjointness of the above operator is preserved under relatively bounded perturbation with a bound less than 1.

If each element of the potential matrix V above is an infinitely differentiable function i.e. $V_{ij} \in C^\infty(\mathbb{R}^3)$, then $H_0 = H_{00} + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)^4$. This follows from the fact that H_0 is an elliptic differential operator of first order [47]. This means that the essential self adjointness of Dirac operators on $C_0^\infty(\mathbb{R}^3)$ does not depend on the growth of V at ∞ but rather on the local singularity near 0. This is not true for Schrödinger operators, the nonrelativistic counterpart of Dirac operators, because a force field which increases too fast as $|x| \to \infty$ can accelerate a particle so much that it escapes to infinity in a finite time. This in turn would require a boundary condition at infinity. This cannot happen to Dirac operators since the relativistic bound on the velocity prevents such an escape to infinity.

The spectrum of the Dirac operator H_0 is the set of allowed energies which is a subset of real numbers. In most cases of physical importance, the spectrum consists of a continuous part and a set of eigenvalues of H_0. Usually the eigenvalues are associated to the bound states and the absolutely continuous spectrum is associated to the scattering states. An isolated point of the spectrum is always an eigenvalue of the Dirac operator H_0.

In perturbation theory, one usually considers the essential spectrum since it is known to be stable under relatively compact potentials. For relatively bounded perturbations, isolated eigenvalues will be shifted and there is the well known Kato-Rellich perturbation theory to compute the shifts. For singular perturbations, an eigenvalue may be absorbed by the continuum. For singular perturbation, the concept of stability describes the reasonable behaviour of eigenvalues under perturbation. Thus, stability of these eigenvalues remain a critical issue.

In the sequel, I am mainly interested in the radial Dirac operator. Therefore, by Dirac operator I mean the radial Dirac operator unless otherwise stated.

Whenever the potential vanishes at infinity, the essential spectrum of the Dirac operator H_0 is the set $(-\infty, -m] \cup [m, \infty)$. This is also similar to the essential spectrum of the free Dirac operator H_{00}.

All the eigenvalues of H_0 lie in the gap $(-m, m)$. Estimates on the number of eigenvalues in this gap have already been obtained by Birman [14]. Hinton and Shaw [35] have shown that for the case of Coulomb potentials, there are infinitely many eigenvalues that accumulate at the right end point m (or $-m$ for repulsive Coulomb potentials). For the Coulomb potential or more general reasonably smooth potentials, one even knows that the continuous spectrum is even absolutely continuous with multiplicity 1.

It should be stressed that the spectral properties of Dirac operators depend very much on the matrix structure of the potentials.
If one takes into account the anomalous magnetic moment of the electron, the situation changes completely. We will see later that the solutions in this case do not admit a power series expansion like (1.17) and an expression of the bound state energies (1.18) has not been found.

1.1.2.3 Dirac equation with anomalous magnetic moment

The most general Dirac equation with anomalous magnetic moment is given by (1.2). For spherically symmetric potentials, in particular, the Coulomb potential we have, for a one-dimensional Dirac Hamiltonian,

$$H_a(\kappa) = \begin{pmatrix} V_e + m & -D + \frac{\kappa}{r} + aV_e' \\ D + \frac{\kappa}{r} + aV_e' & V_e - m \end{pmatrix} \text{ on } L^2((0,\infty))^2 \tag{1.20}$$

with $D = \frac{d}{dr}$, V_e the electric potential and $aV_e' =$ the anomalous magnetic moment potential. Using the Coulomb potential defined above, the anomalous magnetic potential is given by $aV_e' = \frac{a}{r^2}$ and a measures the size of the anomalous magnetic moment. Clearly, the Coulomb problem with the anomalous magnetic moment potential introduces an essential singularity of $\frac{a}{r^2}$ near 0.
The bulk of chapter 2 is therefore devoted to the matrix operator

$$H_a(\kappa) = H_a = \begin{pmatrix} \frac{c}{r} + m & -D + \frac{\kappa}{r} + \frac{a}{r^2} \\ D + \frac{\kappa}{r} + \frac{a}{r^2} & \frac{c}{r} - m \end{pmatrix} \tag{1.21}$$

with the domain $\mathcal{D} = C_0^\infty(\mathbb{R}_+)^2$, where $C_0^\infty(\mathbb{R}_+)$ denotes the infinitely differentiable functions with compact support in $\mathbb{R}_+$. Note that equation (1.21) has the form given in (1.13).
If $a \neq 0$, $\mathcal{D}$ is a common core of H_a and H_0 for all $c^2 \leq \kappa^2 - \frac{1}{4}$ and H_a is therefore essentially self adjoint on this domain, see [1, 27, 37, 47]. This is due to the fact that the anomalous magnetic moment term acts on the gradient of the electric field in a repulsive manner causing the wave function to vanish to infinite order near the origin.
Mathematically, this term represents a singular perturbation. Thus, the regular perturbation theory breaks down because once this most singular term is switched on, it changes the domain of the underlying operator. In that case, computations

of the eigenvalues and eigenfunctions perturbatively is bound to fail, at least for angular momentum $\kappa \leq 3$, see [3].

The Coulomb potential $\frac{c}{r}$ only introduces a regular singularity so that the eigenfunctions of H_0 allow a type of power series representation as already seen in (1.17). On the other hand, the anomalous magnetic moment term introduces an essential singularity near 0 causing the eigenfunctions to behave like $\exp(-ax^{-1})$ near 0, thus prohibiting a power series representation.

The essential spectrum $\sigma_{ess}(H_a)$ of H_a coincide with that of the limiting operator H_0 for a wide range of potentials including the Coulomb potential [2], and for mildly regular potentials, it is even absolutely continuous with multiplicity 1. There are infinitely many eigenvalues that accumulate at most at the right end point m [8]. The closure of H_a which is self adjoint will be denoted again by H_a. Both H_a and H_0 are assumed to be limit point at 0 and at ∞ . More information on the limit point cases can be found in [1, 54].

The strong singularity caused by the anomalous magnetic moment term near the origin and its minute size, raises the question of stability of the point spectrum of the unperturbed operator H_0 if one has to employ perturbation theory. Perturbation here, will only make sense if the eigenvalues are stable. Stability in this case, only applies to isolated eigenvalues of H_0 if one considers the anomalous magnetic moment term as a perturbation to H_0. This is only possible if H_0 is self adjoint. Chapters 2 and 3 are devoted to this problem. As a result, some general spectral results are also obtained.

1.1.3 Stability of Eigenvalues

The book of Kato [38] gives several stability criterion results among them the stability of eigenvalues of a self adjoint operator.

The following Kato-Rellich theorem, concerning the stability of self-adjointness or essential self-adjointness plays an important role.

Recall that a linear operator B in $\mathcal{H}$ is said to be relatively bounded with respect to A or $A-$bounded, if $D(A) \subseteq D(B)$ and there exists non-negative numbers a, b such that

$$||Bu|| \leq a||Au|| + b||u||, \text{ for all } u \in D(A). \tag{1.22}$$

The infimum of the constants a satisfying (1.22) for some $b \geq 0$ is called the $A-$bound of B. If B is $A-$bounded, satisfies (1.22) and is closable, then $\bar{B}$ is

$\bar{A}-$bounded and

$$||\bar{B}u|| \leq a||\bar{A}u|| + b||u||, \text{ for all } u \in D(\bar{A}).$$

If the relative bound is zero, we say that B is infinitesimally small compared to A.

Theorem 1.5. *(Kato-Rellich theorem) Suppose A is self-adjoint, B is symmetric, and B is A-bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A. Further, if A is bounded below by M, then $A+B$ is bounded below by $M - \max\{\frac{b}{1-a}, a|M| + b\}$ where a and b are as in (1.22).*

Proof. For the proof see ([42], Theorem X.12) □

From theorem 1.5, one even has $def(A + B) = def(A)$.
A similar result can also be formulated for operators with eigenvalues in a gap, for instance the Dirac operators.
In case of the spectrum, one has the following criteria for the spectral convergence.

Theorem 1.6. *Let T and T_n $(n \in \mathbb{N})$ be self-adjoint, and assume that $D(T) = D(T_n)$. Assume furthermore, that there are null-sequences (a_n) and (b_n) from $\mathbb{R}$ for which*

$$||(T - T_n)f|| \leq a_n||f|| + b_n||Tf|| \ \ \forall\ f \in D(T).$$

Then $\sigma(T) = \lim_{n\to\infty} \sigma(T_n)$ and $\sigma_{ess}(T) = \lim_{n\to\infty} \sigma_{ess}(T_n)$

Proof. The proof can be found in ([53], Theorem 9.5) □

Theorem (1.5) only applies to cases where the perturbing operator is small compared to the unperturbed operator. This is not the case with our operator H_a since the perturbing term $\frac{a}{r^2}$ is very large near the origin. In that case the only convergence which will be useful to us is the convergence in the resolvent, in particular, the strong resolvent convergence.

Definition 1.7. Let $A_n,\ n = 1, 2, \cdots$ and A be self-adjoint operators. Then A_n is said to converge to A in the strong resolvent sense (or strong generalized sense) if $(A_n - \lambda)^{-1} \to (A - \lambda)^{-1}$ strongly for all λ with $Im\lambda \neq 0$.
Thus, for $A_n \overset{srs}{\to} A$ it implies that for every $\lambda \in \sigma(A)$, there are $\lambda_n \in \sigma(A_n)$ with $\lambda_n \to \lambda$. But, on the other hand, from $\lambda_n \in \sigma(A_n)$ with $\lambda_n \to \lambda$, it does not follow that $\lambda \in \sigma(A)$.

A useful criterion for strong resolvent convergence is given in the following theorem.

Theorem 1.8. *Let T_n, $n \in \mathbb{N}$ and T be self-adjoint operators on a complex Hilbert space $\mathcal{H}$. The sequence (T_n) converges to T in the sense of the strong resolvent convergence if one of the following assumptions is satisfied:*

i) There is a core D_0 of T such that for every $f \in D_0$ there exists an $n_0 \in \mathbb{N}$ with the properties that $f \in D(T_n)$ for $n \geq n_0$ and $T_n f \to Tf$.

ii) The operators T_n and T are bounded and $T_n \xrightarrow{s} T$.

iii) $D(T_n) = D(T)$ for all $n \in \mathbb{N}$ and there are null-sequences (a_n) and (b_n) such that

$$||(T - T_n)f|| \leq a_n||f|| + b_n||Tf|| \;\; \forall\, f \in D(T)$$

Proof. The proof of this theorem can be found in ([53], Theorem 9.16.) □

With a singular perturbation, isolated eigenvalues may get absorbed into the continuous spectrum and this really complicates this theory. However, for our case general results shows that H_a has an absolutely continuous spectrum $\sigma_{ac}(H_a) = [-m, m]^c$ of multiplicity 1 for all $a \neq 0$.
It is known that H_a converges to H_0 in the strong resolvent sense [42] at least for $c^2 \leq \kappa^2 - \frac{1}{4}$ and by theorem 1.8, $H_a \xrightarrow{s} H_0$ so that any discrete eigenvalue of H_0 (i.e any isolated eigenvalue of finite multiplicity) is stable in the following sense:

Definition 1.9. [38] A discrete eigenvalue λ_0 of H_0 is stable with respect to a family of operators H_a if

i) given any sufficiently small $r > 0$,

$$\Gamma_r = \{z : |z - \lambda_0| = r\} \subset \rho(H_a)$$

for all a in some neighbourhood of $a = 0$, and

ii) $\lim_{a\to 0} ||P_a - P_0|| = 0$ where $P_a = (2\pi i)^{-1} \oint_{\Gamma_r} dz R(z, a)$ is the spectral projection of H_a corresponding to the part of the spectrum enclosed in the circle Γ_r.

Condition (ii) implies $dimP_a = dimP_0$ for all a close to 0. A stable eigenvalue is the limit of a group of perturbed eigenvalues with the same total algebraic multiplicity. For more details we refer to ([38], Chapter VIII).

As mentioned in the introduction, the first stability result for Dirac equation with anomalous magnetic moment was obtained by Behncke [3] for large enough angular momentum. Later, Kalf and Schmidt [37] by using Prüfer transformation and the Ricatti equation approach extended the results of Behncke to hold for all angular momenta κ except for some exceptional coupling values. The occurrence of these exceptional values, maybe as a result of their method.

Another approach to stability different from that of Behncke [3] and of Kalf and Schmidt [37], is presented by Vock and Hunziker [52]. Though they study Schrödinger operators, their method can easily be extended to hold also for Dirac operators but only for potentials which are regular at the origin. They work directly with the operator rather than with the resolvent so that strong continuity of the operator on a suitable domain suffices to prove stability. The Vock and Hunziker results will not be of great help to us in this study since our potentials are very singular near the origin.

As stated in [37], $C_0^\infty(\mathbb{R}_+)^2$ is a common core for both H_a and H_0 at least for $c^2 \leq \kappa^2 - \frac{1}{4}$. By theorem 1.8, the spectrum of H_a cannot expand suddenly as $a \to 0$ for this range of c and κ. Therefore, one can expect the eigenvalues of H_a to converge to those of H_0 in the limit $a \to 0$. This fact also follows from the following theorem due to Kato.

Theorem 1.10. *Let T_n, T be self-adjoint operators in a Hilbert space H and let T_n converge to T strongly in the generalized sense. Then every open set containing a point of $\sigma(T)$ contains at least a point of $\sigma(T_n)$ for sufficiently large n.*

Proof. For the proof, see ([38], Chapter VIII, Theorem 1.14). □

Using Prüfer angle technique and the fact that H_a converges to H_0 in the strong resolvent convergence, Kalf and Schmidt [37] obtained the following stability results

Theorem 1.11. *[37]*

i) (Spectral convergence and stability for κ negative) *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 $0 < \varepsilon < \frac{dist(\lambda_0, \sigma(H_0)\setminus\{\lambda_0\})}{2}$. *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 λ_a *in* $(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$.

ii) (Spectral convergence and stability for positive κ). *Let* $\kappa > 0$*; then there are at least* $\left[\frac{\kappa \log 4}{\pi - 1}\right]$ *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* λ_0 *[not] be an eigenvalue of* H_0. *Let* $0 < \varepsilon < \frac{dist\,(\lambda_0, \sigma(H_0)\setminus\{\lambda_0\})}{2}$. *Then for* $a < 0$ *with sufficiently small* $|a|$, H_a *has exactly one [no] eigenvalue* λ_a *in* $(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$.

Proof. For the proof see [37]. □

Kalf and Schmidt only gave a qualitative analysis in their study based on the Prüfer angle techniques. They had to exclude some exceptional values of c.
Chapters 2 and 3 of this thesis can be seen as a follow up to Kalf and Schmidt work [37]
In this thesis another proof for stability based also on strong resolvent convergence of H_a to H_0 is developed. This is achieved by increasingly employing the use of asymptotic integration in conjunction with the Prüfer angle techniques. These techniques are supplemented by the decomposition method.

1.1.3.1 The decomposition method

The decomposition method has been used in the study of defect indices and spectra of differential operators, see [7, 10]. In this study, we use the decomposition method to study the spectral stability. In that case, we choose an arbitrary but fixed point $R \in (0, \infty)$ so that the interval $(0, \infty)$ is decomposed into the intervals $(0, R]$ and $[R, \infty]$. On the operator level H_a with domain restricted by Dirichlet boundary

conditions at R decomposes into a direct sum of operators $H_{a-} \oplus H_{a+}$, where $H_{a-} = H_a|_{L^2((0,R])^2}$ and $H_{a+} = H_a|_{L^2([R,\infty))^2}$ are the corresponding restrictions. Note that the direct sum space $L^2((0,R])^2 \oplus L^2([R,\infty))^2$ can be naturally identified with the space $L^2((0,\infty))^2$ by defining the operator H_a as

$$\begin{aligned} D(H_a) &= \left\{ u : \begin{array}{c} u(t) = u_1(t), \;\; t \in (0,R] \\ u(t) = u_2(t), \;\; t \in [R,\infty), \; u_1 \in D(H_{a-}), \; u_2 \in D(H_{a+}) \end{array} \right\} \\ H_a u &= H_{a-} u_1, \; t \in (0,R], \; H_a u = H_{a+} u_2, \; t \in [R,\infty), \; u \in D(H_a) \end{aligned}$$

It can be verified that $H_{a-} \oplus H_{a+}$ is densely defined, closed, essentially self adjoint in $L^2((0,\infty))^2$ if and only if both H_{a-} and H_{a+} are densely defined, closed, essentially self adjoint in $L^2((0,R])^2$ and $L^2([R,\infty))^2$ respectively.
Since H_{a-} and H_{a+} are real operators in this study, they admit self adjoint extensions $\tilde{H}_{a-}$ and $\tilde{H}_{a+}$ by imposing appropriate boundary conditions at R. These boundary conditions need not be identical. In this case one would have interface conditions. The simplest examples of boundary conditions for $\begin{pmatrix} u \\ v \end{pmatrix}$ would be $u(R) = 0$ or $v(R) = 0$. Since the resolvents of the self adjoint extensions $\tilde{H}_a$ respectively $\tilde{H}_{a-} \oplus \tilde{H}_{a+}$ differ at most by an operator of rank 4 (or an operator of rank 2 in case of identical boundary conditions), $\tilde{H}_a$ and $\tilde{H}_{a-} \oplus \tilde{H}_{a+}$ have identical absolutely continuous spectra and the point spectrum of $\tilde{H}_a$ is infinite if and only if this holds for the point spectrum of $\tilde{H}_{a-} \oplus \tilde{H}_{a+}$. If they are infinite, they will even accumulate at the same value. We emphasize again that this is independent of the boundary condition imposed at R. For the deficiency indices one has

$$def \; H_a = def \; H_{a-} + def \; H_{a+} - (2,2)$$

This formula goes back to Kodaira. It will not be stated explicitly in the sequel the boundary conditions at R, though $u(R) = 0$ seems to be the most natural condition.
It is essentially important that the perturbed (unperturbed) operator is essentially self adjoint if one wants to study stability of the eigenvalues. An easier way of showing essential self adjointness is by use of the deficiency index method. Therefore the behaviour of the solutions in the above intervals will be very crucial. These solutions will be obtained using the techniques of asymptotic integration and the Prüfer angle.
To employ asymptotic integration near 0, the $(0,R]$ interval is transformed into the

interval $[R', \infty)$. To the original as well as the transformed equation, asymptotic integration is applied. At the point where asymptotic integration breaks down, we invoke the Prüfer angle technique to bridge the gap.

1.1.3.2 Asymptotic Integration

The aim of asymptotic integration is to give the asymptotics of eigenfunctions which are then used to determine the deficiency index and the absolutely continuous spectrum with the aid of the now famous Weyl-Titchmarsh M-matrix. Moreover, this technique is one of the tools best suited for studying stability of differential systems. This motivates its choice as one of the tools in this thesis. In physics, asymptotic integration goes by the name WKB method for systems of order two.

In this thesis, we will use asymptotic integration to determine the behaviour of solutions of a differential equation $u' = C(x)u$. For this, the matrix C is diagonalized by a linear transformation T such that $T^{-1}CT = \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ for an $n \times n$ matrix C. This is possible if all the eigenvalues are distinct and the columns of T are the eigenvectors of C corresponding to the $\lambda_{i's}$. The transformation $Tw = u$ yields

$$w' = (\Lambda - T^{-1}T')w$$

If C is reasonably smooth, then $T^{-1}T'$ is small. The diagonalization may be repeated if C is sufficiently differentiable and if higher order derivatives decay faster. The diagonalization of the system will be performed until the system is in Levinson's form

$$w' = [\Lambda + R]w, \quad \Lambda = \text{diag}(\lambda_1(x), \ldots \lambda_n(x)), \; R_{ij} \in L^1([0, \infty)) \tag{1.23}$$

Levinson's Theorem can then be applied. It states that the solutions of the system (1.23) behave like the solutions of the unperturbed system $w' = \Lambda w$ if Λ satisfies a dichotomy condition and if the remainder term R is small in the Levinson's sense. The dichotomy condition amounts to: $Re\lambda_i(x)$ and $Re(\lambda_k(x) - \lambda_j(x)), \quad k \neq j$, have an approximately constant sign modulo L^1 for large x. If the dichotomy condition holds, then the solutions of (1.23) have the form

$$w_k = (e_k + r_k(x)) \exp \int_0^x \lambda_i(s)ds \tag{1.24}$$

In this thesis, we are dealing with two-dimensional systems of the form

$$y' = \begin{pmatrix} V & V_1 \\ V_2 & -V \end{pmatrix} y \tag{1.25}$$

where V, V_1, V_2 are smooth functions. The eigenvalues of this matrix are $\pm\mu$ with $\mu = (V^2 + V_1 V_2)^{\frac{1}{2}}$. The sign of the eigenvalues $\pm\mu$ will be chosen such that it matches the sign of V. For $V > 0$, the corresponding eigenvectors are $(1, c_+)^t$ and $(c_-, 1)^t$ with $c_+ = \frac{\mu - V}{V_1}$ and $c_- = \frac{\mu - V}{-V_2}$ and the diagonalizing matrix T is chosen such that it preserves the structure of the system in (1.25). For that reason, we require that $(T^{-1}T')_{11} = -(T^{-1}T')_{22}$ which gives T as

$$T = (1 - c_+ c_-)^{-\frac{1}{2}} \begin{pmatrix} 1 & c_- \\ c_+ & 1 \end{pmatrix} \tag{1.26}$$

For $V < 0$, we choose

$$T = (1 - c_+ c_-)^{-\frac{1}{2}} \begin{pmatrix} 1 & c_+ \\ c_- & 1 \end{pmatrix} \tag{1.27}$$

with $c_+ = \frac{\mu + V}{V_2}$ and $c_- = \frac{\mu + V}{-V_1}$.
The dichotomy condition will obviously hold in this case since μ has a fixed sign. It will therefore not be mentioned in the sequel. The main problem is therefore to transform the system (1.25) into Levinson's form (1.23). Terms which are mapped into R will be called Levinson terms. They are irrelevant for the asymptotics of the solutions.
For a smooth application of asymptotic integration, one requires that the coefficients of the differential system, which correspond to entries of the associated matrix, satisfy some regularity (decay and smoothness) conditions. For the case at hand, we will require that each coefficient admits a decomposition of the form

$$f = f_0 + f_1 + f_2 + f_3 \tag{1.28}$$

near infinity, where f_0 is a constant, f_1 twice differentiable, f_2 once differentiable with

$$f_1'^2, f_1'', f_2', f_3 \in L^1 \tag{1.29}$$

Since the operator we are studying is defined on the interval $(0, \infty)$ with singularity at both end points, we need two sets of regularity conditions: one at ∞ and the

other at 0. For the singularity at infinity, the above condition suffices. At zero, we will assume approximate power behaviour. These regularity conditions will be stated explicitly later. For a more general exposition to asymptotic integration theory, we refer to [4, 8, 23] and references therein.
One can also study spectral stability based on the the m-function. Stability of the eigenvalues in our case would mean continuity of the functions $m_\pm$ at the point R. This may need the implicit function theorem for these functions which at the moment is still an open question. Therefore, this mode of stability will be postponed for the time being.

1.1.3.3 Prüfer Transformation

The Prüfer transformation is a tool for analysing the zeros and eigenvalues of second order differential equations. It can also be used to analyse zeros of coupled first order differential equations and even help in counting the zeros. One can also apply the comparison results available for first order differential equations.
For the Dirac system, we define this transformation as

$$u = \rho\cos\theta, \quad v = \rho\sin\theta \text{ where } \rho = \sqrt{u^2+v^2}, \quad \theta = \arctan\left(\frac{v}{u}\right). \tag{1.30}$$

u and v are the asymptotic solutions of the separated Dirac equation and θ is the phase function. Using (1.30) in the eigenvalue equation defined by (1.21) with eigenvalue λ, give rise to two non-linear first order equations

$$\theta'(r) = \frac{c}{r} - \lambda + \left(\frac{\kappa}{r} + \frac{a}{r^2}\right)\sin 2\theta + m\cos 2\theta \tag{1.31}$$

$$(\ln\rho(r))' = m\sin 2\theta - \left(\frac{\kappa}{r} + \frac{a}{r^2}\right)\cos 2\theta \tag{1.32}$$

in which comparison results can be used. In particular, we will need

Lemma 1.12. *[37] 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 $f_1(x,y) \le f_2(x,y)$ $(x \in I, y \in \mathbb{R})$. Furthermore, let $y_1^0 \le y_2^0$, 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, $y_1(x) \le y_2(x)$ $(x \in I,\ x \ge x_0)$.

An immediate consequence of this lemma is the following stability criterion.

Lemma 1.13. *[37] 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 $f(x, y_1) > 0,\ f(x, y_2) < 0\ \ (x \in I)$.

There is a unique solution of (1.31) corresponding to the asymptotic solution of the original system defined by (1.21). We even know that for $r \to 0$, θ is continuously decreasing [37]. The uniqueness of θ also follows from the existence and uniqueness theorem for first order differential equations [34, 44]. If $a = 0$, one can even compute the eigenvalues numerically using (1.31) with $a = 0$, see [50]. Note that if one knows u and v, then the size of ρ can be obtained using (1.30). By these methods except the M-function method, we have obtained stability for all values of κ. Precise estimates of the energy shifts $|\lambda_a - \lambda_0|$ are also obtained. This was not possible by the methods used in [37]. The angles can also be computed more explicitly whenever asymptotic integration is possible than in [37]. These results are then extended to a larger class of interactions. As a consequence, some general spectral results are also obtained. All these results are contained in chapters 2 and 3.

