THE BOUND STATES
OF DIRAC EQUATION WITH A SCALAR POTENTIAL

BY

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THESIS
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Abstract

We study the bound states of the 1 + 1 dimensional Dirac equation with a scalar potential, which can also be interpreted as a position dependent “mass”, analytically as well as numerically. We derive a Prüfer-like representation for the Dirac equation, which can be used to derive a condition for the existence of bound states in terms of the fixed point of the nonlinear Prüfer equation for the angle variable. Another condition was derived by interpreting the Dirac equation as a Hamiltonian flow on $\mathbb{R}^4$ and a shooting argument for the induced flow on the space of Lagrangian planes of $\mathbb{R}^4$, following a similar calculation by Jones (Ergodic Theor Dyn Syst, 8 (1988) 119-138). The two conditions are shown to be equivalent, and used to compute the bound states analytically and numerically, as well as to derive a Calogero-like upper bound on the number of bound states. The analytic computations are also compared to the bound states computed using techniques from supersymmetric quantum mechanics.
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And finally: *Muss es sein? Es muss sein*...
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Notation

The Pauli matrices are defined as

\[ \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]

These matrices also form the generators of su(2), the Lie algebra of SU(2), and satisfy

\[ \sigma^i \sigma^j = \delta^{ij} I + i \epsilon^{ijk} \sigma^k, \]

which leads to the commutator and the anticommutator

\[ [\sigma^i, \sigma^j] \equiv \sigma^i \sigma^j - \sigma^j \sigma^i = 2i \epsilon^{ijk} \sigma^k, \]
\[ \{\sigma^i, \sigma^j\} \equiv \sigma^i \sigma^j + \sigma^j \sigma^i = 2 \delta^{ij} I, \]

where \( \epsilon^{ijk} \) is the Levi-Civita tensor with \( \epsilon^{123} = 1 \). We shall always use the square brackets \([,]\) for commutators and the curly braces \(\{,\}\) for the anticommutators, as defined above.

The \( n \) dimensional real and complex Euclidean spaces are denoted by \( \mathbb{R}^n \) and \( \mathbb{C}^n \). The Grassmannian \( G_{r,2n} \) denotes the set of \( r \) dimensional subspace of \( \mathbb{R}^{2n} \), while \( \mathcal{L}(n) \subset G_{n,2n} \) denotes the set of Lagrangian subspaces.

The angled brackets \( \langle, \rangle \) always denote the inner product on \( \mathbb{R}^n \), i.e., \( \langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T \cdot \mathbf{w} \). The inner products on \( \mathbb{C}^n \) is denoted by \( \langle, \rangle_\mathbb{C} \), i.e., \( \langle \mathbf{v}, \mathbf{w} \rangle_\mathbb{C} = \mathbf{v}^\dagger \cdot \mathbf{w} \). The symplectic form \( \Omega(\cdot, \cdot) \) on \( \mathbb{R}^{2n} \) is defined as

\[ \Omega(\mathbf{v}, \mathbf{w}) = \langle \mathbf{v}, \mathcal{J} \mathbf{w} \rangle, \quad \mathcal{J} = \begin{pmatrix} 0_{n \times n} & \mathbb{I}_{n \times n} \\ -\mathbb{I}_{n \times n} & 0_{n \times n} \end{pmatrix}. \]

The spectrum, i.e, the set of eigenvalues of a linear operator \( T \) is denoted by \( \sigma[T] \).

The Greek lowercase symbols \( \psi, \phi \) are used for vectors in \( \mathbb{C}^2 \) and the corresponding uppercase characters
\( \Psi, \Phi \) for vectors in \( \mathbb{R}^4 \). The boldface characters (\( \psi, \phi, S, U \)) are used for 2-dimensional subspaces of \( \mathbb{R}^4 \), either indicated as the span of a pair of linearly independent vectors or as their wedge product.

The independent variables for the ODEs is taken as \( x \), unless stated otherwise. For a function \( f(x) \), the prime always denotes the derivative w.r.t \( x \), i.e., \( f'(x) = df/dx \). We have also used subscripts to denote partial derivatives where it is unambiguous, for instance, \( f_x = \partial f/\partial x \), etc.
Since its inception in 1929[1, 2], the Dirac equation has been of much interest, both to physicists and to mathematicians, and has often helped in bridging the two disciplines. The Dirac operator and its analogues have been a source of interesting results in fields ranging from particle physics[3, 4] and condensed matter physics[5] to dynamical systems[6]. Spinors, the objects a Dirac operator acts on, have also been studied extensively from algebraic[7] as well as geometric[8] perspectives.

In the crudest sense, bound states are the nontrivial $L_2$ (in physics parlance, “normalizable”) solutions of a differential equation, which then typically need to decay exponentially[9]. In physical systems, these correspond to the solutions which are “localized”, as opposed to delocalized plane wave solutions. Thus, physically, the bound state spectrum is simply the “allowed” energy levels for the system. Often, one can physically access these states using a variety of techniques, from scanning and tunneling microscopy to various scattering experiments.

In dynamical systems context, the bound states are most relevant for the inverse scattering transform[10], which is used to describe the evolution of soliton solutions. The essential idea is to treat the soliton at a given time as a potential to an eigenvalue problem (often Schrödinger or Dirac-like equations) to compute the transmission and scattering data, which can then be evolved under an operator under which the flow is isospectral, so that the spectrum is independent of time. The time-evolved soliton solution can then be reconstructed from the transmission and reflection data using the inverse scattering transform.

Furthermore, the bound state spectra of the linear operators are also of much interest in studying the stability of solutions of nonlinear differential equations, esp soliton solutions. Given a soliton solution, one typically linearizes the the system around that solution to obtain an eigenvalue problem. Thus, the existence of an $L_2$ solution to the linearized system about a given soliton solution would imply the instability of that soliton[11, 12, 13].

The bound state spectrum of the Dirac equation with a scalar potential, or alternatively, a position-dependent mass term has been of relevance lately with the advent of topological phases of matter[5, 14], where the Dirac equation is often the low-energy effective theory of a system, with the “mass” being a system parameter that can vary with position. One dramatic manifestation of this fact is the existence of
the topologically protected "edge states", which are essentially bound states to a scalar potential at the point of its zero crossing[15].

The bound state spectrum of Dirac equation is also relevant for the study of the Zakharova-Shabat eigenvalue problem[16], which emerges quite generally as the eigenvalue problem whose isospectral flow corresponds to a soliton solution for the AKNS hierarchy[10]. This context also gives rise to somewhat more exotic colleagues of the Dirac equation, like the Faddeev-Takhtajan eigenvalue problem[17, 18] for the sine-Gordon equation, where the “eigenvalue” parameter enters in a nonlinear fashion.

In this work, we study the bound state solutions for the 1 + 1 dimensional Dirac equation with a scalar potential (equivalently, a position dependent mass) $m(x)$ that tends to a constant value $\mu_{\pm}$ as $x \to \pm \infty$. We have two classes of potentials in mind: potential wells, where $\mu_+$ and $\mu_-$ have the same sign, and instantons, where they have an opposite sign. We use a variety of techniques to compute the spectra both analytically and numerically, as well as to derive a Calogero-like upper bound on the number of bound states, similar to one derive for the 3 + 1 dimensions in Ref [19].

Outline: The rest of this thesis is organized as follows: In the rest of this chapter, we provide a brief (and quite superficial, for the most part) overview of some of the interesting aspects of the Dirac equation known to physicists and mathematicians. In Chapter 2, we formulate the 1+1 dimensional Dirac eigenvalue problem with eigenvalue $E \in \mathbb{R}$ as as an ODE on $\mathbb{C}^2$

$$i\psi'(x) = M(E, x)\psi(x), \quad M(E, x) = im(x)\sigma^2 - E\sigma^3,$$  

and derive a representation reminiscent of the well-known Prüfer representation for real ODEs. In Chapter 3, we analytically solve the Dirac equation for the square well and an instanton potential using the corresponding Klein-Gordon equation. In Chapter 4, following Jones[12, 13], we map the Dirac equation to a flow on $\mathbb{R}^4$ and subsequently on the space of its Lagrangian subspaces. In Chapter 5, we derive two conditions for the existence of bound states; one from the stability characteristics of the Prüfer equations and the other from a shooting argument, and show their equivalence. We employ these conditions to analytically and numerically compute the bound state spectrum and compare the results with the exact calculations, when they are available. Finally, we use the conditions so obtained to prove a Calogero-like upper bound on the number of bound states for a given scalar potential:

$$N_B \leq N_0 + \frac{1}{\pi} \int_{-\infty}^{\infty} dx \sqrt{1 - m^2(x)}$$  

(1.2)
In Chapter 6, we present our conclusions and possible directions of future work. In Appendix A, we discuss the geometry associated with the subspaces of $\mathbb{R}^{2n}$ relevant to the constructions of Chapter 4 and construct a parametrization of the space of Lagrangian subspaces.

1.1 History and lore

In this section, we present a brief overview of the history and lore pertaining to Dirac equation in the physics and mathematics literature. A large part of this discussion is not directly relevant to the problem at hand; however, it should help put the problem in context. The description is bound to be brief and nonrigorous, owing in part to the space constraint and in part to the author’s limited comprehension of many of the ideas.

1.1.1 Quantum mechanics and symmetries

The quantum mechanical description of nature is undoubtedly one of the greatest landmarks of 20th century physics. The essential physical notion, following from the works of Planck, Einstein, Bohr and de Broglie, was the particle-wave duality. Mathematically, the particles are described by a “wavefunction” $\psi : \mathbb{R}^{d-1,1} \rightarrow \mathbb{C}$, where $\mathbb{R}^{d-1,1}$ is the underlying Lorentzian spacetime. The physically meaningful quantity is $|\psi(x)|^2$, which is interpreted as a probability distribution function for the position of the particle in question. In this picture, the “wave” nature of particles is encoded in the interference terms arising from the superposition of two wavefunctions, as $|\psi_1 + \psi_2|^2 \neq |\psi_1|^2 + |\psi_2|^2$.

The earliest proposal to describe this duality was the Schrödinger equation, a wave equation of the form $(i\partial_t - \nabla^2)\psi = 0$ proposed to describe the wavelike behavior of nonrelativistic particle. This can be thought of as simply “quantizing” the Newtonian dispersion relation, $E = |p|^2/2m$ by the replacement $E \mapsto i\hbar \partial_t$ and $p \mapsto -i\hbar \nabla$. Despite its great successes in explaining elementary atomic spectra (except for the fine structure), it was not compatible with Einstein’s special relativity. The first step in that direction was simply quantizing the relativistic dispersion relation, $E^2 = p^2 + m^2$, in a similar fashion, which leads to the Klein-Gordon equation, a wave equation of the form $(\Box + m^2)\psi = (\partial_\tau^2 - \nabla^2 + m^2)\psi = 0$.

The Dirac equation, $D\psi = 0$, which would go on to explain the fine structure of atomic spectra[20, 21] and spin and predict the existence positrons [2], was originally derived in an attempt to obtain a linear operator with only first order derivatives, that is the “square root” of the d’Alembertian operator in the wave equation. Explicitly, Dirac was seeking an operator of the form $D = i\gamma^\mu \partial_\mu - m$. where $\mu = 1, 2, \ldots, d$ is summed over (Einstein summation), such that $D^2 = \Box + m^2$. This was motivated from the fact that the Schrödinger equation has only first order time derivative. However, such an operation in $d$ dimensions necessitates that
\(\gamma^\mu\)'s, the \(d\) coefficients of the derivatives in the resulting \textit{Dirac operator} \(\mathcal{D}\) satisfy \(\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu}\), where \(\eta^{\mu\nu} = \text{diag}\{1, -1, \ldots, -1\}\) is the Lorentzian metric on \(\mathbb{R}^{d-1,1}\). Dirac identified these objects as matrices, which are often known as Dirac matrices in physics literature. This algebraic structure is also a special case of Clifford algebras, which we briefly discuss in the next subsection.

The form and behavior of these equations is intimately connected to the symmetries of the underlying spacetime, owing to the physical requirement that the system be invariant under translations as well as Lorentz transform (or Galilean transform in case of the Schrödinger equation). The underlying spacetime is typically the Lorentzian manifold \(\mathbb{R}^{d-1,1}\), so that the system is required to be invariant under the Lorentz group, \(\text{SO}(d-1,1)\) and the wavefunction \(\psi : \mathbb{R}^{d-1,1} \to \mathbb{C}^k\) may transforms under a representation of the Lorentz group. For Klein-Gordon equation, the wavefunction typically transforms under a scalar or vector representation of \(\text{SO}(d-1,1)\), however, for the Dirac equation, consistency demands that it transform under the spin representation. Such a wavefunction is then referred to as a \textit{spinor}.

\subsection{1.1.2 Spin Representations and Clifford algebra}

The spin representations are essentially the representations of the \textit{spin groups}, which are double covers of the group of rotations. Explicitly, \(\text{Spin}(d)\) is defined by the short exact sequence

\[
1 \to \mathbb{Z}_2 \to \text{Spin}(d) \to \text{SO}(d) \to 1.
\] (1.3)

A lot of physics applications of the relatively obscure spin group stem from the accidental isomorphisms\cite{22}

\[
\text{Spin}(2) \cong \text{U}(1), \quad \text{Spin}(3) \cong \text{SU}(2), \quad \text{Spin}(4) \cong \text{SU}(2) \times \text{SU}(2),
\] (1.4)

which let one study the representation theory of \(\text{Spin}(d)\) for physically relevant cases (as \(d \leq 4\) for physical systems) in terms of the well-known representation theory of \(\text{U}(1)\) and \(\text{SU}(2)\). For Lorentzian manifolds, we have the corresponding double covers of \(\text{SO}(d-1,1)\) as \(\text{Spin}(d-1,1)\), and the accidental isomorphisms

\[
\text{Spin}(1,1) \cong \text{GL}(1, \mathbb{R}), \quad \text{Spin}(2,1) \cong \text{SL}(2, \mathbb{R}), \quad \text{Spin}(3,1) \cong \text{SL}(2, \mathbb{C}).
\] (1.5)

The spinors are essentially vectors in a vector space that carries a representation of the spin group.

