SELF-ADJOINT EXTENSIONS TO THE DIRAC COULOMB HAMILTONIAN

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Chapter 1

Introduction

The Dirac equation is the relativistic generalization of the Schrödinger equation for spin 1/2 particles. It is written in the form

$$-i\hbar c\left(\sum_{i=1}^{3}\alpha^i\frac{\partial\psi}{\partial x^i}\right)+\beta mc^2\psi=i\hbar\frac{\partial\psi}{\partial t}, \tag{1.1}$$

where ψ is a four component Dirac spinor and the coefficients α^i and β are 4×4 matrices. Like the Schrödinger equation, the Dirac equation can be written as a time-independent eigenvalue equation $\hat{H}\psi=E\psi$ for a Hamiltonian operator $\hat{H}$ and energy eigenvalue E through separation of variables. The energy eigenvalues obtained by solving this equation must be real– one of the axioms of quantum mechanics is that physical observables, in this case energy, correspond to self-adjoint operators, in this case the Hamiltonian operator $\hat{H}$, acting on the Hilbert space $\mathcal{H}$ which describes the system in question. It can easily be shown that self-adjoint operators must have real eigenvalues.

The reality of the energy eigenvalues becomes important when examining hydrogenic atoms using the Dirac equation. These atoms can be described by a Coulomb potential, $V(r)=-Ze^2/r$, where Z is the number of protons in the nucleus and e is the elementary charge. When the nonrelativistic Schrödinger equation is solved for a

Coulomb potential, the energy levels are given by the familiar Rydberg formula

$$E_n = -\frac{Z^2\alpha^2 mc^2}{2}\frac{1}{n^2} \tag{1.2}$$

where Z is the number of protons in the atomic nucleus, α is the fine structure constant, m is the electron mass, c is the speed of light, and n a positive integer. Note that this formula assumes a stationary positive charge of infinite mass at the center of the atom, and that the energy levels for a more realistic model of an atom with a nucleus of finite mass M are given by replacing m with the reduced mass $\mu = mM/(m+M)$ in Eq. (1.2).

When the Dirac equation in a Coulomb potential is used instead of the nonrelativistic Schrödinger equation, the energy levels are instead given by

$$E_{n,j} = mc^2\left[1 + \frac{\alpha^2 Z^2}{\left(n' - j - \frac{1}{2} + \sqrt{\left(j+\frac{1}{2}\right)^2 - \alpha^2 Z^2}\right)^2}\right]^{-1/2}, \tag{1.3}$$

where n' is a positive integer and j is the total angular momentum of the electron. The total angular momentum j can take on values in the range $1/2, 3/2, \ldots, n' - 1/2$. The eigenvalues in Eq. (1.3) match those in Eq. (1.2) in the limit $\alpha Z \ll 1$, noting that in Eq. (1.2), a free electron is considered to have an energy of 0, while in Eq. (1.3), a free electron has energy mc^2.

A problem arises with Eq. (1.3) when $\alpha Z > j + \frac{1}{2}$. The quantity $\sqrt{\left(j+\frac{1}{2}\right)^2 - \alpha^2 Z^2}$ is imaginary, causing Eq. (1.3) to yield complex energy eigenvalues. Since the eigenvalues of a self-adjoint operator must all be real, this indicates that the Hamiltonian cannot be self-adjoint when $\alpha Z > j + \frac{1}{2}$.

This issue raises two questions. The first is whether there is a physical explanation for the failure of Eq. (1.2) for large Z. The second is whether this problem can be addressed mathematically by defining a new, self-adjoint operator $\hat{H}_{\text{ex}}$ which is constructed from the old Hamiltonian $\hat{H}$ as a self-adjoint extension. In this thesis, I will answer both of these questions in the affirmative, relying and building upon work

done by others on these questions. I will show how the failure of Eq. (1.2) can be motivated by physical considerations, and I will examine a family of self-adjoint extensions to the Dirac Coulomb Hamiltonian constructed using von Neumann's method of deficiency indices.

Chapter 2

Theoretical Background

2.1 The Dirac Equation

The usual Schrödinger equation for a single particle in three spatial dimensions,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{2.1}$$

make use of a nonrelativistic Hamiltonian operator $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{\vec{x}})$, which is derived by quantizing the Hamiltonian for a classical nonrelativistic particle. To incorporate the effects of special relativity, the Hamiltonian must be altered to incorporate the relativistic energy-momentum relation

$$E = \sqrt{p^2c^2 + m^2c^4}, \tag{2.2}$$

where $p^2 = p_x^2 + p_y^2 + p_z^2$ is the total momentum squared. Following the prescriptions of canonical quantization, we replace E with $\hat{H}$ and p with $\hat{p}$ in Eq. (2.2) to find

$$\hat{H} = \sqrt{\hat{p}^2c^2 + m^2c^4}. \tag{2.3}$$

From canonical quantization, we assume that the action of $\hat{p}$ on a state $|\psi\rangle$ is given by

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial\psi}{\partial x}. \tag{2.4}$$

From Eqs. (2.3) and (2.4), we can calculate the action of $\hat{H}$ on a state $|\psi\rangle$. We find

$$\langle x|\hat{H}|\psi\rangle = \left(\sqrt{\sum_{i=1}^{3} -\hbar^2 c^2 \frac{\partial^2}{\partial x_i^2} + m^2c^4}\right)\psi(x). \tag{2.5}$$

The only way to make sense of the expression in the parenthesis is to write it as a series expansion. Using the series expansion

$$\sqrt{p^2c^2 + m^2c^4} = mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \ldots, \tag{2.6}$$

we find

$$\langle x|\hat{H}|\psi\rangle = \left(mc^2 - \frac{\hbar^2}{2m}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2} + \frac{\hbar^4}{8m^3c^2}\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{\partial^4}{\partial x_i^2 x_j^2} + \ldots\right)\psi(x). \tag{2.7}$$

so that the relativistic version of the Schrödinger equation is given by

$$i\hbar\frac{\partial\psi}{\partial t} = \left(mc^2 - \frac{\hbar^2}{2m}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2} + \frac{\hbar^4}{8m^3c^2}\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{\partial^4}{\partial x_i^2 x_j^2} + \ldots\right)\psi(x). \tag{2.8}$$

We see that there is a problem. The series expansion in Eq. (2.6) does not terminate, which means that Eq. (2.8) is a partial differential equation of infinite order. Besides being difficult to solve, partial differential equations of infinite order are nonlocal. This makes them unsuitable to describe physics which we believe is local. Note that this problem only occurs when working in position space. In momentum space, there is no problem with the factor $\sqrt{p^2c^2 + m^2c^4}$, since the $\hat{p}$ operator does not correspond to a differential operator. However, for the sake of finding an equation which we can use when working in position space, we abandon Eq. (2.8).

There are multiple ways to circumvent this problem. One method is to abandon the requirement that the equation for the wavefunction be given in the Schrödinger form

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle. \tag{2.9}$$

Instead, we can use the relation $E^2 = p^2c^2 + m^2c^4$ to write an equation which is

second order in time. We replace $E \rightarrow i\hbar(\partial/\partial t)$ and $p_i \rightarrow -i\hbar(\partial/\partial x_i)$ to get the Klein-Gordon equation,

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \left(\sum_{i=1}^{3} \frac{\partial^2 \psi}{\partial x_i^2} \right) + mc^2 \psi. \tag{2.10}$$

However, it is found that the Klein-Gordon equation describes the behavior of spin-0 particles. Electrons are spin 1/2 particles, so the Klein-Gordon equation will not give the correct behavior of electrons bound to an atomic nucleus.

Paul Dirac developed a different approach which is more appropriate for describing the behavior of spin 1/2 particles. He noted that the problem of the infinite Taylor series due to the square root in the relativistic energy-momentum relation would disappear if we were able to write

$$p^2 c^2 + m^2 c^4 = \left(\sum_{i=1}^{3} c\alpha^i p_i + \beta mc^2 \right)^2 \tag{2.11}$$

for some coefficients α^i and β. Expanding out the square in Eq. (2.11), we find that this is only possible if α^i and β fulfill the conditions

$$\left\{ \alpha^i, \beta \right\} = 0, \tag{2.12}$$

$$\beta^2 = I, \tag{2.13}$$

$$\left\{ \alpha^i, \alpha^j \right\} = 2\delta^{ij} I, \tag{2.14}$$

where the curly brackets denote the anticommutator, δ^{ij} is the Kronecker delta function, and I is the multiplicative identity. This is not possible if α^i and β are scalars. However, if they are matrices, these relations can be fulfilled. For $3+1$ dimensional spacetime, the smallest such matrices for which this factorization is possible are 4×4. One possible choice of these matrices is

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

where σ^i are the Pauli matrices and I_2 is the 2×2 identity matrix.