1.2 The nonrelativistic limit of the Dirac equation

It is well known that, in the quantum mechanics of a particle, Schrödinger's equation can be obtained as a limiting form of the Dirac's relativistic equation by letting c, the velocity of light, tend to infinity. This of course happens after subtracting the rest energy mc^2, which is a purely relativistic term. The relativistic formulae can then be considered as a perturbed form of the nonrelativistic one, depending on the perturbation parameter c^{-1}. This expectation has been verified by many authors among them [18, 33, 36, 40, 47].
One way of studying the nonrelativistic limit is via the Foldy-Wouthuysen method,

where the Dirac equation is expanded to order c^{-2} . This method played an important role in the physical interpretation of the Dirac equation. It also lead to the first definition of the relativistic corrections to eigenvalues of a Dirac particle, see [24, 40]. However, this method cannot be justified rigorously despite being popular with physicists.

The second method, introduced by Hunziker [36] and later used by Gesztesy, Grosse and Thaller [26, 47] is based on working with the Dirac resolvent rather than the Dirac operator itself. Gesztesy, Grosse and Thaller [26], using the approach introduced in [36], proved holomorphy of the Dirac resolvent in c^{-1} under general conditions on the potentials. Moreover, their approach led to the first rigorous derivation of an explicit formula for relativistic corrections to eigenvalues of the Dirac operator to order $O(c^{-2})$.

The most common method in quantum mechanics books is the Pauli elimination method. This method reproduces the Pauli-Schrödinger equation to first order. For higher order terms one requires normalization on the wave functions. The normalization procedure is rather complicated and makes the method undesirable.

1.2.1 Pauli elimination method

To highlight the Pauli elimination method, let $\Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}$ be a 4-component spinor with ϕ and χ representing the large and small components respectively. Then we have for the eigenvalue E

$$(H_0 - m)\Psi = E_{nrl}\Psi,$$

c is taken as unity as have been assumed earlier. Decoupling this equation and taking $\chi = \sum_{k=0}^{\infty}(-1)^k \frac{(E_{nrl}-V)^k}{(2m)^{k+1}}\sigma \cdot (p - eA)\phi, \quad E_{nrl}, V \ll m$, one obtains further relativistic corrections to the Dirac operator if a proper normalization is applied to ϕ. Taking only the first term in the expansion, one obtains the Pauli- Schrödinger equation

$$\left[\frac{1}{2m}(p - eA)^2 - \frac{e}{2m}(\sigma \cdot \mathbf{B}) + V\right]\phi = E_{nrl}\phi \tag{1.33}$$

Thus, the Pauli-Schrödinger equation can be considered as a first order approximation to the Dirac equation with mass m and charge e. The term $\frac{e}{2m}\sigma$ is called the intrinsic angular momentum and it shows that an electron has an intrinsic

magnetic moment. $\mathbf{B} = \nabla \times A$ is the magnetic field. This is one of the successes of the Dirac theory as it also predicts its correct value, see [13].
The other methods mentioned above for obtaining further relativistic corrections to the Dirac operator will be discussed in chapter 4. We refer to [12, 40, 47] for a detailed account on the nonrelativistic theory of the Dirac equation.

Chapter 2

The Dirac equation with Anomalous Magnetic Moment

In this chapter, we study the Coulomb-Dirac equation with the anomalous magnetic moment potential. To realize the effects of the anomalous magnetic moment, we study the behaviour of the eigenfunctions at both the singular points 0 and infinity. The singularity caused by the anomalous magnetic moment near 0, may have some effects on the stability of the eigenvalues of the unperturbed operator H_0 if this term is considered as a perturbation on H_0 . In the last section of this chapter, we show that the eigenvalues of H_0 are stable with respect to the anomalous magnetic moment potential for all κ. Moreover, the energy shifts are shown to be proportional to a.

2.1 Dirac Equation with Coulomb potential

We will now analyze the eigenfunctions of H_a with the Coulomb potential $V_e = \frac{c}{x}$ by use of asymptotic integration method. The change from r to x is done out of convention. The interval $(0, \infty)$ is decomposed into $(0, R]$ and $[R, \infty)$. The analysis is then done on these intervals separately.
The starting point is the Dirac radial operator

$$H_a = \begin{pmatrix} \frac{c}{x} + m & -\frac{d}{dx} + \frac{\kappa}{x} + \frac{a}{x^2} \\ \frac{d}{dx} + \frac{\kappa}{x} + \frac{a}{x^2} & \frac{c}{x} - m \end{pmatrix} \tag{2.1}$$

on $L^2(\mathbb{R}_+)^2$ with the underlying domain taken as $\mathcal{D} = C_0^\infty(\mathbb{R}_+)^2$.
Here, a measures the size of the anomalous magnetic moment. c is the coupling constant and it will be assumed negative throughout this chapter. The choice of sign here has some physical significance.
The eigenvalue equation

$$H_a \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix} \tag{2.2}$$

leads to

$$\begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} -V & V_1 \\ V_2 & V \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \tag{2.3}$$

with $V = \frac{\kappa}{x} + \frac{a}{x^2}$, $V_1 = -\frac{c}{x} + m + \lambda$, $V_2 = \frac{c}{x} + m - \lambda$. We will denote $m \pm \lambda$ by $m_\pm$ in the sequel and $'$ denotes $\frac{d}{dx}$.

Interchanging u and v in (2.3) results in an equation like (2.3) with V_1 and V_2 interchanged and $V \leftrightarrow -V$. Thus we may fix the sign of a near 0 suitably.
Near infinity, $m_\pm$ are dominant. Near zero, these terms are comparatively small and may be omitted. The terms in V and $\frac{c}{x}$ only play a dominant role near zero. In what follows, we study the behaviour of the eigenfunctions near these two singular points, i.e. near 0 and near ∞ by use of asymptotic integration together with the Prüfer angle method. The behaviour of the solutions will later be useful in proving stability of the eigenvalues.

2.1.1 Behaviour near infinity

We will now analyse the eigenfunctions of H_a near infinity with the $a-$ term included. This is only done to see the effects of this term on the Prüfer angles near infinity. Otherwise, this term contributes very little at infinity. In addition, the anomalous magnetic moment term is a regular perturbation on $[R, \infty)$ and asymptotic integration can be used to give rather general result. The study of stability of the eigenvalues of H_0 in this interval with respect to the $a-$term is therefore superfluous. Nevertheless, we proceed to give the form of the solutions and subsequently evaluate the corresponding angle for the decaying solution.
To apply asymptotic integration, we need two distinct eigenvalues in order to diagonalize the system in (2.3).
Since $m_\pm$ are dominant, the eigenvalues of the coefficient matrix in (2.3) are given

by $\pm\mu$ with

$$\mu = \left[m_- m_+ + \frac{2c\lambda}{x} + \frac{\kappa^2 - c^2}{x^2} + \frac{2a\kappa}{x^3} + \frac{a^2}{x^4} \right]^{\frac{1}{2}}$$

μ can be expanded for large x as

$$\mu \approx (m_+ m_-)^{\frac{1}{2}} \left(1 + \frac{c\lambda}{m_+ m_- x} + \frac{\kappa^2 - c^2}{2m_+ m_- x^2} + \frac{\kappa a}{m_+ m_- x^3} + \dots \right) \tag{2.4}$$

The corresponding eigenvectors can easily be evaluated and are given by

$$\begin{pmatrix} 1 \\ b_+ \end{pmatrix} \text{ for } \mu > 0 \text{ and } \begin{pmatrix} b_- \\ 1 \end{pmatrix} \text{ for } \mu < 0,$$

with

$$\begin{aligned} b_+ &= \frac{\mu + \frac{a}{x^2} + \frac{\kappa}{x}}{-\frac{c}{x} + m_+} \\ &\approx \left(\frac{m_-}{m_+} \right)^{\frac{1}{2}} + \frac{b_1}{x} + \frac{b_2}{x^2} + O(x^{-3}) \end{aligned} \tag{2.5}$$

where

$$b_1 = \frac{c\lambda}{m_+^{\frac{3}{2}} m_-^{\frac{1}{2}}} + \frac{m_-^{\frac{1}{2}} c}{m_+^{\frac{3}{2}}} + \frac{\kappa}{m_+}$$

and

$$b_2 = \frac{\kappa^2 - c^2}{2m_+^{\frac{3}{2}} m_-^{\frac{1}{2}}} + \frac{c^2\lambda}{m_+^{\frac{5}{2}} m_-^{\frac{1}{2}}} + \frac{m_-^{\frac{1}{2}} c^2}{m_+^{\frac{5}{2}}} + \frac{c\kappa}{m_+^2} + \frac{a}{m_+}$$

The other term b_- can be computed in a similar manner. It is given by

$$b_- \approx -\left(\frac{m_+}{m_-} \right)^{\frac{1}{2}} - \frac{\tilde{b}_1}{x} - \frac{\tilde{b}_2}{x^2} + O(x^{-3}) \tag{2.6}$$

where

$$\tilde{b}_1 = \frac{c\lambda}{m_+^{\frac{1}{2}} m_-^{\frac{3}{2}}} - \frac{m_+^{\frac{1}{2}} c}{m_-^{\frac{3}{2}}} + \frac{\kappa}{m_-}$$

and

$$\tilde{b}_2 = \frac{\kappa^2 - c^2}{2m_+^{\frac{1}{2}} m_-^{\frac{3}{2}}} - \frac{c^2\lambda}{m_+^{\frac{1}{2}} m_-^{\frac{5}{2}}} + \frac{m_+^{\frac{1}{2}} c^2}{m_-^{\frac{5}{2}}} - \frac{c\kappa}{m_-^2} + \frac{a}{m_-}$$

Thus, the diagonalizing matrix T takes the form (1.26) and is given by

$$T = (1 - b_+b_-)^{-\frac{1}{2}} \begin{pmatrix} 1 & b_- \\ b_+ & 1 \end{pmatrix} \tag{2.7}$$

T here is chosen in such away that $(T^{-1}T')_{11} = -(T^{-1}T')_{22}$. This is done in order to preserve the structure of our system.
Together with the transformation $y = Tz$, the resultant system becomes

$$z' = (\Lambda - T^{-1}T')z, \qquad \Lambda = \mathrm{diag}(\mu, -\mu), \tag{2.8}$$

and the correction term $T^{-1}T'$ is given by

$$T^{-1}T' = \frac{1}{2}(1 - b_+b_-)^{-1} \begin{pmatrix} b_+b'_- - b'_+b_- & 2b'_- \\ 2b'_+ & b'_+b_- - b_+b'_- \end{pmatrix} \tag{2.9}$$

From (2.5) and (2.6), it is clear that $b'_\pm = O(x^{-2})$. The correction term $T^{-1}T'$ is thus of order x^{-2}. This shows that the correction to the diagonal term Λ is integrable and the off diagonal terms are small in the sense of Levinson. A second diagonalization, if necessary will give correction terms of order x^{-3}. However, in our case, the first diagonalization is sufficient since the system is already in Levison's form.
The square integrable solution thus has the form

$$\begin{pmatrix} u \\ v \end{pmatrix} = (1 - b_+b_-)^{-\frac{1}{2}} \left[\begin{pmatrix} b_- \\ 1 \end{pmatrix} + r(x) \right] \exp - \int_R^x \mu(s)ds. \tag{2.10}$$

The remainder term $r(x) = o(x^{-2})$ and for large x, this term vanishes. Thus, the solutions near infinity behaves like $\exp\left(\pm(m_+m_-)^{\frac{1}{2}}x\right)$. This behaviour is already known for those solutions of the unperturbed Dirac equation in (1.17) when $a = 0$. This shows that the anomalous magnetic moment potential only has effects on the behaviour of the solutions near the origin.
To compute the corresponding angle for the decaying solution, we use (2.10) and define the phase function $\theta(a, x)$ using the vector $\begin{pmatrix} u \\ v \end{pmatrix}$ as

$$\tan\theta(a, x) = \frac{v}{u} \tag{2.11}$$

Assuming $r(x) = 0$ in (2.10), then the phase function $\theta(a, x)$ satisfies

$$\tan\theta(a,x) = \frac{1}{b_-}$$

in which the vector $\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} b_- \\ 1 \end{pmatrix}$. Note that the other terms cancels out. Thus, we have

Proposition 2.1. *For $x > R$ and $a \neq 0$, the angle $\theta(a, x)$ corresponding to the square integrable solution satisfies*

$$\tan\theta(a,x) = \tan\theta(0,x) + \frac{a}{m_+ x^2} + O(x^{-3}).$$

One even has $\theta_\infty < \theta(a, x) < \theta(0, x)$ for all κ

Proof. From (2.6), (2.10) and (2.11) we have

$$\begin{aligned} \tan\theta(a,x) &= b_-^{-1} \\ &= -\left(\frac{m_-}{m_+}\right)^{\frac{1}{2}} + \frac{a_1}{x} + \frac{a_2}{x^2} + \frac{a}{m_+ x^2} \end{aligned} \tag{2.12}$$

where

$$a_1 = \frac{1}{m_+^{\frac{3}{2}} m_-^{\frac{1}{2}}} \left[\kappa(m_+ m_-)^{\frac{1}{2}} - cm\right]$$

and

$$a_2 = \frac{\kappa^2 - c^2}{2m_+^{\frac{3}{2}} m_-^{\frac{1}{2}}} - \frac{c^2\lambda}{(m_+ m_-)^{\frac{3}{2}}} + \frac{c^2}{m_+^{\frac{1}{2}} m_-^{\frac{3}{2}}} - \frac{c\kappa}{m_+ m_-}.$$

We can simplify a_1 further by inserting the expression for $\frac{\lambda}{m}$ from (1.18),

$$\frac{\lambda}{m} = (1+z)^{-\frac{1}{2}}, \quad z = \frac{c^2}{\left(n' + \sqrt{\kappa^2 - c^2}\right)^2}.$$

n' is the index for which the power series expansion terminates. Hence

$$a_1 = \frac{m}{m_+^{\frac{3}{2}} m_-^{\frac{1}{2}}} \left[\kappa\left(1 - \frac{\lambda^2}{m^2}\right)^{\frac{1}{2}} - c\right]$$

By assumption, $|\kappa| > |c|$ and $c < 0$. We have then $\kappa^2\left(1 - \frac{\lambda^2}{m^2}\right) \leq c^2$. This implies that $n'^2 + 2n'\sqrt{\kappa^2 - c^2} \geq 0$. This happens if $n' \geq 0$. If $n' \geq 1$, one has a strict

inequality. Thus, for all κ, a_1 remains positive. For $\kappa > 0$, a_1 is larger compared to the case when $\kappa < 0$. a_2 is similarly positive.
Define

$$\tan\theta(0,x) = -\left(\frac{m_-}{m_+}\right)^{\frac{1}{2}} + \frac{a_1}{x} + \frac{a_2}{x^2} \tag{2.13}$$

if $a = 0$. Therefore, $\tan\theta(a,x)$ has an expansion in x^{-1} of the form

$$\begin{aligned}\tan\theta(a,x) &= -\left(\frac{m_-}{m_+}\right)^{\frac{1}{2}} + \frac{a_1}{x} + \frac{a_2}{x^2} + \frac{a}{m_+x^2} + O(x^{-3}) \\ &= \tan\theta(0,x) + \frac{a}{m_+x^2} + O(x^{-3})\end{aligned}$$

The last claim follows easily since $a_{1/2} > 0$ and $a < 0$.
As $a \to 0$, $\theta(a,x) \to \theta(0,x)$ as expected, because for any point $x = R > 0$, $H_a|_{[R,\infty)}$ is analytic in a
It follows from (2.12) that the limiting Prüfer angle θ_∞ for the square integrable solution is given by

$$\tan\theta_\infty = -\left(\frac{m_-}{m_+}\right)^{\frac{1}{2}} \tag{2.14}$$

From (2.12), we see that $\theta(a,x)$ approaches the $\theta_\infty-$asymptote from above. Since the tangent, $\sin 2\theta$ and $\cos 2\theta$ are $\pi-$ periodic, we can fix θ_∞ to be

$$-\frac{\pi}{4} < \theta_\infty < 0 \tag{2.15}$$

From (2.14), the limiting vector is given by $(2m_-)^{-\frac{1}{2}}\begin{pmatrix} -m_+^{\frac{1}{2}} \\ m_-^{\frac{1}{2}} \end{pmatrix}$.
Thus, $\cos 2\theta_\infty = \frac{1}{2m}(m_+ - m_-) = \frac{\lambda}{m}$ and $\sin 2\theta_\infty = -\left(1 - \frac{\lambda^2}{m^2}\right)^{\frac{1}{2}}$. Now, $\theta'(a,x)$ at $\theta = \theta_\infty$ is given by

$$\theta'(a,x) = \frac{c}{x} - \left(\frac{\kappa}{x} + \frac{a}{x^2}\right)\left(1 - \frac{\lambda^2}{m^2}\right)^{\frac{1}{2}} < 0 \tag{2.16}$$

since the first summand dominates and $c < 0$ by assumption. Thus, $\theta(a,x)$ lies above the $\theta_\infty-$asymptote. □

Remark 2.2. The above proposition shows that for a fixed point $R > 0$, the angles θ_a and θ_0 stay closer for a suitably small. It also gives the precise size of the limiting angle near infinity.

In most cases, especially for n' large, $\lambda \approx m$ and therefore θ_∞ is rather small. In fact, from (2.14), $\theta_\infty \approx 0$.

It is known that the sine function is monotonic and so is $\sin 2x$. Thus, from the Prüfer equation, we can compute $\cos 2\theta_\infty$ and $\sin 2\theta_\infty$. This has already been done in the above proof and we see that $\sin 2\theta_\infty = -\left(1 - \frac{\lambda^2}{m^2}\right)^{\frac{1}{2}} > -1$. This shows that $\theta_\infty > -\frac{\pi}{4}$ and for n' large enough it is close to zero. This justifies (2.15).

If θ does not cross the line $\theta = 0$, we will have $\frac{c}{x} + \frac{\kappa}{x}\sin 2\theta(x) \to 0$ since $m - \lambda$ will be very small. This implies that $\sin 2\theta(0, x) = -\frac{c}{k}$ for $\kappa < 0$ since by assumption $\theta(0, x) < 0$.

If $\kappa > 0$, then the two summands $\frac{c}{x}$ and $\frac{\kappa}{x}\sin 2\theta$ are both negative as long as $\theta(x) < 0$. Thus eventually the line $\theta = 0$ is crossed with a negative slope. This happens when

$$\frac{c}{x} + m - \lambda < 0$$

i.e. for $x < -\frac{c}{m-\lambda}$. Unfortunately, this may be large since m_- is small for n' large. At θ_∞ we have $\frac{1}{x}\left\{c - \left(\kappa - \frac{a}{x}\right)\left(1 - \frac{\lambda^2}{m^2}\right)^{\frac{1}{2}}\right\}$. Here the $c-$term is dominant. The $a-$term decreases the decay and still θ_a lies below θ_0. For $\kappa < 0$, $\frac{\kappa}{x} + \frac{a}{x^2} = V < 0$. So if θ_a remains below the line $\theta = 0$ then we would have a violation of the first part of the Prüfer equation for very small a since the $c-$term dominates the $\kappa-$term for $n' > 0$. Thus θ_0 will also eventually cross the $\theta = 0$ line and since by assumption $|\kappa| > |c|$, θ_a will increase beyond $\theta = 0$ towards $\theta = \frac{\pi}{2}$. In case $\kappa > 0$, θ_a will cross $\theta = 0$ line much faster.

Once the line $\theta = 0$ is crossed, θ cannot turn back, however. It will increase to a value θ_1 where

$$\sin 2\theta_1 \approx -\frac{c}{\kappa}, \tag{2.17}$$

θ_1 here is the limiting value for $\theta(0, x)$, $a = 0$ and m, λ are negligible. This is exactly the behaviour near 0 which will be discussed below.

2.1.2 Behaviour of solutions near 0

Since the potentials we are considering are bounded at infinity, only the behaviour of the potentials near zero is important if one wants to determine the point spectrum and subsequently its stability with respect to the anomalous magnetic moment potential. For the case at hand, stability of the eigenvalues only make sense near zero as the anomalous magnetic moment term is regular on $[R, \infty)$. For that reason, a control of the solutions near zero is therefore necessary. These solutions will form the building blocks for proving our stability result.

To get some insights into the form of the solutions, we analyze the system in (2.3) by means of asymptotic integration. The terms m and λ are bounded near 0. They will not therefore affect the asymptotics of the solutions significantly. These terms will then be neglected, though it is not difficult to include them. Their inclusion will only obstruct our line of analysis.

To study the behaviour of the eigenfunctions of the resultant system, it is advantageous to introduce a new variable $t = x^{-1}$. This changes the interval of definition from $(0, R]$ to $[R^{-1}, \infty)$ because as $x \searrow 0,\ t \nearrow \infty$.

Thus, the transformed system becomes

$$\frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \tilde{V} & \tilde{V}_1 \\ -\tilde{V}_1 & -\tilde{V} \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}, \tag{2.18}$$

with $\tilde{V}(t) = a + \frac{\kappa}{t},\ \tilde{V}_1 = \frac{c}{t}$.

The system (2.18) will now be diagonalized repeatedly to bring it to the Levinson's form. The two distinct eigenvalues are given by $\pm\tilde{\mu}$ with

$$\tilde{\mu} = \left(\tilde{V}^2 - \tilde{V}_1^2\right)^{\frac{1}{2}} = \left[\left(a + \frac{\kappa}{t}\right)^2 - \frac{c^2}{t^2}\right]^{\frac{1}{2}}. \tag{2.19}$$

Difficulties arise when diagonalizing (2.18). This happens when the radicand in (2.19) changes sign making the diagonalizing matrix singular at some points as will be seen later. This occurs when $\kappa > 0$ because a and κ work against each other. Therefore, there is need to analyze the case $\kappa > 0$ and the case $\kappa < 0$ separately.

Case 1. $\kappa < 0, a < 0$

This is the simpler case. Here, κ and a act in parallel and $\tilde{\mu}$ is always positive. Note that the term $|at+\kappa| > |c|$ in (2.19). Since both $\tilde{V}$ and $\tilde{V}_1$ are all negative, we have

a fast and a smooth decay of the eigenfunctions as $t \to \infty$ (resp. $x \to 0$). Since $\tilde{V} < 0$, the diagonalizing matrix takes the form (1.27) with $c_+ = c_- = -\frac{(\tilde{\mu}+\tilde{V})}{\tilde{V}_1}$. The transformation $Tw = \begin{pmatrix} u \\ v \end{pmatrix}$ yields

$$w' = (\Lambda - T^{-1}T')w, \ \Lambda = \mathrm{diag}(-\tilde{\mu}, \tilde{\mu}) \tag{2.20}$$

where the correction term $T^{-1}T'$ is given by

$$T^{-1}T' = (1 - c_-^2)^{-1} \begin{pmatrix} 0 & c_-' \\ c_-' & 0 \end{pmatrix}$$

with

$$(1 - c_-^2)^{-1} c_-' = \frac{1}{2\tilde{\mu}^2}[\tilde{V}_1\tilde{V}' - \tilde{V}\tilde{V}_1'] = \frac{ca}{2\tilde{\mu}^2 t^2} \tag{2.21}$$

For t sufficiently large, the expression $\frac{ca}{2\tilde{\mu}^2 t^2}$ has the form

$$\frac{ca}{2\tilde{\mu}^2 t^2} \approx \frac{c}{2at^2} - \frac{c\kappa}{a^2 t^3} + o(t^{-4})$$

This shows that the remainder term is of order t^{-2}. A second diagonalization shows that the remainder term is of order $o(t^{-3})$. Since by the first diagonalization, the remainder term is already of order t^{-2}, a second diagonalization is harmless. Though, for better remainder term estimates, further diagonalizations is required. Thus, by the Levinson's theorem, the square integrable solution is given by

$$\begin{pmatrix} u \\ v \end{pmatrix} = (1 - c_-^2)^{-\frac{1}{2}} \left[\begin{pmatrix} 1 \\ c_- \end{pmatrix} + r(t) \right] \exp\left(- \int_{R^{-1}}^{t} \tilde{\mu}(s) ds \right) \tag{2.22}$$

where $r(t) = o(t^{-2})$.
In order to obtain the the Prüfer angle corresponding to this solution, a control of the remainder term $r(t)$ is therefore necessary. A detailed study of this term has already been done by Behncke [5]. The following lemma shows that $r(t)$ can be made as small as desired if t is chosen sufficiently large.

Lemma 2.3. *For any $\epsilon > 0$ there exist $a_0 < 0$ so that $|r(t)| < \epsilon$ uniformly for all $a_0 < a < 0$ and $t \geq t_{1+}$*

Proof. The proof of this lemma follows closely Eastham's proof of the Levinson's Theorem.