The spin groups are intimately linked to the Clifford algebras\(\text{see, for instance, Chapter 2 of [8] or Chapter 5 of [23]}\), allowing for a purely algebraic construction of spinors\cite{7}. Recall that a Clifford algebra \(\mathcal{Cl}(V, Q)\) is generated by a vector space \(V\) equipped with a symmetric nondegenerate quadratic form \(Q : V \times V \to \mathbb{R}\).
Given the objects \( v, w \) corresponding to the vectors (denoted in boldface characters) \( v, w \in V \), we define a binary operator \( * \) which satisfies
\[
v * w + w * v = -2Q(v, w) 1,
\]  
where 1 is the identity element of the algebra. For \( \dim(V) = n < \infty \), the Clifford algebra is \( 2^n \)-dimensional, which, given a basis \( \{ e_i, \ i = 1, 2, \ldots n \} \) of \( V \), is spanned by
\[
\{ e_{i_1} * e_{i_2} * \ldots * e_{i_k} \mid 1 \leq i_1 < i_2 < \ldots < i_k \leq n, \ 0 \leq k \leq n \}.
\] (1.7)

Clearly, the coefficients \( i \gamma^\mu \) satisfy a relation of this type, with \( V = \mathbb{R}^d \) and \( Q(v, w) = \eta^{\mu\nu} v_\mu w_\nu \). The Clifford algebras have representations in terms of finite real or complex matrices. In this picture, the Dirac matrices are the induced representation of the Clifford algebra \( C\ell(V, Q) \) on an even-dimensional complex vector space \( \mathbb{C}^{2n} \), the corresponding \( \psi \in \mathbb{C}^{2n} \) being the spinors.

Given a real vector space \( V \cong \mathbb{R}^n \) with a definite bilinear form \( Q \), the short exact sequence that defines \( \text{Spin}(d) \) naturally emerges when one tries to embed \( O(n) \), the subgroup of the automorphism group of \( V \) that leaves \( Q \) invariant, into the algebra \( C\ell(V, Q) \). The Clifford algebras are \( \mathbb{Z}_2 \) graded, as there exists an involution \( \alpha : C\ell(V, Q) \to C\ell(V, Q) \), which acts as \( \alpha(e_{i_1} * e_{i_2} * \ldots * e_{i_k}) = e_{i_k} * \ldots * e_{i_2} * e_{i_1} \). The embedding works as follows: One defines a group action \( g : C\ell(V, Q) \times V \to V \) corresponding to
\[
\varphi \mapsto g(\varphi, v) = \varphi * v * \alpha(\varphi), \quad v \in V, \ \varphi \in C\ell(V, Q).
\] (1.8)

To expose its action, let us take a negative definite \( Q \) and \( \{ e_i \} \) as the basis of \( V \) that diagonalizes \( Q \), so that \( Q(e_i, e_j) = -\delta_{ij} \). If \( \varphi = e_j \), then \( g \) acts as
\[
g(e_j, v) = e_j * v^t e_i * e_j = v^t e_j * (2\delta_{ij} 1 - e_j e_i) = v^t (2\delta_{ij} e_j - e_i),
\] (1.9)

so that \( v \to 2 \langle v, e_j \rangle - v \), which is a reflection about the hyperplane normal to \( e_j \). Thus, the action of \( g \) for \( \varphi = w_1 * w_2 * \cdots * w_k \) corresponds to a sequence of \( k \) reflections about the hyperplanes in \( \mathbb{R}^n \) normal to the vectors \( w_j \).

As rotations can be implemented as a sequence of reflections about different hyperplanes, \( g \) defines a map from \( C\ell(V, Q) \) to \( O(n) \supset SO(n) \), the group of rotations on \( V \). By the Cartan–Dieudonné theorem[7, 8], this map is surjective. Furthermore, \( g(\kappa, v) = \kappa^2 v, \ \kappa \in \mathbb{R} \), so that \( 1^1 \ker(g(\cdot, v)) = \{1, -1 \} \cong \mathbb{Z}_2 \), which leads to the short exact sequence that defines \( \text{Spin}(n) \).

\(^1\)Here, the kernel simply refers to the set of elements \( \varphi \in C\ell(V, Q) \) such that \( g(\varphi, \cdot) : V \to V \) is the identity map.
1.1.3 Integrable systems and AKNS formalism

We briefly discuss the Dirac operator and its variants arising in the Lax pair picture of certain integrable systems, most notable of which is the sine-Gordon model. Recall that two operators $L$ and $H$ are said to form a Lax pair\cite{10,24} if they satisfy the operator equation

$$\frac{dL}{dt} + [L, H] = 0,$$  \hspace{1cm} (1.10)

and the spectrum of $L$ is invariant under $H$, i.e.,

$$L\phi = \lambda \phi, \quad \frac{\partial}{\partial t} \phi = H \phi \implies \frac{\partial \lambda}{\partial t} = 0, \quad \phi : \mathbb{R} \times \mathbb{R} \to \mathbb{C}. \hspace{1cm} (1.11)$$

Hence, every eigenvalue of $L$ is a (local) constant of motion for the time evolution by $H$, typically termed as an *isospectral* flow. As integrable systems typically have an infinite number of local constants of motion, we can potentially represent them as a pair of operators satisfying the Lax compatibility condition.

If $L$ and $H$ are linear differential operators, we can rewrite eq. (1.11) as

$$\psi_x = U \psi, \quad \psi_t = V \psi; \quad \psi : \mathbb{R} \times \mathbb{R} \to \mathbb{C}^n, \quad U, V \in \mathbb{C}^{n \times n}. \hspace{1cm} (1.12)$$

Since $\psi_{xt} = \partial_x \psi_t = \partial_t \psi_x$, these satisfy

$$\partial_t U - \partial_x V - [U, V] = 0 \iff D\Omega = d\Omega - \Omega \wedge \Omega = 0, \hspace{1cm} (1.13)$$

which is a *zero curvature* condition on the matrix valued 1-form $\Omega = U dx - V dt$. A class of Lax pairs can then be defined under the so-called AKNS formalism\cite{10} by taking

$$U(x,t) = \begin{pmatrix} i\lambda & q \\ r & -i\lambda \end{pmatrix} = \frac{q + r}{2} \sigma^1 + \frac{q - r}{2} (i\sigma^2) + \lambda (i\sigma^3), \hspace{1cm} (1.14)$$

where $\lambda \in \mathbb{C}$ and $q, r : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$. Expanding $V = \sum_{k=0}^{N} V_k \lambda^k$, one can solve the compatibility condition of eq. (1.13) order by order in $\lambda$. One gets $N+1$ equations, which can be solved for the $N$ $V_k$’s. Once we have obtained the $2 \times 2$ matrices $U$ and $V$ corresponding to a given integrable system, the local constants of motion are given by the Dirac eigenvalue problem $\partial_x \psi = U \psi$, typically referred to as the Zakharov-Shabat\cite{16,17} system.
In the following, we work out the case for the sine-Gordon equation. Setting

\[ U = \lambda i \sigma^3 + U_0 = \begin{pmatrix} i \lambda & q \\ r & -i \lambda \end{pmatrix}, \quad V = \lambda^{-1} V_{-1} = \frac{1}{\lambda} \begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix}, \] (1.15)

the zero curvature condition at \( O(\lambda) \) is trivial (\( \partial_x \sigma^3 = 0 \)), while the remaining equations becomes

\[
O(1) : \partial_t U_0 - [i \sigma^3, V_{-1}] = 0 \implies \begin{pmatrix} 0 \\ \partial_t r + 2i v_{21} \end{pmatrix} = 0;
\]
\[
O(\lambda^{-1}) : - \partial_x V_{-1} - [i \sigma^3, V_{-1}] = 0 \implies \begin{pmatrix} \partial_x v_{11} + (qv_{21} - rv_{12}) & \partial_x v_{12} - (v_{11} - v_{22})q \\ \partial_x v_{21} + (v_{11} - v_{22})r & \partial_x v_{22} - (qv_{21} - rv_{12}) \end{pmatrix} = 0. \quad (1.16)
\]

These are a total of 6 differential equations, 4 of which can be solved to get

\[ V = \frac{i}{2\lambda} \begin{pmatrix} w \\ -q_t \\ r_t \\ -w \end{pmatrix}, \quad w_x = (qr)_t. \quad (1.17)\]

Including the remaining 2 equations, we have a set of 3 differential equations in \( q, r, w \):

\[ w_x = (qr)_t, \quad q_{xt} + 2wq = 0, \quad r_{xt} + 2wr = 0. \quad (1.18)\]

As the \( q \) and \( r \) equations are identical and complex, let us substitute \( q = -r = -im \), \( m : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R} \), which reduces the system to

\[ w_x = (m^2)_t, \quad m_{xt} + 2wm = 0. \quad (1.19)\]

Multiplying the latter by \( 2m_t \), we get

\[ 0 = \partial_x (m_t)^2 + 2w(m^2)_t = \partial_x (m_t)^2 + 2ww_x = \partial_x ((m_t)^2 + w^2). \quad (1.20)\]

Thus, \( m_t^2 + w^2 = C^2 \). We can substitute \( m_t = C \sin u \) and \( w = C \cos u \), to get

\[ 0 = m_{xt} + 2wm = C \cos u \ u_x + 2C \cos u \ m \implies m = \frac{1}{2} u_x. \quad (1.21)\]

But \( m_t = C \sin u \), so that substituting \( C = 1/2 \), we get

\[ u_{xt} = \sin u, \quad (1.22)\]

which is the sine-Gordon equation. Thus, the sine-Gordon equation is equivalent to the isospectral flow of
the eigenvalue equation

\[ \psi_x = U\psi \implies i\psi_x = \begin{pmatrix} -\lambda & m \\ -m & \lambda \end{pmatrix} \psi = [im\sigma^2 - \lambda\sigma^3] \psi. \]  

(1.23)

This is precisely the form of the Dirac equation that we analyze in this work.

Similarly, taking \( V = \lambda^2 V_2 + \lambda V_1 + V_0 \) and \( q = \pm r^* \), we get the nonlinear Schrödinger equation with the same \( U \) but a different \( V \). Thus, in general, we can think of our “scalar potential” for the Dirac equation as a soliton solution of some integrable system at a fixed time. Knowing its spectrum, we can evolve the system in time according to the “Hamiltonian” \( V \), and then use the inverse scattering transform to compute the time evolution of the soliton.

1.1.4 Physics of mass domain wall

In particle physics, the parameter \( m \) in the Dirac equation is taken to be a positive constant, as it is interpreted as the “mass” of the fermion. The spectrum of the Dirac operator is then unbounded from both above and below, but it has a “mass gap” \( E \in (-m, m) \), a reflection of the fact that \( E^2 = p^2 + m^2 \geq m^2 \).

Clearly, the gap closes if \( m = 0 \). Furthermore, we note that the spectrum is invariant under \( m \rightarrow -m \).

In certain contexts, it is useful to let \( m \) be a (continuous) function of position, \( x \), in which context it is also referred to as a scalar potential\(^2\). Consider such a configuration where \( m(x) \rightarrow \pm \mu \) as \( x \rightarrow \pm \infty \), so that \( m(x) \) must cross zero at some \( x_0 \in \mathbb{R} \). Such a point is termed a mass domain wall (between the two “domains” with opposite signs of mass), and is known to harbor a localized fermion mode at zero energy\(^1\) that cannot be removed by any local transformations. As the authors of Ref \([15]\) point out, there are potentially other normalizable solution to this equation, which, in part, motivates our study of profiles of \( m(x) \) which are of a similar form, i.e, \( m(x) \rightarrow \mu_\pm \) as \( x \rightarrow \pm \infty \), and \( \mu_- < 0 < \mu_+ \).

A particular physical situation which realizes such a mass domain wall is the instanton\([25, 26]\) potential. The physical setup is a scalar background field, \( \phi \), which couples to the fermions. Due to a separation of scales, the fermion sees the scalar potential \( \phi(x) \) as a mass term, so that a nontrivial configuration of \( \phi(x) \) can correspond to a mass domain wall. The instanton is just such a solution of an eigenvalue problem of the form \((\partial^2 + E - V(\phi))\phi = 0\) with the boundary condition \( \phi(x) \rightarrow \pm \phi_0 \) as \( x \rightarrow \pm \infty \), where \( V(x) \) is a double-well potential of the form \( V(x) \sim V_0(\phi^2 - \phi_0^2)^2 \).

A more recent realization of this physics is in topological phases in condensed matter physics, which, being the author’s “day job”, gets a disproportionately large discussion in the following. The physical

\(^2\)As opposed to the “vector” potential. The terminology comes from the coupling of the Dirac equation for \( d > 1 \) to the electromagnetic field, which has a “scalar” component along the time direction and a “vector” component along the space direction.
realization of these systems in materials like graphene has led to detailed investigations of Dirac equation in tabletop experiments, including phenomenon that are all but inaccessible as far as electrons are concerned, like \textit{zitterbewegung}\cite{27} and Klein tunneling\cite{28, 29, 30}. It has also led to the realization of aspects of Dirac equation that are not usually realizable in a particle physics context, for instance, a mass domain wall.

Typically, one considers a model Hamiltonian on a lattice, \((\mathbb{Z}^d \text{ in } d \text{ spatial dimensions})\), whose eigenvalues correspond to the physically allowed energies. For a system on a periodic lattice, it is convenient to represent the Hamiltonian in the plane wave basis, \(e^{i(k \cdot r)}\), where the “quasimomentum” \(k \in T^d\), the \(d\)-dimensional torus. For noninteracting system, the Hamiltonian is block diagonal in \(k\), so that one obtains the “Bloch Hamiltonian”, \(H(k)\) indexed by \(k\), whose eigenvalues, \(E(k)\), correspond to the physical dispersion relation. However, if the system is finite along one (or more) of the directions, then the system must be described by the coordinate along that direction (\(x\), say) and the remaining transverse momentum \(k_{\perp}\).

The Dirac equation has been realized as a low-energy effective theory of certain condensed matter systems\cite{5, 14}, often termed “topological” in physics literature. For instance, a simple model Hamiltonian in \(2 + 1\) dimensions is

\[
H(k) = \sin k_x \sigma^1 + \sin k_y \sigma^2 + (2 + M - \cos k_x - \cos k_y) \sigma^3, \quad (1.24)
\]

Here, \(M\) acts as the mass of the Dirac fermion, which, being a system parameter, can be position dependent. The spectrum of the Bloch Hamiltonian is given by

\[
E(k) = \sqrt{\sin^2 k_x + \sin^2 k_y + (2 + M - \cos k_x - \cos k_y)^2}, \quad (1.25)
\]

so that the gap closes at \(k = 0\) for \(M = 0\), at \(k = (0, \pi), (\pi, 0)\) for \(M = -2\) or at \(k = (\pi, \pi)\) for \(M = -4\).

Now, one says that two Hamiltonians \(\mathcal{H}_1\) and \(\mathcal{H}_2\) are topologically equivalent if there exists a homotopy \(\tilde{\mathcal{H}}(t), t \in [0, 1]\) such that \(\tilde{\mathcal{H}}(0) = \mathcal{H}_1, \tilde{\mathcal{H}}(1) = \mathcal{H}_2\) and the spectrum is gapped for all \(\tilde{\mathcal{H}}(t)\). Thus, thinking of \(M\) as a parameter in \(\mathcal{H}\), we have 4 distinct classes, viz; \(M \in (-\infty, -4), (-4, -2), (-2, 0)\) and \((0, \infty)\).