Using this factorization, the Dirac equation for a free particle is thus

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\left(\sum_{i=1}^{3}\alpha^i\frac{\partial\psi}{\partial x^i}\right) + \beta mc^2\psi, \tag{2.15}$$

where ψ is a four component Dirac spinor. For particles in a potential, the Dirac equation is modified according to the nature of the potential. For a scalar potential $V(r)$, the Dirac equation is

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\left(\sum_{i=1}^{3}\alpha^i\frac{\partial\psi}{\partial x^i}\right) + \beta\left(mc^2 + V(r)\right)\psi. \tag{2.16}$$

Electromagnetic interactions are described by a four-vector potential, $\left(\phi(r), \vec{A}(r)\right)$, where $\phi(r)$ is the electric potential and $\vec{A}(r)$ is the magnetic vector potential. For such potentials, the free particle Dirac equation is modified according to the prescription

$$i\hbar\frac{\partial}{\partial t} \rightarrow i\hbar\frac{\partial}{\partial t} - q\phi(r), \tag{2.17}$$

$$-i\hbar\frac{\partial}{\partial x_i} \rightarrow -i\hbar\frac{\partial}{\partial x^i} - qA_i(r), \tag{2.18}$$

where q is the charge of the particle.

For the Coulomb problem, we take $\phi(r) = Ze/r$ and $A_i(r) = 0$, and note that we are working with an electron of charge $q = -e$. This yields the equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-i\hbar c\sum_{i=1}^{3}\alpha^i\frac{\partial}{\partial x^i} + \beta mc^2 - \frac{Ze^2}{r}\right]\psi, \tag{2.19}$$

so that the appropriate Hamiltonian is given by

$$\hat{H} = -i\hbar c\left(\sum_{i=1}^{3}\alpha^i\frac{\partial}{\partial x^i}\right) + \beta mc^2 - \frac{Ze^2}{r} \tag{2.20}$$

2.2 Operator Domains

In quantum theory, states of a physical system corresponds to elements of a Hilbert space $\mathcal{H}$. In the case of the Dirac Coulomb problem in 3+1 dimensions, the Hilbert space $\mathcal{H}$ is the space of continuous, square integrable functions from $\mathbb{R}^3$ to $\mathbb{C}^4$. Given two such functions $\phi(\vec{r})$ and $\psi(\vec{r})$ corresponding to states $|\phi\rangle$ and $|\psi\rangle$, we define the inner product

$$\langle\phi|\psi\rangle = \int d^3r \sum_{i=1}^{4} \phi_i^*(\vec{r})\psi_i(\vec{r}) \tag{2.21}$$

where $\phi_i(\vec{r})$ and $\psi_i(\vec{r})$ are the ith components of $\phi(\vec{r})$ and $\psi(\vec{r})$.

A operator $\hat{A}$ on $\mathcal{H}$ acts on element $|\psi\rangle$ of $\mathcal{H}$ to return another element, $\hat{A}|\psi\rangle$, of $\mathcal{H}$. A linear operator $\hat{A}$ is an operator which satisfies the requirement

$$\hat{A}(a|\psi_1\rangle + b|\psi_2\rangle) = a\hat{A}|\psi_1\rangle + b\hat{A}|\psi_2\rangle \tag{2.22}$$

for all $|\psi_1\rangle$, $|\psi_2\rangle$ in $\mathcal{H}$ and complex numbers a and b.

Not all operators of interest in quantum physics can be defined on the entire space $\mathcal{H}$. For example, consider the Hilbert space $\mathcal{H}$ of square integrable functions $f(x)$ which take $\mathbb{R}$ to $\mathbb{C}$. This Hilbert space is frequently used in nonrelativistic single dimensional quantum mechanics for systems like the harmonic oscillator . Given an element $|f\rangle$ of $\mathcal{H}$, which corresponds to a square integrable function $f(x)$, the position operator $\hat{x}$ acts on $|f\rangle$ to yield a state $\hat{x}|f\rangle$, which corresponds to a function $xf(x)$. However, even though $f(x)$ is square integrable, it may not be that $xf(x)$ is square integrable. For example, the function

$$f(x) = \frac{1}{\sqrt{1+x^2}}, \tag{2.23}$$

is square integrable, but

$$xf(x) = \frac{x}{\sqrt{1+x^2}}, \tag{2.24}$$

is not square integrable. The action of the operator $\hat{x}$ on a state $|f\rangle$ cannot be defined for all $|f\rangle$ in $\mathcal{H}$.

We see some operators cannot be defined on the whole of $\mathcal{H}$. Instead, the operator is assigned a domain, which is in general a subspace of $\mathcal{H}$. For example, we can define the domain of $\hat{x}$ to be the space of all functions $f(x)$ which take $\mathbb{R}$ to $\mathbb{C}$ such that $xf(x)$ is square integrable.

When we define an operator, we must take care to specify the domain of the operator. For many operators, the domain can be defined as those functions which satisfy a certain boundary condition. For the three dimensional Dirac Coulomb problem, we can define the domain of our Hamiltonian $\hat{H}$ to be those $|\psi\rangle$ for which the function corresponding to $\hat{H}\,|\psi\rangle$ is square integrable.

When we solve the Dirac equation in the Coulomb potential, we will separate variables to get angular and radial equations. The radial equations will be of most interest, and can be written in the form

$$\hat{H}_{\mathrm{r}}\,|\phi\rangle = E\,\phi\rangle \tag{2.25}$$

for a radial Hamiltonian $\hat{H}_{\mathrm{r}}$, where $|\phi\rangle$ is an element of the Hilbert space $\mathcal{H}_{\mathrm{r}}$ of functions $\phi(r)$ from the nonnegative real numbers $\mathbb{R}^+$ to $\mathbb{C}^2$. The domain of the operator $\hat{H}_{\mathrm{r}}$ is defined to be those functions $\phi(r)$ which satisfy $\phi(0) = 0$.

2.3 Operator Adjoints and Self-Adjoint Operators

Given an operator $\hat{A}$ on a Hilbert space $\mathcal{H}$ with domain $\mathrm{Dom}(\hat{A})$, we can define another operator $\hat{A}^\dagger$ called the adjoint of $\hat{A}$. The action of the adjoint operator on an element of $\mathcal{H}$ is defined by the requirement

$$\langle\phi|A\psi\rangle = \langle A^\dagger\phi|\psi\rangle \tag{2.26}$$

for all $|\psi\rangle$ in $\mathrm{Dom}(\hat{A})$ and $|\phi\rangle$ in $\mathrm{Dom}(\hat{A}^\dagger)$. The domain $\mathrm{Dom}(\hat{A}^\dagger)$ is defined to be all $|\phi\rangle$ such that for every $|\psi\rangle$ in $\mathrm{Dom}(\hat{A})$, Eq. 2.26 holds. In general, the domain $\mathrm{Dom}(\hat{A})$ and the domain $\mathrm{Dom}(\hat{A}^\dagger)$ are different.

A self-adjoint operator is an operator $\hat{A}$ such that $\hat{A} = \hat{A}^\dagger$. This equality has two

conditions: (i) $\hat{A}\,|\psi\rangle = \hat{A}^\dagger\,|\psi\rangle$ for all $|\psi\rangle$ in $\mathrm{Dom}(\hat{A})$, and (ii) $\mathrm{Dom}(\hat{A}) = \mathrm{Dom}(\hat{A}^\dagger)$. Condition (i) alone is not sufficient for self-adjointness.

Some operators which appear naively to be self-adjoint are not. For example, consider momentum operator $\hat{p}$ in the one dimensional infinite square well. The Hilbert space $\mathcal{H}_{\mathrm{sw}}$ consists of differentiable square integrable functions $f(x)$ on the interval $[0, L]$. The momentum operator acts on a function $f(x)$ to give $(\hbar/i)f'(x)$. The domain of the momentum operator $\hat{p}$ is defined to be those functions $f(x)$ which meet the boundary conditions $f(0) = f(L) = 0$. We see that the domain of the adjoint consists of all functions $g(x)$ which meet the condition

$$\langle g|\hat{p}f\rangle - \langle \hat{p}^\dagger g|f\rangle = \int_0^L g^*(x)\frac{\hbar}{i}\frac{df}{dx}(x) - (\hat{p}^\dagger g)^*(x)f(x)dx = 0. \tag{2.27}$$

Integrating by parts, we see that this condition will be met if we have

$$\frac{\hbar}{i}g^*(x)f(x)\Big|_{x=0}^{L} - \int_0^L \left[\frac{\hbar}{i}\frac{dg^*}{dx}(x) + \left(\hat{p}^\dagger g\right)^*(x)\right] f(x)dx = 0. \tag{2.28}$$

We find that this will be only if

$$\left(\hat{p}^\dagger g\right)(x) = \frac{\hbar}{i}\frac{dg}{dx}(x), \tag{2.29}$$

and

$$g^*(L)f(L) = g^*(0)f(0). \tag{2.30}$$

We see that Eq. 2.30 is true even if $g^*(L)$ and $g^*(0)$ are nonzero, because $f(L) = f(0) = 0$. Thus the domain of $\hat{p}^\dagger$ is larger than that of $\hat{p}$, because $\mathrm{Dom}(\hat{p}^\dagger)$ includes functions which do not have to vanish at the endpoints of the interval.