Consider the system (2.18) over an interval $[t_{1+}, \infty)$. The transformation $Tw = \begin{pmatrix} u \\ v \end{pmatrix}$ leads to

$$\begin{aligned} w'(t) &= \left[\Lambda(t) - T^{-1}T'\right] w(t) \\ &= \left[\Lambda(t) + B(t)\right] w(t), \quad \Lambda(t) = \operatorname{diag}\left[\tilde{\mu}(t), -\tilde{\mu}(t)\right] \end{aligned} \tag{2.23}$$

The idea is to show that $w(t)$ is uniformly bounded over the interval $[t_{1+}, \infty)$
To prove this, we start by defining the fundamental matrix $\Phi(t)$ of the diagonal system $w'(t) = \Lambda(t)w(t)$ by

$$\begin{aligned} \Phi(t) &= \operatorname{diag}\left(\exp \int_{t_{1+}}^{t} \tilde{\mu}(s)ds, \exp - \int_{t_{1+}}^{t} \tilde{\mu}(s)ds\right) \\ &= \Phi_1(t) + \Phi_2(t) \end{aligned}$$

with $\Phi_1(t) = \operatorname{diag}\left(\exp \int_{t_{1+}}^{t} \tilde{\mu}(s)ds, 0\right)$ and $\Phi_2(t) = \operatorname{diag}\left(0, \exp - \int_{t_{1+}}^{t} \tilde{\mu}(s)ds\right)$.
We see that

$$|\Phi_1(t)\Phi(y)^{-1}| = 1 \; \forall \; t_{1+} < y < t < \infty \text{ and} \tag{2.24}$$

$$|\Phi_2(t)\Phi(y)^{-1}| = 1 \; \forall \; t_{1+} < t < y < \infty \tag{2.25}$$

because of the form of $\Lambda(t)$ above.
By the variation of parameters formula we have

$$w(t) = e_k + \Phi_1(t) \int_{t_{1+}}^{t} \Phi^{-1}(y)B(y)w(y)dy - \Phi_2(t) \int_{t}^{\infty} \Phi^{-1}(y)B(y)w(y)dy \tag{2.26}$$

Apply now the method of successive approximation to (2.26) with $w_1(t) = e_k$ and

$$w_{n+1}(t) = e_k + \Phi_1(t) \int_{t_{1+}}^{t} \Phi^{-1}(y)B(y)w_n(y)dy - \Phi_2(t) \int_{t}^{\infty} \Phi^{-1}(y)B(y)w_n(y)dy \tag{2.27}$$

for all $n = 1, 2, 3, \ldots$. We need that each $w_n(t)$ is bounded in $[t_{1+}, \infty)$. Assume that $|w_n(t)| \leq C_n$ for some constant C_n by induction on n. Then, using (2.24) and (2.25) in (2.27) we have

$$\begin{aligned} |w_{n+1}(t)| &\leq 1 + C_n \int_{t_{1+}}^{t} |B(y)|dy + C_n \int_{t}^{\infty} |B(y)|dy \\ &\leq 1 + 2C_n \int_{t_{1+}}^{\infty} |B(y)|dy \end{aligned}$$

This implies that $|w_{n+1}(t)| \leq C_{n+1}$ with $C_{n+1} = 1 + 2C_n \int_{t_{1+}}^{\infty} |B(y)|dy$. This shows that $w_n(t)$ is bounded for each n since by assumption $w_1(t) = e_k$.
It remains to show that $w_n(t)$ converges uniformly to the limiting function $w(t)$. To prove this, consider now

$$\begin{aligned} |w_{n+2}(t) - w_{n+1}(t)| &\leq \int_{t_{1+}}^{t} |B(y)||w_{n+1}(y) - w_n(y)|dy + \\ &\quad \int_{t}^{\infty} |B(y)||w_{n+1}(y) - w_n(y)|dy \\ &\leq 2\int_{t_{1+}}^{\infty} |B(y)||w_{n+1}(y) - w_n(y)|dy \end{aligned}$$

and by induction again, we see that

$$|w_{n+1}(t) - w_n(t)| \leq \left(2\int_{t_{1+}}^{\infty} |B(y)|dy\right)^n \tag{2.28}$$

For t_{1+} chosen suitably large, we can arrange so that

$$2\int_{t_{1+}}^{\infty} |B(y)|dy < 1 \tag{2.29}$$

and hence by extension $w(t)$ is bounded in $[t_{1+}, \infty)$. Moreover, $w_n(t) \to w(t)$ as $n \to \infty$. □

The angle corresponding to the square integrable solution can thus be computed using the relation $\tan\theta = \frac{v}{u}$, where the vector $\begin{pmatrix} u \\ v \end{pmatrix}$ is obtained from (2.22). Since $r(t)$ can be made small by Lemma 2.3, then for t large enough, the angle $\theta_a(t)$ satisfies,

$$\begin{aligned} \tan\theta_a &\approx c_- \\ &= \frac{at + \kappa + [(at+\kappa)^2 - c^2]^{\frac{1}{2}}}{-c} \end{aligned} \tag{2.30}$$

An expansion of (2.30), shows that $c_- \to 0$ as $t \to \infty$. This means that $\theta_a(t) \to 0 + n\pi,\ n = 0, 1, 2, \ldots$ as $t \to \infty$ and θ_a is rather smooth near zero because a and κ act in parallel. The other angle corresponding to the non-square integrable solution tends to $\frac{\pi}{2} + n\pi,\ n = 0, 1, 2, \cdots$. This agrees well with the results in [37] after a slight transformation given in the remark below.

Remark 2.4. Kalf and Schmidt based their Pruefer angle on $\begin{pmatrix} u \\ v \end{pmatrix} = \rho \begin{pmatrix} \sin\theta \\ -\cos\theta \end{pmatrix}$ while ours is based on $\begin{pmatrix} u \\ v \end{pmatrix} = \rho \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$. To get same results as those in [37], one needs to add $\frac{\pi}{2}$ to our angles.

If $a = 0$, the case for the unperturbed operator H_0, then it is convenient to change variables using the transformation $t = -\ln x$. The transformed system is therefore given by

$$\begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} \kappa & c \\ -c & -\kappa \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \tag{2.31}$$

because $\frac{df}{dt} = -e^{-t}\frac{df}{dx}$. The diagonalizing matrix is a constant and the decaying solution is given by

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) = (1 - c_0^2)^{-\frac{1}{2}} \begin{pmatrix} 1 \\ c_0 \end{pmatrix} \exp -\mu_0 t = C x^{\mu_0}, \tag{2.32}$$

where $c_- = c_0 = \frac{\kappa+\mu_0}{-c}$, $\mu_0 = (\kappa^2 - c^2)^{\frac{1}{2}}$ and C is a constant.
This behaviour is already known from the Coulomb-Dirac problem for all $x \in (0, R]$. The limiting angle $\theta_0(t)$ corresponding to (2.32) satisfies

$$\tan\theta_0 = \frac{\kappa + \sqrt{\kappa^2 - c^2}}{-c}. \tag{2.33}$$

Case $\kappa > 0,\ a < 0$.
Here, κ and a act in opposite directions. Therefore, the first summand of $\tilde{\mu}$ can be zero. If that happens, then (2.19) becomes imaginary, i.e. $\tilde{\mu}$ changes sign in some region. The change in sign occurs at the points $t_{1/2} = \frac{\kappa \mp c}{|a|}$ where $\tilde{\mu} = 0$. This creates what we call the transition interval (t_2, t_1), over which the eigenfunctions are oscillatory. This interval is also responsible for the increase in angles in [37] and we believe this is also the cause of existence of the exceptional values of c in [37].
The corresponding points in $x-$space can be obtained using the transformation $t = x^{-1}$. This will be done without mention in the sequel.
Diagonalization as in case 1 is not possible for this case because of the singularities at $t_{1/2}$. Asymptotic integration is therefore only possible outside the transition region. In order to estimate the behaviour of the eigenfunctions, we divide the interval $[R^{-1}, \infty)$ into three regions and then study the behaviour of the solutions

in these three regions separately. The interval $[R^{-1}, \infty)$ is divided as follows:

I) The region near zero where the $a-$term is dominant. We call it the $a-$domain.

II) The region where $|a + \frac{\kappa}{t}| < |c|$ i.e. $\tilde{\mu}_r$ is imaginary. This is the transition region.

III) The region where the $\kappa-$term is dominant. This is the classical region.

For regions I and III, the radicand of $\tilde{\mu}$ is positive and the eigenfunctions have a similar behaviour as in the case when $\kappa < 0$ though the decay is slower due to the opposing action of the angular momentum $\frac{\kappa}{t}$. In these regions, asymptotic integration is possible.
For region II, we have $|at + \kappa| < |c|$ and $\tilde{\mu}$ is imaginary leading to the transition region

$$\frac{\kappa + c}{-a} < t < \frac{\kappa - c}{-a}. \tag{2.34}$$

From (2.34), we see that the length of the interval (t_2, t_1) is proportional to $|a|$. This fact will later be useful in proving the stability of the eigenvalues.
For $\kappa > 0$, the function $\tilde{\mu}$, has to be analysed then more carefully. In particular, we need a better understanding of the diagonalizing transformation before and after the transition interval. Note that $\tilde{\mu}^2$ changes sign from positive-negative-positive as $t \to \infty$ (resp. $x \to 0$). On the interval (t_2, t_1), $\tilde{\mu}$ is purely imaginary. The solutions of the Dirac equation are oscillatory but they remain bounded. It is not known if these solutions are also $|a|-$ uniformly bounded. Later, we will show that the decaying solutions remain $a-$uniformly bounded on the interval (t_2, t_1).
Now, we define the regions above more explicitly as follows:

$$I = [t_{1+}, \infty),\ II = [t_{2-}, t_{1+}] \text{ and } III = [R^{-1}, t_{2-}],\ \text{ where}$$

$$\begin{aligned} t_{2\pm} &= \frac{\kappa + c \pm \delta}{-a}, \\ t_{1\pm} &= \frac{\kappa - c \pm \delta}{-a} \ \text{ for some } \ 0 < \delta < \kappa + c. \end{aligned}$$

Then $R^{-1} < t_{2-} < t_2 < t_{2+} < t_{1-} < t_1 < t_+ < \infty$.
We begin by studying the behaviour of solutions in region III.
Solutions on $[R^{-1}, t_{2-}]$

Here, κ is dominant and a is small though its effects cannot be ignored. Because κ dominates, the term $\tilde{V}$ is positive. Due to the change of sign for κ, we alter the transformation T accordingly so that sign $\tilde{\mu}$ = sign $\tilde{V}$. Thus, for t large enough, we have from (1.26) with $c_+ = c_- = \frac{\tilde{\mu}-\tilde{V}}{\tilde{V}_1}$. The transformation $Tw = \begin{pmatrix} u \\ v \end{pmatrix}$ yields

$$w' = \begin{pmatrix} \tilde{\mu} & d_1 \\ d_1 & -\tilde{\mu} \end{pmatrix} w \tag{2.35}$$

with $d_1 = -(1-c_-^2)^{-1}c_-' = \frac{ca}{-2\tilde{\mu}^2 t^2} < 0$ and $\tilde{\mu}$ is uniformly bounded away from zero. Thus, $d_1 \in L^1$ as long as $\tilde{\mu}^{-1}$ is bounded.
A second diagonalization with a matrix T_1 of the form

$$T_1 = (1+e^2)^{-\frac{1}{2}} \begin{pmatrix} 1 & e \\ -e & 1 \end{pmatrix}, \quad e = \frac{\mu_1 - \tilde{\mu}}{-d_1}$$

with $T_1 w_1 = w$ leads to a system in Levinson form

$$w_1' = \begin{pmatrix} \mu_1 & d_2 \\ -d_2 & -\mu_1 \end{pmatrix} w_1,$$

where $\mu_1 = (\tilde{\mu}^2 + d_1^2)^{\frac{1}{2}}$ and $d_2 = -(1+e^2)^{-1}e' = \frac{1}{2\mu_1^2}(d_1'\tilde{\mu} - d_1\tilde{\mu}')$. Note that this second diagonalization is unproblematic because $\mu_1 \neq 0$. Therefore, T_1 is bounded. Thus, the decaying solution is given by

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) = (1-c_-^2)^{-\frac{1}{2}}(1+e^2)^{-\frac{1}{2}} \left[\begin{pmatrix} e+c_- \\ ec_-+1 \end{pmatrix} + r(t) \right] \exp\left(-\int_{R^{-1}}^t \mu_1(s)ds \right) \tag{2.36}$$

for all $t \in [R^{-1}, t_{2-}]$ and a suitably small.
If $a = 0$, then the system in (2.18) can be diagonalized by a constant matrix T_0 of the form (1.26) with $c_+ = c_- = c_0 = \frac{\kappa - \sqrt{\kappa^2 - c^2}}{-c}$. The decaying solution takes the form

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) = (1-c_0^2)^{-1/2} \begin{pmatrix} c_0 \\ 1 \end{pmatrix} t^{-\left[\kappa^2 - c^2\right]^{1/2}} \tag{2.37}$$

In this case, the angle corresponding to (2.37) is a constant and it satisfies

$$\begin{aligned} \tan\theta_0 &\approx \frac{-c}{\kappa - \sqrt{\kappa^2 - c^2}} \\ &= \frac{x}{1-\sqrt{1-x^2}} = f(x), \quad x = \frac{-c}{\kappa} \end{aligned} \tag{2.38}$$

A similar expression as (2.37) can also be realized by means of the Prüfer equation because the explicit form of the angle corresponding to the square integrable solution can be obtained.

To show this, we begin by stating the Prüfer equations for the reduced system,

$$\theta'(\kappa,t) = -\frac{c}{t} - \left(a + \frac{\kappa}{t}\right)\sin 2\theta \tag{2.39}$$

and

$$(\ln\rho)' = \left(a + \frac{\kappa}{t}\right)\cos 2\theta \tag{2.40}$$

If $a = 0$, then the $\rho-$ Prüfer equation (2.40) reduces to

$$(\ln\rho(t))' = \frac{\kappa}{t}\cos 2\theta \tag{2.41}$$

and it can be shown using (2.38) that

$$(\ln\rho(t))' = -\frac{\sqrt{\kappa^2 - c^2}}{t}, \tag{2.42}$$

which has same form as (2.37).

If $a \approx \frac{-\delta}{t}$, one obtains from (2.42) that

$$(\ln\rho(t))' = -\frac{\sqrt{(\kappa-\delta)^2 - c^2}}{t}$$

Solutions on $[t_{1+}, \infty)$

Here, the anomalous magnetic moment term is dominant turning $\tilde{V}$ negative. The diagonalizing matrix is chosen such that sign $\tilde{V}$ = sign $\tilde{\mu}$. Thus, the diagonalizing matrix T takes the form (1.27) with $c_+ = c_- = f_- = \frac{\tilde{\mu}+\tilde{V}}{-\tilde{V}_1}$. The transformation $\tilde{T}w = \begin{pmatrix} u \\ v \end{pmatrix}$ leads to

$$w' = \begin{pmatrix} -\tilde{\mu} & d_3 \\ d_3 & \tilde{\mu} \end{pmatrix} w \tag{2.43}$$

with $d_3 = -(1 - f_-^2)^{-1} f_-'$. An explicit evaluation of d_3 for all $t > t_1$ gives

$$d_3 = \frac{ca}{-2\tilde{\mu}^2 t^2} \approx \frac{-c}{2at^2} + \frac{c\kappa}{a^2 t^3} + o(t^{-4})$$

This shows that the remainder term is of order t^{-2} for all $\tilde{\mu}$ bounded away from zero and for t sufficiently large. A second diagonalization with diagonalizing matrix of

the form

$$\tilde{T}_1 = (1+g_-^2)^{-\frac{1}{2}} \begin{pmatrix} 1 & -g_- \\ g_- & 1 \end{pmatrix}, \quad g_- = \frac{\mu_1 + \tilde{\mu}}{-d_3}$$

with $\tilde{T}_1 w_1 = w$ leads to

$$w_1' = \begin{pmatrix} -\mu_1 & d_4 \\ -d_4 & \mu_1 \end{pmatrix} w_1 \tag{2.44}$$

where $\mu_1 = (\tilde{\mu}^2 + d_3^2)^{\frac{1}{2}}$ and $d_4 = \left(1+g_-^2\right)^{-1} g_-' = \frac{1}{-2\mu_1^2}\left(d_3'\tilde{\mu} - d_3\tilde{\mu}'\right)$.
An explicit evaluation of d_4 for large t shows that it is of order t^{-3}. Thus, the second diagonalization is harmless. The decaying solution is given by

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) = \left(1-f_-^2\right)^{-\frac{1}{2}} \left(1+g_-^2\right)^{-\frac{1}{2}} \left[\begin{pmatrix} 1+f_-g_- \\ f_-+g_- \end{pmatrix} + r(t) \right] \exp - \int_{t_{1+}}^{t} \mu_1(s)ds, \tag{2.45}$$

with $r(t) = o(t^{-3})$.
For t large enough, the $a-$term is dominant and $\mu_1 \approx \pm t^{-1}\left[(at+\kappa)^2 - c^2\right]^{\frac{1}{2}} \approx \pm|a|$. From (2.45) we have that

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) \approx C_1 \exp -|a|t, \quad C_1 \text{ is a constant} \tag{2.46}$$

near the origin.
By Lemma 2.3, t can be chosen large enough so that $r(t)$ is small and therefore it can be neglected when computing the associated angle. Thus, the corresponding angle satisfies

$$\tan\theta_a \approx \frac{f_- + g_-}{1 + f_- g_-} \tag{2.47}$$

Prüfer angle method
To extend (2.36) directly to t_1 is bound to fail because the term $(1-c_-^2)^{-1} = \frac{\tilde{V}_1^2}{-2\tilde{\mu}(\tilde{\mu}-\tilde{V})}$ is singular when $\tilde{\mu}=0$ and the diagonalizing matrix becomes singular at t_2 and t_1. Asymptotic integration therefore does not know how to continue this solution. The triangularization method of Gingold [30] or partial diagonalization does not help here either since these methods require $\tilde{\mu}_r \neq 0$. To overcome this difficulty, we make good use of the Prüfer angle equation, particularly, the angle part. The advantage of using the Prüfer angle method stems from the fact that the two solutions of (2.18) belong to different branches of $\theta_a(\kappa, t)$ so that the above ambiguity does not arise. Moreover, one can employ the comparison results for first order differential equations. We know also from the Prüfer equations that the

solutions of (2.18) are regular at the points $t_{2/1}$. Hence, these singularities are just artifacts of this method. The Prüfer equation especially the $\rho-$equation (2.40) can then be used to estimate the growth in norm of the solutions over the interval (t_{2-}, t_{1+}) as already been seen in (2.42). Therefore, a control of the angles near t_2 and t_1 is necessary. Near t_2, we use the fact that a is smaller than κ/t. The advantage we have over this transition interval is that its length is proportional to $-a^{-1}$. Now, denote by $\theta_a(\kappa, t)$ the Prüfer angle for the decaying solution (2.36). If $a = 0$, then it follows from (2.38) that $\theta_0(\kappa, t)$ is a constant and it satisfies

$$\tan\theta_0 = \frac{x}{1-\sqrt{1-x^2}} = f(x), \quad x = \frac{-c}{\kappa}$$

If $x \approx 0$, then $f(x) \approx \frac{2}{x}$ and if $x \approx 1$, then $f(x) \approx 1$. Thus, $\theta_0(\kappa, t) \in \left(\frac{\pi}{4}, \frac{\pi}{2}\right)$ for all $t \in [R^{-1}, t_{2-}]$. One even has $\theta_0(\kappa, R^{-1}) \in \left(\frac{\pi}{4}, \frac{\pi}{2}\right)$ for suitably small R. Thus, by the comparison Lemma 1.12 we can choose $0 < \delta < \kappa + c$ such that

$$\theta_0(\kappa - \delta, R^{-1}) < \theta_a(\kappa, R^{-1}) < \theta_0(\kappa, R^{-1})$$

Since a is small, it can be considered as a small perturbation on $\frac{\kappa}{t}$ so that $\theta_a \leq \theta_0$. Thus, for $t \leq \frac{\delta}{-a}$, we can achieve

$$\frac{\pi}{4} < \theta_0(\kappa - \delta, t) < \theta_a(\kappa, t) < \theta_0(\kappa, t) < \frac{\pi}{2}$$

This inequality will hold also for all $t \in [R^{-1}, t_{2-}]$. By the comparison Lemma 1.12, we can choose $\delta < \kappa + c$ such that

$$\pi/4 + \delta < \theta_a(\kappa, t) < \pi/2$$

near t_2.

From (2.45) we see that for t large , the Prüfer angle corresponding to the square integrable solution is given by (2.47). An evaluation of f_- and g_- for large t gives

$$f_- \approx \frac{-c}{2at} + \frac{c\kappa}{2a^2t^2} + o(a^{-3}), \quad g_- \approx \frac{ac}{-4\tilde{\mu}^3t^2}$$

In this case, we can assume $\tilde{\mu} = o(a)$. An expansion of f_- and g_- near t_1, shows that θ_a is almost $\pi/4$ and then it decreases to 0 as $t \to \infty$. Thus, $0 < \theta_a < \pi/4$. The Prüfer $\rho-$ equation shows that ρ decreases. Moreover, $\delta > 0$ can be chosen such that $\theta_a < \pi/4 - \delta$ near t_1.

The intervals $(\pi/4, \pi/2)$ and $(0, \pi/4)$ remain stable by Lemma 1.13. Thus, we have the following

Lemma 2.5. *For $\kappa > 0$, the square integrable solution grows by a finite factor independent of a over the interval (t_{2-}, t_{1+}). Moreover,*

$$\ln\left(\frac{\rho(t_{1+})}{\rho(t_{2-})}\right) \leq \kappa\left(\ln(\mu_\delta^2\kappa^{-2})\right), \quad \mu_\delta^2 = \kappa^2 - (c-\delta)^2 \tag{2.48}$$

Proof. The starting point is (2.40). The function $\tilde{V}(t) = a + \frac{\kappa}{t}$ changes sign over the interval (t_2, t_1). The change occurs at the point $t = t_{max} = \kappa/|a|$. This is the point where $\tilde{V}(t) = 0$. The behaviour of solutions near t_2 and near t_1 have been discussed above and the associated angles given. The size of the angles near these points will then give the right sign for $\cos 2\theta$ in the ρ-Prüfer equation. Thus,

$$\begin{aligned}
\int_{t_{2-}}^{t_{1+}} \ln\rho(t)'dt &= \int_{t_{2-}}^{t_{1+}} \left(a + \frac{\kappa}{t}\right)\cos 2\theta dt \\
&\leq \int_{t_{max}}^{t_{2-}} \left(a + \frac{\kappa}{t}\right)dt + \int_{t_{max}}^{t_{1+}} \left(a + \frac{\kappa}{t}\right)dt \\
\ln\left(\frac{\rho(t_{1+})}{\rho(t_{2-})}\right) &\leq \kappa\ln\left(\frac{\kappa^2 - (c-\delta)^2}{\kappa^2}\right)
\end{aligned}$$

The right hand side is independent of a. □

This result will be improved later for the general Dirac-type operators.

2.2 Stability of the Coulomb Dirac Hamiltonian

So far, we have studied the operator H_a on $[R, \infty)$ and on $(0, R]$. In either case, asymptotic integration leads directly to rather general results. This method also shows that the absolutely continuous spectrum of H_a is determined by a combination of smoothness and decay conditions near infinity. The point spectrum on the other hand is determined by the behaviour near 0.

From asymptotic integration over $[R, \infty)$, we know that H_a and H_0 have absolutely continuous spectrum of multiplicity 1 in $[-m, m]^c$, see [2, 3]. Moreover, the point spectrum of H_0 lies in the interval $(-m, m)$. The problem is how to determine the point spectrum of H_a. It is quite obvious that in general, this will be a rather hopeless task since even the eigenfunctions are not known in closed form.

The next simpler problem would be to determine the point spectrum of H_0 and prove its stability with respect to the anomalous magnetic moment. This, however, will make sense if H_0 is essentially self-adjoint, because otherwise the point spectrum of any extension $\tilde{H}_0$ will depend on the boundary conditions, whereas H_a has a fixed well defined point spectrum.
Since zero is the only finite singularity for the Coulomb Dirac equation, any eigenfunction will be analytic in a on $[R, \infty)$ for any fixed point $R > 0$. We know from [3] that the inequality

$$H_{a-}^2 \geq V_3^2 - |V_3'| - 2|V_e V_3|, \quad V_3 = \frac{\kappa}{x} + \frac{a}{x^2} \tag{2.49}$$

holds in the form sense. This shows that the domain $D(H_a)$ of H_a, $a \neq 0$ is given by

$$D(H_a) = D(H_0) \cap D\left(\frac{1}{x^2}\right). \tag{2.50}$$

It also implies that an operator $H_{a'}$ can be considered a relatively bounded perturbation of H_a if $a \neq 0$ and if $|a - a'|$ is small. Thus, if λ_a is an eigenvalue of H_a, then there is a continuous family $a' \to \lambda_{a'}$ of eigenvalues of $H_{a'}$ for $a' \neq 0$. These families $a \to \lambda_a$ will not intersect for $a \neq 0$, because the eigenvalues are simple. Thus, stability in this case amounts to stability at 0.
It is known that $C_0^\infty((0,\infty))^2$ is a core for H_0 and H_a if and only if $c^2 \leq \kappa^2 - \frac{1}{4}$, hence H_a converges to H_0 in the strong resolvent sense as $a \to 0$ [[41], Theorem VIII. 25(a)]. By [[38], Chapter VIII, Theorem 1.14], this means that for any $\lambda_0 \in \sigma_p(H_0)$ and a suitably small, there exist at least one family of eigenvalues λ_a of H_a so that $\lambda_a \to \lambda_0$ as $a \to 0$. So each λ_0 is a limit of at least one continuous family $a \to \lambda_a$ of eigenvalues λ_a of H_a with $\lambda_a \to \lambda_0$. These families cannot intersect or coalesce for $a \neq 0$. Stability thus amounts to show that there is at most one such family λ_a for which $\lambda_a \to \lambda_0$.
The following Lemma is the key to our stability criteria. It uses the fact that H_a eigenfunctions are almost H_0 eigenfunctions because $\frac{a}{x^2}$ is only singular at zero. It is rather a general differential operator result and will therefore hold in much more general situations.