The mass domain wall physics comes from the realization that the vacuum can be thought of as described by a Dirac Hamiltonian with \(M \to \pm \infty\). Thus, a Hamiltonian with \(M \in (-4, -2), (-2, 0)\) is not homotopically connected to the vacuum. The standard lore is that whenever this happens, the edge between our system and the vacuum hosts localized states, which are protected by the fact that the Hamiltonians on the two sides of the edge are topologically distinct.

For concreteness, let us consider a system with \(M = M_0 \in (-2, 0)\), so that the linearized Hamiltonian

\[9\]
around $k = 0$ can be written as

$$
\mathcal{H}(k) = k_x \sigma^1 + k_y \sigma^2 + M_0 \sigma^3.
$$

(1.26)

This is the low energy effective model, which is essentially a continuum Hamiltonian, as the system does not see the lattice, encoded in the periodicity of $k$ in the original expression. Now, let the system have an edge along $x$, we have the “topologically nontrivial” system with $M = M_0$ for $x < 0$ and vacuum with $M = M_{\text{vac}} > 0$ for $x > 0$. Inverse Fourier transforming along $x$, the Hamiltonian becomes

$$
\mathcal{H}(x, k_y) = (-i \partial_x) \sigma^1 + k_y \sigma^2 + m(x) \sigma^3, \quad m(x) = \begin{cases} 
M_0, & x < 0 \\
M_{\text{vac}}, & x > 0
\end{cases}
$$

(1.27)

Thus, we have obtained a mass domain wall. For $k_y = 0$, this corresponds to a zero energy mode localized at the interface, which cannot be removed by any local deformations of the Hamiltonian. This is essentially the sense in which these systems are “topological”: the boundary has a localized mode dependent only on the topology, and not the geometry, of the bulk.

### 1.2 The Dirac Equation

The Dirac equation in $d + 1$ dimensional spacetime can be written as

$$
[i \gamma^\mu \partial_\mu - m(x)] \psi(x, t) = 0,
$$

(1.28)

where the coordinate $(t, x) \in \mathbb{R}^{1,d}$, the $d + 1$ dimensional real space with the Minkowski metric, $\eta_{\mu\nu} = \text{diag}\{1, -1, \cdots -1\}$. The index $\mu$ runs from 0 to $d$ and the sum over repeated indices (Einstein summation) is implied. Typically, the coordinate $x^0$ is interpreted as time, while the rest of the $x^\mu$’s are interpreted as space coordinates. As we are interested in the bound states, we assume that the mass/scalar potential is independent of time. The $d + 1$ Dirac matrices $\gamma^\mu$ satisfy $\{\gamma_\mu, \gamma_\nu\} = \eta_{\mu\nu}$, generally taken to be Hermitian or anti-Hermitian matrices (depending on $(\gamma^\mu)^2 = \pm 1$) of order $n = 2^{\left[\frac{d+1}{2}\right]}$. Hence, the Dirac equation is a first order linear partial differential equation in $\psi : \mathbb{R}^{1,d} \rightarrow \mathbb{C}^n$.

The Dirac equation can also be written as the saddle point of the action functional

$$
S[\psi, \bar{\psi}] = \int d^dx \bar{\psi}(i \gamma^\mu \partial_\mu - m)\psi,
$$

(1.29)

where we have introduced $\bar{\psi} = \psi^\dagger \gamma^0$. Typically, $\psi$ and $\bar{\psi}$ are treated as the independent variables, so that the Dirac equation is equivalent to setting the variation of $S$ w.r.t $\bar{\psi}$ as zero. Furthermore, it can be written
in a Hamiltonian form by splitting the sum over $\mu$ and premultiplying by $\gamma^0$, as

\[
i \partial_t \psi = \mathcal{H}_{\text{Dirac}} \psi = [\gamma^0 \gamma^j (i \partial_j) + m(x) \gamma^0] \psi, \quad j = 1, 2, \ldots d,
\]

(1.30)

where $\gamma^0$ and $\gamma^0 \gamma^j$ are Hermitian matrices.

Being linear in $\psi$, the Dirac equation is clearly invariant under multiplication of $\psi$ by arbitrary constants $\zeta \in \mathbb{C}$. A multiplication by a real $\zeta$ is simply a scaling, which can be rid off by considering the solution on a real projective space, or alternatively, by normalizing the solution. Physically, as $\psi^\dagger \psi$ denotes a probability density function, it must integrate to unity, which fixes $\psi$ up to a phase. However, the system is still invariant under $\psi(x) \rightarrow e^{i\theta} \psi(x), \theta \in \mathbb{R}$, which is referred to as the global U(1) symmetry. A famous theorem by Emmy Noether states that there is a conserved current corresponding to every differentiable symmetry of the action. The current corresponding to this global U(1) symmetry is given by

\[
j^\mu = \bar{\psi} \gamma^\mu \psi = \psi^\dagger \gamma^0 \gamma^\mu \psi, \quad \mu = 0, 1, \ldots d.
\]

(1.31)

The zeroth component, $j^0 = \bar{\psi} \gamma^0 \psi = \psi^\dagger \psi \equiv \rho$, is simply the probability density, while the remaining components forming the $d$ vector $\mathbf{j}$ denote the probability current. This current is conserved in the sense that

\[
0 = \partial_\mu j^\mu = \frac{\partial \rho}{\partial t} - \nabla \cdot \mathbf{j},
\]

(1.32)

which is simply the continuity equation for the probability. Hence, the global U(1) symmetry ensures a local conservation of probability.
In this chapter, we describe the Dirac equation in 1+1 dimensions, which forms the basis of the rest of this work. We also construct a representation of the 1+1 dimensional Dirac equation reminiscent of the Prüfer representation (or “action-angle variables”), which essentially decomposes the Dirac spinor into an amplitude and an angle variables. Analyzing the decay characteristics of the amplitude, we can study the possibility of bound states.

2.1 Dirac equation in 1+1 dimensions

For the Dirac equation on $\mathbb{R}^{1,1}$ (“in 1 + 1 dimensions” in physics parlance), the Dirac matrices take a particularly nice form in terms of the Pauli matrices. Defining

$$\gamma^0 = \sigma^1, \gamma^1 = i\sigma^2,$$ (2.1)

so that $(\gamma^0)^2 = -(\gamma^1)^2 = 1$, the Dirac equation becomes

$$\mathcal{H}_{\text{Dirac}} = i\partial_t \psi(x,t) = \sigma^1 \left[ -\sigma^2 \partial_x + m(x) \right] \psi(x,t)$$

$$= \left[ \sigma^3(-i\partial_x) + m(x)\sigma^1 \right] \psi(x,t)$$ (2.2)

The eigenvalue condition for the Hamiltonian is

$$\left[ \sigma^3(-i\partial_x) + m(x)\sigma^1 - EI \right] \psi(x) = 0,$$ (2.3)

which can be written explicitly as

$$\begin{pmatrix} -i\partial_x & m(x) \\ m(x) & i\partial_x \end{pmatrix} \psi(x) = E\psi(x).$$ (2.4)

---

1In physics parlance, this is termed the “chiral basis”, as the chirality operator, $\gamma^5 = \gamma^0\gamma^1 = -\sigma^3$ is diagonal in this basis. Thus, if $\psi = (u, v)^T$, then $u$ and $v$ are the two chiral sectors, often termed “left-moving” and “right moving” modes.

2This is equivalent to substituting $\psi(x,t) = \psi(x)e^{-iEt}$, $E \in \mathbb{R}$ in eq. (2.2)
We are only interested in $E \in \mathbb{R}$, as $E$ is interpreted as the energy of a state, which must be real for a physical system\(^3\). We rearrange the Dirac equation as

$$i \psi'(x) = (im(x)\sigma^2 - E\sigma^3) \psi(x) \equiv M(E, x)\psi(x), \quad (2.5)$$

where

$$M(x) = im(x)\sigma^2 - E\sigma^3 = \begin{pmatrix} -E & m(x) \\ -m(x) & E \end{pmatrix}. \quad (2.6)$$

Thus, the Dirac equation represents a flow on $\mathbb{C}^2$ under $x$. A salient feature of this choice of the $\gamma$ matrices is that $M(E, x)$ is real. We consider following hypotheses on $m(x)$:

1) $m(x) : \mathbb{R} \rightarrow \mathbb{R}$ is piecewise $C^1$.

2) $m(x) \rightarrow \mu_\pm \in \mathbb{R}$ as $x \rightarrow \pm \infty$, where $\mu_\pm \neq 0$.

3) $m(x)$ approaches its asymptotic values monotonically and exponentially, i.e, $|m(x) - \mu_\pm|$ monotonically decreases to zero as $x \rightarrow \pm \infty$ and $\exists k > 0$ such that $\lim_{x \rightarrow \pm \infty} e^{k|x|} (m(x) - \mu_\pm) = 0$.

We shall term the cases where $\mu_+ - \mu_- > 0$ as a potential well, while the cases with $\mu_+ - \mu_- < 0$ will be referred to as instanton potentials.

**Remark 2.1.** Defining $\mu_0 = \min (|\mu_+|, |\mu_-|)$, we generally need $E \in [-\mu_0, \mu_0]$ for the existence of a bound state. The argument is essentially similar to the case of Schrödinger equation, where the (WKB) solution asymptotes to $e^{\pm \sqrt{E^2 - \mu_0^2}}$, which does not decay if $|E| > |\mu_0|$.

### 2.1.1 Bound states and discrete symmetries

In this thesis, we seek the bound states to the Dirac equations, i.e, the nontrivial solutions $\psi(x)$ that decay exponentially as $x \rightarrow \pm \infty$. We shall impose one further physical conditions that they do not carry any current, i.e, they are stationary in time\(^4\). The probability current in 1 + 1 dimension is given by

$$j^1 = \bar{\psi} \gamma^1 \psi = \bar{\psi} \gamma^0 \gamma^1 \psi = \psi^\dagger \gamma^1 (i\sigma^2) \psi = -\psi^\dagger \sigma^3 \psi. \quad (2.7)$$

For this to vanish, we shall demand that our solutions $\psi = (u, v)^T$, $u, v : \mathbb{R} \rightarrow \mathbb{C}$, satisfy

$$\psi^\dagger \sigma^3 \psi = |u|^2 - |v|^2 = 0. \quad (2.8)$$

\(^3\)In principle, the “energy” can have an imaginary part, which implies that the total probability of finding the particle in the entire space decays with time. Clearly, that is no way for any self-respecting particle to behave; however, such states were used by Gamow to model the $\alpha$-decay of heavy nuclei\([31, 32]\).
Next, we recall that from the linearity of the Dirac equation, it is clear that if $\psi(x)$ is a solution, then so is $e^{i\theta}\psi$; this is just the global $U(1)$ symmetry. Additionally, there are discrete symmetries, obtained by multiplying the Dirac equation by Pauli matrices to the left and/or complex conjugation. In the following, we state a few of these symmetries of some relevance in physics, esp condensed matter physics. If $\psi(x)$ solves the Dirac equation, then:

- $K\psi(x) = \psi^*(x)$ solves the Dirac equation with $x \to y = -x$, as
  \[
i\partial_y \psi^* = -i\partial_x \psi^* = (im(-y)\sigma^2 - E\sigma^3) \psi^*.
  \tag{2.9}
\]

This essentially follows from the fact that $M(E, x)$ is real.

- $\sigma^1\psi(x)$ also solves the Dirac equation with $x \to y = -x$, as
  \[
i\partial_y (\sigma^1\psi) = -\sigma^1 (im(-y)\sigma^2 - E\sigma^3) \psi = (im(-y)\sigma^2 - E\sigma^3) \sigma^1\psi.
  \tag{2.10}
\]

Hence, the Dirac spectrum is invariant under $x \to -x$ if $m(-x) = m(x)$. This is usually the case in particle physics as $m$, the bare fermionic mass, is taken to be a constant. This symmetry is referred to as “parity” (P).

- $\sigma^1 K\psi(x) = \sigma^1 \psi^*(x)$, where $K$ denotes complex conjugation, solves the Dirac equation as it is:
  \[
i\partial_x (\sigma^1\psi^*) = -\sigma^1 (im(x)\sigma^2 - E\sigma^3) \psi^* = (im(x)\sigma^2 - E\sigma^3) \sigma^1\psi^*.
  \tag{2.11}
\]

Hence, if $\psi(x)$ is a solution with energy $E$, so is $\sigma^1\psi^*(x)$. This is typically referred to as “time reversal” (T).

- $\sigma^2\psi(x)$ also solves the Dirac equation with $\tilde{E} = -E$, as
  \[
i\partial_x (\sigma^2\psi) = \sigma^2 (im(x)\sigma^2 - E\sigma^3) \psi = (im(x)\sigma^2 + E\sigma^3) \sigma^2\psi.
  \tag{2.12}
\]

Hence, given a solution at energy $E$, there is another solution with similar decay characteristics at energy $-E$. The spectrum of $\mathcal{H}_{\text{Dirac}}$ is therefore symmetric about $E = 0$. This symmetry is referred to as “energy-reflection” (ER) (or chirality).

---

4Strictly speaking, we can have stationary solutions that carry a constant nonzero current, but these are simply plane waves. Furthermore, we can have states which have a current that does not vanish everywhere but integrates to zero over $\mathbb{R}$. We shall not deal with such cases in this work.

5This is legitimate as the Pauli matrices have trivial kernels, so that $\sigma^i v = 0 \implies v = 0$. 

14
\[ \sigma^3 K \psi(x) = \sigma^3 \psi^*(x) \text{ solves the Dirac equation with } E \to -E, \text{ as} \]

\[ i\partial_x (\sigma^3 \psi^*) = -\sigma^3 (im(x)\sigma^2 - E\sigma^3) \psi^* = (im(x)\sigma^2 + E\sigma^3) \sigma^3 \psi^*. \]  \tag{2.13} \]

This is typically referred to as “charge conjugation” (C).

As \( \sigma^3 = i\sigma^2 \cdot \sigma^1 \), the last three symmetries are not independent. We shall usually concern ourselves only with ER and T. We also note that all the symmetries square to \( \mathbb{I} \). Furthermore, \( P \) and \( ER \) are unitary, while \( C \) and \( T \), containing the complex conjugation, are antiunitary.