2.4 Self-Adjoint Extensions to an Operator

Given an operator $\hat{A}$ with domain $\mathrm{Dom}(\hat{A})$ such that $\mathrm{Dom}(\hat{A}) \subset \mathrm{Dom}(\hat{A}^\dagger)$, it is sometimes possible to construct a new operator $\hat{A}_{\mathrm{ex}}$ which satisfies the following requirements: (i) $\hat{A}_{\mathrm{ex}}\,|\psi\rangle = \hat{A}\,|\psi\rangle$ for all $|\psi\rangle \in \mathrm{Dom}(\hat{A})$, (ii) $\mathrm{Dom}(\hat{A}) \subset \mathrm{Dom}(\hat{A}_{\mathrm{ex}}) \subset$

$\mathrm{Dom}(\hat{A}^\dagger)$, and (iii) $\hat{A}_{\mathrm{ex}}^\dagger = \hat{A}_{\mathrm{ex}}$. When this is possible, the operator $\hat{A}_{\mathrm{ex}}$ is called a self-adjoint extension of $\hat{A}$.

One technique [4] for obtaining a self-adjoint extension of an operator $\hat{A}$ is the method of deficiency indices, discovered by John von Neumann. We define a symmetric operator to be an operator $\hat{A}$ such that $\langle \hat{A}\phi|\psi\rangle = \langle \phi|\hat{A}\psi\rangle$ for all $|\phi\rangle$ and $|\psi\rangle$ in $\mathrm{Dom}(\hat{A})$. For such an operator, we will have $\hat{A}\,|\psi\rangle = \hat{A}^\dagger\,|\psi\rangle$ for all $|\psi\rangle$ in $\mathrm{Dom}(\hat{A})$, though we will not necessarily have $\mathrm{Dom}(\hat{A}) = \mathrm{Dom}(\hat{A}^\dagger)$. We solve the eigenvalue equations

$$\hat{A}^\dagger\,|\phi_\pm\rangle = \pm i\,|\phi_\pm\rangle \tag{2.31}$$

and examine the solution spaces $\mathcal{S}_\pm = \left\{|\phi\rangle : \hat{A}^\dagger\,|\phi\rangle = \pm i\,|\phi\rangle\right\}$. Let $\mathcal{N}_\pm$ be the dimension of $\mathcal{S}_\pm$. Assume $\mathcal{N}_+ = \mathcal{N}_-$. We define an isometry to be a function $U : \mathcal{S}_+ \to \mathcal{S}_-$ such that $\langle\phi|\phi\rangle = \langle U\phi|U\phi\rangle$ for all $|\phi\rangle$ in $\mathcal{S}_+$. If $\mathcal{N}_+ = \mathcal{N}_- = n$, the set of all isometries is isomorphic to $U(n)$, the set of $n \times n$ unitary matrices.

For every isometry U, we can define a self-adjoint extension $\hat{A}_U$. The extension is defined by the conditions

$$\hat{A}_U\,|\phi\rangle = \hat{A}^\dagger\,|\phi\rangle\,, \tag{2.32}$$

for all $|\phi\rangle$ in $\mathrm{Dom}(\hat{A}_U)$, and

$$\mathrm{Dom}(\hat{A}_U) = \left\{|\phi_0\rangle + c\,(|\phi_+\rangle + U\,|\phi_+\rangle) : |\phi_0\rangle \in \mathrm{Dom}(\hat{A}), c \in \mathbb{C}, |\phi_+\rangle \in \mathcal{S}_+\right\}.$$

In the special case that $\mathcal{N}_+ = \mathcal{N}_- = 1$, we can write

$$\mathrm{Dom}(\hat{A}_U) = \left\{|\phi_0\rangle + c\left(|\phi_+\rangle + e^{i\theta}\,|\phi_-\rangle\right) : |\phi_0\rangle \in \mathrm{Dom}(\hat{A}), c \in \mathbb{C}\right\},$$

where $\hat{A}^\dagger\,|\phi_\pm\rangle = \pm i\,|\phi_\pm\rangle$ and $\langle\phi_\pm|\phi_\pm\rangle = 1$.

2.5 The Dirac Equation in the Coulomb Potential

The Dirac equation for a Coulomb potential is given by

$$\left[-i\left(\sum_{i=1}^{3}\alpha^i\frac{\partial}{\partial x^i}\right)+\beta-\frac{\alpha Z}{r}\right]\Psi=i\frac{\partial\Psi}{\partial t} \tag{2.33}$$

where we have set $\hbar = c = m = 1$, α is the fine structure constant $\alpha = e^2/\hbar c \approx 1/137$, and we have defined

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

where the σ^i are the Pauli matrices and I_2 is the two dimensional identity matrix. We can separate out the time variable by setting $\Psi(\vec{r},t) = \psi(\vec{r})T(t)$, yielding the time independent Dirac equation

$$\left[-i\left(\sum_{i=1}^{3}\alpha^i\frac{\partial}{\partial x^i}\right)+\beta-\frac{\alpha Z}{r}\right]\psi=E\psi, \tag{2.34}$$

as well as the familiar time dependence, $T(t) = e^{-iEt}$.

Following [2], we can separate variables to eliminate the time and angular variables. We separate

$$\psi(\vec{r}) = \begin{pmatrix} irg(r)\Theta_{j\ell m}(\Omega) \\ -rf(r)\Theta_{j\ell' m}(\Omega) \end{pmatrix} \tag{2.35}$$

where $\Theta_{j\ell m}(\Omega)$ is a two component spinor with definite total angular momentum j, orbital angular momentum ℓ, and spin angular momentum m, and $\ell' = 2j - \ell$. After some algebra, this gives rise to the eigenvalue equation

$$\begin{pmatrix} 1-\frac{Z\alpha}{r} & -\frac{d}{dr}+\frac{\kappa}{r} \\ \frac{d}{dr}+\frac{\kappa}{r} & -1-\frac{Z\alpha}{r} \end{pmatrix}\begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = E\begin{pmatrix} f(r) \\ g(r) \end{pmatrix}, \tag{2.36}$$

where $\kappa = j + 1/2$. We note that this has the form of an eigenvalue equation for a

radial Hamiltonian $\hat{H}_r$ whose action on a state $|\phi\rangle$ is given by

$$\langle r|\hat{H}_r|\phi\rangle = \begin{pmatrix} 1-\frac{Z\alpha}{r} & -\frac{d}{dr}+\frac{\kappa}{r} \\ \frac{d}{dr}+\frac{\kappa}{r} & -1-\frac{Z\alpha}{r} \end{pmatrix} \begin{pmatrix} \phi_1(r) \\ \phi_2(r) \end{pmatrix} = E \begin{pmatrix} \phi_1(r) \\ \phi_2(r) \end{pmatrix}, \tag{2.37}$$

where

$$\langle r|\phi\rangle = \begin{pmatrix} \phi_1(r) \\ \phi_2(r) \end{pmatrix}. \tag{2.38}$$

Eq. (2.36) is a system of two first-order differential equations, so there are in general two linearly independent solutions. For arbitrary E, one solution is given by

$$\begin{aligned} \phi_1(r) &= \sqrt{1+E}\exp(-\rho/2)\rho^{\lambda} \\ &\times \left[F(\lambda - E\delta_E|1+2\lambda|\rho) + \frac{E\delta_E-\lambda}{\chi-\delta_E}F(\lambda-E\delta_E+1|1+2\lambda|\rho)\right], \end{aligned} \tag{2.39}$$

$$\begin{aligned} \phi_2(r) &= \sqrt{1-E}\exp(-\rho/2)\rho^{\lambda} \\ &\times \left[-F(\lambda - E\delta_E|1+2\lambda|\rho) + \frac{E\delta_E-\lambda}{\chi-\delta_E}F(\lambda-E\delta_E+1|1+2\lambda|\rho)\right], \end{aligned} \tag{2.40}$$

where $F(a|b|c)$ is the confluent hypergeometric function (see Appendix A) [1] and we have defined $\rho = 2r\sqrt{1-E^2}$, $\delta_E = \alpha Z/\sqrt{1-E^2}$, and $\lambda = \sqrt{\kappa^2-\alpha^2Z^2}$. We denote this solution as $\phi^+_E(r)$ and its components by $\phi^+_{E,1}(r)$ and $\phi^+_{E,2}(r)$. The other linearly independent solution is denoted by $\phi^-_E(r)$ and its components by $\phi^-_{E,1}(r)$ and $\phi^-_{E,2}(r)$. The solution $\phi^-_E(r)$ is obtained by replacing λ with $-\lambda$ in Eq. (2.39) and (2.40). The hypergeometric functions diverge as ρ tends towards infinity unless

$$\lambda - E\delta_E = -n' \tag{2.41}$$

[1] The confluent hypergeometric function is defined as a power series, $F(a|b|x) = 1+\frac{a}{b}x+\frac{a(a+1)}{b(b+1)}\frac{x^2}{2!}+\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^3}{3!}+\ldots$. As x tends to infinity, we have $F(a|b|x) \sim \frac{\Gamma(b)}{\Gamma(a)}\exp[(a-b)x]$. If a is a nonpositive integer, the series will have only finitely many terms, so that $F(a|b|x)$ is a polynomial.

for some nonnegative integer n, yielding the energy eigenvalues

$$E_{n',\kappa} = \left[1 + \frac{\alpha^2 Z^2}{\left(n' + \sqrt{\kappa^2 - \alpha^2 Z^2}\right)^2}\right]^{-1/2}, \tag{2.42}$$

when $\alpha Z < \kappa$. If we set $n' = n - j - 1/2$, we recover the well-known Sommerfeld fine structure formula

$$E_{n,\kappa} = \left[1 + \frac{\alpha^2 Z^2}{\left(n - \kappa + \sqrt{\kappa^2 - (\alpha Z)^2}\right)^2}\right]^{-1/2}. \tag{2.43}$$

We find the linear combination of $\phi_E^+(r)$ and $\phi_E^-(r)$ which is consistent with the boundary condition $\phi_E(0) = 0$ by noting that $\phi_E^-(r)$ diverges at the origin when λ is positive, i.e. when $\alpha Z < \kappa$. Thus the energy eigenfunction for the energy $E_{n,\kappa}$ is $\phi^+_{E_{n,\kappa}}(r)$, normalized appropriately.