Lemma 2.6. *Assume there is a continuous family $a \to \lambda_a$ of eigenvalues of H_a, $a < 0$ with $\lambda_a \to \lambda_0$ as $a \to 0$, so that for some $R > 0$ and $a_0 > 0$, the associated normalized eigenfunctions w_a of H_a are $a-$uniformly small on $[0, R]$ for $a \in [-a_0, 0)$. Then $\lambda_0 \in \sigma_p(H_0)$.*

Proof. For an indirect proof, let $\tilde{\chi}$ be an infinitely differentiable monotonic function with

$$\tilde{\chi}(x) = 0 \text{ for } x \leq \frac{1}{2} \text{ and } 1 \text{ for } x \geq 1. \text{ Assume } \lambda_0 \notin \sigma_p(H_0).$$

Then for $a \in [-a_0, 0)$ and $\chi(x) = \tilde{\chi}(\frac{x}{R})$

$$\begin{aligned}(H_0 - \lambda_0)\chi w_a &= (H_a - \lambda_a)\chi w_a - aA\chi w_a + (\lambda_a - \lambda_0)\chi w_a \\ &= [H_a, \chi]w_a - aA\chi w_a + (\lambda_a - \lambda_0)\chi w_a\end{aligned}$$

where $H_a = H_0 + aA$. For $a \to 0$, the last two terms become arbitrarily small. The first summand can be estimated by $C||\chi' w_a||_{[0,R]}$ which becomes small for R small by assumption. Assume $||(H_0 - \lambda_0)\psi|| < \epsilon$ for $\psi = \frac{\chi w_a}{|\chi w_a|}$. Then, the spectral theorem shows $\sigma(H_0) \cap (\lambda_0 - \epsilon, \lambda_0 + \epsilon) \neq \emptyset$. However, since $(-m, m)$ contains only eigenvalues, which cluster at most at $\pm m$, we see that $\lambda_0 \in \sigma_p(H_0)$ if ϵ is small enough. This has to be an eigenvalue because the continuous spectrum is located in $[-m, m]^c$. Thus, $\lambda_0 \in \sigma_p(H_0)$ contrary to our earlier assumption. □

If in applications $\lambda_a \to \lambda_0 \in \sigma_p(H_0)$, then the lemma shows that λ_0 is an approximate eigenvalue. However, $\sigma_p(H_0)$ is discrete of multiplicity one. So, λ_0 will have to be an eigenvalue.
If there are several branches $\lambda_a \to \lambda_0$, $\lambda'_a \to \lambda_0, \ldots,$ then λ_0 would have a multiplicity strictly larger than one because eigenfunctions for different families $\lambda_a, \lambda_{a'}, \ldots$ are linearly independent.

Remark 2.7. Lemma 2.6 remains valid if the sup-norm replaced by the L^2-norm on $[0, R]$ is uniformly small. It will also be valid for more general Dirac-type operators. This Lemma in fact suffices for stability, because if $\lambda_0 \in \sigma_p(H_0)$ is approximated by two or more continuous branches of eigenvalues $\lambda_a \to \lambda_0$, one would derive with this Lemma that λ_0 have a multiplicity larger than two.

In our particular case, standard perturbation theory will provide more details for the interval $[R, \infty)$, $R > 0$, because, there, the perturbing term $\frac{a}{x^2}$ is regular. This in turn implies that, the eigenfunctions and the eigenvalues are analytic in a.
Lemma 2.6 also shows that a control of the eigenfunctions near zero is essential.
For $\kappa < 0, a < 0$, $\tilde{\mu}$ can be expressed as

$$\tilde{\mu}(a, t) = \left[a^2 + \frac{2a\kappa}{t} + \frac{\kappa^2 - c^2}{t^2}\right]^{\frac{1}{2}},$$

showing that $\tilde{\mu}(a,t) \geq [\kappa^2 - c^2]^{\frac{1}{2}}\, t^{-1}$ so that the λ_a-eigenfunction vanishing at zero can be estimated a uniformly on $(0,R]$ by

$$|w(x)|_\infty \leq Cx^\nu, \quad \nu = \left[\kappa^2 - c^2\right]^{\frac{1}{2}} \tag{2.51}$$

where C is a constant independent of a. Equation (2.51) suffices for stability in the case of $\kappa < 0$.

For $a = 0$ and $\kappa > 0$ asymptotic integration of (2.18) causes no problem and the transformation T of the form (1.26) gives for the solutions of (2.18)

$$\begin{pmatrix} u \\ v \end{pmatrix}_{\pm} (t) = (Te_\pm + r_\pm(t)) \exp \pm \int_{t_0}^{t} \mu_1(s)ds \qquad \text{with} \tag{2.52}$$

$e_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $e_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $r_\pm = o(1)$.

To apply this result, we choose some large point $t_0 = R^{-1}$ (resp. $x_0 = R$) such that $R^{-1} > \frac{-c}{m_-}$ and integrate the exponent in (2.52) from t_0 to t with $t > t_0$. Then the solution decaying with respect to x is given by

$$\begin{pmatrix} u \\ v \end{pmatrix}_{-} (x) = (1 - c_+c_-)^{-\frac{1}{2}} \left(\begin{pmatrix} c_- \\ 1 \end{pmatrix} + r_-(x) \right) \left(\frac{x}{x_0} \right)^\nu \tag{2.53}$$

with ν as defined in (2.51).

This behaviour is well known since for $a = 0$, explicit solutions are known. This behaviour also follows from (2.42).

Thus, we have the following stability result:

Theorem 2.8. *The eigenvalues of the Coulomb Dirac Hamiltonian are stable and the H_a-eigenfunctions almost satisfy (2.53). More precisely this means that there exist an $a-$independent $R > 0$, an $a_0 < 0$ and $\delta < \kappa + c$ so that any H_a eigenfunction $\begin{pmatrix} u \\ v \end{pmatrix}$ satisfies*

$$\left| \begin{pmatrix} u \\ v \end{pmatrix} (x) \right|_\infty \leq Cx^\varrho \quad \textit{with } \varrho = \left((\kappa - 2\delta)^2 - c^2 \right)^{\frac{1}{2}} \tag{2.54}$$

uniformly in $a_0 < a < 0, x \leq R$ *and for some* $\delta > 0$. *Close to 0, where* $x \approx |a|$, *one even has*

$$\left| \begin{pmatrix} u \\ v \end{pmatrix}(x) \right|_\infty \leq C \exp^{-\frac{|a|}{x}},\ C = \rho(x_4)$$

Proof. The main aim is to show that the decaying solutions of H_a are $a-$ uniformly small near the origin. For $\kappa < 0$, (2.54) holds and thus stability follows by asymptotic integration. So it remains to consider the case $\kappa > 0$. The proof will be a kind of perturbation result of the $a = 0$ case.

Denote by $\theta(\kappa, a, t)$ the Prüfer angle for the square integrable solution of H_a with angular momentum κ. Choose an $R > 0$ so small with $R^{-1} > \frac{-c}{m_-}$. Since the term $\frac{a}{x^2}$ is a bounded perturbation of H_a on $[R, \infty)$, all relevant quantities for H_a restricted to the interval $[R, \infty)$ are analytic in a. Thus, we can find for any $\eta > 0$ an $a_0 < 0$ such that

$$|\theta(a, \kappa, R^{-1}) - \theta(0, \kappa, R^{-1})| < \eta$$

uniformly for $a_0 < a \leq 0$.

It follows from (2.38) that $\tan\theta(0, \kappa, t) \approx c_0^{-1}$ has the asymptotics $c_0^{-1} = \frac{-c}{\kappa - \sqrt{\kappa^2 - c^2}} = f(\frac{-c}{\kappa})$ with $f(x) = \frac{x}{1-\sqrt{1-x^2}}$ and $x = \frac{-c}{\kappa}$. $f(x)$ defined on $(0, 1)$ is monotonically decreasing to 1 as $x \to 1$. Thus, $\theta(0, \kappa, R^{-1}) \in (\frac{\pi}{4}, \frac{\pi}{2})$ for suitably small R. From Lemma 1.12 we have for some $\delta < \frac{\kappa + c}{2}$

$$\theta(0, \kappa - 2\delta, R^{-1}) < \theta(a, \kappa, R^{-1}) < \theta(0, \kappa, R^{-1}).$$

This can be achieved by adjusting R whenever necessary. This will remain valid as long as $t \approx -\frac{2\delta}{a}$. The solutions over $(0, R]$ for $\kappa > 0$ are given by (2.36), (2.45) and Lemma 2.5. Since $m_\pm t^{-2}-$ terms contribute at most finite factors, the result then follows by Lemma 2.6 since $t = O(|a|^{-1})$. □

2.2.1 Energy shift

The result in theorem 2.8 can also be used to estimate the energy shift due to the anomalous magnetic moment.

It is quite clear that the naive approach of applying the anomalous magnetic moment term to eigenfunctions of H_0 is going to work only for sufficiently large angular momenta [[3], Theorem 3]. This is because the singularity due to ax^{-2} prohibits an application to H_0. However, we may turn the analysis around and

perturb H_a by $a'x^{-2}$, because H_a-eigenfunctions are in the domain of x^{-2}. In this case $a'x^{-2}$ can be considered a relatively bounded perturbation of H_a if $|a'-a|$ is small. Thus, we have

Proposition 2.9. *The shift on the bound state energy can be estimated by* $-C|a|^{2\varrho-1}$ *with* $\varrho > \frac{1}{2}$. *Thus, a charge* c *less than* $\frac{\sqrt{3}}{2}$ *would correspond to an energy shift proportional to* a *for* $\kappa = 1$.

Proof. The typical first order eigenvalue shift of the eigenvalue λ_0 with respect to the perturbation $S = a'x^{-2}$ is given by $\langle Sw_0, w_0\rangle$, [43]. Here w_0 is the normalized λ_a eigenfunction of H_a, see [38], chapter VIII, Theorem 2.6]. Then we can write

$$\langle Sw_0, w_0\rangle = \int_0^\infty a'x^{-2}w_0^2(x)dx = I_1 + I_2 + I_3 + I_4$$

The integrals $I_i,\ i = 1, 2, 3, 4$ are defined over the intervals $(0, x_4], [x_4, x_3], [x_3, R]$ and $[R, \infty)$ respectively. The first integral can be estimated as

$$\begin{aligned} I_1 = \int_0^{x_4} \frac{a'}{x^2}|w(x)|^2 e^{\frac{C'a}{x}}dx &\le C_1\frac{a'}{|a|^2}|w(x_4)|^2 \\ &\le C_2\frac{a'}{|a|^2}x_4^{2\varrho},\quad \varrho = \left(\kappa^2 - (c-\delta)^2\right)^{\frac{1}{2}} \end{aligned} \tag{2.55}$$

Similarly, using Lemma 2.5 and (2.42), the second integral is estimated as

$$I_2 = \int_{x_4}^{x_3} \frac{a'}{x^2}|w(x)|^2 dx \le C_3\frac{a'}{|a|^2}|w(x_3)|^2$$

I_3 can be estimated similarly, whereas I_4 is proportional to a. Note that $|w(x_i)| = \rho(x_i)$ and $x_3,\ x_4 = O(|a|)$.
For $\kappa < 0$ this estimate will hold with $\delta = 0$. Thus, the shift of the bound state energy can be estimated by $-C|a|^{2\varrho-1}$ respectively Ca, if $\varrho > \frac{1}{2}$.
Therefore a charge of $c < \frac{\sqrt{3}}{2}$ corresponding to $Z = 118$, would amount to an energy shift proportional to a for $\kappa = 1$. □

Remark 2.10. The estimates for $\kappa < 0$ are less problematic. However, the estimate for I_1 cannot be improved substantially.

Chapter 3

General Dirac-type operators

We now extend the results from the Coulomb-Dirac case to a larger class of potentials. Since the starting point of this study is the separated Coulomb Dirac Hamiltonian, we will consider only potentials which are bounded near infinity, though asymptotic integration also allows to study unbounded potentials at infinity as in [4]. This, however, would give no additional information about the effects of the anomalous magnetic moment. The most general operator which we will study here, is given by

$$H_a = \begin{pmatrix} V_e + V_s & -D + V_r + aV_a \\ D + V_r + aV_a & V_e - V_s \end{pmatrix}, \quad D = \frac{d}{dx} \tag{3.1}$$

where V_e is the electric potential, V_s is the scalar potential, V_r is the potential due to radial angular momentum while V_a is the anomalous magnetic moment potential. These potentials V_e, V_s, V_r, V_a are assumed to be real-valued and locally integrable i.e they are in $L^1_{loc}(\mathbb{R}_+)$. The restriction to $\mathbb{R}_+$ allows potentials which are rather singular near zero. L^p_0 denotes all $p-$integrable functions vanishing at infinity. With these assumptions, H_a is obviously a symmetric operator and will act on $L^2(\mathbb{R}_+)^2$ in the obvious fashion.
Near infinity, these potentials are supposed to admit a representation $f = V_\ell,\ \ell = a, e, r, s$ of the form

$$f = f_0 + f_1 + f_2 + f_3 \ \text{ with } f_0 \text{ constant and } f_1'', f_1'^2, f_2', f_3 \in L^1_0 \tag{3.2}$$

for all $x \geq R > 0$ and assume $V_{a0} = 0$. Here, the subscript $a0$ represent the limiting form. Such functions we call almost constant.

It is also possible to allow highly oscillatory terms f_4 or Wigner von Neumann terms, see [6]. It is likewise possible to generalize the decomposition (3.2) by allowing terms f_k with $f_k \in L_0^{\frac{k}{i}}$, $i = 0, \ldots, k$. This, however, can be improved hardly because there are decaying $C^\infty-$ potentials giving rise to singular continuous spectra. Our main technique here will be the decomposition method and asymptotic integration.

The interval $(0, \infty)$ is decomposed as before into $(0, R]$ and $[R, \infty)$. On the operator level H_a with domain restricted by the Dirichlet boundary conditions at R decomposes into a direct sum of operators $H_{a-} \oplus H_{a+}$, where $H_{a-} = H_a|_{L^2((0,R])^2}$ and $H_{a+} = H_a|_{L^2([R,\infty))^2}$.

We emphasize again that this is independent of the boundary condition imposed at R. Thus it will not be stated explicitly below, though $u(R) = 0$ seems to be the most natural condition.

To study the behaviour near origin, the interval $(0, R]$ is transformed into $[R', \infty)$ using a suitable transformation and then asymptotic integration is applied. The conditions near infinity will have to be supplemented by conditions near 0. The conditions near 0 will be stated later.

The flow of this chapter is patterned as in chapter 2.

3.1 Behaviour near infinity

To begin with, we consider $H_{a+} = H_a|_{[R,\infty)}$. Here the results of Behncke and Hinton [8], allow us to determine the deficiency index and the spectra without much effort. The results on the deficiency indices goes back to Kodaira [22] and as regards the spectrum, one can decompose the operator H_a as $H_a = H_{a-} \oplus H_{a+}$ with $H_{a-} = H_a|_{L^2((0,R])^2}$, see [29].

The limiting operator has the form

$$H_0 = \begin{pmatrix} V_{e0} + V_{s0} & -D + V_{r0} \\ D + V_{r0} & V_{e0} - V_{s0} \end{pmatrix} \tag{3.3}$$

The main result for H_{a+} over the interval $[R, \infty)$ is a consequence of the results in [8].

Lemma 3.1. *Let $m^2 = V_{s0}^2 + V_{r0}^2$. Then one has def $H_{a+} = (1, 1)$ and the self adjoint extensions $\tilde{H}_{a+}$ satisfy*

a) $m^2 = 0$ *implies* $\sigma_{ac}(\tilde{H}_{a+}) = \mathbb{R}$ *with no embedded eigenvalues, with a possible exception of an isolated eigenvalue at* V_{e0}.

b) $m^2 > 0$ *implies* $\sigma_{ac}(\tilde{H}_{a+}) = [V_{e0} - m, V_{e0} + m]^c$. *The continuous spectrum is absolutely continuous of multiplicity one with no embedded eigenvalues. Eigenvalues may only accumulate at the boundary of the absolutely continuous spectrum. All eigenvalues are simple.*

Proof. This result is a special case of [[8], Theorem 2.4]. It states that the continuous spectrum of $\tilde{H}_{a+}$ agrees with that of the constant coefficient limiting operator. For a proof, one employs asymptotic integration by performing successive diagonalizations . Thus, consider the eigenvalue equation $H_a \begin{pmatrix} u \\ v \end{pmatrix} = z \begin{pmatrix} u \\ v \end{pmatrix}$ or

$$\begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} -V_r - aV_a & -V_e + V_s + z \\ V_e + V_s - z & V_r + aV_a \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -V & V_1 \\ V_2 & V \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \quad (3.4)$$

For $z \in \mathbb{R}$ and constant coefficients, the eigenfunctions will be exponentials and the continuum eigenfunctions will be multiples of $e^{i\lambda x}$. To determine the corresponding spectral values z, consider the Fourier polynomial $\mathcal{P}$

$$\begin{aligned} \mathcal{P}(\lambda, z) &= det \begin{pmatrix} V_{e0} + V_{s0} - z & -i\lambda + V_{r0} \\ i\lambda + V_{r0} & V_{e0} - V_{s0} - z \end{pmatrix} \\ &= (V_{e0} - z)^2 - V_{s0}^2 - V_{r0}^2 - \lambda^2 \end{aligned} \quad (3.5)$$

Recall that $V_{a0} = 0$ and $De^{i\lambda x} = i\lambda e^{i\lambda x}$. Here the discriminant is given by $D(z) = 4[(V_{e0} - z)^2 - (V_{s0}^2 + V_{r0}^2)]$. Choosing $z = Ki$ with K large leads to eigenvalues λ with nontrivial imaginary part. If $Im\lambda > 0$ then the corresponding solution decays exponentially while the other grows exponentially. Thus, $def\ H_{a+} = (1, 1)$. The absolutely continuous spectrum is therefore given by all real z for which $(V_{e0} - z)^2 - m^2 \geq 0$. This result remains valid also for almost constant coefficient. In this case the continuum eigenfunctions are of the form

$$\begin{pmatrix} u \\ v \end{pmatrix}(x) = \left(\begin{pmatrix} u \\ v \end{pmatrix}_0 + r(x) \right) \exp \int_1^x i\lambda(t, z)dt \quad \text{with } r(x) = o(1), \quad (3.6)$$

where $i\lambda(x)$ is a root of the Fourier polynomial $\mathcal{P}(x, \lambda, z)$ which is formed with the differentiable part of the coefficient and $\begin{pmatrix} u \\ v \end{pmatrix}_0$ is the eigenvector associated

to the limiting eigenvalue. This follows by asymptotic integration; see for example [8]. The continuum eigenfunctions are thus almost plane waves. In particular, they are bounded, which also shows that the spectrum is absolutely continuous [6, 8]. For the bound states (3.6) is still valid, but now $\mathcal{P}(x, \lambda, z)$ has two complex conjugate roots and only one of these satisfies $Im\lambda > 0$, thus leading to an exponentially decaying solution. The fact that $\sigma_{ac}(\tilde{H}_{a+})$ does not contain any embedded eigenvalues and that all eigenvalues are simple, follows from the fact that $\mathcal{P}(x, \lambda, z)$ is a polynomial of degree two in λ with real coefficients and also from the local unique continuation theorem for Dirac operators [11] . Note that for $z = m$ or $z = -m$, it is not difficult to construct square integrable solutions of (3.4) for $0 = V_{r0} = V_{e0}$ and $V_{s0} = o(1)$. □

Remark 3.2. It should be noted that this latter result is shown by asymptotic integration and a refinement of the Levinson's Theorem.
Note that Lemma 3.1 is independent of V_a, because $V_{a0} = 0$ by assumption. Also, a simple shift of the spectrum by $-V_{e0}$ allows one to assume $V_{e0} = 0$. For the case at hand we will assume there are no embedded eigenvalues. This then renders the study of stability of eigenvalues in this region superfluous.

3.2 Behaviour near zero

It remains to study H_{a-}, i.e the restriction of H_a to the interval $(0, R]$, $R > 0$. This is done by transforming $(0, R]$ to $[R', \infty)$ and analyzing the transformed system by means of asymptotic integration.
To achieve this, we introduce two functions $h(x)$ and $k(x)$ and assume $h(x)$, $k(x) \nearrow \infty$ as $x \to 0+$ monotonically. These two functions are used in defining the potentials near zero. Moreover, we assume $h(x)$ is a three times differentiable function on $(0, R]$ while $k(x)$ is two times differentiable such that

$$\frac{k(x)}{-h'(x)} \to 0 \text{ monotonically near } 0. \tag{3.7}$$

Thus, $h'(x)$ is more singular than $k(x)$ and it will be used to describe the singularity of the anomalous magnetic moment term V_a. $k(x)$ will therefore describe the other potentials which are less singular than the anomalous magnetic moment potential term. In the classical Coulomb-Dirac case, one would take $h(x) = x^{-1}$ and $k(x) = x^{-1}$.

Now we transform the variables using the transformation

$$t = h(x). \tag{3.8}$$

This transforms the interval $(0, R]$ to $[R', \infty)$ where $R' = h(R)$. By the chain rule we see that $\frac{df}{dx} = h'(x)\frac{df}{dt}$. Note that $h'(x)$ is negative by definition.
For smooth potentials near zero, one can show as in [3] that

$$H_{a-}^2 \geq V_3^2 - |V_3'| - 2|V_e V_3|, \text{ if } V_3 = V_r + aV_a,\ V_a' = o(V_a^2). \tag{3.9}$$

This implies $D(H_a) = D(H_0) \cap D(V_a)$ and V_a is more singular than x^{-1} if $a \neq 0$. It also implies that $H_{a'}$ can be considered as a relatively bounded perturbation of H_a if $a \neq 0$ and if $|a - a'|$ is small. Thus if λ_a is an eigenvalue of H_a, then there is a continuous family $a' \to \lambda_{a'}$ of eigenvalues of $H_{a'}$ for $a' \neq 0$. These families $a \to \lambda_a,\ a \in (0, a_0)$ for some a_0, will not intersect for $a \neq 0$, because the eigenvalues are simple.
With the properties of V_a alluded to above, the potentials near zero assume a factorization of the form

$$\begin{gathered} V_a(x) = -h'(x) + U_a(x),\ \ V_\ell(x) = b_\ell k(x) + U_\ell(x),\ \ell = e, r, s, \\ U_\ell^{(i)}(x) = o(k^{(i)}),\ i = 0, 1, 2,\ \ell = a, e, r, s,\ b_\ell \text{ const.},\ xk(x) \geq d > 0 \end{gathered} \tag{3.10}$$

Using (3.8) and (3.10) in (3.4) with the spectral parameter z absorbed into V_e, the transformed system becomes

$$\frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \tilde{V} & \tilde{V}_1 \\ \tilde{V}_2 & -\tilde{V} \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} \tag{3.11}$$

where $\tilde{V}(t) = a + b_r\tilde{k} + \tilde{U},\ \ \tilde{V}_1(t) = (b_e - b_s)\tilde{k} + \tilde{U}_1,\ \tilde{V}_2(t) = -(b_e + b_s)\tilde{k} + \tilde{U}_2,\ \tilde{k} = -\frac{k}{h'}(x(t))$. Note that $\tilde{V}_\ell(t) \sim \tilde{V}_\ell(x(t)),\ \ \ell = a, e, r, s$.

The system (3.11) will now be diagonalized repeatedly using transformations of the form (1.26) and (1.27) in order to transform it into Levinson's form. For this we need integrability conditions on the diagonal and the off diagonal entries.