**Remark 2.2.** For a fixed \( E \), only \( T \) is a genuine symmetry of the Hamiltonian, i.e., if \( \psi(x) \) solves the Dirac equation with eigenvalue \( E \), so does \( T\psi(x) \), so that we can take a basis of the eigenspace as \( \psi_{\pm}(x) \equiv \psi(x) \pm T\psi(x) \). But these solutions satisfy \( T\psi_{\pm}(x) = \pm \psi_{\pm}(x) \), so that we can restrict our analysis to the solutions that are the eigenvalues of \( T \), i.e., the solutions that satisfy \( \sigma^1 \psi^*(x) = \psi(x) \). Furthermore, one can explicitly check that if \( T\psi = \psi \), then \( T(i\psi) = -i\psi \).

**Remark 2.3.** If \( m(-x) = m(x) \) (for instance, in the case of a potential well), then parity is a genuine symmetry, so that if \( \psi(x) \) is a solution with eigenvalue \( E \), then so is \( \sigma^1 \psi(-x) \). Thus, \( E \) is degenerate, unless \( \psi(x) = \sigma^1 \psi(-x) \).

### 2.1.2 Exact solution for \( E = 0 \)

An interesting feature of the \( d = 1 \) system is the existence of an explicit bound state solution for \( E = 0 \) for a nontrivial \( m(x) \). Substituting \( E = 0 \) and the ansatz \( \psi(x) = \exp \{ \xi \int^x m(x')dx' \} \psi_0 \), where \( \psi_0 \in \mathbb{C}^2 \) is a constant, the Dirac equation becomes

\[ i\xi m(x) \psi_0 = im(x)\sigma^2 \psi_0 \implies \sigma^2 \psi_0 = \xi \psi_0. \]  \tag{2.14} \]

The eigenvalue condition for \( \psi_0 \) can be solved for \( \xi = \pm 1 \); however, not all \( m(x) \) will lead to a bound state solution. Considering \( m(x) \) such that \( \mu_\pm \geq 0 \) (instanton potential) and demanding that the resulting bound state decays exponentially as \( x \to \pm\infty \), we get the closed form solution

\[ \psi(x) = \zeta_0 \exp \left\{ -\int^x m(x')dx' \right\} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \]  \tag{2.15} \]
A typical instanton potential of this form is \( m(x) = \tanh \left( \frac{x}{a} \right), \ a > 0, \) for which the bound state solution becomes

\[
\psi(x) = \zeta \text{sech}^a \left( \frac{x}{a} \right) \psi_0. \tag{2.16}
\]

We plot this solution as well as the potential for \( a = 1 \) in the adjacent figure.

We can explicitly check that this solution satisfies the bound state condition of eq. (2.8). Furthermore, it satisfies \( \sigma^2 \psi = \psi, \) so that it is an eigenstate of the ER symmetry. Hence, all states \( \psi \) with eigenvalue \( E \) have their chiral partners \( \sigma^2 \psi \) with eigenvalue \(-E\), except for the zero mode. Thus, the number of zero modes is also the index of the Dirac operator.

Furthermore, this solution is clearly symmetric under \( C \) as \( \sigma^3 \psi^*(x) = \psi(x), \) and can be reduced to a to a \( T \)-invariant form as \( \psi \rightarrow \tilde{\psi} = e^{i\pi/4} \psi, \) so that

\[
\tilde{\psi}(x) = \zeta_0 \exp \left\{ - \int_0^x m(x') dx' \right\} \begin{pmatrix} e^{i\pi/4} \\ e^{-i\pi/4} \end{pmatrix}, \tag{2.17}
\]

which clearly satisfies \( \sigma^1 \tilde{\psi}^*(x) = \tilde{\psi}(x). \)

### 2.2 A Pr"{u}fer-type representation

The Pr"{u}fer representation was originally\(^{[33]} \) derived for the analysis of Strum-Liouville equations of the form

\[
\frac{d}{dx} \left( k(x) \frac{du}{dx} \right) + q(x) u = 0, \tag{2.18}
\]

where \( k, q, u : \mathbb{R} \rightarrow \mathbb{R}. \) Pr"{u}fer analysis then involves writing

\[
\phi(x) = \begin{pmatrix} u(x) \\ k(x)u'(x) \end{pmatrix} = \zeta(x) \begin{pmatrix} \cos \theta(x) \\ \sin \theta(x) \end{pmatrix}, \quad \phi : \mathbb{R} \rightarrow \mathbb{R}^2, \tag{2.19}
\]

so that

\[
\phi(x) = M(\lambda, x)\phi, \quad M(x) = \begin{pmatrix} 0 & \frac{1}{k(x)} \\ -q(x) & 0 \end{pmatrix}, \tag{2.20}
\]
and \( \zeta \) and \( \theta \) satisfy

\[
\begin{align*}
\zeta' &= \left( \frac{1}{k(x)} - q(x) \right) \zeta \sin \theta \cos \theta, \\
\theta' &= \frac{1}{k(x)} \cos^2 \theta + q(x) \sin^2 \theta.
\end{align*}
\]

The equation for \( \zeta(x) \) can clearly be integrated, while the equation for \( \theta(x) \) can be reduced to a Riccati equation

\[ \eta' = \frac{1}{k(x)} + q(x) \eta^2 \]  

by the substitution \( \eta = \tan \theta \). These equation are then quite useful in the analysis of the zeros of solutions as well as the boundary value problems[33, 6].

An equivalent representation is not possible for the Dirac equation as \( \psi : \mathbb{R} \to \mathbb{C}^2 \cong \mathbb{R}^4 \), which, in principle, has 4 degrees of freedom. However, the bound state condition, \(|u(x)|^2 = |v(x)|^2 \) (eq. (2.8)), can be used to derive a Prüfer-like representation of the Dirac equation. Consider the ansatz

\[
\psi(x) = \zeta(x) e^{i\varphi(x)} \left( \begin{array}{c} e^{i\theta(x)} \\ e^{-i\theta(x)} \end{array} \right), \quad \zeta, \varphi, \theta : \mathbb{R} \to \mathbb{R}.
\]

The Dirac equation, \( i\psi' = M\psi \), leads to

\[
\begin{pmatrix}
\zeta' \\
\frac{\zeta}{\zeta} - \varphi'
\end{pmatrix}
\begin{pmatrix}
e^{i\theta} \\
e^{-i\theta}
\end{pmatrix} - \begin{pmatrix}
\theta' \\
\theta'
\end{pmatrix}
\begin{pmatrix}
e^{i\theta} \\
e^{-i\theta}
\end{pmatrix} = \begin{pmatrix}
-Ee^{i\theta} + me^{i\theta} \\
-m e^{-i\theta} + E e^{-i\theta}
\end{pmatrix},
\]

which can be rewritten as

\[
-i \zeta' \frac{\zeta}{\zeta} - \varphi' = \theta' - E + m e^{-2i\theta} = -\theta' + E - m e^{2i\theta}.
\]

The latter equality gives

\[
\theta' = E - m \cos 2\theta \implies \frac{\zeta'}{\zeta} + i\varphi' = -m \sin 2\theta.
\]

Simply taking the real and imaginary part of the last equation, we get \( \varphi' = 0 \), so that \( \varphi(x) \) is a constant function (which can be made zero by a global \( U(1) \) rotation).

**Remark 2.4.** This simplification can also be explained in terms of the \( T \)-symmetry of the system, as for \( \varphi = 0 \), our ansatz satisfies \( T\psi = \psi \). This suffices for the given \( T \) symmetric system\(^6\), as per Remark 2.2.

---

\(^6\)If we break the \( T \) symmetry by adding a gauge field as \( i\partial_x \rightarrow i\partial_x + A \), we get \( \varphi' = A \), so that \( \varphi \) is not a constant anymore.
The Prüfer equations become

\[ \zeta'(x) = -\zeta(x)m(x)\sin 2\theta(x), \]
\[ \theta'(x) = E - m(x)\cos 2\theta(x). \quad (2.27) \]

We shall hereafter refer to \( \zeta(x) \) and \( \theta(x) \) as Prüfer “amplitude” and “phase” variables. The equation for \( \zeta(x) \) can be solved to get

\[ \zeta(x) = \zeta(x_0) \exp \left\{ -\int_{x_0}^{x} m(x')\sin 2\theta(x')dx' \right\}. \quad (2.28) \]

Interestingly, as \( \theta(x) \) determines \( \zeta(x) \) and hence \( \psi(x) \) completely, analyzing this equation is enough for the analysis of bound states.

**Remark 2.5.** Eq. (2.28) implies that \( \zeta(x) \) is either uniformly zero or it does not vanish anywhere. The former implies \( \psi(x) \equiv 0 \), which is not normalizable and hence unphysical. Hence, a bound state will have \( \zeta(x) \neq 0 \) \( \forall x \in \mathbb{R} \) and \( \zeta(x) \to 0 \) as \( x \to \pm\infty \).

**Remark 2.6.** The solutions to the Dirac equation are invariant under \( \theta \to \theta + n\pi \). As \( \psi(x) \) depends only on \( e^{i\theta(x)} \), it is clearly invariant under \( \theta(x) \to \theta(x) + 2n\pi \), but furthermore, under \( \theta(x) \to \theta(x) + \pi \), \( \psi(x) \to i\psi(x) \), which can be rotated back to the original solution using the global U(1) symmetry.

**Remark 2.7.** The action of discrete symmetries of the Dirac equation leaves the amplitude \( \zeta(x) \) invariant. Under \( P \) and \( T \) symmetries,

\[ P : \theta(x) \to -\theta(-x), \quad T : \theta(x) \to \theta(x), \quad (2.29) \]

while under \( C \) and \( \text{ER} \), we need an extra \( \text{U}(1) \) transform to get the wavefunction back to Prüfer form, with

\[ C : \theta(x) \to \theta(x) + \frac{\pi}{2}, \quad \text{ER} : \theta(x) \to -\theta(x) \frac{\pi}{2}. \quad (2.30) \]

### 2.2.1 Asymptotic behavior

In this section, we study some essential features of the Prüfer phase equation from a dynamical systems perspective. The equation \( \theta' = f(x, \theta) \), where \( f(x, \theta) = E - m(x)\cos 2\theta \), describes a nonlinear, nonautonomous flow on \( \mathbb{R} \). Let \( m(x) \to \mu \) as \( x \to \infty \), and we assume \( \mu > 0 \) without loss of generality. Clearly, \( f \) is \( C^1 \) in \( \theta \) and piecewise \( C^1 \) in \( x \), so that there is a solution to the system. The solution is unique[34], which follows from the fact that \( f(x, \theta) \) is Lipschitz continuous in \( \theta \), since

\[ |f(x, \theta_1) - f(x, \theta_2)| = |m(x)||\cos 2\theta_1 - \cos 2\theta_2| \leq 2\mu |\theta_1 - \theta_2|, \quad (2.31) \]
since $|m(x)| \leq \mu$ and $\|\cos 2\theta\|_{C^1} = 2$.

As $\theta$ and $\theta + \pi$ correspond to the same solution of the Dirac equation (Remark 2.6), we identify $\theta \sim \theta + \pi$, so that the Prüfer phase equation now describes a flow on $S^1$. Consider a constant $m(x) = \mu > 0$ and define $\tilde{f}(\theta) = E - \mu \cos 2\theta$, so that the system $\theta' = \tilde{f}(\theta)$ is autonomous. Its fixed points are obtained by setting $\tilde{f}(\theta) = 0$, whose stability is governed by $\partial_\theta \tilde{f}(\theta)$ evaluated at the fixed point. Explicitly, we have 2 fixed points at

$$\theta_s^* = \gamma, \quad \theta_u^* = \pi - \gamma; \quad \gamma = \frac{1}{2} \cos^{-1}\left(\frac{E}{\mu}\right) \in \left[0, \frac{\pi}{2}\right],$$

(2.32)

where the subscripts $s$ and $u$ denote the stable and unstable, respectively.

As the flow is defined on a compact manifold $S^1$, any solution of $\theta' = \tilde{f}(\theta)$ will tend to one of these fixed points as $x \to \infty$. Formally, let $\widetilde{\omega}(\theta_0)$ denote the $\omega$-limit set of the solution to $\theta' = \tilde{f}(\theta)$ with initial condition $\theta(x_0) = \theta_0$. Recall that the $\omega$-limit set of a trajectory $\theta(x)$ is defined as the set of all points $\theta^* \in S^1$ for which there exists a sequence $\{x_n\}_{n=1}^\infty$ such that

$$\lim_{n \to \infty} x_n = \infty, \quad \lim_{n \to \infty} \theta(x_n) = \theta^*.$$  

(2.33)

Similarly, the $\alpha$ limit is defined for $x \to -\infty$. Strictly speaking, these sets are defined for a trajectory, but as the system is deterministic, given a point $\theta_0 \in S^1$, so that we can define $\omega(\theta_0)$ and $\alpha(\theta_0)$ as the $\omega$- and $\alpha$-limit sets of the (unique) trajectory through $\theta_0$. With a slight abuse of notation\(^7\), define the limit set

$$\bar{\omega}(S^1) \equiv \bigcup_{\theta_0 \in S^1} \widetilde{\omega}(\theta_0) = \{\theta_u^*, \theta_s^*\}.$$  

(2.34)

Now, let $\omega(\theta_0)$ denotes the $\omega$-limit set of the solution to the nonautonomous system $\theta' = f(x, \theta)$ with initial condition $\theta(x_0) = \theta_0$. Then, we seek $\omega(S^1)$, defined in a similar fashion.

**Theorem 2.1.** All solutions of the Prüfer phase equation on $S^1$, where $m(x) \to \mu$ as $x \to \infty$, tend to a fixed point of the corresponding autonomous system with $m(x) = \mu$. Formally, $\omega(S^1) = \bar{\omega}(S^1)$.

**Proof.** The proof essentially hinges on the compactness of $S^1$. Given the two fixed points $\theta_u^*$ and $\theta_s^*$, the complement set $S^1 \setminus \{\theta_u^*, \theta_s^*\}$ is then a disjoint union of two open sets, $S_+$ and $S_-$, defined as

$$S_+ = \{\theta \mid \tilde{f}(\theta) > 0\}, \quad S_- = \{\theta \mid \tilde{f}(\theta) < 0\}.$$  

(2.35)

Next, we note that $E - \mu \leq \tilde{f}(E) \leq E + \mu$. Thus, for $-\mu < E < \mu$, choose a positive $\delta < \min\{\mu + E, \mu - E\}$,\(^7\) We note that $\omega(S^1)$, the “$\omega$-limit set” of $S^1$, does not need to be connected, unlike the $\omega$-limit set of a given trajectory.
and define the open sets $D^\pm_\pm \subset S_\pm$ as

$$D^+_- = \{ \theta \mid \bar{f}(\theta) > \delta \}, \quad D^-_+ = \{ \theta \mid \bar{f}(\theta) < -\delta \}. \tag{2.36}$$

Then, $S^1 \setminus (D^+_+ \cup D^-_-)$, where $D$ denotes the closure of a set $D$, is a disjoint union of sets $D^s_-$ and $D^-_u$, containing at $\theta^*_s$ and $\theta^*_u$, respectively. Define the 1-balls $B^s_\pm$ and $B^u_\pm$ centered at $\theta^*_s$ and $\theta^*_u$, respectively, and with radius $\epsilon(\delta)$, which contain $D^s_\pm$ and $D^-_\pm$, respectively. As $\bar{f}(\theta)$ is smooth, for a small enough $\delta$, we can use the implicit function theorem near $\theta^*$ to find a function $f^{-1}_{\mu,s}$ such that $\epsilon = f^{-1}_{\mu,s}(\delta)$, which ensures that $\epsilon \to 0$ as $\delta \to 0$.