For the ground state, we have $E_{1,1} = \sqrt{1 - (\alpha Z)^2}$ and a wavefunction $\phi(r)$ with components

$$\phi_{E_{1,1},1}(r) = \sqrt{1 + E_{1,1}} \exp(-\rho/2)\rho^{\lambda}, \tag{2.44}$$

$$\phi_{E_{1,1},2}(r) = \sqrt{1 - E_{1,1}} \exp(-\rho/2)\rho^{\lambda}. \tag{2.45}$$

Chapter 3

The Self-Adjoint Extension

3.1 The Problem of Self-Adjointness

There is a problem with the fine structure formula in Eq. (2.43). When $\kappa < \alpha Z$, the energy eigenvalues are complex. Furthermore, the energy eigenfunctions for arbitrary E no longer meet the boundary condition $\phi_E(r) = 0$. Near the origin, we have $\phi^{\pm}_{E,1}(r) \sim \phi^{\pm}_{E,2}(r) \sim r^{\pm\lambda}$, and when $\kappa < \alpha Z$, we see $\lambda = \sqrt{\kappa^2 - (\alpha Z)^2}$ is imaginary. Defining $L = \sqrt{(\alpha Z)^2 - \kappa^2}$, we see that

$$r^{\pm\lambda} = \cos(L \ln r) \pm i \sin(L \ln r). \tag{3.1}$$

As r tends towards 0, the quantity $r^{\pm\lambda}$ does not converge to a limit. Instead, it spins around the unit circle in the complex plane, moving faster and faster the closer r gets to 0. Thus, when $\alpha Z > \kappa$, the Hamiltonian does not have energy eigenfunctions for any value of E which lie in its domain. Our discussion of these problems follows that of [1].

These problems arise because the Hamiltonian $\hat{H}_r$ from Eq. (2.37) is not self-adjoint. The domain of the Hamiltonian $\hat{H}_r$ is all two component continuous functions $\phi(r)$ which are square integrable on $[0, \infty)$ and for which $(\hat{H}_r\phi)(r)$ is also square integrable on $[0, \infty)$. The domain of the adjoint $\hat{H}_r^{\dagger}$ is deduced from Eq. (2.26). We

see

$$\left\langle \hat{H}_r^\dagger \tau | \phi \right\rangle - \left\langle \tau | \hat{H}_r \phi \right\rangle = \tau_2^*(0)\phi_1(0) - \tau_1^*(0)\phi_2(0), \tag{3.2}$$

which vanishes due to the boundary condition $\phi(0) = 0$. There is no requirement for $\tau(0)$ to vanish. Thus the domain of $\hat{H}_r^\dagger$ includes functions which do no vanish at the origin.

In fact, we have a stronger requirement on the functions in $\mathrm{Dom}(\hat{H}_r)$ stemming from the condition $(\hat{H}_r\phi)(r)$ square integrable. Assume that near the origin, $\phi_1(r)$ behaves as r^s and $\phi_2(r)$ behaves as cr^t for some c, s, and t. We see near the origin

$$(\hat{H}_r\phi)(r) \sim \begin{pmatrix} r^s - \alpha Z r^{s-1} + c(\kappa - t)r^{t-1} \\ -cr^t - \alpha Z c r^{t-1} + (s+\kappa)r^{s-1} \end{pmatrix}. \tag{3.3}$$

We find that $|(\hat{H}_r\phi)(r)|^2$ has terms with r^{2s}, r^{2t}, r^{2s-2}, r^{2t-2}, and r^{s+t-2}. Square integrability requires that for each of these terms with a factor of r^k, we have $k > -1$. This yields the condition $s, t > 1/2$.

There is one exception to this requirement. If we pick $s = t$, we find that we can make all of the terms except for the r^s terms cancel if we have

$$\alpha Z = c(s - \kappa), \tag{3.4}$$

$$c\alpha Z = s + \kappa, \tag{3.5}$$

which occurs if we take $s = \lambda$ and $c = (\kappa + \lambda)/\alpha Z$. In this case, we see that $\phi(r)$ can behave like r^λ near the origin, even if $\lambda \leq 1/2$.

With these considerations, we find that functions $\tau(r)$ in $\mathrm{Dom}(\hat{H}_r^\dagger)$ need only fulfill the requirement $\lim_{r\to 0} r^k \tau(r) = 0$ where $k = \min(\lambda, 1/2)$, assuming that λ is real, and $\lim_{r\to 0} r^{1/2}\tau(r) = 0$ otherwise. From this, we can deduce why the Sommerfeld fine structure formula is incorrect for $\alpha Z > \kappa$. The operator $\hat{H}_r$ is not self adjoint because its domain is smaller than the domain of its adjoint $\hat{H}_r^\dagger$. This is true even when λ is real. However, the fact that $\hat{H}_r$ is not self-adjoint does not become important unless λ is imaginary. When λ is real, the domain of $\hat{H}_r$ includes its energy eigenfunctions,,

even though $\hat{H}_r$ is not self-adjoint. When λ is imaginary, the energy eigenfunctions of $\hat{H}_r$ lie outside $\mathrm{Dom}(\hat{H}_r)$, so that a self-adjoint extension of $\hat{H}_r$ must be found.

Consider the class of functions defined by

$$\phi_E^N(r) = A(\lambda, E)\phi_E^+(r) - A(-\lambda, E)\phi_E^-(r), \tag{3.6}$$

where we pick $A(\lambda, E) = \Gamma(\lambda - E\delta_E)\Gamma(1-2\lambda)$. These functions are square integrable for all E when λ is imaginary. Near the origin, they behave as r^λ. This means that they satisfy the boundary conditions of $\mathrm{Dom}(\hat{H}_r^\dagger)$ since $\lim_{r\to 0} r^{\lambda+1/2} = 0$. They decay exponentially at infinity, as can be checked using the asymptotic form of the confluent hypergeometric function (see footnote in section 2.5). This is the only linear combination of $\phi_E^+(r)$ and $\phi_E^-(r)$ (up to a scaling factor) which is normalizable and hence in $\mathrm{Dom}(\hat{H}_r^\dagger)$.

In particular, choosing $E = \pm i$, we see that $\hat{H}_r^\dagger$ has a deficiency index of $\mathcal{N}_+ = \mathcal{N}_- = 1$, implying that we can find a self-adjoint extension to $\hat{H}_r^\dagger$.

3.2 The Self-Adjoint Extension

Using the method described in section 2.3, we can find a family of self-adjoint extensions to the Hamiltonian $\hat{H}_r$. We define new operators $\hat{H}_r^\theta$ as the restriction of $\hat{H}_r^\dagger$ to the domain

$$\mathrm{Dom}(\hat{H}_r^\theta) = \{\phi_0(r) + \beta(\phi_{-i}^N(r) + e^{i\theta}\phi_i^N(r)), \phi_0(r) \in \mathrm{Dom}(\hat{H}_r), \beta \text{ complex}\} \tag{3.7}$$

for $\theta \in [0, 2\pi)$.