Thus, we assume the correction terms satisfy

$$\left(\frac{\tilde{k}'}{\tilde{k}}\right)^2, \frac{\tilde{k}'\tilde{U}_\ell}{\tilde{k}^2}, \frac{\tilde{U}'_\ell}{\tilde{k}}, \frac{\tilde{k}''}{\tilde{k}} \in L^1_t \tag{3.12}$$

All these conditions are stated with respect to t, the new variable. Thus, $\tilde{k}' = \frac{d}{dt}\tilde{k}$ and L^p_t means $p-$integrable with respect to t.
In the framework of (3.2), these conditions correspond to $f = f_0 + f_1$. An extension to a more general setting is possible.
The above conditions (3.12) apply in particular to potentials with an approximate power behaviour near zero. By this, we mean potentials of the form

$$V_\ell(x) = \frac{b_\ell(x)}{x^{\gamma_\ell}}, \quad \ell = e, r, s, a \quad \text{with } b_\ell \text{ bounded and twice differentiable}$$
$$\text{on } (0, h(R)] \text{ and } b'^2_\ell, b''_\ell \in L^1, \quad b_a(0) = 1, \ \gamma_a > \gamma_\ell, 1, \ \ell = e, r, s \tag{3.13}$$

The characteristic equation for the matrix in (3.11) shows that the eigenvalues are given by $\pm\tilde{\mu}$ with

$$\tilde{\mu} = \left(\tilde{V}^2 + \tilde{V}_1\tilde{V}_2\right)^{\frac{1}{2}} \tag{3.14}$$

and $\tilde{V}$, $\tilde{V}_{1/2}$ are as defined in (3.11). The transformations used to obtain the conditions in (3.12) have already been introduced in chapter 1 by equations (1.26) and (1.27). For instance, if $\tilde{V} > 0$ we use the diagonalizing matrix T of the form (1.26),

$$T = (1 - c_+c_-)^{-\frac{1}{2}} \begin{pmatrix} 1 & c_- \\ c_+ & 1 \end{pmatrix} \tag{3.15}$$

with $c_+ = \frac{\tilde{\mu}-\tilde{V}}{\tilde{V}_1}$, $c_- = \frac{\tilde{\mu}-\tilde{V}}{-\tilde{V}_2}$ and $\tilde{V}, \tilde{V}_{1/2}$ are as defined in (3.11). Again, we see that the transformation $Tw = \begin{pmatrix} u \\ v \end{pmatrix}$ leads to

$$w' = \begin{pmatrix} \mu_1 & d_1 \\ d_2 & -\mu_1 \end{pmatrix} w \tag{3.16}$$

with $\mu_1 = \tilde{\mu} - 1/2(1 - c_+c_-)^{-1}(c_+c'_- - c'_+c_-)$ and $d_{1/2} = -(1 - c_+c_-)^{-1}c'_{\mp}$ with the $d_{1/2}$ and the correction to the diagonal entries satisfying the integrability conditions in (3.12). A detailed study of the system (3.11) will be postponed until section 3.3 as we digress a bit to discuss the case when the anomalous magnetic

moment term is absent, the general Coulomb-Dirac case.

Remark 3.3. The solutions of the transformed equation (3.11) behave like $\exp(\pm at) = \exp(\pm ah(x))$ near 0, because all the potential $V_\ell,\ \ell = e, r, s$ are $o(h)$ terms, so that the twice diagonalized system is approximately diagonal. This behaviour also shows that the classical methods like the Frobenius theory are not applicable here. Thus, the system (3.4) with (3.12) defines an essentially self adjoint operator H_a if only one of the solutions is square integrable on $(0, R]$ (resp. $[R', \infty)$) for all $a < 0$. This will hold because of (3.7). The anomalous magnetic moment term aV_a thus enforces essential self adjointness.

If we consider the anomalous magnetic moment term as a perturbation and intend to compute its effect on the eigenvalues, one has to assume that the unperturbed operator H_0, is self adjoint because otherwise its point spectrum will depend on the boundary condition at 0, whereas the point spectrum of $H_a,\ a \neq 0$ is fixed.
In order to study the self adjointness of H_0, we proceed as above and analyze the limiting operator $H_{0-} = H_0|_{(0,R]}$. For this, we assume that V_ℓ are defined via a function $K(x)$ which is a two times differentiable real valued function on $(0, R]$ with $-K' \nearrow \infty$ monotonically near 0. The function $K(x)$ can be chosen such that $-K'(x) = k(x)$ in this case. The transformation $t = K(x)$ of equation (3.4) leads to (3.11) with

$$\tilde{V}_\ell(t) = (K'^{-1}V_\ell)(x(t)),\ \ \ell = e, r, s \text{ and } \tilde{V}_e = K'^{-1}(V_e - z),\ V_a = 0 \tag{3.17}$$

Thus, we assume a factorization of the form

$$\begin{gathered} V_\ell(x) = b_\ell K'(x) + U_\ell(x),\ \ell = e, r, s,\ b_\ell \text{ a const.},\ xK'(x) \geq d \\ U_\ell(x) = o(K') \quad \text{satisfies conditions similar to those in equation (3.12)} \end{gathered} \tag{3.18}$$

Again by the chain rule one has $\frac{df}{dx} = K'(x)\frac{df}{dt}$ and $K'(x)$ is negative. Changing the variables by $t = K(x)$ leads to

$$\frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \left\{ \begin{pmatrix} b_r & b_e - b_s \\ -(b_e + b_s) & -b_r \end{pmatrix} + \tilde{U} \right\} \begin{pmatrix} u \\ v \end{pmatrix}, \tag{3.19}$$

All the lower order terms are assembled in $\tilde{U}$. The lower order terms can be transformed away by successive diagonalizations. Thus, the asymptotics of the solutions of (3.19) is determined by the first summand and the solutions behave asymptotically like $\exp(\pm\mu K(x))$ where $\pm\mu = (b_r^2 + b_s^2 - b_e^2)^{\frac{1}{2}}$ are the eigenvalues of the the first summand in (3.19).
Thus, we have the following result

Lemma 3.4. *a) def* $H_{0-} = \begin{cases} (2,2) & \text{if } b_r^2 + b_s^2 < b_e^2 \\ (1,1) & \text{if } b_r^2 + b_s^2 > b_e^2 \end{cases}$
if $xK'(x) \to \infty$ *monotonically as* $x \to 0+$

b) If $K(x) = x^{-1}c(x)$ *with* $c(x)$ *continuously differentiable and* $\lim_{x\to 0} c(x) = c_0 > 0$ *then*

$$def\ H_{0-} = \begin{cases} (2,2) & \text{if } b_r^2 + b_s^2 - b_e^2 < 1/4 \\ (1,1) & \text{if } b_r^2 + b_s^2 - b_e^2 > 1/4 \end{cases}$$

c) If $K(x)$ *is bounded i.e. if* K' *is integrable, one has def* $H_{0-} = (2,2)$.

Proof. a) If $b_r^2 + b_s^2 < b_e^2$, μ is purely imaginary and H_{0-} has two bounded solutions. Otherwise, by asymptotic integration, the solutions behave like $\exp(\pm\mu K(x))$ and in that case only one solution is square integrable if $b_r^2 + b_s^2 - b_e^2 > 0$.

b) Assume $c(x)$ to be a constant say c_0. Then the solutions of (3.19) behave approximately like $\exp(\pm\mu \ln(c_0 x^{-1}) = c_0^{\pm\mu} x^{\pm\mu}$. Now the general result follows easily.

c) In this case both solutions are bounded. Thus, *def* $H_{0-} = (2,2)$.

□

Remark 3.5. In case (a) we speak of superstrong potentials while (b) could be called the approximate Coulomb case. In (c), only weak interactions are considered.

If $b_r^2 + b_s^2 = b_e^2$ respectively $b_r^2 + b_s^2 - b_e^2 = 1/4$ in Lemma 3.4 (a) or (b), then the lower order terms will play a crucial role in determining the deficiency index. To show this, we consider the following two examples:

Example 3.1. *Let* $V_\ell(x) = b_\ell x^{-\gamma} + u_\ell x^{-\beta}$, $\ell = e, r, s \quad \gamma > \beta > 1$.
Assume $b_r^2 + b_s^2 - b_e^2 = 0$. *Changing variables with* $t = x^{-(\gamma-1)}$, *system (3.4) is transformed into*

$$y'(t) = \frac{1}{\gamma - 1} \begin{pmatrix} b_r + u_r t^\delta & b_e + u_e t^\delta - (b_s + u_s t^\delta) \\ -[b_e + u_e t^\delta + (b_s + u_s t^\delta)] & -b_r - u_r t^\delta \end{pmatrix} y \tag{3.20}$$

where $\delta = \frac{\beta - \gamma}{\gamma - 1}$.
The lower order terms are bounded and the system is almost constant. Thus, one diagonalization will suffice. The eigenvalues of this matrix are $\pm\mu$ *with*

$$\mu = \pm(\gamma - 1)^{-1} \left(2At^\delta + dt^{2\delta}\right)^{1/2} \tag{3.21}$$

where $A = 2(b_r u_r + b_s u_s - b_e u_e)$ *and* $d = u_r^2 + u_s^2 - u_e^2$.
Neglecting the second summand in (3.21), we see that the two eigenfunctions will behave like

$$\exp\left(\pm(\gamma - 1)^{-1}(1 + \frac{\delta}{2})^{-1}\sqrt{2A}t^{1+\frac{\delta}{2}}\right)$$

If $A > 0$ *and* $\beta + \gamma > 2$, *then only one of these eigenfunctions is square integrable i.e def* $\tilde{H}_{0-} = (1, 1)$. *If* $A < 0$, *then both solutions will be bounded and thus def* $\tilde{H}_{0-} = (2, 2)$.

Example 3.2. *Let* $V_r = (1 + g)x^{-1}$, $V_e = \sqrt{\frac{3}{4}}x^{-1}$, $V_s = 0$ *and choose* $R = 1$ *with* g *smooth and* $o(1)$. *Then with* $t = -\ln x$, *we have*

$$\frac{d}{dt}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 + g & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -1 - g \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

and the eigenvalues are $\lambda = \pm\left(\frac{1}{4} + 2g + g^2\right)^{\frac{1}{2}} \approx \pm(\frac{1}{2} + 2g)$. *Now, if we choose* $g(x) = B(\ln x)^{-1}$ *with* $B > 0$ *a constant. The solutions take the form* $t^{\mp 2B}\exp(\pm\frac{1}{2}t)$ *and we see that for* $B > 0$ *all the solutions are square integrable, while for* $B = 0$ *only one of the solutions is square integrable.*

We summarize the above results in the following theorem:

Theorem 3.6. *a) Consider the operator* H_a *on* $\mathcal{H} = L^2((0, \infty))^2$ *with potentials* V_r, V_s, V_e *and* V_a *satisfying (3.2), (3.10) and (3.12). Then* H_a, $a \neq 0$ *is essentially self-adjoint on* $C_0^\infty(\mathbb{R}_+)^2$ *and its spectrum is absolutely continuous of multiplicity 1 as defined in Lemma 3.1. It has no embedded eigenvalues*

and these can at most accumulate at the boundaries of the absolutely continuous spectrum.

b) H_0, $a = 0$, *is essentially self-adjoint on* $C_0^\infty(\mathbb{R}_+)^2$ *if* H_{0-} *has deficiency index* $(1,1)$ *otherwise* H_0 *has deficiency index* $(1,1)$. *Let* $\tilde{H}_0$ *denote the closure respectively any self-adjoint extension of* H_0. *Then for* $\tilde{H}_0$, *the same spectral results as in part* (a) *hold.*

Proof. We use the decomposition technique on H_a and write $H_a = H_{a-} \oplus H_{a+}$ where H_{a-} (H_{a+}) is the restriction of H_a to $(0, R]$ ($[R, \infty)$) induced by Dirichlet boundary conditions at R.
Then $def H_a = def H_{a-} + def H_{a+} - (2,2)$. As noted above, any extension $\tilde{H}_{a\mp}$ of H_{a-} (H_{a+}) has discrete (absolutely continuous) spectrum and the resolvents of $\tilde{H}_{a-} \oplus \tilde{H}_{a+}$ and of any extension of H_a differ at most by a rank 4 operator. Thus, these operators have identical absolutely continuous spectra independent of the boundary conditions at R. Part (b) follows directly from Lemma 3.4. Lack of embedded eigenvalues follows from Lemma 3.1. □

Remark 3.7. The decomposition method splits the study of these general Dirac operators to that on $[R, \infty)$ and on $(0, R]$. In either case, asymptotic integration leads directly to rather general results. It is obvious that the conditions on the potentials can be extended quite far, as long as asymptotic integration is possible. Thus, we could consider exponential or oscillatory terms to obtain Wigner von Neumann type results. From this study, it is clear that the absolutely continuous spectrum is determined by a combination of smoothness and decay conditions near infinity. In particular, we see again that the boundedness of eigenfunctions results in an absolutely continuous spectrum. The point spectrum on the other hand, is determined by the behaviour near 0, though the tunnel effect makes the point spectrum finite if the potentials decay faster than x^{-2} near infinity.

Thus, it remains to determine the point spectrum of these Dirac operators $H_a, a \neq 0$, with anomalous magnetic moment. It is quite obvious as in chapter 2, that in general, this will be a rather hopeless task. So the next simpler problem would be to determine the point spectrum of H_0 and prove its stability. This, however, makes sense for essentially self-adjoint H_0 only, because otherwise the point spectrum of any extension $\tilde{H}_0$ will depend on the boundary conditions, whereas H_a has a fixed well defined point spectrum.

A particular case of this, the Coulomb Dirac Hamiltonian has already been studied. Stability of the eigenvalues of H_0 for a larger class of Dirac-type operators will follow closely from that of the Coulomb-Dirac case.

3.3 Stability For General Dirac Operators

The stability results of the previous chapter will now be extended to a more larger class of potentials. The approach will follow closely that of the Coulomb Dirac case. For stability study of the eigenvalues of H_0 with respect to the family H_a to make sense, we require that the unperturbed operator H_0 is self adjoint and has a gap in the spectrum. Conditions for self adjointness and the spectrum are given in Lemma 3.4 and Lemma 3.1 respectively.

Since all eigenfunctions are exponentially decreasing at infinity, stability based on Lemma 2.6 reduces essentially to a study of H_{a-}. Note that Vock and Hunziker's stability results [52] are essentially studies of H_{a+} because they are mainly interested in potentials with singularities at infinity. In order to reduce the multitude of cases somewhat, we will assume that the four potentials define two classes of singularities. In the Coulomb-Dirac case, these were $V_a \sim x^{-2}$ and $V_r,\ V_e \sim x^{-1}$. For the case at hand, these potentials $V_\ell,\ \ell = a, e, r, s$ have already been defined in (3.10) and they have to satisfy the conditions in (3.12) near zero. Since V_a is the most singular term, we require that it also satisfies condition (3.7).

All potentials are assumed to be real valued, so that the operator H_{a-} is symmetric. It is also possible to extend these assumptions as in (3.2) to more general conditions which combine smoothness and decay but this would only obstruct the line proof unnecessarily. Therefore, we will abstain from this generalization.

Before we state the main result, we fix some constants. As in the previous section, we will assume that

$$a, b_e < 0.$$

For the self adjointness of H_0, we also need

$$b_e^2 \neq b_s^2 \ \text{ and } \begin{cases} b_r^2 > b_e^2 \ \text{ if } \ xK'(x) \to \infty \text{ as } x \to 0 \ \text{ or} \\ b_r^2 > b_e^2 + \frac{1}{4} \ \text{ if } \ K'(x) = x^{-1} \end{cases} \tag{3.22}$$

The case when $b_e^2 = b_s^2$ will depend critically on the lower order terms.
From (3.14), we see that $\tilde{\mu}$ is given by

$$\tilde{\mu} = \left((a + b_r\tilde{k})^2 + (b_s^2 - b_e^2)\tilde{k}^2 + \tilde{U}\right)^{\frac{1}{2}}, \tag{3.23}$$

and all the lower order terms are assembled in $\tilde{U}$.
Before we continue, we introduce a simplification which allow us to consider (3.23) with either $b_s = 0$ or $b_e = 0$. This is done only for simplification purposes, otherwise one can carry along all the terms.

Simplification
Here, we introduce a useful simplification, which uses the fact that $\tilde{V}_s$ and $\tilde{V}_e$ have the same singularity near the origin. Thus, we apply a constant transformation S where $S = \mathrm{diag}(1, A)$ to the system (3.11). With $y = \begin{pmatrix} u \\ v \end{pmatrix}$ this leads to

$$\left(S^{-1}y\right)' = \left\{ \begin{pmatrix} a + b_r\tilde{k} & (b_e - b_s)A\tilde{k} \\ -(b_e + b_s)A^{-1}\tilde{k} & -(a + b_r\tilde{k} \end{pmatrix} + S^{-1}\tilde{U}S \right\} S^{-1}y$$

If $b_s^2 < b_e^2$, we can set $A = \left(\frac{b_e+b_s}{b_e-b_s}\right)^{\frac{1}{2}}$ and the transformed system looks as if it had an effective electric potential of $-(b_e^2 - b_s^2)^{\frac{1}{2}}\tilde{k}$ modulo lower order terms. If $b_s^2 > b_e^2$ one chooses $A = ((b_e + b_s)(b_s - b_e)^{-1})^{\frac{1}{2}}$ in order to remove the b_e term. Thus, one may assume $b_e = 0$ or $b_s = 0$.
Here and in the remainder $\tilde{U}$ will always denote lower order terms derived from $\tilde{U}_\ell$, $\ell = a, e, r, s$.

Remark 3.8. The lower order terms in this case will be dropped whenever necessary. This will not affect our results since only the leading terms contribute significantly to the asymptotics of the eigenfunctions.
If $b_e^2 = b_s^2$, then the oscillation interval collapses otherwise one will require the lower order terms to proceed with the analysis.

In addition to conditions in (3.12), we will assume initially that

$$\tilde{k}' = o(\tilde{k}^2) \tag{3.24}$$

Although this condition excludes the case $\tilde{k} = O(t^{-1})$, it will simplify asymptotic integration a great deal. The condition that includes the case $\tilde{k} = O(t^{-1})$ is given

at the end of Theorem 3.9
The major result in this section is:

Theorem 3.9. *The eigenvalues $\lambda_0 \in (-m, m)$ of the general Dirac operator are stable.*

Proof. Because of Lemma 2.6, we have to show that the system (3.11) has a square integrable solution vanishing $a-$uniformly as $t \to \infty$ (respectively $x \to 0$). For the proof one has to consider several subcases, otherwise the proof is patterned on the proof of the Coulomb-Dirac case.

Case 1. $a < 0,\ b_r < 0,\ b_e = 0, b_s \neq 0$.
Here, the radicand of $\tilde{\mu}$ reduces to

$$\tilde{\mu} = \left[\left(a + b_r\tilde{k})\right)^2 + b_s^2\tilde{k}^2 + \tilde{U}\right]^{\frac{1}{2}}, \tag{3.25}$$

and is always positive mod $\tilde{U}$. The result would follow by Lemma 2.6 if asymptotic integration is possible. For this, we use the diagonalizing matrix T of the form (1.27) with $c_{\mp} = \mp\frac{\tilde{\mu}+\tilde{V}}{\tilde{V}_{1/2}}$ where $\tilde{V}_1 = b_s\tilde{k} + \tilde{U}_1,\ \tilde{V}_2 = b_s\tilde{k} + \tilde{U}_2$.
For suitably small R, the term $(1 - c_+c_-)^{-1} = \frac{\tilde{V}_1\tilde{V}_2}{2\tilde{\mu}(\tilde{\mu}+\tilde{V})}$ exists finitely and is $a-$uniformly bounded for $t \to \infty$ (respectively $x \to 0$) since $\tilde{\mu}$ is always positive and stays bounded away from zero. Essentially, it is the boundedness of $\tilde{\mu}$ that makes asymptotic integration possible. Note that c_+ and c_- differ only in lower order terms.
The transformation $Tw_1 = \begin{pmatrix} u \\ v \end{pmatrix}$ leads to

$$w_1' = \begin{pmatrix} -\mu_1 & b_1 \\ b_2 & \mu_1 \end{pmatrix} w_1$$

with $\mu_1 = \tilde{\mu} - 1/2(1 - c_+c_-)^{-1}(c_+'c_- - c_-'c_+)$ and $b_{1/2} = -(1 - c_+c_-)^{-1}c_{\pm}'$. The off diagonal entries $b_{1/2}$ are integrable because of (3.12). A further diagonalization finally leads to the desired Levinson form with diagonal terms $\pm\mu_1$ where $\tilde{\mu} - \mu_1 \in L_t^1$. Thus, the eigenfunctions can be estimated $a-$uniformly by $\exp \pm \int_{R'}^t \mu_1(s)ds$. Lemma 2.6 can now be used to deduce the stability.
The case $b_r > 0$ is shown in a similar manner with T having the form given by

(3.15).

Case 2. $a < 0, b_r < 0, b_e < 0, b_s = 0$.
Here again the diagonalizing matrix T takes the form (1.27). In order that the terms $c_\pm$ be well defined, R (R') must be chosen small(large) enough. Since $b_r < 0$, $\tilde{\mu}$ is always positive because aV_a and V_r work in parallel. The proof then proceeds in the same manner as in case 1 above.

Case 3. $a < 0, b_r > 0, b_e < 0, b_s = 0$.
This is the most difficult case since V_r and aV_a act against each other. In that case, $\tilde{\mu}^2$ changes sign and $\tilde{\mu}$ becomes imaginary creating a transition region again. We will proceed along the lines of the $\kappa > 0$ Coulomb-Dirac case. However, now asymptotic integration is much more complicated because $\tilde{k}$ is much general. Thus, the proof will be spread over several subcases. In the proof we will assume $\tilde{U}$, $\tilde{U}_{1/2} = 0$ and take this terms into account in the Prüfer angle discussion. Note that it is not difficult to modify the proof to include these smaller perturbing terms.
As in the Coulomb-Dirac case, the function $\tilde{\mu}^2$ changes sign at $(a + b_r\tilde{k})^2 = b_e^2\tilde{k}^2$ giving a transition region (t_2, t_1) where the critical points t_1 and t_2 are defined implicitly by

$$\tilde{k}(t_{1/2}) = \frac{-a}{b_r \mp b_e}, \quad t_2 < t_1. \tag{3.26}$$

The $t-$values become increasingly large as $|a| \to 0$, because $\tilde{k}(t) \to 0$ as $t \to \infty$. In particular, the perturbing terms become relatively small as $|a| \to 0$.
Now fix a point $R' = h(R)$ and choose $\delta > 0$ small, such that $\delta < b_r + b_e$. Since the lower order terms satisfy $\tilde{U}_\ell = o(\tilde{k})$, we may choose $a_0 < 0$ so small so that $\tilde{U}_\ell(t) \leq \delta\tilde{k}(t)$ for all $t \geq t_{2-}$ and all $a < a_0$.
Asymptotic integration is only possible whenever $\tilde{\mu}^{-1}$ is bounded. Thus, for some arbitrary but fixed $\delta > 0$ we can define

$$t_{1\pm} \text{ by : } \quad \tilde{k}(t_{1\pm}) = \frac{-a}{b_r - b_e \pm \delta} \tag{3.27}$$

$$t_{2\pm} \text{ by : } \quad \tilde{k}(t_{2\pm}) = \frac{-a}{b_r + b_e \pm \delta} \tag{3.28}$$

From (3.27), we see that $t_{1+} > t_1 > t_{1-} > t_{2+} > t_2 > t_{2-} > R'$.
Asymptotic integration is then possible in $[R', t_{2-}]$, $[t_{2+}, t_{1-}]$ and $[t_{1+}, \infty)$.

The a-small domain

In the interval $[R', t_{2-}]$, one has $\tilde{k}(t) \geq -a(b_r + b_e - \delta)^{-1}$ which implies $\tilde{\mu}^2 \geq -2\delta b_e \tilde{k}^2 + \delta^2 \tilde{k}^2 > 0$ and hence asymptotic integration is possible. In this interval, the terms $b_r\tilde{k}$ and $b_e\tilde{k}$ are dominant. The anomalous magnetic moment term a is small but cannot be ignored. Thus, we assume it can be estimated by $a \approx -\delta\tilde{k}$. The system (3.11) with $\tilde{U}_\ell = 0$, $\ell = a, e, r, s$, is then diagonalized by T in (3.15) with $c_+ = c_- = \frac{\tilde{\mu}-\tilde{V}}{\tilde{V}_1}$. The transformation $Tw = \begin{pmatrix} u \\ v \end{pmatrix}$ gives with $\tilde{\mu} = \left(\tilde{V}^2 - \tilde{V}_1^2\right)^{\frac{1}{2}}$

$$w' = \begin{pmatrix} \tilde{\mu} & d_1 \\ d_1 & -\tilde{\mu} \end{pmatrix} w \tag{3.29}$$

where $d_1 = -(1 - c_-^2)^{-1} c_-'$. An explicit evaluation of d_1 gives $d_1 = \frac{ab_e\tilde{k}'}{2\tilde{\mu}^2}$. Because of (3.24), d_1 is approximately constant since $\tilde{\mu} = o(\tilde{k})$. This will hold in general modulo integrable terms. A second diagonalization with a matrix T_1 of the form (3.15)

$$T_1 = \left(1 + e_-^2\right)^{-\frac{1}{2}} \begin{pmatrix} 1 & e_- \\ -e_- & 1 \end{pmatrix}, \quad e_- = \frac{\mu_1 - \tilde{\mu}}{-d_1} \tag{3.30}$$

with $T_1 w_1 = w$ leads to a system in Levinson form

$$w_1' = \begin{pmatrix} \mu_1 & d_2 \\ -d_2 & -\mu_1 \end{pmatrix} w_1, \quad \mu_1 = \left(\tilde{\mu}^2 + d_1^2\right)^{\frac{1}{2}} \tag{3.31}$$

with $d_2 = -\left(1 + e_-^2\right)^{-1} e_-'$. An explicit evaluation of d_2 gives $d_2 = (2\mu_1^2)^{-1}[\tilde{\mu}d_1' - d_1\tilde{\mu}']$ which is square integrable because of (3.12) and (3.24). This second diagonalization is unproblematic because $\mu_1 \neq 0$ so that T_1 is bounded. The decaying solution is thus given by

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) = \left(1 - c_-^2\right)^{-\frac{1}{2}} \left(1 + e_-^2\right)^{-\frac{1}{2}} \left[\begin{pmatrix} c_- + e_- \\ c_- e_- + 1 \end{pmatrix} + r(t) \right] \exp - \int_{R'}^{t} \mu_1(s) ds \tag{3.32}$$

where $r(t) = o(1)$. This holds for all $R' \leq t \leq t_{2-}$,

To extend directly (3.32) to t_{2+} is bound to fail because $(1 - c_-^2)^{-1} = \frac{\tilde{V}_1^2}{-2\tilde{\mu}(\tilde{\mu}-\tilde{V})}$ becomes singular as $\tilde{\mu} \to 0$. Asymptotic integration therefore does not know how to continue the above solution. At this point we invoke the Prüfer angle method because the solutions corresponding to $+\tilde{\mu}$ and $-\tilde{\mu}$ belong to different branches of the Prüfer equation.