Finally, note that for the compact set $D^s_-\pm$, we have $|\theta'| = |\bar{f}(\theta)| \geq \delta$, so that any trajectory that enters $D^s_-\pm$ must leave it after $\Delta x \sim \delta^{-1}$. Furthermore, as the $\omega$ limit set does not contain any limit cycles, it must be contained in $B^s_+ \cup B^u_-$. Take a sequence $\{\delta_n\}$ such that $\delta_n \to 0$ as $n \to \infty$. Thus,

$$\omega(S^1) \in \bigcap_{n=1}^{\infty} (B^s_n \cup B^u_n) = \{ \theta^*_s, \theta^*_u \} = \bar{\omega}(S^1). \tag{2.37}$$

Thus, all trajectories in $S^1$ tend to one of the fixed points of $\theta' = \bar{f}(\theta)$. \qquad \Box

### 2.2.2 Prüfer and Riccati

The Prüfer equation for $\theta(x)$ can be converted to a Riccati equation

$$y' = (E + m(x)) + y^2 (E - m(x)). \tag{2.38}$$

by substituting $y(x) = -\cot \theta(x)$. We can obtain another useful representation by substituting $y(x) = -f(m(x)) \cot \varphi(x)$, where $f(m)$ is a function of $m(x)$ to be determined later. This is equivalent to substituting $\theta = \cot^{-1}(f(m) \cot \varphi)$, up to a choice of the branch of the cotangent. Then, $\varphi$ satisfies

$$-f'(m)m' \cot \varphi + f(m) \csc^2 \varphi \varphi' = (E + m) + f^2(m) \cot^2 \varphi (E - m), \tag{2.39}$$

which can be rearranged as

$$\varphi' = \frac{E + m}{f(m)} \sin^2 \varphi + \frac{f(m)(E - m) \cos^2 \varphi + f'(m)}{f(m)} m' \sin^2 \varphi \cot \varphi. \tag{2.40}$$

---

8This is a generalization of the substitution used to obtain the Calogero bound for the Schrödinger equation in Reed and Simon[9], Theorem XIII.9.
We can choose \( f(m) \) to remove the \( \varphi \) dependence from the first two terms, by setting

\[
\frac{E + m}{f(m)} = f(m)(E - m) \implies f(m(x)) = \sqrt[\uparrow]{\frac{E + m(x)}{E - m(x)}},
\]

(2.41)

where \( f: (-1, 1) \to \mathbb{R}^+ \), as \( m(x) \in (-E, E) \). Thus,

\[
\varphi' = \sqrt{E^2 - m^2(x)} + \frac{m'(x)}{E^2 - m^2(x)} \sin^2 \varphi \cot \varphi.
\]

(2.42)

This is an alternative representation of the Prüfer equation. The term independent of \( \varphi \) is always positive, a feature that will be useful for deriving inequalities.
3 Exact solutions

In this chapter, we consider certain cases where an exact solution to the 1+1 dimensional Dirac equation can be obtained by transforming it to the corresponding Klein-Gordon (KG) equation. We compute the bound state conditions as well as the exact wavefunctions for the case of a square well and a tanh instanton potential. These results will be useful to compare with the corresponding results obtained in this thesis by relatively indirect means.

3.1 Klein-Gordon equation

The Dirac equation \( \psi' = -iM(E, x)\psi \) can be differentiated w.r.t \( x \) to get

\[
\psi'' = -iM'\psi - iM\psi' = -(iM' + M^2)\psi. \tag{3.1}
\]

This is the KG equation. Substituting \( M(E, x) = m(x)i\sigma^2 - E\sigma^3 \), we get

\[
\psi'' = \left[ (m^2(x) - E^2) \mathbb{1} + m'(x)\sigma^2 \right] \psi = \begin{pmatrix} m^2(x) - E^2 & -im'(x) \\ im'(x) & m^2(x) - E^2 \end{pmatrix} \psi. \tag{3.2}
\]

Let \( \psi = (u, v)^T \) and \( w_\pm = u \pm iv \), in terms of which the KG equation becomes

\[
\left( -\frac{d^2}{dx^2} + m^2(x) \mp m'(x) - E^2 \right) w_\pm = 0. \tag{3.3}
\]

Define the operators

\[
\hat{a} = \frac{d}{dx} + m(x) \implies \hat{a}^\dagger = -\frac{d}{dx} + m(x), \tag{3.4}
\]

which reduces the Klein-Gordon equation to

\[
(\hat{a}^\dagger \hat{a} - E^2) w_+ = 0, \quad (\hat{a} \hat{a}^\dagger - E^2) w_- = 0. \tag{3.5}
\]
We can define the “Hamiltonians” \( H_1 = \hat{a} \hat{a}^\dagger \) and \( H_2 = \hat{a}^\dagger \hat{a} \), which satisfy

\[
\hat{a} H_1 = H_2 \hat{a}, \quad H_1 \hat{a}^\dagger = \hat{a}^\dagger H_2,
\]

from which we deduce that if \( w(x) \) is an eigenvector of \( H_1 \) with eigenvalue \( E^2 \), then \( \hat{a} w \) is an eigenvector of \( H_2 \) with the same eigenvalue, unless \( \hat{a} w = 0 \).

In physics literature, such a pair of “Hamiltonians” \( H_1 \) and \( H_2 \) are often referred to as supersymmetric partners [35] and \( m(x) \) is termed the “superpotential”. The supersymmetry interpretation comes from defining

\[
H = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & 0 \\ \hat{a} & 0 \end{pmatrix}.
\] (3.7)

These satisfy the supersymmetry algebra

\[
[Q, H] = [Q^\dagger, H] = 0, \quad \{Q, Q\} = H.
\] (3.8)

Furthermore, we can rewrite \( Q = \hat{a} \xi, Q^\dagger = \hat{a}^\dagger \bar{\xi} \), where \( \xi, \bar{\xi} \) are the \( 2 \times 2 \) matrices as above, which satisfy

\[
\{\xi, \xi\} = \{\bar{\xi}, \bar{\xi}\} = 0, \quad \{\xi, \bar{\xi}\} = 1.
\] (3.9)

These are simply a representation of the Grassmann numbers. Thus, we have \( \hat{a} \), the “bosonic” degree of freedom, and \( \xi \), the “fermionic” degree of freedom, with \( Q = \hat{a} \xi \) rotating between the two. These are our supersymmetric partners.

The essential result of this factorization is that \( H_1 \) and \( H_2 \) have the same eigenvalues, \( E^2 \), corresponding to an eigenvalue \( E \) of the Dirac equation. Furthermore, as the solutions are related by \( \hat{a} \), this reduces solving the Dirac equation to solving one of the two second order differential operators (say, \( (H_1 - E^2)w_+ = 0 \)); the other solution can then be written in general as \( w_- = \kappa^{-1} \hat{a} w_+ \), where \( \kappa \in \mathbb{C} \setminus \{0\} \) is an arbitrary constant.

By differentiating the Dirac equation, we have introduced an extra degree of freedom, which we now need to fix by plugging

\[
\psi(x) = \begin{pmatrix} u \\ v \end{pmatrix} = A \begin{pmatrix} w_+ + w_- \\ -i(w_+ - w_-) \end{pmatrix} = \frac{A}{2\kappa} \begin{pmatrix} \kappa + \hat{a} \\ -i(\kappa - \hat{a}) \end{pmatrix} w_+(x)
\] (3.10)
back in the Dirac equation. Here $A$ is a normalization constant. Using $a = \partial_x + m$ and eq. (3.5), we get

$$0 = (\partial_x I + iM)\psi(x)$$

$$= \left( \begin{array}{cc} \partial_x - iE & im \\ -im & \partial_x + iE \end{array} \right) \left( \begin{array}{c} \kappa + \partial_x + m \\ -i\kappa + i\partial_x + im \end{array} \right) w_+(x)$$

$$= \left( \begin{array}{c} \kappa \partial_x + \partial_x^2 + m' + m \partial_x + \kappa(m - iE) + (-iE - m)(\partial_x + m) \\ -i\kappa \partial_x + i(\partial_x^2 + m') + im \partial_x + \kappa(E - im) + (-im - E)(\partial_x + m) \end{array} \right) w_+(x)$$

$$= \left( \begin{array}{c} (\kappa + \mu - iE - \mu\partial_x + \mu^2 - E^2 + km - i\kappa E - iEm - \mu\partial_x^2 \\ -i(\kappa - \mu + \mu - iE)\partial_x + i(\mu^2 - E^2) + \kappa E - i\kappa m - i\mu \partial_x^2 + mE \end{array} \right) w_+(x)$$

$$= \left( \begin{array}{c} (\kappa - i\mu)(\partial_x - iE + m) \\ -i(\kappa - i\mu)(\partial_x + iE + m) \end{array} \right) w_+(x). \quad (3.11)$$

Clearly, the only solution is $\kappa = iE$. We can write the normalized general solution as

$$\psi(x) = \frac{1}{2E \|w_+\|_2} \left( \begin{array}{c} \hat{a} + iE \\ i(\hat{a} - iE) \end{array} \right) w_+(x), \quad (3.12)$$

where the normalization constant was computed using

$$1 = \|\psi\|_2^2 = A^2 \int_{-\infty}^{\infty} w_+(x) (\hat{a}^\dagger - iE, -i(\hat{a}^\dagger + iE)) \left( \begin{array}{c} \hat{a} + iE \\ i(\hat{a} - iE) \end{array} \right) w_+(x)$$

$$= 2A^2 \int_{-\infty}^{\infty} w_+(x) (\hat{a}^\dagger \hat{a} + E^2) w_+(x)$$

$$= 4A^2 E^2 \int_{-\infty}^{\infty} |w_+(x)|^2 = 4A^2 E^2 \|w_+\|_2^2. \quad (3.13)$$

We shall often absorb this normalization constant in the other arbitrary constants for a given solution, with the tacit assumption that we can always normalize the solution at the end of the day.

At this point, we have the immense literature of exact solutions for the Schrödinger equation to draw upon (see, for instance, pp 40 of Ref [35] for a list). However, we shall consider only a few simple cases, which are particularly relevant to this work.

1) **Constant potential** ($m(x) = \mu$): In this case, the Klein-Gordon equation reduces to a Schrödinger equation

$$\left( -\frac{d^2}{dx^2} + q^2 \right) w_+ = 0, \quad q = \sqrt{\mu^2 - E^2}, \quad (3.14)$$

The most general solution is given by

$$w_+(x) = C_1 e^{qx} + C_2 e^{-qx}, \quad (3.15)$$
where $C_1$ and $C_2$ are (in general complex) constants, and $q$ is purely real for $|E| \leq |\mu|$ and purely imaginary for $|E| > |\mu|$.

2) **Linear potential** ($m(x) = \lambda x$): In this case, the Klein-Gordon equation reduces to the Weber differential equation:

$$\left( \frac{\partial^2}{\partial z^2} + \nu + \frac{1}{2} - \frac{z^2}{4} \right) w_+(z) = 0, \quad x = \frac{z}{\sqrt{2} \lambda}, \quad \nu = \frac{E^2}{2 \lambda}. \quad (3.16)$$

The most general solution of this equation is

$$w_+(z) = C_1 D_{\nu}(z) + C_2 D_{\nu}(-z), \quad (3.17)$$

where $D_{\nu}(z)$ denotes the parabolic cylinder function of order $\nu$. For $\nu = n$, a positive integer, these reduce to

$$D_n(z) = 2^{-n/2} e^{-z^2/4} H_n \left( \frac{z}{\sqrt{2}} \right), \quad (3.18)$$

where $H_n(x)$ are the Hermite polynomials. Thus, a linear potential is the analogue of the harmonic oscillator for the Dirac equation, which contains an infinite number of bound states$^1$.

3) **Tanh potential** ($m(x) = \tanh \left( \frac{x}{a} \right)$, $a > 0$): The Klein-Gordon equation becomes a Schrödinger equation with the Pöschl-Teller potential$^{[37]}$:

$$\left( -\frac{d^2}{dx^2} + \tanh^2 \left( \frac{x}{a} \right) - \frac{1}{a} \text{sech}^2 \left( \frac{x}{a} \right) - E^2 \right) w_+ = 0, \quad (3.19)$$

which, on substituting

$$z = \tanh \left( \frac{x}{a} \right) \implies \partial_x = \frac{dz}{dx} \partial_z = \frac{1}{a} \text{sech}^2 \left( \frac{x}{a} \right) \partial_z = \frac{1 - z^2}{a} \partial_z,$$

becomes

$$\left[ -\frac{1 - z^2}{a} \frac{d}{dz} \left( \frac{1 - z^2}{a} \frac{d}{dz} \right) + z^2 - \frac{1 - z^2}{a} - E^2 \right] w_+ = 0. \quad (3.20)$$

This is simply the generalized Legendre equation:

$$\left[ \frac{d}{dz} \left( 1 - z^2 \frac{d}{dz} \right) + a(a + 1) - \frac{\nu^2}{1 - z^2} \right] w_+ = 0, \quad \nu = a \sqrt{1 - E^2} \quad (3.21)$$

$^1$We do not go into the details of this potential as we are only concerned with potentials that asymptote to a constant value as $x \to \pm \infty$. The details of the solution can be found in Ref $[36]$
whose general solution is given by

$$w_+(z) = C_1 P\nu_a(z) + C_2 Q\nu_a(z),$$

(3.22)

where $P\nu_a$ and $Q\nu_a$ denote the associated Legendre functions of the first and second kind, respectively.

### 3.2 Specific cases

We solve for the bound state spectrum for two specific cases:

#### 3.2.1 Square well potential

We start off with the (finite) square well, or “particle in a box”, the first potential one typically encounters for the Schrödinger equation in introductory quantum mechanics\(^2\). Somewhat surprisingly, its Dirac analogue is not as commonly studied, possibly owing to various problems of interpretations, as well as issues like Klein paradox and the existence of a double-sided spectrum.