With our new operators $\hat{H}_r^\theta$ defined, we can solve the eigenvalue equation

$$\hat{H}_r^\theta |\phi\rangle = E |\phi\rangle , \tag{3.8}$$

by writing $|\phi\rangle = |\phi_0\rangle + \beta(|\phi_{-i}\rangle + e^{i\theta}|\phi_i\rangle)$. We can rewrite the equation as

$$(\hat{H}_r^\theta - E)|\phi_0\rangle = \beta[(E-i)|\phi_{-i}\rangle + e^{i\theta}(E+i)|\phi_i\rangle] \tag{3.9}$$

where we have $\phi_0(0) = 0$. This gives rise to the solution

$$\phi_0(r) = \phi_E^N(r) - \beta[\phi_{-i}^N(r) + e^{i\theta}\phi_i^N(r)], \tag{3.10}$$

and boundary condition

$$\phi_E^N(0) = \beta[\phi_{-i}^N(0) + e^{i\theta}\phi_i^N(0)]. \tag{3.11}$$

Eq. (3.10) tells us that the solution $\phi_E(r)$ is given by

$$\phi_E(r) = \phi_E^N(r), \tag{3.12}$$

as expected, and Eq. (3.11) can be manipulated by eliminating β into the boundary condition

$$\phi_{E,2}^N(0)\left[\phi_{i,1}^N(0) + e^{i\theta}\phi_{-i,1}^N(0)\right] = \phi_{E,1}^N(0)\left[\phi_{i,2}^N(0) + e^{i\theta}\phi_{-i,2}^N(0)\right]. \tag{3.13}$$

The boundary condition Eq. (3.13) relates two parameters: the energy E and the extension parameter θ. After some algebra, Eq. (3.13) can be turned into an implicit equation for E in terms of θ,

$$-\left(\frac{\kappa + iL}{\sqrt{\kappa^2 + L^2}}\right)\left(\frac{-\kappa + (1+E)\delta_E + iL}{-\kappa + (1+E)\delta_E + iL}\right)\left(\frac{\Gamma(-iL - E\delta_E)}{\Gamma(iL - E\delta_E)}\right) = \tag{3.14}$$

$$\frac{(2\delta_i - \kappa + L)^{1/2}\Gamma(-iL - i\delta_i)e^{i\theta/2} + (2\delta_i - \kappa - L)^{1/2}\Gamma(-iL + i\delta_i)e^{-i\theta/2}\sigma}{(2\delta_i - \kappa + L)^{1/2}\Gamma(iL + i\delta_i)e^{-i\theta/2} + (2\delta_i - \kappa - L)^{1/2}\Gamma(iL - i\delta_i)e^{i\theta/2}\sigma},$$

where $\sigma = \text{sign}(\delta_i - \kappa)$ and $\ell = \text{Im}(\lambda)$. This information allows us to compute both the energy eigenvalues for a given value of θ and the corresponding eigenfunctions $\phi_E^N(r)$.

3.3 Self-Adjointness and the Dirac Equation

It is instructive to go through the proof that self-adjoint operators have real eigenvalues in order to see where the argument breaks down for the Dirac Coulomb Hamiltonian. We start with the eigenvalue equation

$$\begin{pmatrix} 1-\frac{\alpha Z}{r} & -\frac{d}{dr}+\frac{\kappa}{r} \\ \frac{d}{dr}+\frac{\kappa}{r} & -1-\frac{\alpha Z}{r} \end{pmatrix} \begin{pmatrix} \phi_{E,1}(r) \\ \phi_{E,2}(r) \end{pmatrix} = E \begin{pmatrix} \phi_{E,1}(r) \\ \phi_{E,2}(r) \end{pmatrix}, \tag{3.15}$$

and take the complex conjugate to obtain

$$\begin{pmatrix} \phi^*_{E,1}(r) & \phi^*_{E,2}(r) \end{pmatrix} \begin{pmatrix} 1-\frac{\alpha Z}{r} & \frac{\overleftarrow{d}}{dr}+\frac{\kappa}{r} \\ -\frac{\overleftarrow{d}}{dr}+\frac{\kappa}{r} & -1-\frac{\alpha Z}{r} \end{pmatrix} = E^* \begin{pmatrix} \phi^*_{E,1}(r) & \phi^*_{E,2}(r) \end{pmatrix}, \tag{3.16}$$

where the differential operator $\overleftarrow{d}/dr$ acts to the left so that $f(r)\overleftarrow{d}/dr = df/dr$. Multiplying Eq. (3.15) by $\phi^*(r)$ on the left and Eq. (3.16) by $\phi(r)$ on the right and subtracting the latter from the former, we obtain

$$\frac{d}{dr}\left(\phi_{E,1}(r)\phi^*_{E,2}(r) - \phi_{E,2}(r)\phi^*_{E,1}(r)\right) = (E-E^*)\left[|\phi_{E,1}(r)|^2 + |\phi_{E,2}(r)|^2\right] \tag{3.17}$$

We can integrate Eq. (3.17) with r ranging from 0 to positive infinity, yielding

$$\phi_{E,1}(0)\phi^*_{E,2}(0) - \phi_{E,2}(0)\phi^*_{E,1}(0) = E^* - E, \tag{3.18}$$

where we have assumed $\phi_E(r)$ is properly normalized. When $\phi_E(r)$ meets the boundary condition $\phi_E(0) = 0$, the left hand side of Eq. 3.18 vanishes, yielding $E = E^*$. However, when $\alpha Z > \kappa$, there are no energy eigenfunctions which fulfill the boundary condition $\phi_E(r) = 0$. All energy eigenfunctions will be proportional to a linear combination of r^λ and $r^{-\lambda}$ near the origin, where λ is imaginary, and no nontrivial linear combination of r^λ and $r^{-\lambda}$ approaches a limit as r tends to 0. The proof of self-adjointness does not go through because the energy eigenfunctions do not fulfill the boundary condition which causes the left hand side of Eq. (3.18) to vanish.

Chapter 4

Numerical Analysis of Self-Adjoint Extension Eigenfunctions

4.1 Computer Generated Plots of Eigenfunctions

In this section, we provide plots of the components of the energy eigenfunctions, the probability density corresponding to those eigenfunctions, and the probability density for a nonrelativistic electron by comparison. The plots were generated in Mathematica version 7.0.1.0, using the formulae derived in chapter 3.

The energy eigenfunctions for $\hat{H}_r^\theta$ are two component spinors given by $\phi_E^N(r)$ from Eq. (3.6). The components of $\phi_E^N(r)$ are denoted by $\phi_{E,1}^N(r)$ and $\phi_{E,2}^N(r)$. Each component corresponds to a possible spin that the electron can have. The probability of finding the electron in either spin state at a distance from the nucleus between r and $r+dr$ is given by $|\phi_E^N(r)|^2 dr = \left(|\phi_{E,1}^N(r)^2| + |\phi_{E,2}^N(r)|^2\right) dr$. The non-relativistic Schrödinger equation for the three dimensional Coulomb problem yields a one component radial wavefunction, $r\psi_{\rm nr}(r)$, with the probability of finding the electron at a distance of r to $r+dr$ from the radius given by $r^2|\psi_{\rm nr}(r)|^2$. Plots comparing $|\phi(r)|^2$ and $r^2|\psi_{\rm nr}(t)|^2$ for an electron in the ground state of a hydrogenic atom are shown for $Z = 1, 50$, and 130 in Fig. 4-1, 4-2, and 4-3, where $\phi_E^N(r)$ has been normalized for comparison to $r\psi_{\rm nr}(r)$. This corresponds to the choice $\kappa = -1$. We see that as Z increases, the relativistic corrections become more significant. The relativis-

tic wavefunction is focused more tightly around the nucleus than the nonrelativistic wavefunction. The behavior of the peak of the probability density is discussed in section 5.3.

The behavior of the wavefunction $\phi_E^N(r)$ is qualitatively different in the regimes $\alpha Z < |\kappa|$ and $\alpha Z > |\kappa|$. In the $\alpha Z < |\kappa|$ regime, each component of the ground state radial wavefunction is a smooth function with no roots, behaving similarly to the non-relativistic Schrödinger wavefunction. The wavefunction components $\phi_{E,1}^N(r)$ and $\phi_{E,2}^N(r)$ vanish at $r = 0$, meeting the same boundary condition as the radial wavefunction for the nonrelativistic Schrödinger radial wavefunction $r\psi_{\text{nr}}(r)$.

In the regime where $Z \geq 1/\alpha$, we must choose a radial wavefunction which corresponds to a self-adjoint extension of the Hamiltonian. The wavefunction depends on the extension parameter θ implicitly as the energy eigenvalues vary with the extension parameter. The energy eigenfunctions depend on θ implicity, since the eigenfunctions depend on the energy eigenvalue E and the energy eigenvalues depend on the choice of θ. In Figure 2, we show the components of the ground state wavefunction for $\kappa = -1$ with $Z = 136.999$ and $Z = 137.001$, where we have approximated $\alpha = 1/137$. For the extension wavefunction with $Z = 137.001$, the parameter θ has been chosen so that the ground state energy E considered as a function of Z is continuous across $Z = 1/\alpha$. This corresponds to a value of $\theta = 326.318° = 5.69532$, as discussed in [1]. The phase of the self-adjoint wavefunctions is constant but arbitrary. We choose those wavefunctions to be real valued with the sign chosen so that $\phi_1(r)$ is positive.