The interval $[t_{2-}, t_{2+}]$

The Prüfer equation for the transformed system (3.11) is given by

$$\theta' = -\tilde{V}\sin 2\theta - b_e\tilde{k} - \tilde{U}_1\sin^2\theta + \tilde{U}_2\cos^2\theta \tag{3.33}$$

$$(\ln\rho)' = \tilde{V}\cos 2\theta + \frac{1}{2}(\tilde{U}_1 + \tilde{U}_2)\sin 2\theta \tag{3.34}$$

A control of the angles near t_2 is therefore necessary. We proceed as in the Coulomb-Dirac case with $\tilde{k}$ instead of t^{-1}. If $a = 0$, then the system in (3.11) can be diagonalized by a constant matrix. In this case, the Prüfer angle $\theta_0(b_r, t)$ is a constant and it satisfies

$$\tan\theta_0 = \frac{-b_e}{b_r - \sqrt{b_r^2 - b_e^2}} = \frac{x}{1-\sqrt{1-x^2}} = f(x), \quad x = \frac{-b_e}{b_r} \tag{3.35}$$

From (3.35), we see that if $x \to 0$, then $f(x) \to \infty$ and if $x \to 1$, then $f(x) \to 1$ monotonically. Thus, $\theta_0(b_r, t) \in (\pi/4, \pi/2)$. Considering a as a perturbation to b_r makes b_r smaller and x bigger so that $\theta_0 \to \pi/4$ with a negative slope. Thus, one even has $\theta_0(b_r \pm \delta, t) \in (\pi/4, \pi/2)$.

Since the anomalous magnetic moment term is a regular perturbation of the operator H_a restricted to $[R, \infty)$, we can find for any $\eta > 0$ an $a_0 < 0$ such that

$$|\theta(a, b_r, R') - \theta(0, b_r, R')| < \eta, \quad \forall\, a_0 < a \leq 0. \tag{3.36}$$

By adjusting R' if necessary, we can even achieve $\theta(0, b_r \pm 2\delta, R') \in (\frac{\pi}{4}, \frac{\pi}{2})$.

Therefore, for any $0 < \delta < (b_r + b_e)/2$ we have

$$\pi/4 < \theta_0(t, b_r - 2\delta) < \theta_a(t, b_r) < \theta_0(t, b_r) < \pi/2$$

for all $t \in [R', t_{2-}]$. In addition, we can choose δ such that $\theta_a(b_r, t) \geq \frac{\pi}{4} + \delta$ in the neighbourhood of t_2. The comparison Lemma then shows that

$$\pi/4 + \delta < \theta_a(b_r, t) < \theta_0(b_r, t) < \pi/2$$

for all $t \leq t_{2+}$. This also follows from (3.32), because $c_-,\ e_- > 0$ and the remainder term $r(t)$ can be made arbitrarily small for $a \to 0$ by Lemma 2.3. In this case, the angle satisfies

$$\tan\theta_a = \frac{c_- e_- + 1}{c_- + e_-}$$

Therefore, as long as $\theta_a > \pi/4 + \delta$, one has that $\cos 2\theta \geq -2\delta$. Since $\tilde{V}$ is positive

in $[R', t_{2+}]$, it follows from the Prüfer equations that $(\ln \rho)' \leq 0$ there which implies that $\rho(t_{2+}) \leq \rho(t_{2-})$. Thus, for $\theta_a \geq \pi/4 + \delta$, we have

$$\begin{aligned} \ln \frac{\rho(t_{2+})}{\rho(t_{2-})} &= \int_{t_{2-}}^{t_{2+}} (a + b_r \tilde{k}) \cos 2\theta dt \\ &\leq -2\delta \int_{t_{2-}}^{t_{2+}} (a + b_r \tilde{k}) dt, \quad \text{because} \\ &\quad \cos 2\theta \geq -2\delta \end{aligned} \tag{3.37}$$

which is $a-$uniformly small because of the negative sign before the integrand.

The Oscillation interval $[t_{2+}, t_{1-}]$

Here, we see that $\tilde{k}(t) \leq -a(b_r + b_e + \delta)^{-1}$ and $\tilde{k}(t) \geq -a(b_r - b_e - \delta)^{-1}$. This implies $\tilde{\mu}^2 \leq (\delta^2 + 2b_e\delta)\tilde{k}^2 < 0$ showing that $\tilde{\mu}$ is purely imaginary. This is due to the fact that the V_e-term is dominant since the effects from the aV_a-term and the V_r-term cancel out. The eigenfunctions are therefore oscillatory. Asymptotic integration, then shows that ρ will grow by a fixed constant because the successive diagonalization generate only integrable contributions to the diagonal. Therefore, they will stay $a-$uniformly bounded for all sufficiently small a.

It is rather hopeless to follow the angles through to t_1. Therefore, to cross the interval $[t_{1-}, t_{1+}]$, we will follow the angles from t_{1+}. For that reason, we need first the solutions on $[t_{1+}, \infty)$.

The near zero interval $[t_{1+}, \infty)$

Here, the anomalous magnetic moment term is dominant and $\tilde{V}$ is negative. Moreover, $\tilde{k}(t) \leq -a(b_r - b_e + \delta)^{-1}$ so that $\tilde{\mu}^2 \geq (-2b_e\delta + \delta^2)\tilde{k}^2 > 0$ and we see again that asymptotic integration is possible. Arguing as above, the diagonalizing matrix T takes the form in (1.27) with $c_+ = c_- = f = \frac{\tilde{\mu}+\tilde{V}}{-\tilde{V}_1}$. The transformation $\tilde{T}w = \begin{pmatrix} u \\ v \end{pmatrix}$ yields

$$w'(t) = \begin{pmatrix} -\tilde{\mu} & d_3 \\ d_3 & \tilde{\mu} \end{pmatrix} w(t)$$

with $d_3 = -(1 - f^2)^{-1} f' = \frac{ab_e\tilde{k}'}{2\tilde{\mu}^2}$.

Because a is dominant here, we can assume in addition to (3.24) that $\tilde{\mu} = o(a)$ for all $t \geq t_{1+}$. In that case, $d_3 \approx \frac{b_e\tilde{k}'}{2a} - \frac{b_e b_r \tilde{k}\tilde{k}'}{2a^2}$ is small. A second diagonalization

with $\tilde{T}_1 w_1 = w$ where

$$\tilde{T}_1 = (1+g^2)^{-\frac{1}{2}} \begin{pmatrix} 1 & -g \\ g & 1 \end{pmatrix}, \quad g = \frac{\mu_1 - \tilde{\mu}}{-d_3}, \ \mu_1 = \sqrt{\tilde{\mu}^2 + d_3^2}$$

leads to

$$w_1' = \begin{pmatrix} -\mu_1 & d_4 \\ -d_4 & \mu_1 \end{pmatrix} w_1$$

where $d_4 = (1+g^2)^{-1} g' = -(2\mu_1^2)^{-1}(d_3'\tilde{\mu} - d_3\tilde{\mu}')$.
The system is thus in Levinson form because $d_{3/4} \in L_t^2$. The square integrable solution is then given by

$$\begin{pmatrix} u \\ v \end{pmatrix}(t) = (1-f^2)^{-\frac{1}{2}}(1+g^2)^{-\frac{1}{2}} \left[\begin{pmatrix} 1+fg \\ f+g \end{pmatrix} + r(t) \right] \exp - \int_{t_{1+}}^{t} \mu_1(s) ds \quad (3.38)$$

with $r(t) = o(\tilde{k}')$. This holds for all $t \geq t_{1+}$.
An evaluation of g and f based on the above assumptions gives

$$g \approx \frac{b_e \tilde{k}'}{4a^2} - \frac{b_e b_r \tilde{k} \tilde{k}'}{2a^3} + \cdots$$
$$f \approx \frac{b_e \tilde{k}}{-2a} + \frac{b_e b_r \tilde{k}^2}{2a^2}$$

It is clear from (3.38) that the decaying solutions are $a-$uniformly small.
Because of Lemma 2.3, $r(t)$ can be made small and the Prüfer angle corresponding to the decaying solution satisfies

$$\tan \theta_a \approx \frac{f+g}{1+fg} \quad (3.39)$$

An expansion of f and g near t_1 shows that the Prüfer angle θ_a of the decaying solution is almost $\pi/4$ near t_1 and it converges to 0 as $t \to \infty$. The $\rho-$Prüfer equation then shows that $\rho \to 0$ in $[t_1, \infty)$ which gives stability by Lemma 2.6.
Thus, the H_a-eigenfunctions converge $a-$uniformly near zero so that all the eigenvalues $\lambda_0 \in (-m, m)$ of H_0 are stable. □

Remark 3.10. If $\tilde{k}' \neq o(\tilde{k}^2)$, the we write

$$\frac{\tilde{k}'}{\tilde{k}^2} = f$$

with f uniformly bounded. In this case, $\tilde{k}(t) = \left(\int_0^t f(s)ds\right)^{-1}$. This is an almost Coulomb-Dirac case and can be treated as in the Coulomb-Dirac case.

As before, we will also estimate to first order the spectral shift due to the anomalous magnetic moment

Proposition 3.11. *To first order, the energy shift due to the anomalous magnetic moment $-ah'(x)$ can be estimated by $C \cdot |a|$, where C is a constant and h is more singular than x^{-1}.*

Proof. By first order perturbation theory, we have to estimate $\langle a'h'(x)w(x), w(x)\rangle$ where $w(x)$ is a normalized λ_a-eigenfunction of H_a with $a < a' < 0$. Thus, we have to estimate

$$\int_0^\infty a'h'(x)|w(x)|^2dx = \int_0^R a'h'(x)|w(x)|^2dx + \int_R^\infty a'h'(x)|w(x)|^2dx$$

The integral $[R, \infty)$ can be estimated by $a'C_1|w|^2$ since all relevant quantities are analytic in $a < a' < 0$. It remains to estimate the integral on $(0, R]$. Thus, by the transformation $t = h(x)$, we have

$$\int_0^R a'h'(x)|w(x)|^2dx = \int_{R'}^\infty a'|w(t)|^2dt$$

The integral on the right hand side can be separated as

$$\int_{R'}^\infty a'|w(t)|^2dt = I_1 + I_2 + I_3$$

The integrals I_i are defined over the intervals $[t_{1+}, \infty)$, $[t_{2-}, t_{1+}]$ and $[R', t_{2-}]$ respectively. The first integral can be estimated as

$$\int_{t_{1+}}^\infty a'|w(t)|^2e^{2at}dt \leq C_2a'|w(t_{1+})|^2 \leq C_3a' \exp -2\left(b_r^2 - b_e^2\right)^{1/2} \int^{t_{2-}} \tilde{k}(t)dt$$

for all $a < a' < 0$ with t_{2-} proportional to a^{-1}. I_2 and I_3 can be estimated similarly using Theorem 3.9. It is also possible to analyze the integral as in Proposition 2.9 for potentials with power behaviour. This completes the proof. □

Chapter 4

Relativistic Correction to the energy

In this chapter, we study the non-relativistic approximation of the Dirac Hamiltonian by the method of Foldy and Wouthuysen (FW) and by the method of Gesztesy, Grosse and Thaller. We give explicitly the terms to order $O(c^{-4})$ in the case the Gesztesy, Grosse and Thaller method and give terms to order c^{-6} for the FW method. The second relativistic correction to the bound state energy is then computed.

4.1 The Nonrelativistic Limit of the Dirac equation

It is well known that, in the quantum mechanics of a particle, Schrödinger's equation can be obtained as a limiting form of the Dirac relativistic equations by letting c, the velocity of light, tend to infinity. This of course happens after subtracting the rest energy mc^2, which is purely a relativistic term. The relativistic formulae can then be considered as a perturbed form of the nonrelativistic one, depending on the perturbation parameter c^{-1}. This expectation has so far been verified by various authors, see [18, 33, 36, 40, 47].

One way of studying the nonrelativistic limit of a Dirac Hamiltonian is via the FW method, where the Dirac equation is expanded to any order of c^{-2} . This method has played an important role in the physical interpretation of the Dirac

equation, particularly the first order approximation to the Dirac equation. It also lead to the first definition of the relativistic corrections to eigenvalues of Dirac operators for spin-1/2 particles, see [24, 40]. However, this method cannot be justified rigorously despite being popular with physicists. The notion of analyticity of the eigenvectors and the eigenvalues were assumed.
The second method, which was first introduced by Hunziker [36], is based on the resolvent of the Dirac operator. Gesztesy, Grosse and Thaller [26], using an abstract approach as introduced in [36], proved the holomorphy of the Dirac resolvent in c^{-1} under general conditions on the potentials. Moreover, their approach led to the first rigorous derivation of an explicit formula for relativistic corrections to bound state energies to $O(c^{-2})$ terms .

4.2 Relativistic expansion of the Dirac Operator.

A relativistic expansion of the Dirac equation up to order c^{-2} is treated in almost all quantum mechanics books with relativistic quantum theory though, in some books the p^4-term, (the first order correction to the kinetic energy) is mostly left out making the resultant Hamiltonian non self adjoint. This expansion is not only useful in getting the nonrelativistic limit but also in computing nonrelativistic corrections to bound state energies of the Schrödinger Hamiltonian. One way to carry out this expansion is by use of the old Pauli elimination method which has been discussed already in the introductory chapter.
A second way of getting the expansion to any desired order of c^{-2} is by use of the Foldy-Wouthuysen unitary transformation which eliminates odd operators in the Dirac equation to any desired order, see [24, 40]. In the FW method, the normalization condition is taken into account automatically since a unitary transformation does not affect normalization.
These first two methods, which were the first ones to be developed, use directly the Dirac Hamiltonian in the expansion. They were also preferred by physicists, because the first order approximations to the Dirac equation have direct physical interpretation.
The best method so far of deriving relativistic corrections to bound-state energies to any order has been given by Gesztesy, Grosse and Thaller [26]. Using an abstract setting, Gesztesy, Grosse and Thaller have given a relativistic correction

to bound state energy to order c^{-2}. They used the Dirac Hamiltonian resolvent rather than the Hamiltonian itself as in the previous methods. We will extend these two approaches in the sequel and compute the corresponding energy correction to the bound state energy.

We begin by studying the Dirac operator in an abstract setting and extend the results in [26] in which terms of order $O(c^{-4})$ are given explicitly. These terms have not been given explicitly in the available literature. A formula for the second order relativistic correction to the bound state energy can then be written easily using regular perturbation theory.

In the second part, we give a higher order non-relativistic approximation to the Dirac Hamiltonian up to order $O(c^{-6})$ using the FW method. The relative sizes of the corrections are evaluated and we show that only the first order relativistic correction to the bound state energy is necessary. The mystery surrounding computation of eigenvalues for the Pauli Hamiltonian, which somehow don't exist but results obtained agree well with the experimental results, is explained via the concept of spectral concentration.

4.2.1 The Dirac operator in an abstract setting

The central object in the definition of an abstract Dirac operator is a self adjoint unitary operator β, with the properties

$$\beta^*\beta = \beta\beta^* = \beta^2 = 1 \tag{4.1}$$

Thus, β has eigenvalues ± 1 giving rise to eigenspaces $\mathcal{H}_\pm$ so that a Hilbert space $\mathcal{H}$ decomposes into $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. The corresponding orthogonal projections $P_\pm$ are defined as

$$P_\pm = 1/2(1 \pm \beta) \quad \text{with} \quad P_\pm \mathcal{H} = \mathcal{H}_\pm \tag{4.2}$$

Now let $\tilde{A}$ be an unbounded self adjoint operator such that

$$\tilde{A}\beta + \beta\tilde{A} = 0 \tag{4.3}$$

Then, $\tilde{A}, \beta$ can be represented in an operator matrix form as

$$\tilde{A} = \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.4}$$

where A is assumed to be a densely defined closed operator from $\mathcal{H}_+$ to $\mathcal{H}_-$ taking the form of an odd matrix.
The abstract free Dirac operator is then defined as

$$H^0(c) = c\tilde{A} + \beta mc^2, \;\; \mathcal{D}(H^0(c)) = \mathcal{D}(\tilde{A}) \tag{4.5}$$

Let V be the operator representing the potential such that V is self adjoint and commutes with β. Then, V has the form of an even matrix

$$V = \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix}. \tag{4.6}$$

Furthermore, V is assumed to be relatively bounded with respect to $\tilde{A}$ and thus bounded relative to $H^0(c)$ with a bound less than 1. This implies that V_+ (resp V_-) is relatively bounded with respect to A (resp A^*).
Next, we introduce the operator $\tilde{B}$ representing the magnetic potential. $\tilde{B}$ is taken to be a perturbation on $\tilde{A}$ and it assumes a form similar to $\tilde{A}$ and assumed to be relatively bounded with respect to $\tilde{A}$ with a bound less than 1. Thus, $\tilde{B}$ has the form

$$\tilde{B} = \begin{pmatrix} 0 & B^* \\ B & 0 \end{pmatrix}$$

and satisfies the same commutation relation in (4.3), in particular it anticommutes with β.
The operator $\tilde{A} + \tilde{B}$ is self adjoint by results in [38] since V is $\tilde{A} + \tilde{B}-$bounded.
The abstract Dirac operator with both magnetic and electric potentials is given by

$$\tilde{H}(c) = c(\tilde{A} + \tilde{B}) + \beta mc^2 + V, \tag{4.7}$$

and for c large enough, (4.7) is self adjoint. Moreover, this form is more general as to include the Dirac operator on curved spaces as well as the usual the Dirac operator on $\mathbb{R}^n$, see [18]. Equation (4.7) is in fact in the form studied by Hunziker [36].
Another form of abstract Dirac operator with supersymmetry is discussed in the book of Thaller [[47], Chapter 5].
If $\tilde{B} = 0$ then one obtains from (4.7) the Dirac operator without the magnetic potential,

$$H(c) = c\tilde{A} + \beta mc^2 + V. \tag{4.8}$$

Since we will be interested mainly in (4.8) in the nonrelativistic limit, we need to determine the associated free Pauli-Schrödinger operators. These are defined as follows:
Let

$$H_+^0 = \frac{A^*A}{2m} \text{ and } H_-^0 = \frac{AA^*}{2m} \tag{4.9}$$

be the free abstract Pauli-Schroedinger operators. Then, the corresponding abstract Pauli-Schrödinger operators are given by

$$H_+ = H_+^0 + V_+ \quad \mathcal{D}(H_+) = D(A^*A) \tag{4.10}$$

$$H_- = H_-^0 + V_- \quad \mathcal{D}(H_-) = D(AA^*) \tag{4.11}$$

Relative boundedness of $V_\pm$ implies that the operators $H_\pm$ are self adjoint.
Note that the operators $A^*(AA^* - z)^{-1}$ and $A(A^*A - z)^{-1}$ are everywhere defined i.e. they are bounded by the closed graph theorem [20].
The following commutation formulas given in [20] will be useful later in simplifying a number of terms.

$$\begin{aligned} (A^*A - z)^{-1}A^* &= A^*(AA^* - z)^{-1} \\ (AA^* - z)^{-1}A &= A(A^*A - z)^{-1} \\ A(A^*A - z)^{-1}A^* &= 1 + z(AA^* - z)^{-1} \\ A^*(AA^* - z)^{-1}A &= 1 + z(A^*A - z)^{-1} \end{aligned} \tag{4.12}$$

for all $z \in \rho(A^*A)\backslash\{0\} = \rho(AA^*)\backslash\{0\}$. We also have

$$\begin{aligned} (H_+^0 - z)^{-1}V_+(H_+ - z)^{-1}) &= (H_+^0 - z)^{-1} - (H_+ - z)^{-1} \\ z(H_-^0 - z)^{-1} &= \frac{1}{2m}A(H_+^0 - z)^{-1}A^* - 1 \end{aligned} \tag{4.13}$$

It is expected that the relativistic theory is similar to the nonrelativistic counterpart if one allows c to be very large.
The above Dirac operator $H(c)$ describes the energy of the electron with rest energy mc^2 included. This term has to be subtracted in the nonrelativistic limit since it is a purely relativistic term. Even though the rest energy is subtracted, the resultant Dirac Hamiltonian $H(c) - mc^2$ still makes no sense as $c \to \infty$. The best way to study the $c-$dependence on $H(c) - mc^2$ is by studying its resolvent $(H(c) - mc^2 - z)^{-1}$ for one and hence for all $z \in \mathbb{C}\backslash\mathbb{R}$ with $Imz \neq 0$. This has already been done in [26, 47]. The expansion that appeared in [26] only gives the

terms up to c^{-2} terms. Here, we give terms up to order c^{-4}.
Thus, we can state the following result which gives the resolvent expansion up to terms of order c^{-4}.

Theorem 4.1. *a) Let $H(c)$ be as in (4.8). Then $(H(c) - mc^2 - z)^{-1}$ is holomorphic in c^{-1} around $c^{-1} = 0$ in a $z-$dependent neighbourhood. Moreover,*

$$(H(c) - mc^2 - z)^{-1} = \sum_{n=0}^{4} c^{-n} R_n(z) + O(c^{-5}) \tag{4.14}$$

b) Let $S(c) = \begin{pmatrix} 1 & 0 \\ 0 & c \end{pmatrix}$ be a nonsingular matrix. Then $S(c)(H(c) - mc^2 - z)^{-1} S(c)^{-1}$ is holomorphic in c^{-2}

Proof. The aim is to write $(H(c) - mc^2 - z)^{-1}$ as a converging power series in c^{-1}. The proof follows closely that of [26] with terms in c^{-3}, c^{-4} added.
Let $z \in \mathbb{C}\backslash\mathbb{R}$, then

$$(H(c) - mc^2 - z)^{-1} = \left\{ \begin{pmatrix} -z & cA^* \\ cA & -2mc^2 \end{pmatrix} + \begin{pmatrix} V_+ & 0 \\ 0 & V_- - z \end{pmatrix} \right\}^{-1} \tag{4.15}$$

Now, using equations (4.12) and (4.13), we can write (4.15) in the form

$$[1 + M^{-1}N]^{-1} M^{-1}$$

with

$$M^{-1} = \begin{pmatrix} (H_+^0 - z)^{-1} & \frac{1}{2mc}(H_+^0 - z)^{-1} A^* \\ \frac{1}{2mc} A (H_+^0 - z)^{-1} & \frac{z}{2mc^2}(H_-^0 - z)^{-1} \end{pmatrix}, \quad N = \begin{pmatrix} V_+ & 0 \\ 0 & V_- - z \end{pmatrix} \tag{4.16}$$

Further simplification using (4.13) yields

$$(H(c) - mc^2 - z)^{-1} = \sum_{n=0}^{4} \frac{1}{c^n} R_n(z) + O(c^{-5})$$

with

$$
\begin{aligned}
R_0(z) &= \begin{bmatrix} (H_+ - z)^{-1} & 0 \\ 0 & 0 \end{bmatrix} \\
R_1(z) &= \begin{bmatrix} 0 & \frac{1}{2m}(H_+ - z)^{-1}A^* \\ \frac{1}{2m}A(H_+ - z)^{-1} & 0 \end{bmatrix} \\
R_2(z) &= \begin{bmatrix} {}_2R_{11} & 0 \\ 0 & {}_2R_{22} \end{bmatrix} \\
R_3(z) &= \begin{bmatrix} 0 & {}_3R_{12} \\ {}_3R_{21} & 0 \end{bmatrix} \\
R_4(z) &= \begin{bmatrix} {}_4R_{11} & 0 \\ 0 & {}_4R_{22} \end{bmatrix}
\end{aligned}
$$

where

$$
\begin{aligned}
{}_2R_{11} &= \frac{1}{4m^2}(H_+ - z)^{-1}A^*(z - V_-)A(H_+ - z)^{-1} \\
{}_2R_{22} &= \frac{1}{2m}\left[\frac{1}{2m}A(H_+ - z)^{-1}A^* - 1\right] \\
{}_3R_{12} &= \frac{1}{4m^2}\left[\frac{1}{2m}A(H_+ - z)^{-1}A^* - 1\right](H_+ - z)^{-1}A^*(V_- - z) \\
{}_3R_{21} &= \frac{1}{4m^2}\left[\frac{1}{2m}A(H_+ - z)^{-1}A^* - 1\right](z - V_-)A(H_+ - z)^{-1} \\
{}_4R_{11} &= \frac{1}{8m^3}(H_+ - z)^{-1}A^*(V_- - z)\left[\frac{1}{2m}A(H_+ - z)^{-1}A^* - 1\right] \cdot \\
&\quad (V_- - z)A(H_+ - z)^{-1} \\
{}_4R_{22} &= \frac{1}{4m^2}\Bigg\{z - V_- + \frac{1}{2m}\left[(V_- - z)A(H_+ - z)^{-1}A^* + \right. \\
&\quad \left. A(H_+ - z)^{-1}A^*(V_- - z)\right] - \frac{1}{4m^2}A(H_+ - z)^{-1}A^* \cdot \\
&\quad (V_- - z)A(H_+ - z)^{-1}A^*\Bigg\}
\end{aligned}
$$

For the second part, note that $S(c)$ leaves the main diagonal entries of $(H(c) - mc^2 - z)^{-1}$ unchanged but multiplies the up and the down off diagonal entries by $\frac{1}{c}$ and c respectively. This eliminates the odd powers of c^{-1}. Thus,

$$
S(c)(H(c) - mc^2 - z)^{-1}S(c)^{-1} = \tilde{R}_0(z) + \frac{1}{c^2}\tilde{R}_1(z) + \frac{1}{c^4}\tilde{R}_2(z) + O(c^{-6}) \quad (4.17)
$$

with

$$\tilde{R}_0(z) = \begin{bmatrix} (H_+ - z)^{-1} & 0 \\ \frac{1}{2m}A(H_+ - z)^{-1} & 0 \end{bmatrix} \tag{4.18}$$

$$\tilde{R}_1(z) = \begin{bmatrix} {}_2R_{11} & \frac{1}{2m}(H_+ - z)^{-1}A^* \\ {}_3R_{21} & {}_2R_{22} \end{bmatrix} \tag{4.19}$$

$$\tilde{R}_2(z) = \begin{bmatrix} {}_4R_{11} & {}_3R_{12} \\ 0 & {}_4R_{22} \end{bmatrix} \tag{4.20}$$

$\tilde{R}_1$ have been determined explicitly in [26]. The $\tilde{R}_2$ entries are new in the literature. These entries will later be used in computing the second order relativistic correction to the bound state energy. Note that higher order terms can be obtained in a similar manner and so do higher order corrections to the bound state energies.