Consider a square potential well\(^3\), defined as

$$m(x) = \begin{cases} 
  b\mu, & x \in [-a, a] \\
  \mu, & \text{otherwise,} 
\end{cases} \quad a \in (0, \infty), \ b \in (-\mu^2, \mu^2), \ \mu > 0. \quad (3.23)$$

We can write down the solution in each region where $m(x)$ is constant using eq. (3.12). We demand that these solutions match at the boundaries and decay as $x \to \pm\infty$. As the bound states can occur only for energies $|b\mu| < |E| < \mu^2$, we define $q = \sqrt{\mu^2 - E^2} \in \mathbb{R}$ and $k = \sqrt{E^2 - (b\mu)^2} \in \mathbb{R}$.

For $x \in (-a, a)$, $\dot{a} = \partial_x + b\mu$, and the general solution can be written as

$$\psi(x) = C_1 e^{i\pi/4} \begin{pmatrix} e^{-i\pi/4} (b\mu + i(E + k)) \\
  e^{i\pi/4} (b\mu - i(E - k)) \end{pmatrix} e^{ikx} + C_2 e^{i\pi/4} \begin{pmatrix} e^{i\pi/4} (b\mu + i(E - k)) \\
  e^{i\pi/4} (b\mu - i(E + k)) \end{pmatrix} e^{-ikx}. \quad (3.24)$$

We seek to express $e^{-i\pi/4}(b\mu + i(E \pm k))$ in the polar form. Use

$$|b\mu + i(E \pm k)|^2 = (b\mu)^2 + E^2 + k^2 \pm 2kE = 2E(E \pm k)$$

\(^2\)The particle-in-a-box problem typically refers to a potential that is infinite everywhere except for a finite region, i.e., the potential well. For Dirac, this situation is problematic, as such walls would continuously radiate.
to write

\[ e^{-i\pi/4}(b\mu + i(E + k)) = \sqrt{2E(E + k)}e^{i\alpha}, \quad \alpha = \frac{1}{2} \cos^{-1} \left( \frac{b\mu}{E} \right) \]

\[ e^{-i\pi/4}(b\mu + i(E - k)) = \sqrt{2E(E - k)}e^{i\beta}, \quad \beta = \frac{1}{2} \cos^{-1} \left( \frac{b\mu}{E} \right). \quad (3.25) \]

We have used the fact that if \( e^{-i\pi/4}z = e^{-i\pi/4}(x + iy) = |z|e^{i\phi} \), then

\[ \tan \left( \phi + \frac{\pi}{4} \right) = \frac{y}{x} \implies \cos(2\phi) = \frac{2xy}{x^2 + y^2} = \frac{2xy}{|z|^2}. \quad (3.26) \]

Clearly, \( \cos(2\alpha) = \cos(2\beta) \), but \( \alpha \neq \beta + n\pi \), as that would imply \( E + k = E - k \), which is not true. Thus, we instead take \( \beta = -\alpha \). The wavefunction becomes

\[ \psi(x) = C_1 e^{i\pi/4} \left( \sqrt{2E(E + k)}e^{i\alpha} \right) e^{ikx} + C_2 e^{i\pi/4} \left( \sqrt{2E(E - k)}e^{-i\alpha} \right) e^{-ikx}. \quad (3.27) \]

Absorbing all the overall constants in \( C_1 \) and \( C_2 \), we get

\[ \psi(x) = A \left( \begin{array}{c} 1 \\ \nu \end{array} \right) e^{ikx} + B \left( \begin{array}{c} \nu \\ 1 \end{array} \right) e^{-ikx}, \quad \nu = \sqrt{\frac{E - k}{E + k}} = \frac{b\mu}{E + k}. \quad (3.28) \]

For \( x \notin (-a, a) \), \( \hat{a} = \partial_x + \mu \), and the general solution can be written as

\[ \psi(x) = \frac{C_1 e^{i\pi/4}}{2iE} \left( e^{-i\pi/4}(q + \mu + iE) \right) e^{ikx} + \frac{C_2 e^{i\pi/4}}{2iE} \left( e^{i\pi/4}(-q + \mu + iE) \right) e^{-ikx}. \quad (3.29) \]

By a calculation similar to the case of \( x \in (-a, a) \), we get

\[ \psi(x) = C \left( \begin{array}{c} e^{i\gamma} \\ e^{-i\gamma} \end{array} \right) e^{qx} + D \left( \begin{array}{c} e^{-i\gamma} \\ e^{i\gamma} \end{array} \right) e^{-qx}, \quad \gamma = \frac{1}{2} \cos^{-1} \left( \frac{E}{\mu} \right). \quad (3.30) \]

Thus, the most general solution can be written as

\[ \psi(x) = \begin{cases} 
C \left( \begin{array}{c} e^{i\gamma} \\ e^{-i\gamma} \end{array} \right) e^{qx}, & x \in (-\infty, -a), \\
A \left( \begin{array}{c} 1 \\ \nu \end{array} \right) e^{ikx} + B \left( \begin{array}{c} \nu \\ 1 \end{array} \right) e^{-ikx}, & x \in [-a, a], \\
D \left( \begin{array}{c} e^{-i\gamma} \\ e^{i\gamma} \end{array} \right) e^{-qx}, & x \in (a, \infty). 
\end{cases} \quad (3.31) \]
At the boundaries, \( x = \pm a \), we demand that \( \psi(\pm a^-) = \psi(\pm a^+) \). which leads to the matching condition

\[
e^{ia} \begin{pmatrix} A \\ B \end{pmatrix} = C \left( \begin{array}{cc} e^{-ika} & \nu e^{ika} \\ \nu e^{-ika} & e^{ika} \end{array} \right)^{-1} \left( \begin{array}{c} e^{i\gamma} \\ e^{-i\gamma} \end{array} \right) = D \left( \begin{array}{cc} e^{ika} & \nu e^{-ika} \\ \nu e^{ika} & e^{-ika} \end{array} \right)^{-1} \left( \begin{array}{c} e^{-i\gamma} \\ e^{i\gamma} \end{array} \right),
\]

where the inverse exists as the determinant, \( 2/k(E + k) \), is nonvanishing. Thus, the matching condition simplifies to

\[
\begin{pmatrix} e^{i(ka+\gamma)} - \nu e^{i(ka-\gamma)} & -e^{-i(ka+\gamma)} + \nu e^{-i(ka-\gamma)} \\ e^{-i(ka+\gamma)} - \nu e^{-i(ka-\gamma)} & -e^{i(ka+\gamma)} + \nu e^{i(ka-\gamma)} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = 0,
\]

so that by Cramer’s rule, the determinant of the matrix must vanish for a bound state, i.e

\[
e^{2ika}(e^{i\gamma} - \nu e^{-i\gamma})^2 = e^{-2ika}(\nu e^{i\gamma} - e^{-i\gamma})^2.
\]

This can be further simplified using

\[
\tan \gamma = -i \frac{e^{i\gamma} - e^{-i\gamma}}{e^{i\gamma} + e^{-i\gamma}} \iff e^{2i\gamma} = \frac{1 + i \tan \gamma}{1 - i \tan \gamma}
\]

so that

\[
e^{2ika} = \left( \frac{\nu e^{2i\gamma} - 1}{e^{2i\gamma} - \nu} \right)^2 = \left( \frac{(1 - \nu) + (1 + \nu)i \tan \gamma}{(1 - \nu) - (1 + \nu)i \tan \gamma} \right)^2.
\]

Define

\[
\lambda \equiv \frac{1 - \nu}{1 + \nu} = \sqrt{E + k} - \sqrt{E - k} = \frac{E - b\mu}{k} = \sqrt{\frac{E - b\mu}{E + b\mu}},
\]

so that

\[
\frac{1 + i\lambda \tan \gamma}{1 - i\lambda \tan \gamma} = \pm e^{2ika} = e^{2i(ka + \frac{n\pi}{2})} \implies \lambda \tan \gamma = \tan \left( ka + \frac{n\pi}{2} \right).
\]

This is a transcendental equation, whose solutions are the bound state energies. Using \( E = \mu \cos(2\gamma) \), we can also rewrite it as

\[
\cos(2ka + n\pi) = \frac{E(1 + \lambda) + \mu(1 - \lambda)}{E(1 - \lambda) + \mu(1 + \lambda)},
\]

For \( b = 0, k = E \) and \( \lambda = 1 \), so that the bound state condition reduces to

\[
E = \cos(2Ea + n\pi) = \pm \cos(2Ea).
\]

These expression agree with the bound state conditions derived in Ref. [39]. Similar expressions are obtained for the Dirac equation in 3 + 1 dimensions in Chapter 9 of Ref. [40].
3.2.2 Tanh Instanton

We now compute the spectrum of the well-known Tanh instanton potential, which has no direct analogue in the case of Schrödinger equation, as it has no classical “turning points”. We begin by writing out the general solution for the Dirac equation with the instanton potential \( m(x) = \tanh \left( \frac{x}{a} \right), \ a > 0 \). Using the recurrence relation for the associated Legendre functions,

\[
(1 - z^2) \frac{d}{dz} P_\nu^\mu(z) = (\nu + a) P_\nu^\mu(z) - az P_\nu^\mu(z),
\]

we get

\[
\hat{a} P_\nu^\mu(z) = \left( \frac{d}{dx} + \tanh \left( \frac{x}{a} \right) \right) P_\nu^\mu(z) = \frac{1 - z^2}{a} \frac{d}{dz} z + z P_\nu^\mu(z) = \left( 1 + \frac{\nu}{a} \right) P_\nu^\mu(z - 1),
\]

where \( z = \tanh x \) and \( \nu = a \sqrt{1 - E^2} \in [0, a] \). We have an identical expression for \( Q_\nu^\mu \). Finally, using eq. (3.12), the most general solution is

\[
\psi(x) = C_1 \left( (1 + \frac{\nu}{a}) P_{\nu - 1}^\mu(z) + iE P_\nu^\mu(z) \right) + C_2 \left( (1 + \frac{\nu}{a}) Q_{\nu - 1}^\mu(z) + iEQ_\nu^\mu(z) \right).
\]

This expression is reasonably ugly, but as we expect the bound states to decay as \( x \to \pm \infty \), we are only interested in its asymptotics. As \( x \to \pm \infty \),

\[
z = \tanh x \approx \pm (1 - e^{-2|x/a|}) = \pm (1 - 2\epsilon), \quad \epsilon \equiv e^{-|x/a|}.
\]

Using Mathematica\textsuperscript{TM}, we compute the series expansions of the associated Legendre functions

\[
\begin{align*}
P_\nu^\mu(1 - 2\epsilon) & \sim e^{-\frac{\pi}{2}} \left( \frac{1}{\Gamma(1 - \nu)} + O(\epsilon^\nu) \right), \\
P_\nu^\mu(-1 + 2\epsilon) & \sim -e^{-\frac{\pi}{2}} \left( \frac{\sin(\pi a)}{\sin(\pi \nu)\Gamma(1 - \nu)} + O(\epsilon^\nu) \right), \\
Q_\nu^\mu(1 - 2\epsilon) & \sim e^{-\frac{\pi}{2}} \left( \frac{\cot(\pi \nu) + 2}{\pi \nu \Gamma(1 - \nu)} + O(\epsilon^\nu) \right), \\
Q_\nu^\mu(-1 + 2\epsilon) & \sim -e^{-\frac{\pi}{2}} \left( \frac{\cos(\pi a)}{\sin(\pi \nu)\Gamma(1 - \nu)} + O(\epsilon^\nu) \right).
\end{align*}
\]
The crucial point to note here is that the singularity, $\epsilon^{-\nu/2} = e^{[\nu x/2a]}$, is independent of $a$. Thus, the leading order term in $\psi(x)$ can be written as

$$
\psi(x) \sim e^{\nu x/2a} \sin(\pi \nu) \frac{\Gamma(\nu)}{\pi} \left[ C_1 + C_2 \frac{\pi}{2} \cot(\pi \nu) \right] \left( \frac{1 + \frac{\nu}{a} + iE}{i(1 + \frac{\nu}{a} - iE)} \right), \quad x \to \infty,
$$

$$
\sim e^{\nu x/2a} \sin(\pi a) \frac{\Gamma(\nu)}{\pi} \left[ C_1 + C_2 \frac{\pi}{2} \cot(\pi a) \right] \left( \frac{1 + \frac{\nu}{a} - iE}{i(1 + \frac{\nu}{a} + iE)} \right), \quad x \to -\infty,
$$

(3.41)

where we have used the reflection formula for the Euler Gamma function

$$
\Gamma(\nu)\Gamma(1 - \nu) = \frac{\pi}{\sin(\pi \nu)}.
$$

Defining $\varphi = \tan^{-1} \left( \frac{\pi C_2}{2C_1} \right)$,

$$
\psi(x) \sim e^{\nu x/2a} \sin(\pi \nu + \varphi) \frac{\Gamma(\nu)}{\pi} \left( \frac{1 + \frac{\nu}{a} + iE}{i(1 + \frac{\nu}{a} - iE)} \right), \quad x \to \infty,
$$

$$
\sim e^{-\nu x/2a} \sin(\pi a + \varphi) \frac{\Gamma(\nu)}{\pi} \left( \frac{1 + \frac{\nu}{a} - iE}{i(1 + \frac{\nu}{a} + iE)} \right), \quad x \to -\infty.
$$

(3.42)

Thus, the solution diverges as $x \to \pm \infty$, unless

$$
\sin(\pi \nu + \varphi) = \sin(\pi a + \varphi) = 0.
$$

(3.43)

As $\varphi$ is arbitrary, we just need

$$
\pi a + \varphi = \pi \nu + \varphi + n\pi \implies \nu = a - n,
$$

(3.44)

so that the spectrum becomes

$$
a\sqrt{1 - E^2} = a - n \implies E_n = \pm \sqrt{1 - \left(1 - \frac{n}{a}\right)^2}.
$$

(3.45)

Thus, we have an analytic expression for the spectrum of the Tanh potential, which in agreement with Ref [35]. There are a total of $[a]$ bound states for $E \in (0, 1)$, corresponding to $n = 0, 1, 2, \ldots [a]$. 

30
4 Dirac Equation and Geometry

An interesting perspective on the existence of bound states is the shooting argument by Jones[12, 13] for the stability of traveling wave solutions of the nonlinear Schrödinger equation. In this section, we derive a similar formalism for the Dirac equation. We begin by mapping the Dirac equation, thought of as a flow on $\mathbb{C}^2$, to a Hamiltonian flow on $\mathbb{R}^4$, and consider the induced flows on $G_{2,4}$, the space of 2-dimensional subspaces of $\mathbb{R}^4$. However, using the global $U(1)$ symmetry of the Dirac equation, we can actually map the individual solutions of the Dirac equation to the trajectories of the flow induced on $G_{2,4}$. The vanishing current condition for a bound state turns out to be equivalent to the condition that these subspaces be Lagrangian, so that we construct the flows explicitly on $\mathcal{L}(2)$, the set of Lagrangian planes, and $C(2)$, its universal covering space, using the parametrization derived in Appendix A.