As Z increases past $1/\alpha$, the maximum of the wavefunction moves back away from the origin, as can be seen comparing Figures 4-6 through and 4-7 with $Z = 150$ to Figures 4-4 and 4-5 with $Z = 137.001$. These plots are somewhat misleading as they mask the behavior of the wavefunction as $r \to 0$. Near the point $r = 0$, the wavefunction is proportional to $\sin(\ell \ln r + \delta)$ for a phase shift δ. Contrary to the impression given by the plot, the limit $\lim_{r\to 0} \phi(r)$ does not exist. The dependence on $\ln r$ makes this behavior difficult to see on a linearly scaled plot. The period of the oscillations as a function of $\ln(r)$ is given by $\frac{2\pi}{\ell}$, which decreases as Z increases past 137. This can also be seen by comparing Figures 4-4 and 4-5 to 4-6 and 4-7.

The period of the sinusoid as a function of $\ln(r)$ is much shorter for $Z = 150$.

We also show in Figure 4-14 the dependence of the ground state energy E on Z for the extension parameter $\theta = 5.69532$.

There is no clear physical meaning for the oscillations near the origin for wavefunctions in the $\alpha Z > |\kappa|$ regime. As discussed in [2], the problem occurs when the binding energy of the electron exceeds the threshold necessary for creation of e^+e^- pairs, so the single particle Dirac equation may not be applicable. Furthermore, though a unique value of the extension parameter θ can be found so that E depends continuously on Z across the boundary $\alpha Z = |\kappa|$, there is no physical reason why θ cannot vary with Z. As discussed in Chapter 5, there are reasons to believe that the problems here are not merely a mathematical problem. Even in classical physics, there are hints that bound states should be problematic for strong enough fields in $1/r$ potentials.

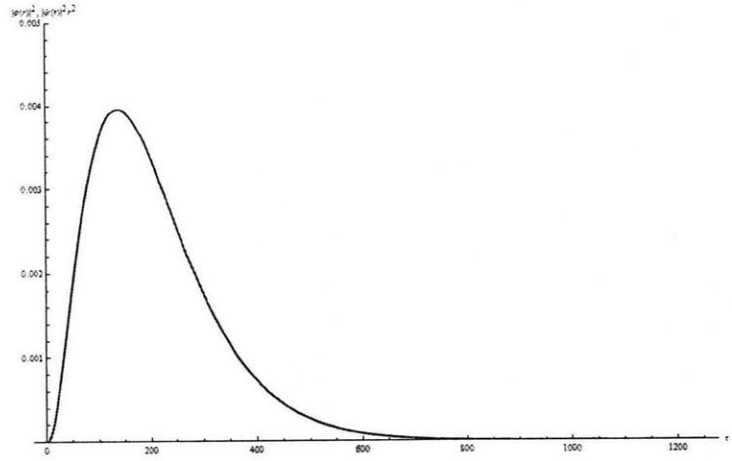

Figure 4-1: Probability densities of relativistic and nonrelativistic orbitals for $Z = 1$, with units of $\hbar/m_e c$ for r. In Figs. 4-1, 4-2, and 4-3, the dashed line is the nonrelativistic probability density and the solid line is the relativistic probability density. In Fig. 4-1, these are indistinguishable.

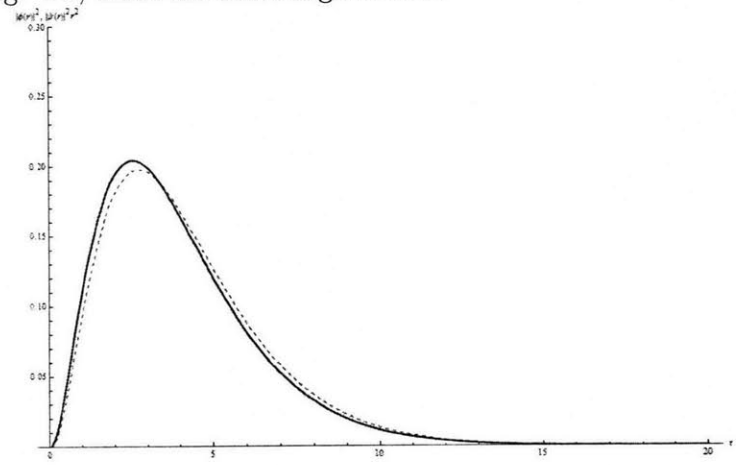

Figure 4-2: Relativistic and nonrelativistic probability densities for $Z = 50$.

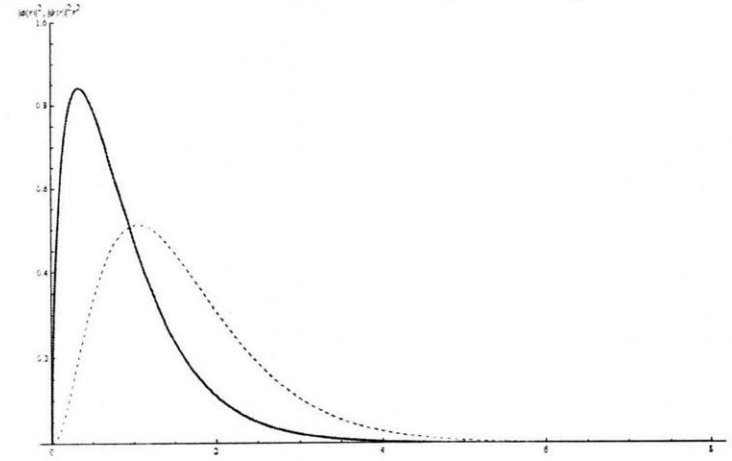

Figure 4-3: Relativistic and nonrelativistic probability densities for $Z = 130$.

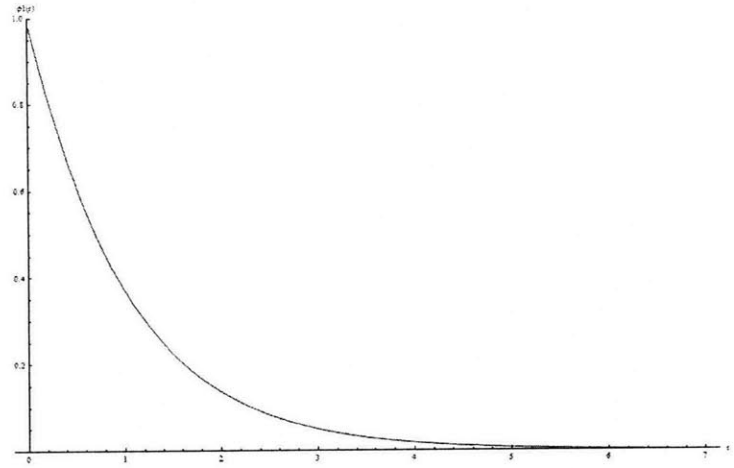

Figure 4-4: $\phi^{+}_{E,1}(r)$ for $Z = 136.999$, with units of $\hbar/m_e c$ for r.

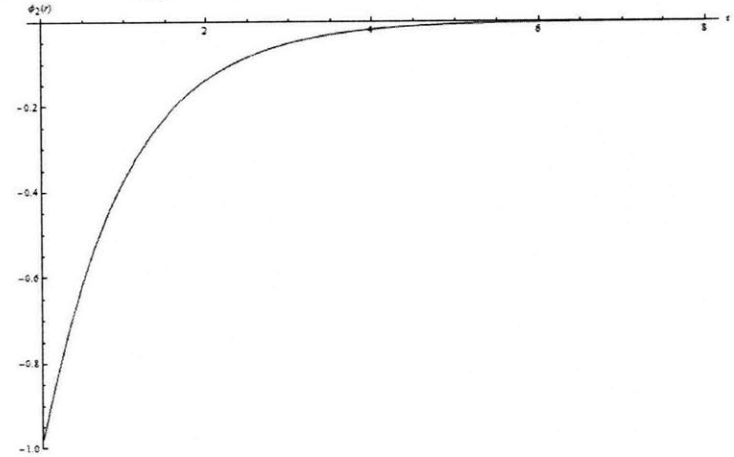

Figure 4-5: $\phi^{+}_{E,2}(r)$ for $Z = 136.999$.

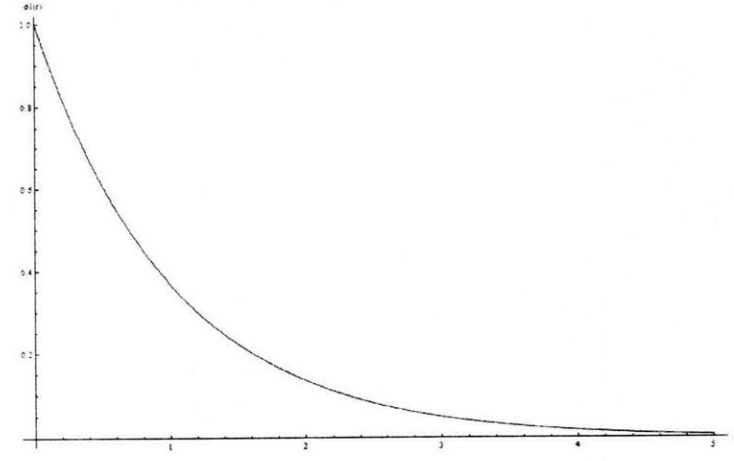

Figure 4-6: $\phi^{N}_{E,1}(r)$ for $Z = 137.001$.