□

Remark 4.2. Note that $S(c)$ is a similarity transformation. Hence $S(c)(H(c) - mc^2 - z)^{-1}S(c)^{-1}$ and $(H(c) - mc^2 - z)^{-1}$ have the same eigenvalues. Thus, the eigenvalues of $S(c)(H(c) - mc^2 - z)^{-1}S(c)^{-1}$ are analytic in c^{-2}.

Corollary 4.3. $(H(c) - mc^2 - z)^{-1} \to R_0(z)$ *as* $c \to \infty$ *in the norm resolvent sense.*

The proof follows from the above Theorem 4.1 by taking $c \to \infty$.
This corollary shows that the Dirac operator $H(c) - mc^2$ converges in norm resolvent sense to the Pauli operator H_+ times the projector P_+. One also speaks of pseudoresolvents in this case.
The norm resolvent convergence, implies that there exist a sequence of numbers $E(c)$ of $\sigma_d(H(c) - mc^2)$ such that $E(c) \to E_0 \in \sigma_d(R_0(z))$ as $c \to \infty$ [53].
If $A = A^* = \sigma \cdot (p - eA)$, the discrete case, then one obtains a similar expansion as in Theorem 4.1 with H_+ replaced by H_p. In that case $\tilde{R}_0(z)$ becomes

$$\tilde{R}_0(z) = \begin{bmatrix} (H_p - z)^{-1} & 0 \\ \frac{1}{2m}\sigma \cdot (p - eA)(H_p - z)^{-1} & 0 \end{bmatrix}$$

It is now known that the eigenvalues of $\hat{H}(c) = H(c) - mc^2$ are analytic in c^{-1}. This follows from analytic perturbation theory as seen in the following theorem.

Theorem 4.4. *[38] Let $\hat{H}(c)$ be a family of operators in a finite dimensional Hilbert space, such that $\hat{H}(c)$ is analytic in a neighbourhood of $c = \infty$. Suppose that $\hat{H}(c)$ is self adjoint for a real c and let E_0 be an eigenvalue of $\hat{H}(0)$ with multiplicity m. Then there are $k < m$ distinct functions, $E_1(c^{-1}), \ldots, E_k(c^{-1})$, which are analytic in c^{-1} in a neighbourhood of $c = \infty$, and which are all eigenvalues of $\hat{H}(c)$ with multiplicities m_j, such that $\sum_{j=1}^{k} m_j = m$.*

From this theorem we see that $(H(c) - mc^2 - z)^{-1}$ and its eigenvalues admit an expansion of the form

$$\begin{aligned} (H(c) - mc^2 - z)^{-1} &= \sum_{n=0}^{\infty} \frac{1}{c^n} R_n \\ E(c^{-1}) &= \sum_{n=0}^{\infty} \frac{1}{c^n} E_n \end{aligned} \tag{4.21}$$

This form of expansion is useful when one wants to compute the relativistic corrections to the eigenvalue of the Dirac operator by perturbation theory.

4.2.1.1 Relativistic corrections to bound state energy

We can use the nonrelativistic expansion (4.17) not only to compute the nonrelativistic limit, but also to obtain the first and the second order corrections to the nonrelativistic eigenvalue problem. By the analyticity theorem above, the eigenvalues admit an expansion of the form (4.21).
Since we are using the Dirac operator resolvent, we reformulate the computation of the the eigenvalues in the resolvent sense.
Let $\lambda(c^{-2}) = [E(c^{-2}) - z]^{-1}$ be the eigenvalues of $S(c)(H(c) - mc^2 - z)^{-1}S(c)^{-1}$ if $E(c^{-2})$ is an eigenvalue of $H(c) - mc^2$. Let E_0 be a nondegenerate eigenvalue of the Pauli Hamiltonian H_+. One can expand $\lambda(c^{-2})$ and $E(c^{-2})$ as in (4.21). Thus, we have

$$\lambda(c^{-2}) = \sum_{n=0}^{\infty} \frac{1}{c^{2n}} \lambda_n \tag{4.22}$$

$$E(c^{-2}) = \sum_{n=0}^{\infty} \frac{1}{c^{2n}} E_n \tag{4.23}$$

Using (4.23) in (4.22) one obtains

$$(E(c^{-2})-z)^{-1} = (E_0-z)^{-1} - \frac{1}{c^2}(E_0-z)^{-2}E_1 - \frac{1}{c^4}\left[(E_0-z)^{-2}E_2 + (E_0-z)^{-3}E_1^2\right] + O(c^{-6}) \tag{4.24}$$

One therefore needs to analyze the spectral properties of $\tilde{R}_0(z)$ in relation to those of $(H_+ - z)^{-1}$. A direct computation shows that if λ_0 is an eigenvalue of $(H_+ - z)^{-1}$ with eigenvector f_0, then λ_0 is also an eigenvalue of $\tilde{R}_0(z)$ with eigenvector $\phi_0 = \begin{pmatrix} f_0 \\ \frac{A}{2m}f_0 \end{pmatrix}$ where $f_0 \in \mathcal{H}_+$. The converse of this statement is also true. This can be seen easily by looking at the resolvent of $\tilde{R}_0(z)$ in which case $(H_+ - z)^{-1}$ has a pole at λ_0. Thus,

$$(H_+ - z)^{-1} f_0 = \lambda_0 f_0$$

implies

$$\tilde{R}_0(z)\begin{pmatrix} f_0 \\ \frac{A}{2m}f_0 \end{pmatrix} = \lambda_0 \begin{pmatrix} f_0 \\ \frac{A}{2m}f_0 \end{pmatrix}$$

Note that $\tilde{R}_0(z)^*$ and $\tilde{R}_0(z)$ have the same eigenvalues but different eigenvectors. A direct computation shows that $\varphi_0 = \begin{pmatrix} f_0 \\ 0 \end{pmatrix}$ is an eigenvector of $\tilde{R}_0(z)^*$ corresponding to the simple eigenvalue $(E_0 - \bar{z})^{-1}$.
First order perturbation theory then gives

$$\lambda_1 = \langle \varphi_0, \tilde{R}_1(z)\phi_0 \rangle \tag{4.25}$$

where φ_0 is the normalized eigenvector of $\tilde{R}_0(z)^*$ and $\phi_0 \neq 0$ is the normalized eigenvector of $\tilde{R}_0(z)$ associated with the eigenvalue $\lambda_0 \neq 0$. Using (4.24), one obtains an explicit formula for the first order correction to the nonrelativistic bound state energy as

$$E_1 = \langle \frac{A}{2m}f_0, (V_- - E_0)\frac{A}{2m}f_0 \rangle \tag{4.26}$$

if E_0 is a nondegenerate eigenvalue of H_+ with the corresponding normalized eigenvector f_0. This formula has already been given in [26].
The second order relativistic correction E_2 can be computed in a similar manner.

Thus,

$$E_2 = \langle \varphi_0, \tilde{R}_2(z)\phi_0 \rangle + \langle \varphi_0, \tilde{R}_1\phi_1 \rangle \tag{4.27}$$

where ϕ_1 can be expressed in terms of ϕ_0, see ([47], pp. 185).
A more general result concerning the relativistic corrections is given in the following theorem.

Theorem 4.5. *[15] Let $H(c)$ be defined as in (4.8) and assume $E_0 \in \sigma_d(H_+)$ to be a discrete eigenvalue of H_+ of multiplicity $m_0 \in \mathbb{N}$. Then, for c^{-2} small enough, $H(c) - mc^2$ has precisely m_0 eigenvalues (counting multiplicity) near E_0 which are all holomorphic with respect to c^{-2}. More precisely, all eigenvalues $E_j(c^{-2})$ of $H(c) - mc^2$ near E_0 satisfy*

$$E_j(c^{-2}) = E_0 + \sum_{k=1}^{\infty} (c^{-2})^k E_{j,k}, \qquad j = 1, \dots, j_0, \;\; j_0 \leq m_0 \tag{4.28}$$

and if m_j denotes the multiplicity of $E_j(c^{-2})$ then $\sum_{j=1}^{j_0} m_j = m_0$.
In addition, there exist linearly independent vectors

$$f_{jl}(c^{-1}) = \begin{pmatrix} f_{+jl}(c^{-2}) \\ c^{-1} f_{-jl}(c^{-2}) \end{pmatrix}, \;\; j = 1, \dots, j_0, \;\; l = 1, \dots, m_j \tag{4.29}$$

such that $f_{\pm jl}$ are holomorphic in c^{-2} near $c^{-2} = 0$ and

$$H_+ f_{+jl}(0) = E_0 f_{+jl}(0), \quad f_{-jl}(0) = \frac{A}{2m} f_{+jl}(0) \tag{4.30}$$

and

$$(H(c) - mc^2) f_{jl}(c^{-1}) = E_j(c^{-2}) f_{jl}(c^{-1}), \;\; j = 1, \dots, j_0, \;\; l = 1, \dots, m_j \tag{4.31}$$

The eigenvectors $f_{jl}(c^{-1})$ can be chosen to be orthonormal. Finally, the first-order corrections $E_{j,1}$ in (4.28) are explicitly given as the eigenvalues of the matrix

$$\frac{1}{4m^2} \langle A f_r, (V_- - E_0) A f_s \rangle \;\; r, s = 1, \dots, m_0 \tag{4.32}$$

where $\{f_r\}_{r=1}^{m_0}$ is any orthonormal basis of the eigenspace of H_+ to the eigenvalue E_0.

This theorem is more general and covers the results in [26] in which the authors only considered the case $m_0 = 1$. The only contribution in this line is the explicit

evaluation of the terms of order c^{-3} and c^{-4} which so far have not been given explicitly in the available literature.

4.2.1.2 Dirac operator with an anomalous magnetic moment

The above expansion (4.14) can also be applied to the Dirac equation with the anomalous magnetic moment. This can be achieved by defining the separated Dirac operator with anomalous magnetic moment with rest energy mc^2 subtracted as

$$h(c) = \begin{pmatrix} V(r) & cD^*(c) \\ cD(c) & V(r) - 2mc^2 \end{pmatrix} \tag{4.33}$$

with $D^* = \left(-\frac{d}{dr} + \frac{\kappa}{r} + \frac{a}{c}V'\right)$ and $D = \left(\frac{d}{dr} + \frac{\kappa}{r} + \frac{a}{c}V'\right)$. The study of the nonrelativistic limit for this operator $h(c)$ proceeds as in Theorem 4.1. The calculations in Theorem 4.1 to the Dirac resolvent $(h(c) - z)^{-1}$ is repeated without changes except that now D depends on c, see [47]. The leading term $R_0(z)$ of the Dirac resolvent $(h(c) - z)^{-1}$ now depends on c. However, $(h(c) - z)^{-1} \to (h(p) - z)^{-1}$ in operator norm as $c \to \infty$. If $V(r)$ is the Coulomb potential, the the anomalous magnetic term introduces a r^{-4} term to the associated Schrödinger operator h_p.
Another way of finding the relativistic expansion of the Dirac Hamiltonian is by use of the Foldy-Wouthuysen transformation.

4.2.2 Foldy-Wouthuysen Transformation

In this section, we derive a formula for third-order relativistic correction to the Pauli Hamiltonian by the FW method from which we state explicitly the second-order relativistic correction in the presence of a central potential. The sizes of the corrections are then considered.
By means of a unitary transformation of the wave function, a representation is found where the Dirac Hamiltonian is an even Dirac operator i.e. the Dirac equation splits into two uncoupled Pauli type equations. In the presence of interactions, an infinite sequence of transformations can be made, each of which makes the Hamiltonian even to one higher order in the expansion parameter m^{-1}.
This expansion helps in understanding the nonrelativistic limit of the Dirac Hamiltonian as will be seen later.
The wave function in the Dirac theory is a column vector Ψ with four components

and satisfies the wave equation $i\hbar\frac{d\Psi}{dt} = H\Psi$ where the Dirac Hamiltonian H is given by

$$H = \beta mc^2 + \mathcal{E} + \mathcal{O} \tag{4.34}$$

where $\mathcal{E}$ is the even operator and $\mathcal{O}$ is the odd operator. Note that the product of two even or odd operators is even and product of odd and even is an odd operator. β here anticommutes with $\mathcal{O}$ i.e. $\beta\mathcal{O} = -\mathcal{O}\beta$.

It is known from the Dirac theory that the α matrices are odd thus the operator $c\alpha \cdot (p - eA) = c\alpha \cdot \Pi$, $\Pi = p - eA$ is odd. The interactions normally commute with β and hence are even operators. Therefore, $\mathcal{E} = V$, represent the potential energy and $\mathcal{O} = c\alpha \cdot \Pi$, represent the kinetic energy.

Now consider the unitary transformation $\Psi' = e^{iS}\Psi$, S being unitary. Then Ψ' satisfies the wave equation

$$i\hbar\frac{d\Psi'}{dt} = H'\Psi'$$

where the new Hamiltonian H' is given by

$$\begin{aligned} H' &= e^{iS}He^{-iS} = H + [iS, H] + \frac{1}{2!}[iS, [iS, H]] + \frac{1}{3!}[iS, [iS, [iS, H]]] + \\ &\quad \frac{1}{4!}[iS, [iS, [iS, [iS, H]]]] + \cdots \end{aligned} \tag{4.35}$$

We can expand H' to any desired order in $\frac{1}{m}$. Here, we give the expansion of H' up to order m^{-7}.

By another transformation say S_1, we can obtain a new Hamiltonian using (4.35) by

$$H'' = e^{iS_1}H'e^{-iS_1} \tag{4.36}$$

This procedure can be carried out until all of the odd operators are eliminated to a required order. The generator of the transformation S at each step is chosen to be

$$S = -\frac{i}{2mc^2}\beta \times (\text{odd terms in Hamiltonian of lowest order in } \frac{1}{m}) \tag{4.37}$$

For more details on this scheme, see [24, 40].

In what follows, we give the relativistic expansion of (4.34) up to m^{-7}. Note that the lowest odd term in (4.34) is $\mathcal{O}$. Therefore, we begin with

$$S = \frac{-i}{2mc^2}\beta\mathcal{O}$$

and (4.35) becomes

$$\begin{aligned} H' &= \beta mc^2 + \mathcal{E} + \frac{\beta\mathcal{O}_1}{2mc^2} + \frac{\beta\mathcal{O}^2}{2mc^2} - \frac{\mathcal{O}^3}{3m^2c^2} - \frac{\mathcal{E}_1}{8m^2c^2} - \\ &\frac{\beta\mathcal{O}^4}{8m^3c^6} + \frac{\mathcal{O}^5}{30m^4c^8} + \frac{\mathcal{O}^6}{144m^5c^{10}} + \\ &\frac{\beta\mathcal{O}_2}{48m^3c^6} + \frac{\mathcal{E}_2}{384m^4c^8} + \frac{\beta\mathcal{O}_3}{3840m^5c^{10}} - \\ &\frac{\mathcal{O}^7}{840m^6c^{12}} + \frac{\mathcal{E}_3}{46080m^6c^{12}} - \frac{\beta\mathcal{O}^8}{5760m^7c^{14}} + \frac{\beta\mathcal{O}_4}{92160\times 7m^7c^{14}} \end{aligned}$$

where

$$\begin{aligned} \mathcal{E}_1 = \mathcal{O}^2\mathcal{E} + \mathcal{E}\mathcal{O}^2 - 2\mathcal{O}\mathcal{E}\mathcal{O},\ \mathcal{O}_1 = \mathcal{O}\mathcal{E} - \mathcal{E}\mathcal{O} \\ \mathcal{O}_2 = \mathcal{E}_1\mathcal{O} - \mathcal{O}\mathcal{E}_1,\ \mathcal{E}_2 = \mathcal{O}_2\mathcal{O} - \mathcal{O}\mathcal{O}_2 \\ \mathcal{O}_3 = \mathcal{O}\mathcal{E}_2 - \mathcal{E}_2\mathcal{O},\ \mathcal{E}_3 = \mathcal{O}_3\mathcal{O} - \mathcal{O}\mathcal{O}_3 \\ \mathcal{O}_4 = \mathcal{O}\mathcal{E}_3 - \mathcal{E}_3\mathcal{O},\ \mathcal{O}_5 = \mathcal{O}_1\mathcal{E} - \mathcal{E}\mathcal{O}_1 \end{aligned}$$

If we apply the transformation $S_1 = \frac{\beta\mathcal{O}_1}{2mc^2}$ followed by $S_2 = \frac{-\mathcal{O}^3}{3m^2c^4} + \frac{\mathcal{O}_1\mathcal{E}-\mathcal{E}\mathcal{O}_1}{4m^2c^4}$ followed by $S_3 = \frac{\beta}{48m^3c^6}(\mathcal{O}_2 - 6\mathcal{O}_6 + 8\mathcal{O}_{15} + 6\mathcal{O}_{16})$ followed by the next odd operator in lowest order in $\frac{1}{m}$, where $\mathcal{O}_6 = \mathcal{O}_1\mathcal{O}^2 + \mathcal{O}^2\mathcal{O}_1$, $\mathcal{O}_{15} = \mathcal{E}\mathcal{O}^3 - \mathcal{O}^3\mathcal{E}$ and $\mathcal{O}_{16} = \mathcal{O}_5\mathcal{E} - \mathcal{E}\mathcal{O}_5$, then the expansion of H up to order m^{-7} free of odd operators is given by

$$\begin{aligned} \tilde{H}_{FW} &= \beta mc^2 + \mathcal{E} + \frac{\beta}{2mc^2}\mathcal{O}^2 - \frac{1}{8m^2c^4}(\mathcal{O}^2\mathcal{E} + \mathcal{E}\mathcal{O}^2 - 2\mathcal{O}\mathcal{E}\mathcal{O}) - \\ &\frac{\beta}{8m^3c^6}((\mathcal{O}^4 + \mathcal{O}\mathcal{E}\mathcal{O}\mathcal{E} + \mathcal{E}\mathcal{O}\mathcal{E}\mathcal{O} - \mathcal{E}\mathcal{O}^2\mathcal{E} - \mathcal{O}\mathcal{E}^2\mathcal{O})) + \\ &\frac{1}{128m^4c^8}[11(\mathcal{E}\mathcal{O}^4 + \mathcal{O}^4\mathcal{E}) - 12(\mathcal{O}^3\mathcal{E}\mathcal{O} + \mathcal{O}\mathcal{E}\mathcal{O}^3) + 2\mathcal{O}^2\mathcal{E}\mathcal{O}^2] + \\ &\frac{\mathcal{E}'_3}{32m^4c^8} + \frac{\beta}{16m^5c^{10}}\mathcal{O}^6 - \frac{\beta}{96m^5c^{10}}\mathcal{E}'_4 + \frac{\mathcal{E}'_5}{46080m^6c^{12}} - \frac{5\beta}{128m^7c^{14}}\mathcal{O}^8 + \cdots \end{aligned} \tag{4.38}$$

where

$$\begin{aligned} \mathcal{E}'_3 &= \mathcal{O}\mathcal{E}\mathcal{O}\mathcal{E}^2 - \mathcal{E}\mathcal{O}^2\mathcal{E}^2 - \mathcal{E}^2\mathcal{O}^2\mathcal{E} + \mathcal{E}^2\mathcal{O}\mathcal{E}\mathcal{O} + 2\mathcal{O}\mathcal{E}^3\mathcal{O} - \\ &\quad 3(\mathcal{O}\mathcal{E}^2\mathcal{O}\mathcal{E} + \mathcal{E}\mathcal{O}\mathcal{E}^2\mathcal{O}) + 4\mathcal{E}\mathcal{O}\mathcal{E}\mathcal{O}\mathcal{E} \\ \mathcal{E}'_4 &= 3(\mathcal{E}\mathcal{O}^2\mathcal{E}\mathcal{O}^2 - \mathcal{O}\mathcal{E}\mathcal{O}\mathcal{E}\mathcal{O}^2 + \mathcal{O}^2\mathcal{E}\mathcal{O}^2\mathcal{E} - \mathcal{O}^2\mathcal{E}\mathcal{O}\mathcal{E}\mathcal{O}) + \\ &\quad 4(\mathcal{E}^2\mathcal{O}^4 + \mathcal{O}^4\mathcal{E}^2 + \mathcal{E}\mathcal{O}^4\mathcal{E}) + 5(\mathcal{O}^3\mathcal{E}^2\mathcal{O} - \mathcal{O}\mathcal{E}\mathcal{O}^3\mathcal{E} - \mathcal{E}\mathcal{O}^3\mathcal{E}\mathcal{O}) + \\ &\quad 6(\mathcal{O}\mathcal{E}\mathcal{O}^2\mathcal{E}\mathcal{O} + \mathcal{O}\mathcal{E}^2\mathcal{O}^3) - 10(\mathcal{E}\mathcal{O}\mathcal{E}\mathcal{O}^3 + \mathcal{O}^3\mathcal{E}\mathcal{O}\mathcal{E}) \\ \mathcal{E}'_5 &= 1830\mathcal{O}^5\mathcal{E}\mathcal{O} - 98\mathcal{O}\mathcal{E}\mathcal{O}^5 - 225\mathcal{E}\mathcal{O}^6 - 2145\mathcal{O}^6\mathcal{E} - \\ &\quad 1455\mathcal{O}^4\mathcal{E}\mathcal{O}^2 + 473\mathcal{O}^2\mathcal{E}\mathcal{O}^4 + 1608\mathcal{O}^3\mathcal{E}\mathcal{O}^3 \end{aligned}$$

Thus, (4.38) can be used to obtain the third order relativistic correction to the Pauli Hamiltonian. Its nonrelativistic limit can be obtained by subtracting the rest mass energy βmc^2 from (4.38). Because of the terms involved, we will only give the explicit form of the first two corrections to the Pauli Hamiltonian. To do this, we consider only the upper component by taking $\beta = I$.
Put $\mathcal{O} = c\sigma \cdot p$ and $\mathcal{E} = V$. Using the Pauli identity

$$(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma \cdot (a \times b)$$

and that $[\sigma \cdot p, V] = -i\sigma \cdot \nabla V$, the nonrelativistic limit H_{FW} of H is given by

$$\begin{aligned} H_{FW} &= \frac{p^2}{2m} + V - \frac{1}{c^2}\left\{\frac{p^4}{8m^3} - \frac{\sigma \cdot (\nabla V \times p)}{4m^2} - \frac{\Delta V}{8m^2}\right\} + \\ &\quad \frac{1}{c^4}\left\{\frac{p^6}{16m^5} + \frac{(\nabla V)^2}{8m^3} + \frac{p^2 V p^2}{64m^4} + \frac{11}{128m^4}(Vp^4 + p^4 V) + \right. \\ &\quad \left. \frac{3[p^2(\nabla V \cdot \nabla) + (\nabla V \cdot \nabla)p^2]}{32m^4} + \frac{3[p^2(\sigma \cdot \nabla V \times p) + (\sigma \cdot \nabla V \times p)p^2]}{32m^4}\right\} \\ &= H_0 - \frac{1}{c^2}H_1 + \frac{1}{c^4}H_2 + \cdots \end{aligned} \tag{4.39}$$

The approximation of H to order c^{-6} can be obtained easily from (4.38). Similarly, an electromagnetic field version of (4.39) can be obtained by taking $\mathcal{O} = c\sigma \cdot (p - eA)$ where A is the magnetic vector potential.
H_{FW} is therefore the second order nonrelativistic approximation of H.
We now characterize H_{FW} as follows:

Theorem 4.6. *Let V be p^6-bounded (resp. p^4, p^2- bounded) with a bound less than 1 in (4.39). Then H_{FW} is self adjoint on the domain $D(p^6)$. Moreover, H_{FW} is bounded from below and $\sigma_e(H_{FW}) = [0, \infty) = \sigma_e(H_0)$*

Proof. Self adjointness of H_{FW} follows from the Kato-Rellich Theorem. Boundedness from below of H_{FW} is due to the positive sign before the p^6-term. By Fourier transform, we see that

$$\sigma_e(H_{FW}) = \sigma_e\left(p^2 - c^{-2}p^4 + c^{-4}p^6\right) = [0, \infty)$$

It is known that $H_0 = -\Delta + V \geq 0$ in the sense of quadratic forms. Using Fourier transform, we see that $\sigma_e(H_0) = [0, \infty)$. □

This theorem will also hold if $V \to 0$ as $x \to \infty$. If V satisfies some smoothness conditions, then one even get that $\sigma_e(H_{FW}) = \sigma_{ac}(H_{FW})$ by the results of Behncke and Hinton [8].