4.1 A Hamiltonian flow on $\mathbb{R}^4$

We seek a bijection $\mathcal{R} : \mathbb{C}^2 \to \mathbb{R}^4$ which maps the flow of eq. (2.5) on $\mathbb{C}^2$ corresponding to the Dirac eigenvalue problem to a Hamiltonian flow on $\mathbb{R}^4$. As $M(E, x) \in \mathbb{R}^{2 \times 2}$, defining $\psi = \psi_R + i\psi_I$, $\psi_R, \psi_I \in \mathbb{R}^2$, we can take the real and imaginary parts of eq. (2.5) as

$$\partial_x \psi_R = M \psi_I, \quad \partial_x \psi_I = -M \psi_R. \quad (4.1)$$

Putting these together as a vector in $\mathbb{R}^4$ as

$$\partial_x \begin{pmatrix} \psi_R \\ \psi_I \end{pmatrix} = \mathcal{J} \mathcal{H} \begin{pmatrix} \psi_R \\ \psi_I \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix}, \quad (4.2)$$

does not work as $M$, and hence $\mathcal{H}$, is not Hermitian. Instead, take $\psi = (u, v)^T$ and define $w = -u_I$ so that

$$\partial_x \begin{pmatrix} u_R \\ v_R \end{pmatrix} = \begin{pmatrix} E & m(x) \\ m(x) & E \end{pmatrix} \begin{pmatrix} w \\ v_I \end{pmatrix} \equiv M_+ \begin{pmatrix} w \\ v_I \end{pmatrix}, \quad (4.3)$$
\[
\partial_x \begin{pmatrix} w \\ v_I \end{pmatrix} = - \begin{pmatrix} E & -m(x) \\ -m(x) & E \end{pmatrix} \begin{pmatrix} u_R \\ v_R \end{pmatrix} \equiv -M_- \begin{pmatrix} u_R \\ v_R \end{pmatrix}.
\]

These can be combined as
\[
\Psi' = A(E, x) \Psi := JH \Psi, \quad H = \begin{pmatrix} M_- & 0 \\ 0 & M_+ \end{pmatrix},
\]

where \( H \) is now Hermitian as \( M_\pm = E\mathbb{I} \pm m(x)\sigma^1 \) are Hermitian, and
\[
\psi = \begin{pmatrix} u_R + iu_I \\ v_R + iv_I \end{pmatrix} \in \mathbb{C}^2 \rightarrow \Psi = \mathcal{R}(\psi) = \begin{pmatrix} u_R \\ v_R \\ -u_I \\ v_I \end{pmatrix} \in \mathbb{R}^4.
\]

Hence, the Dirac equation induces a Hamiltonian flow on \( \mathbb{R}^4 \), so that every solution of the original system corresponds to a trajectory on \( \mathbb{R}^4 \).

### 4.1.1 Symmetries

The symmetries of the Dirac equation can be thought of as representations of the symmetry groups on \( \mathbb{C}^2 \), which induces a representation of the corresponding groups in \( \mathbb{R}^4 \) under \( \mathcal{R} \), which we now construct explicitly. To begin with, the global U(1) symmetry
\[
\psi \rightarrow \psi e^{i\theta} = \begin{pmatrix} (u_R \cos \theta - u_I \sin \theta) + i(u_R \sin \theta + u_I \cos \theta) \\ (v_R \cos \theta - v_I \sin \theta) + i(v_R \sin \theta + v_I \cos \theta) \end{pmatrix},
\]

takes \( \Psi \rightarrow \mathcal{R}(\theta) \Psi \), where
\[
\mathcal{R}(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta & 0 \\ 0 & \cos \theta & 0 & -\sin \theta \\ -\sin \theta & 0 & \cos \theta & 0 \\ 0 & \sin \theta & 0 & \cos \theta \end{pmatrix}.
\]

More concisely, \( \mathcal{R}(e^{i\theta} \psi) = \mathcal{R}(\theta) \mathcal{R}(\psi) \). This is the induced representation of \( \mathcal{R} \) of U(1) \( \cong \text{SO}(2) \) on \( \mathbb{R}^4 \), which corresponds to two copies of the fundamental representations of SO(2) with angles \( \theta \) and \(-\theta\). One way to understand this is to notice that \( \mathcal{R} : \mathbb{C}^2 \rightarrow \mathbb{R}^4 \) can be thought of as simply taking \( u \mapsto u^* \) followed by \( \psi = (u, v)^T \mapsto (\psi_R, \psi_I)^T \), so that the action of U(1) now corresponds to \( u^* \mapsto e^{-i\theta} u^* \), \( v \mapsto e^{i\theta} v \), which are the fundamental complex representations of U(1) with angles \( \theta \) and \(-\theta\).
Similarly, the C, P, T and ER symmetries defined in §2.1.1 induce representations of $\mathbb{Z}_2$ on $\mathbb{R}^4$, given by

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$T = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad E = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$  (4.9)

We can explicitly check that $C^2 = P^2 = T^2 = E^2 = I$. Furthermore, they all belong to the Lie group $O(4)$.

Using these symmetries, we have the following results about the system $\Psi' = A(E,x)\Psi$:

**Lemma 4.1.** All eigenvalues of $A(E,x)$ have a geometric multiplicity of at least 2.

**Proof.** This is an immediate consequence of the global U(1) invariance of the Dirac equation\(^1\). For a fixed $E$ and $m(x)$, given a solution $\Psi(x)$ of $\Psi' = A(E,x)\Psi$, any other $\Psi_\theta(x) = R(\theta)\Psi(x)$ also satisfies the equation, so that $\forall \theta \in [0,2\pi)$,

$$\Psi'(x) = A(E,x)\Psi(x) \quad R(\theta)\Psi'(x) = A(E,x)R(\theta)\Psi(x) \quad \Rightarrow \quad A(E,x)R(\theta) = R(\theta)A(E,x). \quad (4.10)$$

Now, if $\Psi_0$ is an eigenvector of $A(E,x)$ for a given $x$ with eigenvalue $\rho$, the commutation of $A(E,x)$ and $R(\theta)$ implies that so is $\Phi_0 = R(\pi/2)\Psi_0$. But an explicit calculation shows that $\Phi_0$ and $\Psi_0$ are orthogonal, so that the eigenspace corresponding to $\rho$ is at least 2-dimensional. Hence, we conclude that every eigenvalue of $A$ has a geometric multiplicity of at least 2.

\[ \square \]

**Lemma 4.2.** $\sigma[A(E,x)]$ is invariant under $E \rightarrow -E$.

**Proof.** This follows from the ER-symmetry of the Dirac equation. For a fixed $m(x)$, given a solution $\Psi(x)$ of $\Psi' = A(E,x)\Psi$, $E\Psi(x)$ also satisfies the equation with $E \rightarrow -E$, so that

$$\Psi'(x) = A(E,x)\Psi(x) \quad E\Psi'(x) = A(-E,x)E\Psi(x) \quad \Rightarrow \quad E A(E,x)E = A(-E,x), \quad (4.11)$$

\(^1\)One gets a similar result, the so-called Kramers’ degeneracy, when the time-reversal operator is defined such that $T^2 = -I$, which hinges on the fact that then $\psi$ and $T\psi$ must be orthogonal. Since we have $T^2 = I$, we may have $T\psi = \psi$, so that $T$ is not sufficient to ensure the degeneracy.
as $\mathcal{E}^2 = 1$. Now, if $\Psi_0(x)$ is an eigenvector of $A(E, x)$ for a given $x$ with eigenvalue $\rho$ and $\Phi_0 = \mathcal{E}\Psi_0$, then

$$\rho \Phi_0 = \mathcal{E}(\rho \Psi_0) = \mathcal{E}A(E, x)\Psi_0 = A(-E, x)\Phi_0,$$

(4.12)

so that $\rho$ is also an eigenvalue of $A(-E, x)$. Hence, $\sigma[A(E, x)]$ is invariant under $E \to -E$. \qed

4.1.2 Compactification

The flow defined by $\Psi' = A(E, x)\Psi$ is non-autonomous, as $A$ depends on $x$. Defining $\tau = \tanh(\kappa x) \in (-1, 1)$, $\kappa > 0$, which compactifies $x \in \mathbb{R}$, we get an autonomous flow $(\Psi(x), \tau(x)) \in \mathbb{R}^4 \times (-1, 1)$ as

$$\Psi' = \tilde{A}(E, \tau)\Psi, \quad \tau' = \kappa(1 - \tau^2).$$

(4.13)

The functions of the compactified variable $\tau$ are written with a tilde, for instance, $\tilde{A}(E, \tau) = A\left(E, \frac{1}{\kappa} \tanh^{-1} \tau\right)$. The fixed points of this flow are formally given by $\Psi' = \tau' = 0$, i.e., by $\tilde{A}\Psi = 0$, $\tau = \pm 1$. But as the system is defined only for $\tau \in (-1, 1)$, we need to extend it to $\tau \in [-1, 1]$ by defining $\tilde{A}(E, \pm 1)$ so that $\tilde{A}(E, \tau)$ is smooth near $\tau = \pm 1$. As $A(E, x)$ depends on $x$ only through $m(x)$, using the hypotheses on $m(x)$, we derive a lemma analogous to Lemma 2.2 of Jones’ paper [12].

Lemma 4.3. A $\kappa \in \mathbb{R}$ can be chosen so that $\tilde{m}(\tau)$ extends to $\tau = \pm 1$ in a $C^1$ fashion.

Proof. Define $\tilde{m}(\pm 1) = \mu_{\pm}$. The continuity follows immediately from the assumptions on $m(x)$, as

$$\lim_{\tau \to \pm 1} |\tilde{m}(\tau) - \mu_{\pm}| = \lim_{x \to \pm\infty} |m(x) - \mu_{\pm}| = 0.$$  

(4.14)

For $\tilde{m}(\tau)$ to be differentiable at, say, $\tau = 1$, we need the existence of the limit

$$\frac{d}{d\tau} \tilde{m}(\tau) \bigg|_{\tau=1} = \lim_{\tau \to 1} \frac{\mu_{+} - \tilde{m}(\tau)}{1 - \tau} = \lim_{x \to \infty} \frac{\mu_{+} - m(x)}{1 - \tanh(\kappa x)} = \lim_{x \to \infty} \frac{1}{2} e^{2\kappa x} (\mu_{+} - m(x)).$$  

(4.15)

But the hypotheses on $m(x)$ imply that $\exists k > 0$ s.t. $\lim_{x \to \infty} e^{kx} (\mu_{+} - m(x)) = 0$. An identical computation shows that this choice of $\kappa$ also ensures the differentiability of $\tilde{m}(\tau)$ at $\tau = -1$. Hence, defining $\tilde{m}(\pm 1) = \mu_{\pm}$ extends $\tilde{m}(\tau)$, and hence $\tilde{A}(E, \tau)$ to $\tau \in [-1, 1]$ in a $C^1$ fashion. \qed

Following the extension to $\tau = \pm 1$, we have a flow on $\mathbb{R}^4 \times [-1, 1]$, described by

$$\Psi' = \tilde{A}(E, \tau)\Psi, \quad \tau' = \kappa(1 - \tau^2).$$

(4.16)
The planes $\tau = \pm 1$ are invariant, on which the system is simply $\Psi'(x) = \tilde{A}(E, \pm 1)\Psi$, which is a linear ODE with constant coefficients. We explicitly compute the spectrum of $\tilde{A}(E, a)$, $a = \pm 1$ as

$$0 = \det(\rho I_4 - \tilde{A}) = \begin{vmatrix} \rho \bar{l}_2 & -\tilde{M}_+ \\ \tilde{M}_- & \rho \bar{l}_2 \end{vmatrix}$$

$$= \det(\rho \bar{l}_2) \det \left( \rho \bar{l}_2 + \tilde{M}_+ \rho^{-1} \tilde{l}_2 \tilde{M}_- \right)$$

$$= \det \left( \rho^2 \bar{l}_2 + \tilde{M}_+ \tilde{M}_- \right)$$

$$= \rho^2 - E^2 + \mu^2_a,$$  \hspace{1cm} (4.17)

where we have used $\tilde{M}_+ \tilde{M}_- = (E^2 - \mu^2_a) I_2$, $a = \pm 1$. The eigenvalues are given by

$$\rho = \pm \sqrt{\mu^2_a - E^2} = \pm \rho_a, \quad \rho_a \equiv \sqrt{\mu^2_a - E^2}.$$  \hspace{1cm} (4.18)

Clearly, both the eigenvalues are doubly degenerate and invariant under $E \rightarrow -E$, as dictated by Lemma 4.1 and 4.2. From Remark 2.1, we are only interested in $|E| \leq \min_a(|\mu_a|)$, and $A(E, a)$ is singular if $|E| = |\mu_a|$.

Consider the nonsingular case first, when the fixed points in the $\tau = \pm 1$ plane are simply $\Psi = 0$. For $|E| < |\mu_a|$, the eigenvalues lie on the real axis, so that $\tilde{A}(E, a)$ is hyperbolic and there is a 2-dimensional unstable subspace $U_a$ corresponding to the eigenspace of $\rho = \rho_a$ and a 2-dimensional stable subspace $S_a$ corresponding to $\rho = -\rho_a$. Explicitly, we can write these subspaces, using the eigenvectors of $\tilde{A}(E, a)$, as

$$U_a = \text{span} \left\{ \frac{1}{\sqrt{2}} (\lambda_a, 0, -\xi_a, 1)^T, \frac{1}{\sqrt{2}} (\xi_a, 1, \lambda_a, 0)^T \right\},$$  \hspace{1cm} (4.19)

$$S_a = \text{span} \left\{ \frac{1}{\sqrt{2}} (0, \lambda_a, -1, \xi_a)^T, \frac{1}{\sqrt{2}} (-1, -\xi_a, 0, \lambda_a)^T \right\},$$  \hspace{1cm} (4.20)

where $\xi_a = E/\mu_a \in (-1, 1)$ and $\lambda_a = \text{sgn}(\mu_a) \sqrt{1 - \xi^2}$.