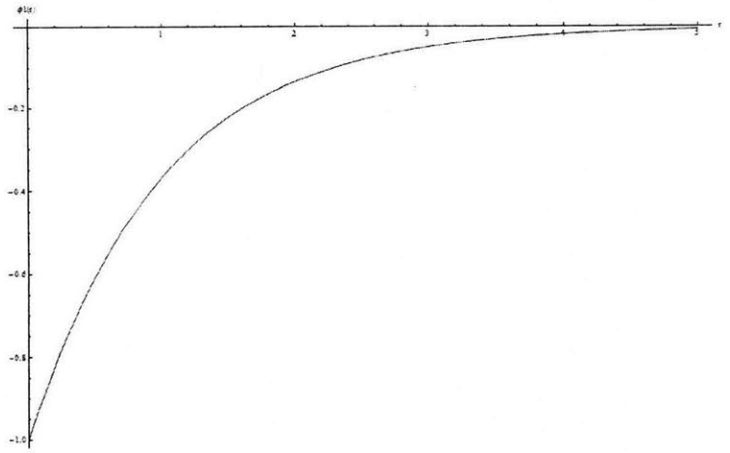

Figure 4-7: $\phi^N_{2,E}(r)$ for $Z = 137.001$.

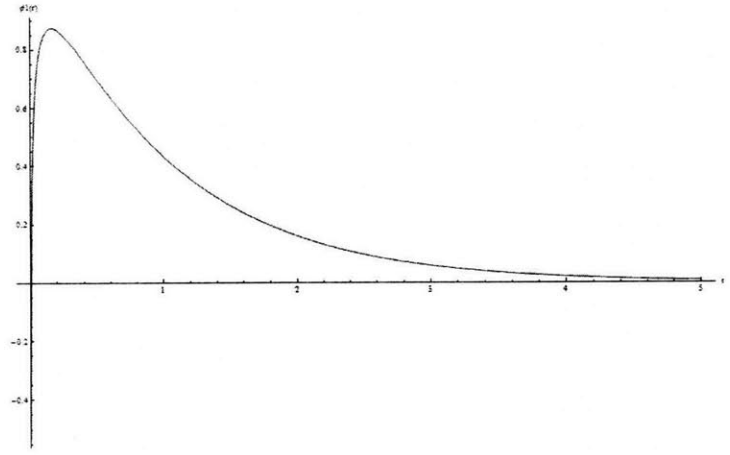

Figure 4-8: $\phi^N_{E,1}(r)$ for $Z = 150$.

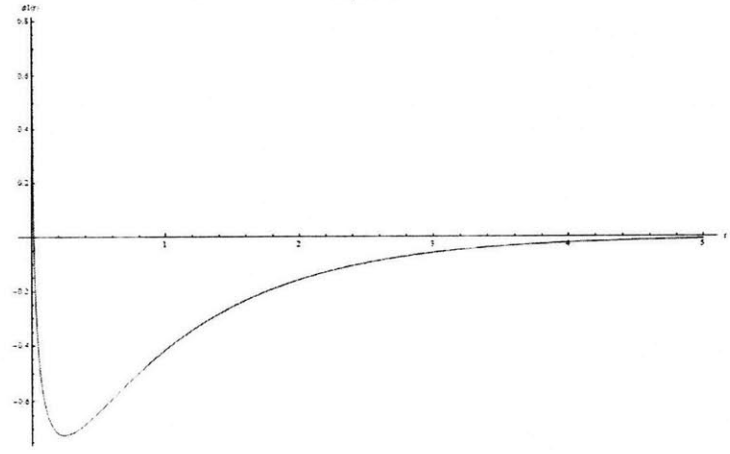

Figure 4-9: $\phi^N_{E,2}(r)$ for $Z = 150$.

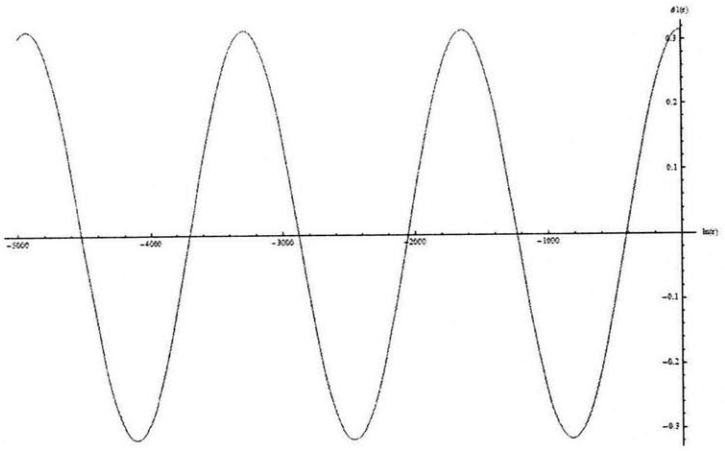

Figure 4-10: $\phi^N_{1,E}(r)$ for $Z = 137.001$, as a function of $\ln(r)$.

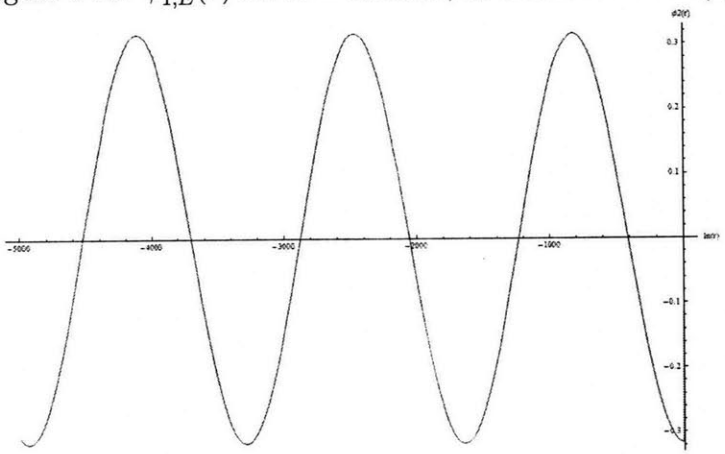

Figure 4-11: $\phi^N_{2,E}(r)$ for $Z = 137.001$, as a function of $\ln(r)$.

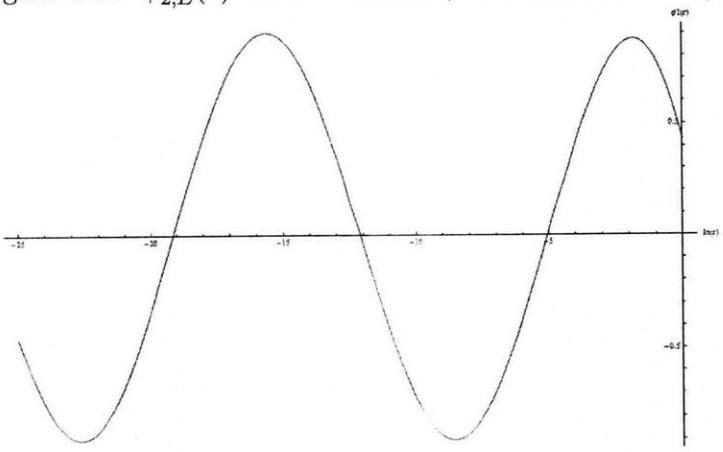

Figure 4-12: $\phi^N_{1,E}(r)$ for $Z = 150.$ as a function of $\ln(r)$.

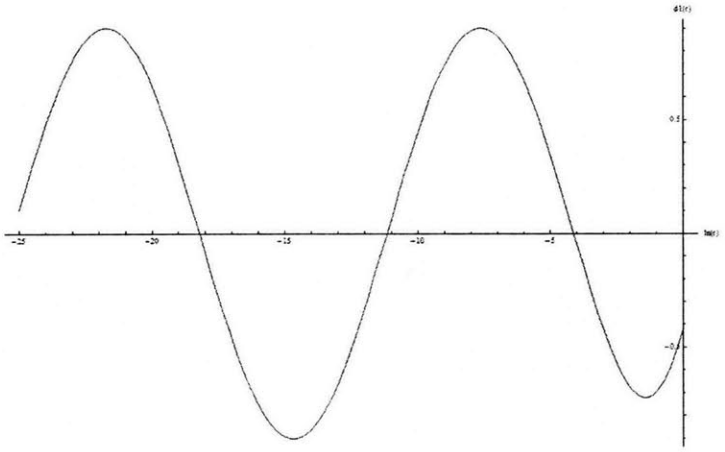

Figure 4-13: $\phi^N_{2,E}(r)$ for $Z = 150$, as a function of $\ln(r)$.