Remark 4.7. The first order nonrelativistic correction to H can be written down easily from (4.39) and is given by

$$H_{FW}(c^{-2}) = H_0 - \frac{1}{c^2}\left[\frac{p^4}{8m^3} - \frac{1}{4m^2}\sigma \cdot (\nabla V \times p) - \frac{\Delta V}{8m^2}\right]. \tag{4.40}$$

This equation is presented in many books which cover relativistic quantum mechanics, see for example [40]. It is very popular with physicists because the various terms involved have physical interpretation. The first term, H_0, is the usual nonrelativistic Schrödinger Hamiltonian. The second term is the relativistic correction to the kinetic energy. The third term is the spin-orbit coupling term while the fourth term is the Darwin term. The Darwin term only affects the $S-$states i.e for the separated equation, the Darwin term is zero for all $l > 0$.
The characterization of this operator has already been done in [27] where it is shown that, $H_{FW}(c^{-2})$ is bounded from above and $\sigma_e(H_{FW}(c^{-2})) = (-\infty, \frac{c^2}{4}]$. The boundedness from above is essentially due to the negative sign before $\frac{p^4}{8m^3}-$term. In fact in general, the spectrum of higher order nonrelativistic corrections to H alternates between bounded above and below as the sign before the highest power of p changes from negative to positive, i.e. $p_+^2, p_+^6,\ p_+^{10}, \ldots$ are all bounded from below where the subscript represent the sign before p while $p_-^4,\ p_-^8, \ldots$ are all bounded from above.

We now apply the FW method to the separated Dirac equation.

4.2.2.1 The separated FW expansion

We will now express the above FW expansion in a central field. For that reason, we consider a spherically symmetric potential

$$V(r) = \frac{\gamma}{r} I_2 + \sigma_1 \frac{a}{r^2} \quad \gamma, a < 0, \tag{4.41}$$

where $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. This is the Coulomb potential with anomalous magnetic moment. The $\sigma_1 \frac{a}{r^2}$ term represents the anomalous magnetic moment potential and

since it appears only in the off-diagonal, it is repulsive and will only contribute to the radial part of the angular momentum. For these central potentials, the underlying Hilbert space is decomposed into its radial and angular parts as has already been seen in the introductory chapter.

To obtain the radial equation of (4.39), we use the relations

$$\begin{aligned} \nabla V &= \frac{1}{r}\frac{dV}{dr}\vec{r} \\ \nabla V \cdot \nabla &= \frac{dV}{dr}\frac{d}{dr} \end{aligned} \tag{4.42}$$

in order to simplify the expression in (4.39).

The spin-orbit term $\frac{1}{4m^2}\sigma \cdot (\nabla V \times p)$ reduces to $\frac{1}{2m^2} S \cdot L \frac{1}{r}\frac{dV}{dr}$ and for computation purposes, we replace $S \cdot L$ by its eigenvalues. In this case we choose the spin up and therefore $S \cdot L = -(\kappa + 1), \quad \kappa = -(l+1)$.

Using (4.42) and the expression for the spin-orbit term in (4.39), we obtain for $l \geq 0$

$$\begin{aligned} h_\kappa(c^{-4}) &= \frac{p_r^2}{2m} + \frac{\gamma}{r} - \frac{1}{c^2}\left\{\frac{p_r^4}{8m^3} - \frac{\gamma(\kappa+1)}{2m^2r^3} - \frac{\gamma}{4m^2r^3}\right\} + \\ &\quad \frac{1}{c^4}\left\{\frac{p_r^6}{16m^5} + \frac{\gamma^2 r^{-4}}{8m^3} + \frac{p_r^2\gamma r^{-1}p_r^2}{64m^4} + \frac{11(\gamma r^{-1}p_r^4 + p_r^4\gamma r^{-1})}{128m^4} + \right. \\ &\quad \frac{3[p_r^2(-\gamma r^{-2}\frac{d}{dr}) + (-\gamma r^{-2}\frac{d}{dr})p_r^2]}{32m^4} + \\ &\quad \left. \frac{3}{16m^4}\left[p_r^2(\gamma(\kappa+1)r^{-3}) + (\gamma(\kappa+1)r^{-3})p_r^2\right]\right\} \\ &= h_0 - \frac{1}{c^2}h_1 + \frac{1}{c^4}h_2 \end{aligned} \tag{4.43}$$

where $p_r^2 = -\frac{d^2}{dr^2} + \frac{\kappa(\kappa+1)}{r^2} + \frac{2a(\kappa+1)}{r^3} + \frac{a^2}{r^4}$

The operator $h_\kappa(c^{-4})$ can be characterized as in Theorem 4.6 and we see that $\sigma_e(h_\kappa(c^{-4})) = [0, \infty)$ and $h_\kappa(c^{-4})$ is bounded below.

By perturbation theory [25], the first and second order nonrelativistic corrections to the bound state energy for the hydrogen atom can be computed using (4.43) and are given by

$$E_1 = \langle f_0, h_1 f_0 \rangle \tag{4.44}$$

$$E_2 = \langle f_0, h_2 f_0 \rangle + \langle f_0, h_1 f_1 \rangle \tag{4.45}$$

for $f_0, f_1 \in D(h_0)$ for the eigenvalue E_0 and $h_{1/2}$ are as defined above. E_0 here is assumed to be nondegenerate.

These corrections have also been obtained through the Dirac resolvent approach in [26]. Comparing (4.45) with equation (4.26), we see that (4.26) is simple and more compact and does not involve partial derivatives of V.

4.2.2.2 Effects of the correction terms h_1 and h_2

We estimate the significance of the higher order correction terms for the hydrogen like atoms. We consider the hydrogen atom and therefore we set $\gamma = Z\alpha$ and $a = 0$ in (4.41). Z here is the atomic number and can be set to $Z = 1$ while $\alpha = \frac{e^2}{\hbar c}$ is the fine structure. It can be seen that α is proportional to c^{-1}, and c is the speed of light.

From (4.43) we see that the first order correction h_1 is of order α^2 while the second order correction h_2 is of order α^4. Due to the small size of α, the energy splitting due to α^4 term is practically negligible in this case because $Z = 1$. Thus, the second order correction terms h_2 are therefore not useful in the computation of the relativistic corrections to the bound state energy of the hydrogen atom. This claim can easily be seen from the Lamb shift point of view.

The eigenvalues for the hydrogen atom in the nonrelativistic limit with $a = 0$ have the expansion [12]

$$\begin{aligned} E_{n\kappa} \approx & -E_0 - \frac{\alpha^2}{n} E_0 \left(\frac{1}{\kappa} - \frac{3}{4n} \right) + \\ & \frac{\alpha^4}{2n} E_0 \left(\frac{1}{2\kappa^3} - \frac{3}{2n\kappa^2} + \frac{3}{n^2\kappa} - \frac{5}{4n^3} \right) + \cdots \end{aligned} \tag{4.46}$$

where $E_0 = -\frac{mc^2\alpha^2}{2n^2}$ is the eigenvalue of the Hamiltonian h_0. n is the principal quantum number given by $n = n' + \kappa$ and κ is as defined before. The second term in (4.46) corresponds to the first order correction E_1 in (4.44). The third term corresponds to the second order correction E_2 in (4.45) above. From (4.46), one can compute the energy difference explicitly.

Taking $n = 2$ in (4.46), the energy difference $\triangle E_{n\kappa}$ between the level with $\kappa = 1$ and with $\kappa = 2$ can be evaluated. For the first order correction, this difference is already given in [[12], equation 17.3] as $\triangle E^1_{n\kappa} = 0.365 cm^{-1}$.

For the second order correction to the eigenvalue $E_{n\kappa}$, we have $\triangle E^2_{n\kappa} = \frac{5}{16}\alpha^4 E_0 = \frac{5}{32}\alpha^4 Ry = 4.86 \times 10^{-5} cm^{-1}$, where $Ry = 109679 cm^{-1}$ is the Rydberg constant

for hydrogen atom. Thus, the contribution due to E_2 is practically negligible and therefore are of no importance to the energy spectrum of light atoms like the hydrogen atom. Thus, only the first order correction E_1 is important. Further corrections $E_2, \ldots$ to the bound state energy are therefore not necessary. This shows that only the first order relativistic correction to the Pauli Hamiltonian is important. For the Coulomb potential with the anomalous magnetic moment potential, we obtain from (4.43) the first order relativistic correction to the separated Dirac operator H as

$$h_\kappa(c^{-2}) = h_0 - \frac{1}{c^2} h_1. \tag{4.47}$$

where $h_0 = \frac{p_r^2}{2m} + \frac{\gamma}{r}$, $h_1 = \frac{p_r^4}{8m^3} - \frac{\gamma(\kappa+1)}{2m^2 r^3} - \frac{\gamma}{4m^2 r^3}$ and $p_r^2 = -\frac{d^2}{dr^2} + \frac{\kappa(\kappa+1)}{r^2} + \frac{2a(\kappa+1)}{r^3} + \frac{a^2}{r^4}$
We show below that the anomalous magnetic moment makes the operator $h_\kappa(c^{-2})$ essentially self adjoint even if the term $\frac{p_r^4}{8m^3}$ is excluded in (4.47). Note that in many physics books the terms $p^4, p^{-6}, \ldots$ in (4.43) are deleted leading to non self adjoint Hamiltonians if $a = 0$.

Theorem 4.8. *a) Let V be as in (4.41), then $h_\kappa(c^{-2})$ is essentially self adjoint for repulsive coupling constants even if the p_r^4-term is excluded in (4.47), i.e. the spin-orbit term does not destroy the self adjointness of $h_\kappa(c^{-2})$.*

b) Let the effective potential in (4.47) be $q(r)$. Then the spectrum of $h_\kappa(c^{-2})$ is absolutely continuous with no embedded eigenvalues

Proof. Note that $h_\kappa(c^{-2})$ is the first order approximation to the Dirac hamiltonian with anomalous magnetic moment. We show essential self adjointness by use of decomposition method. Assume Dirichlet boundary conditions and denote by $h_\kappa(c^{-2})$ the operator without the p_r^4 for all $\kappa < -1$ and write $h_\kappa(c^{-2}) = h_\kappa^-(c^{-2}) + h_\kappa^+(c^{-2})$ where $h_\kappa^-(c^{-2}) = h_\kappa(c^{-2})|_{(0,1]}$. Now for $u \in \mathcal{D}(h_\kappa^-(c^{-2}))$ and consider only the most singular term, then we have $h_\kappa^-(c^{-2})u(r) = u'' - \frac{a^2}{r^4}u = 0, \quad a < 0$. By reducing to first order, we see that $u(r) = C\exp(\pm\frac{|a|}{r})$. Thus, $def h_\kappa^-(c^{-2}) = (1,1)$ and hence the full operator has $def h_\kappa(c^{-2}) = (0,0)$.
Absolute continuity of the spectrum follows from a result in [8]. Lack of embedded eigenvalues can be shown using the virial theorem. Note that $h_\kappa(c^{-2})$ give rise a fourth order differential equation

$$-u^{(iv)}(r) - u''(r) + q(r)u(r) = \lambda u(r) \tag{4.48}$$

where $u(r)$ is the eigenfunction corresponding to λ. If we neglect the boundary terms then the virial theorem for (4.48) can be obtained easily using the general form given in [9] as $\int_0^\infty [4q(r) + rq'(r)]u^2(r)dr = 0 = 4\lambda \int_0^\infty u^2(r)dr \neq 0$ leading to a contradiction. □

Remark 4.9. If $a = 0$, then for all $\kappa < -1$, the spin-orbit term destroys the essential self adjointness of $h_\kappa(c^{-2})$ if the $\frac{p_r^4}{8m^3}$-term is excluded. The situation only improves when the $\frac{p_r^4}{8m^3}$-term is included since by the partial wave Rellich inequality,

$$\int \frac{|f(r)|^2}{r^4} dr \leq \left[l(l+1) - \frac{3}{4} \right]^{-2} \int |(p_r^2 f)(r)|^2 dr, \; l > 0 \tag{4.49}$$

one can show that $\frac{\gamma(\kappa+1)}{2m^2 r^3}$ is infinitesimally form bounded with respect to p_r^4, see [27].

From a physical point of view, the relativistic corrections are generally expected to be small. But, the perturbation $-\frac{1}{c^2}h_1$ in (4.47) is very large. In fact, this term is so singular that regular perturbation theory is not applicable. The Pauli Hamiltonian h_0 is small against its perturbation h_1 and because of the negative sign before h_1, lower semiboundedness is turned into upper semiboundedness. The essential spectrum of $h_\kappa(c^{-2})$ is given by $\sigma_e(h_\kappa(c^{-2})) = (-\infty, c^2/4]$. We expect h_0 and $h_\kappa(c^{-2})$ to have finitely many eigenvalues in $(-\infty, 0)$ and $(c^2/4, \infty)$ respectively. However, discrete eigenvalues of $h_\kappa(c^{-2})$ in $(c^2/4, \infty)$ have no physical significance in the energy regime $E \geq c^2/4$ because the relativistic $c^{-2}-$corrections are by no means small and these eigenvalues escape to ∞ in the nonrelativistic limit. However, physicists prefer the FW method and have used it to compute the first order relativistic correction to the eigenvalues which seemingly don't exist but surprisingly their results agree well with experimental results especially in the case of pure Coulomb potentials $-\frac{Z\alpha}{r}$ as seen above. This mystery can only be explained via the phenomenon of spectral concentration.

4.2.3 Spectral Concentration

In this section, we will discuss the notion of spectral concentration with respect to the pure Coulomb problem.

Given a self adjoint operator H_0 on some Hilbert space $\mathcal{H}$ and a perturbation H_1 such that $H(k) = H_0 + kH_1$ is a family of self adjoint operators converging in the strong resolvent sense to H_0 as $k \to 0$, it may happen that the spectrum of H_0 is

changed drastically as soon as the perturbation H_1 is turned on. For example, a discrete spectrum may become continuous so that there is no perturbed eigenvalue in any neighbourhood of an eigenvalue E_0 of H_0. This had been observed with the Stark effect in which case H_0 describes the hydrogen atom and H_1 a constant electric field. The perturbed spectrum is purely continuous and covers the whole real line. Therefore $H(k)$ has no eigenvalues. However, one still detects sharp lines whose locations can be accurately evaluated using the Rayleigh-Schrödinger perturbation theory. This observation was first explained by Titchmarsh [48] who introduced the notion of spectral concentration.
Titchmarsh showed that the asymptotic series for Stark "eigenvalues" as derived by Schrödinger, defines nested intervals on which the spectrum of $H(k)$ is concentrated. This concept was further developed by Riddell [45] who established the equivalence of spectral concentration with the existence of pseudoeigenvectors. In the framework of the abstract theory of spectral concentration, Riddell [45] gave a criteria for existence of the spectral concentration of order p. He also observed that this phenomenon of spectral concentration holds for a large class of abstract operators, including the family of Dirac and Schrödinger operators corresponding to hydrogen atom in an electric field.
The theory of spectral concentration was developed first for isolated eigenvalues of finite multiplicity say m [33, 38, 45], but as pointed out in [31, 38], the arguments suffice with a few changes for non-isolated eigenvalues as well.

Definition 4.10. [27],([43],pp. 46) Let H_ε on $D(H_\varepsilon)$, $\varepsilon \in [0, A]$, $A > 0$, be a family of self adjoint operators in some Hilbert space $\mathcal{H}$ and assume that H_ε tends to H_0 in the strong resolvent sense as $\varepsilon \to 0$. Furthermore, let $\Omega, I \subset \mathbb{R}$, $I_\varepsilon \subset I$ be Borel sets and denote by $P_\varepsilon(\Omega)$ the family of spectral projections of H_ε associated with Ω. Then

1) The part of the spectrum of H_ε in I is asymptotically in I_ε or, equivalently, the part of H_ε in I_ε is asymptotically the part of the spectrum of H_0 in I if and only if
$$s - \lim_{\varepsilon \to 0} P_\varepsilon(I \setminus I_\varepsilon) = 0. \tag{4.50}$$

2) Assume $E_0 \in \sigma_d(H_0)$ and J is a Borel set such that $E_0 \in J \subset I$ and $\sigma(H_0) \cap \bar{J} = \{E_0\}$. If P_0 denotes the spectral projector of H_0 corresponding to E_0 then:
The spectrum of H_ε contained in J is concentrated to order $p > 0$ on the

Borel sets $\Omega_\varepsilon \subset J$ if and only if $s-\lim_{\varepsilon\to 0} P_\varepsilon(\Omega_\varepsilon) = P_0$ and $\lim_{\varepsilon\to 0} \varepsilon^{-p}|\Omega_\varepsilon| = 0$, where $|\cdot|$ denotes Lebesgue measure on $\mathbb{R}$.

With this definition, one has the following

Theorem 4.11. *[27] Under the conditions described above, the following assertions are equivalent:*

a) The spectrum of H_ε contained in J is concentrated to order $p>0$ on the sets $\Omega_\varepsilon = \bigcup_{j=1}^{dim\ P_0} \left(\lambda_\varepsilon^{(j)} - o(\varepsilon^p), \lambda_\varepsilon^{(j)} + o(\varepsilon^p)\right)$.

b) There exists a set of unit vectors $\left\{\Phi_\varepsilon^{(j)}\right\}$ and a set of real numbers $\left\{\lambda_\varepsilon^{(j)}\right\}$, $1 \le j \le dim\ P_0$, such that

$$\Phi_\varepsilon^{(j)} \in D(\mathcal{H}), \qquad \lim_{\varepsilon\to 0} \|\Phi_\varepsilon^{(j)} - \Phi_0^{(j)}\| = 0,$$
$$\lim_{\varepsilon\to 0} \varepsilon^{-p} \| \left(H_\varepsilon - \lambda_\varepsilon^{(j)}\right) \Phi_\varepsilon^{(j)} \| = 0, \qquad 1 \le j \le dim\ P_0$$

($\left\{\Phi_\varepsilon^{(j)}\right\}$ is called an asymptotic basis of order p for $P_\varepsilon(J)$; $\Phi_\varepsilon^{(j)}, \lambda_\varepsilon^{(j)}$ are called pseudoeigenvectors and pseudoeigenvalues of H_ε).

c) There exists a set of unit vectors $\left\{\Psi_\varepsilon^{(j)}\right\}$ and a set of complex numbers $\left\{\mu_\varepsilon^{(j)}\right\}$, $1 \le j \le dim\ P_0$, such that

$$\lim_{\varepsilon\to 0} \|\Psi_\varepsilon^{(j)} - \Phi_0^{(j)}\| = 0,$$
$$\lim_{\varepsilon\to 0} \varepsilon^{-p} \| \left((H_\varepsilon - i)^{-1} - \mu_\varepsilon^{(j)}\right) \Psi_\varepsilon^{(j)} \| = 0, \qquad 1 \le j \le dim\ P_0.$$

The numbers $\mu_\varepsilon^{(j)}$ can be chosen such that $\lambda_\varepsilon^{(j)} = (\mu_\varepsilon^{(j)})^{-1} + i$ is real and Ω_ε are given by the unionof intervals of length $o(\varepsilon^p)$ centered at $\lambda_\varepsilon^{(j)}$

Proof. For the proof of this theorem see [27] □

Here, we will only give an illustration of this concept for the separated Dirac operator (4.47) with $a = 0$.

Spectral concentration with pure Coulomb potential

Recall that, the usual way to treat relativistic corrections for eigenvalues is to apply first order perturbation theory to (4.47). For the pure Coulomb potential $V = \gamma/r,\ \gamma < 0$, the results can be compared with the exact solution of the Dirac equation. In that case, first order perturbation theory indeed gives the correct expansion of the Dirac eigenvalue up to order c^{-2} [19, 40] which is very surprising because h_0 is an infinitesimally small perturbation of $c^{-2}h_1$. Moreover, the relativistic perturbation converts the discrete spectrum of h_0 which is in $(-\infty, 0)$ into a continuous one extending from $-\infty$ to $c^2/4$. Thus, the perturbation $c^{-2}h_1$ changes the spectrum drastically. As stated above, the discrete eigenvalues of $h_\kappa(c^{-2})$ have no physical significance in the nonrelativistic limit. On the other hand, for the usual nonrelativistic atomic bound states, the expectation value of the kinetic energy p_r^2 is small compared to rest mass of the electron, so that the $-c^{-2}p_r^4$ term will be a small correction. It means that, something like a trace of the bound state(pseudoeigenvector) remains when the relativistic correction $-c^{-1}h_1$ is turned on which points to the notion of spectral concentration and pseudoeigenvalues.

In order to prove spectral concentration of $h_\kappa(c^{-2})$ at the discrete eigenvalue of h_0, one must first state in what sense $h_\kappa(c^{-2})$ approaches h_0 as $c \to \infty$. It turns out that [27]

$$s - \lim_{c\to\infty} \left(h_\kappa(c^{-2}) - z\right)^{-1} = (h_0 - z)^{-1}, \quad Im\ z \neq 0$$

Let E_0 be an isolated nondegenerate eigenvalue of h_0 with associated eigenvector f_0. We say that $E_0 + \frac{1}{c^2}E_1$, where $E_1 = \langle f_0, h_1 f_0\rangle$ is a first-order pseudoeigenvalue of $h_\kappa(c^{-2})$ if and only if there exists $f(c^{-2})$ with [43]

$$f(c^{-2}) \xrightarrow{s} f_0,\ c(h_\kappa(c^{-2}) - E_0 - \frac{1}{c^2}E_1)f(c^{-2}) \xrightarrow{s} 0 \ \text{ as } c^{-2} \to 0 \tag{4.51}$$

Mathematically, the existence of a first-order pseudoeigenvalue of $h_\kappa(c^{-2})$ is equivalent to the notion of first-order spectral concentration [26]. In that case, one says that the spectrum of $h_\kappa(c^{-2})$ is asymptotically concentrated to first order on the union of intervals of length $O(c^{-2})$ centered at the first-order pseudoeigenvalues $E_0 + \frac{1}{c^2}E_1$ [27]. For a detailed construction of these pseudoeigenvalues and the corresponding pseudoeigenvectors we refer to [45] and [48].

To prove that $E_0 + \frac{1}{c^2}E_1$ is a first-order pseudoeigenvalue of $h_\kappa(c^{-2})$, one has to

verify that f_0 lies in the domain of h_1 for all $\gamma \neq 0$. Since $f_0 = O(r^{l+1})$ near the origin, we see that $f_0 \in D(h_1)$ if and only if $l \geq 2$. Thus, we have the following

Theorem 4.12. *Let $V = \gamma/r, \quad l \geq 2 \quad \gamma \neq 0$. If E_0 is an eigenvalue of h_0 with corresponding eigenvector f_0, and $E_1 = \langle f_0, h_1 f_0 \rangle$ then $E_0 + \frac{1}{c^2}E_1$ is a first-order pseudoeigenvalue of $h_\kappa(c^{-2})$ i.e the spectrum of $h_\kappa(c^{-2})$ is asymptotically concentrated to first-order in the interval $\left(E_0 + \frac{1}{c^2}E_1 - O(c^{-2}), E_0 + \frac{1}{c^2}E_1 + O(c^{-2})\right)$ as $c \to \infty$.*

This result which gives a good illustration of the notion of spectral concentration, is a specific case of the following general result given by Gesztesy, Grosse and Thaller [27].

Theorem 4.13. *[27] Let $V(r) = \frac{\gamma}{r}, \quad l \geq 2, \ \gamma \neq 0$. If $E_{n,l}, \ n = 0, 1, 2, \ldots$ are discrete eigenvalues of h_0 with corresponding eigenfunctions $\phi_{n,l}$, then the spectrum of $h_\kappa(c^{-2})$ is concentrated to first order on the union of intervals of length $o(c^{-2})$ centered at the first-order pseudoeigenvalues $E_{n,\kappa}(c) = E_{n,l} + \frac{1}{c^2}E^1_{n,\kappa}$ of $h_\kappa(c^{-2})$.*

For generalization of the concept of spectral concentration to higher order and to isolated eigenvalues of finite multiplicity, we refer to [27, 33, 38, 43, 45].

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