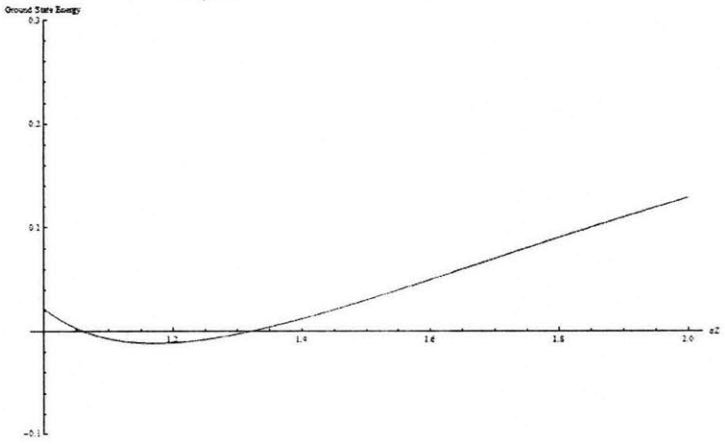

Figure 4-14: Dependence of the ground state energy E on Z for $\theta = 5.69532$. Energy is in units of mc^2.

Chapter 5

Classical Explanations of the Breakdown at $Z = 1/\alpha$

5.1 The Classical Relativistic Kepler Problem

The lack of a physically meaningful bound state for sufficiently large nuclear charges and small angular momenta occurs in classical as well as quantum mechanics. Even in classical physics, the Coulomb potential does not always admit bound states for relativistic particles. This can be seen by analyzing the Kepler problem using relativistic expressions for energy and momentum, following [3]. The energy of a relativistic particle with mass m and charge e in a Coulomb potential is given by

$$E = \sqrt{p^2c^2 + m^2c^4} - \frac{Ze^2}{r}, \tag{5.1}$$

where p is the momentum of the particle. The square of the momentum can be broken into tangential and radial components, $p^2 = p_r^2 + \frac{L^2}{r^2}$, where L is the particle's angular momentum. Substituting this into Eq. (2.1), we find

$$E = c\sqrt{p_r^2 + \frac{L^2}{r^2} + m^2c^2} - \frac{Ze^2}{r}. \tag{5.2}$$

We note that

$$E = c\sqrt{p_r^2 + \frac{L^2}{r^2} + m^2c^2} - \frac{Ze^2}{r} \geq \frac{Lc - Ze^2}{r}, \tag{5.3}$$

and that the right hand side of Eq. (5.3) is always positive if $L > Ze^2/c$. As r approaches 0, $(Lc - Ze^2)/r$ increases without bound. Since $E \geq (Lc - Ze^2)/r$ and E is a fixed constant, we must have that there is some finite minimum value which r can take on.

If $L < Ze^2/c$, then $(Lc - Ze^2)/r$ diverges to negative infinity as r tends to 0. If we choose p_r to diverge to positive infinity as r tends to 0 in Eq. (5.3), we can make the divergences cancel out so that a finite value of E is consistent with arbitrarily small values of r. This indicates that the particle will spiral into the nucleus for sufficiently small L. This phenomenon does not occur in the non-relativistic case. Furthermore, if we get $L \sim \hbar$, we find that the condition for the non-existence of a bound state is $\hbar < Ze^2/c$, which can be rewritten as $Z\alpha > 1$.

This is the same as the condition for the Dirac Coulomb Hamiltonian to fail to be self-adjoint. This gives us a new insight into why this failure of self-adjointness occurs– the problem of a non-self-adjoint Hamiltonian is not merely a mathematical one. There are physical reasons why there should be no bound states when $Z\alpha > 1$.

5.2 Relativistic Bohr Radius

There is another way to see how this problem arises even classically. In Bohr's model of hydrogenic atoms, the spectrum is calculated by assuming that electrons travel in circular orbits around the atomic nucleus with angular momenta that are multiples of $\hbar$. By simultaneously combining Bohr's angular momentum quantization

$$mvr = n\hbar, \tag{5.4}$$

with the requirement that the centripetal force equal the Coulomb force

$$\frac{mv^2}{r} = \frac{Ze^2}{r^2}, \tag{5.5}$$

we obtain

$$v_n = \frac{Ze^2}{\hbar}\frac{1}{n} \tag{5.6}$$

and

$$r_n = \frac{\hbar^2 n^2}{Ze^2 m}. \tag{5.7}$$

For a particle in a $1/r$ potential, the energy is given by

$$E = \frac{1}{2}mv^2 - \frac{Ze^2}{r}. \tag{5.8}$$

Substituting Eqs. (5.6) and (5.7) into Eq. (5.8), we find

$$E_n = -\frac{Z^2 e^4 m}{2\hbar^2}\frac{1}{n^2}, \tag{5.9}$$

which matches the energy spectrum given by solving the nonrelativistic Schrödinger equation.

This technique can be extended to find the spectrum of a relativistic particle in a $1/r$ potential. We replace the mass m in Eqs. (5.4) and (5.5) with the expression γm, where $\gamma = (1 - v^2/c^2)^{-1/2}$, obtaining

$$\frac{mvr}{\sqrt{1 - \frac{v^2}{c^2}}} = n\hbar \tag{5.10}$$

and

$$\frac{mv^2}{r\sqrt{1 - \frac{v^2}{c^2}}} = \frac{Ze^2}{r^2}. \tag{5.11}$$

Solving Eqs. (5.10) and (5.11) yields

$$v_n = \frac{Ze^2}{\hbar}\frac{1}{n} \tag{5.12}$$

and

$$r_n = \frac{\hbar^2 n^2}{Ze^2 m}(1 - Z^2\alpha^2)^{1/2}. \tag{5.13}$$

The relativistic energy is given by

$$E = \frac{mc^2}{\sqrt{1 - v^2/c^2}} - \frac{Ze^2}{r}. \tag{5.14}$$

Substituting Eqs. (5.12) and (5.13) into Eq. (5.14), we obtain the energy spectrum

$$E_n = mc^2 \sqrt{1 - \left(\frac{Z\alpha}{n}\right)^2}.$$

We note that this is the same as the fine structure formula obtained using the Dirac equation under the assumption that $n = \kappa$. We also see that the formula for the Bohr radii,

$$r_n = \frac{n^2\hbar^2}{Ze^2m}\sqrt{1 - (Z\alpha)^2}, \tag{5.15}$$

yields imaginary values for $Z\alpha > 1$. This fact gives us another way of seeing why the Dirac equation should not be expected to yield a sensible ground state when $Z\alpha > 1$. The Bohr quantization condition cannot be met.

5.3 Bohr Radius and Most Probable Radius

In nonrelativistic quantum mechanics, the Bohr radius of an electron in a hydrogenic atom with nuclear charge Z is also the most probable distance of the electron when the wavefunction is found with the Schrödinger equation. The nonrelativistic ground state is given by

$$\psi(r) = \frac{1}{\sqrt{\pi}a_0^{3/2}} \exp\left(-r/a_0\right), \tag{5.16}$$

where $a_0 = \frac{1}{Z}\frac{\hbar}{mc\alpha}$ is the Bohr radius. The most probable radius can be computed,

$$\frac{d}{dr}\left(r^2\left|\psi(r)\right|^2\right) = \frac{d}{dr}\left[\frac{r^2}{\pi a_0^3}\exp\left(-2r/a_0\right)\right] = 0$$

which yields $r = a_0$.

The same property holds in the case of the relativistic hydrogenic atom and the

relativistic Bohr radius. The relativistic Bohr radius for the ground state is given by

$$a_{0,\mathrm{rel}} = \frac{1}{Z}\frac{\hbar^2}{e^2 m}\sqrt{1-(Z\alpha)^2}.$$

The most probable radius can be found by maximizing $|\phi_E^+(r)|^2$, where $\phi_E^+(r)$ is given by Eq. (2.39) with $\lambda - E\delta_E = 0$ and $\kappa = -1$ so that $E = mc^2\sqrt{1-(Z\alpha)^2}$. In this case, the components of $\phi(r)$ can be written as

$$\phi_{E,1}^+(r) = \sqrt{1+E}\rho^\lambda \exp(-\rho/2), \tag{5.17}$$

$$\phi_{E,2}^+(r) = \sqrt{1-E}\rho^\lambda \exp(-\rho/2), \tag{5.18}$$

where as in Eq. (2.39) $\rho = 2(1-E^2)^{1/2}r$, and we have used $H(0|1+2\lambda|\rho) = 1$ and $\lambda - E\delta_E = 0$. Calculating $|\phi(r)|^2$, we find

$$|\phi(r)|^2 = \rho^{2\lambda}\exp(-\rho) = \left[2\sqrt{1-E^2}\right]^{2\lambda} r^{2\lambda}\exp\left(-2r\sqrt{1-E^2}\right). \tag{5.19}$$

Finding the maximum of this, we see that it occurs when

$$r = \frac{\lambda}{\sqrt{1-E^2}} = \frac{1}{Ze^2}\sqrt{1-(Z\alpha)^2}. \tag{5.20}$$

Reinserting the dimensional factors $\hbar$ and m, we find that

$$r = \frac{1}{Z}\frac{\hbar^2}{e^2 m}\sqrt{1-(Z\alpha)^2}, \tag{5.21}$$

which is the same as the expression for the relativistic Bohr radius. Thus, we see that the property that the most probable radius equals the relativistic Bohr radius is preserved in relativistic quantum mechanics.

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