In the singular case ($|E| = |\mu_a|$), all eigenvalues vanish, and $\tilde{A}$ is defective as $\text{rank}(\tilde{A}) = 2 < \text{dim}(\tilde{A})$. Reducing $A$ to its Jordan canonical form, the dynamics on the invariant plane $\tau = a$ is given by

$$\Psi' = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Psi \implies \begin{cases} \Psi_1' = \Psi_2, \\ \Psi_3' = \Psi_4, \\ \Psi_2' = \Psi_4' = 0. \end{cases}$$  \hspace{1cm} (4.21)

Thus, there is no dynamics in the plane given by $\Psi_2 = \Psi_4 = 0$, which acts as a repeller in $\mathbb{R}^4$, as any $\Psi$ outside that plane diverges linearly along a trajectory normal to the plane\(^2\).

\(^2\)Recall that a constant coefficient ODE has a constant and a linear solution for a nontrivial $2 \times 2$ Jordan block.
4.1.3 Global Stable/Unstable manifolds

The bound states, by the requirement that they be normalizable (i.e., have a finite nonzero $L_2$ norm), must decay to $0$ as $x \to \pm \infty$. On $\mathbb{R}^4 \times [-1, 1]$, they correspond to the trajectories that tend to the fixed points $(0, -1)$ as $x \to -\infty$ and to $(0, 1)$ as $x \to \infty$. Define the global stable manifold $W^s_+ \subset \mathbb{R}^4$ as the set of initial conditions which tend to $(0, 1)$ as $x \to \infty$, or, alternatively, as the basin of attraction of $(0, 1)$. Formally\footnote{See §2.2.1 for a definition of the $\omega$- and $\alpha$-limit sets, or Ref [34] for more details.},

$$W^s_+ = \{ (\Psi, \tau) \in \mathbb{R}^4 \times [-1, 1] | \omega((\Psi, \tau)) = (0, 1) \}. \quad (4.22)$$

Similarly, the global unstable manifold $W^u_-$ as the set of initial conditions which tend to $(0, -1)$ as $x \to -\infty$, or, alternatively, as the basin of attraction of $(0, -1)$ for the system running backwards in $x$. Formally,

$$W^u_- = \{ (\Psi, \tau) \in \mathbb{R}^4 \times [-1, 1] | \alpha((\Psi, \tau)) = (0, -1) \}. \quad (4.23)$$

These manifolds are clearly functions of $E$ and $\mu_a$. The bound states correspond to a trajectory (or, equivalently, a point $(\Psi, \tau)$) that lies in $W^u_- \cap W^s_+$. However, the trivial solution $(0, \tanh(\kappa(x - x_0)))$ lies entirely in $W^u_- \cap W^s_+$. Hence, following Jones[12], we have the following lemma:

**Lemma 4.4.** If $W^u_-(E) \cap W^s_+(E) \neq \{0\} \times (-1, 1)$, then there is a bound state of the Dirac equation with energy $E$.

**Remark 4.1.** The global stable/unstable manifolds are 3-dimensional submanifolds of $\mathbb{R}^4$, the $\tau$ slices of which, i.e., $W^s_+ \cap \{\tau = \tau_0\}$ and $W^u_- \cap \{\tau = \tau_0\}$ are 2-dimensional subspaces of $\mathbb{R}^4/[12]$. Indeed,

$$S_+ = W^s_+ \cap \{\tau = +1\}, \quad U_- = W^u_- \cap \{\tau = -1\}. \quad (4.24)$$

Thus, these slices can be thought of as a curve in $G_{2,4}$, the space of 2-dimensional subspace of $\mathbb{R}^4$.

4.2 Subspaces of $\mathbb{R}^4$

We seek to follow Jones’ construction of thinking of the curves on $G_{2,4}$ corresponding to the global stable/unstable manifolds as trajectories of a flow induced on $G_{2,4}$. However, we note that the symmetries of the Dirac equation offer an additional interpretation to the induced flow.

**Lemma 4.5.** Every nontrivial solution $\psi(x)$ of the Dirac equation corresponds to a unique 2-dimensional subspace $\Psi(x) \in G_{2,4}$ for each $x \in \mathbb{R}$ where $\psi(x) \neq 0$. 
Proof. This immediately follows from the induced representation of $U(1)$ on $\mathbb{R}^4$. Given a solution $\psi(x)$, we have a family of solutions $e^{i\theta}\psi(x)$, which correspond to the set of vectors $\{R(\theta)R(\psi) | \theta \in [0,2\pi]\}$. These vectors form a 2-dimensional subspace of $\mathbb{R}^4$ if $R(\psi) \neq 0 \iff \psi \neq 0$, as $R$ is a bijection. \hfill \Box

Lemma 4.6. The zero current condition for $\psi(x)$ is equivalent to the condition that the subspaces $\psi(x)$ are Lagrangian $\forall x \in \mathbb{R}$.

Proof. We begin by invoking Remark 2.5 to note that if $\psi$ satisfies the zero current condition, it is nonzero everywhere, so that from Lemma 4.5, $\exists \psi(x) \in \mathbb{G}_{2,4} \forall x \in \mathbb{R}$. Fix $x$, and for $\psi = (u,v)^T$, construct a basis $\{\Psi, \Phi\}$ of $\psi(x)$ as

$$
\Psi = R(\psi) = (u_R, v_R, -u_I, v_I)^T, \quad \Phi = R(i\psi) = (-u_I, -v_I, -u_R, v_R)^T.
$$

(4.25)

The zero current condition (eq. (2.8)) then implies that

$$
\Omega(\Phi, \Psi) = \langle \Phi, J\Psi \rangle = |v(x)|^2 - |u(x)|^2 = 0.
$$

Thus, each bound state solution of the Dirac equation corresponds to a unique trajectory for the flow on $\mathcal{L}(2)$. We shall see this relation explicitly using a parametrization of $\mathcal{L}(2)$.

4.2.1 The flow on $G_{2,4}$

The dynamical system on $\mathbb{R}^4 \times [-1,1]$ naturally induces a flow on $\Lambda^2(\mathbb{R}^4) \times [-1,1]$, where $\Lambda^2(\mathbb{R}^4) \cong \mathbb{R}^6$ is the second exterior power of $\mathbb{R}^4$. Given $Q = \Phi \wedge \Psi$, by chain rule

$$
Q' = \Phi' \wedge \Psi + \Phi \wedge \Psi' = \tilde{A}\Phi \wedge \Psi + \Phi \wedge \tilde{A}\Psi = \tilde{A}^{(2)}Q,
$$

(4.26)

where we have defined an operator $\tilde{A}^{(2)} : \Lambda^2(\mathbb{R}^4) \to \Lambda^2(\mathbb{R}^4)$ corresponding to $\tilde{A} : \mathbb{R}^4 \to \mathbb{R}^4$. Thus, the induced flow on $\Lambda^2(\mathbb{R}^4) \times [-1,1]$ is

$$
Q' = \tilde{A}^{(2)}Q, \quad \tau' = \kappa(1 - \tau^2).
$$

(4.27)

As this is linear in $Q$, we can project down to $\mathbb{RP}^5 \times [-1,1]$ to get

$$
\psi' = a(E, x, \psi), \quad \tau' = \kappa(1 - \tau^2).
$$

(4.28)
where $\psi = \Pi(Q) \in \mathbb{RP}^5$. As the Grassmannian $G_{2,4}$ is a surface of codimension 1 in $\mathbb{RP}^5$ (see Appendix A, esp Lemma A.1 for details), this further induces a flow on $G_{2,4} \times [-1,1]$. Again, we have invariant planes given by $\tau = \pm 1$.

**Lemma 4.7.** The stable and unstable subspaces $U_{\pm}$ and $S_{\pm}$ are fixed points of the flow on the invariant planes $G_{2,4} \times \{\pm 1\}$.

**Proof.** Consider the plane $\tau = a, a = \pm 1$. Let $\psi(x)$ be a solution to the flow on $G_{2,4}$ with the initial condition $\psi(x_0) = \Psi_1(x_0) \wedge \Psi_2(x_0)$, where $\Psi_i(x_0) \in S_a, \ i = 1, 2$. The $\Psi_i$'s evolve under the flow on $\mathbb{R}^4$ as

\[
\Psi_i' = A(E,a)\Psi_i = -\rho_a \Psi_i \implies \Psi_i(x) = e^{-\rho_a(x-x_0)}\Psi_i(x_0). \tag{4.29}
\]

Thus, if $\Psi_i(x_0) \in S_a$, so is $\Psi_i(x) \forall x$, so that $\psi(x) = \Psi_1(x) \wedge \Psi_2(x) = S_a$. Hence, $S_a$ is invariant under the flow on $G_{2,4}$, and is hence a fixed point. An identical calculation shows that $U_a$ is also a fixed point. \hfill $\square$

Next, we study the stability of these fixed points. We define $\mathcal{D}(\psi)$, the **train** of a space $\psi \in G_{2,4}$, as the set of subspaces of $\mathbb{R}^4$ that have a nontrivial overlap with $\psi$. This is a surface of codimension 1 in $G_{2,4}$ (see Appendix A for details).

**Lemma 4.8.** The set $\mathcal{D}(S_{\pm})$ is a repeller to the flow on $G_{2,4} \times \{\pm 1\}$.

**Proof.** Consider the plane $\tau = a, a = \pm 1$. Reduce $\tilde{A}(E,a)$ to the Jordan canonical form:

\[
\tilde{A}(E,a) = \begin{pmatrix}
-\rho_a & 1 & 0 & 0 \\
0 & -\rho_a & 0 & 0 \\
0 & 0 & \rho_a & 1 \\
0 & 0 & 0 & \rho_a
\end{pmatrix}, \quad \rho_a = \sqrt{\mu_a^2 - E^2}, \tag{4.30}
\]

so that $S_a = \text{span}\{e_1, e_2\}$ and $U_a = \text{span}\{e_3, e_4\}$. In this basis, using eq. (A.22) from Appendix A, the train of the stable subspace becomes

\[
\mathcal{D}(S_a) = \{ \phi \in G_{2,4} \mid \phi_{34} = 0 \}. \tag{4.31}
\]

The flow acts on $\phi = \phi_{34} e^3 \wedge e^4$ as

\[
\phi' = \tilde{A}^{(2)}\phi = \phi_{34} (Ae^3 \wedge e^4 + e^3 \wedge Ae^4) = 2\rho_a \phi_{34} e^3 \wedge e^4, \tag{4.32}
\]

so that $\phi'_{34} = 2\rho_a \phi_{34}$. But as $\rho_a > 0$, we deduce that the set given by $\phi_{34} = 0$ is a repeller. \hfill $\square$
We can also understand the above result intuitively. As $S_a$ and $U_a$ together span $\mathbb{R}^4$, any vector $\Psi$ in $\mathbb{R}^4$ can be written as

$$\Psi = \alpha_s \Psi_s + \alpha_u \Psi_u, \quad |\Psi_s|^2 = |\Psi_u|^2 = 1, \quad \Psi_s \in S_a, \quad \Psi_u \in U_a, \quad \alpha_s, \alpha_u \in \mathbb{R}. \quad (4.33)$$

Then, under the flow on $\mathbb{R}^4$, the stable component decays and the unstable one grows, i.e, $\alpha_s(x) \to 0$ while $\alpha_u(x) \to \infty$ as $x \to \infty$. Thus, intuitively, we would expect that for all vectors $\Psi$ not entirely in $S_a$, the overlap with $S_a$ will decrease under the flow. In terms of subspaces, as $x \to \infty$, we would expect any $\phi \in \mathcal{D}(S_a)$ to drift away from $S_a$ itself, i.e, to get attracted towards $S_a$ if we run $x$ backwards. Hence, $\mathcal{D}(S_a)$ is a repeller in $G_{2,4}$.

4.2.2 The flow on $L(2)$

Finally, we restrict the flow to $L(2) \times [-1, 1] \subset G_{2,4} \times [-1, 1]$. Starting from an initial condition $(\psi_0, \tau_0) \in L(2) \times [-1, 1]$, the flow stays in $L(2) \times [-1, 1]$, which is guaranteed by the following theorem, which lies at the heart of Hamiltonian mechanics:

**Theorem 4.1.** A real Hamiltonian flow preserves the Lagrangian subspaces.

**Proof.** Consider a Hamiltonian system described by $\Psi' = J\mathcal{H}\Psi$, where $\Psi \in \mathbb{R}^{2n}$, and take $n$ solutions $\Psi_i(x), \, i = 1, \ldots, n$ of the flow $\Psi' = J\mathcal{H}\Psi$, with initial conditions $\Psi_i(x_0) = \Psi_i^{(0)}$, so that $\text{span}\{\Psi_i^{(0)}\} \in \mathcal{L}(n)$, i.e, $\Omega(\Psi_i^{(0)}, \Psi_j^{(0)}) = 0 \forall i, j$. Then,

$$\frac{d}{dx} \Omega(\Psi_i, \Psi_j) = (\Psi_i')^T J\Psi_j + \Psi_i^T J\Psi'_j,$$

$$= (J\mathcal{H}\Psi_i)^T J\Psi_j + \Psi_i^T J(J\mathcal{H}\Psi_j),$$

$$= \Psi_i^T \mathcal{H}\Psi_j - \Psi_i^T \mathcal{H}\Psi_j = 0, \quad (4.34)$$

where we have used the facts that $J^T = -J, \mathcal{H}^T = \mathcal{H}$ and $J^2 = -\mathbb{I}$. We have proved that $\Omega(\Psi_i(x), \Psi_j(x))$ stays invariant under the Hamiltonian flow, so that,

$$\Omega(\Psi_i(x), \Psi_j(x)) = \Omega(\Psi_i(x_0), \Psi_j(x_0)) = \Omega(\Psi_i^{(0)}, \Psi_j^{(0)}) = 0 \forall x \in \mathbb{R}. \quad (4.35)$$

Hence, $\text{span}\{\Psi_i(x)\} \in \mathcal{L}(n) \forall x$ under the Hamiltonian flow.

**Remark 4.2.** We prove the invariance of Lagrangian subspace under Hamiltonian flows by a direct computation using tools from the theory of ODEs; however, the statement is essentially tautological under the
An explicit calculation shows that $S_+, U_- \in \mathcal{L}(2)$. As $W^u_+, W^u_-$ are trajectories on $G_{2,4}$ with initial conditions $S_+, U_-$, from Theorem 4.1, they are confined to $\mathcal{L}(2)$. Thus, the flow induced on $\mathcal{L}(2) \times [-1,1]$ suffices to study the global stable/unstable manifolds. The bound state condition of Lemma 4.4 translates to a shooting argument, the essence of which is to start off with a trajectory $\psi(x)$ such that $\psi(x) \to U_-$ as $x \to -\infty$, and figure out if it has any overlap with $S_+$ as $x \to \infty$, i.e., if it “hits” $\mathcal{D}(S_+)$. We set this argument more carefully in §5.1.1.

In Appendix A, we describe the geometry of $\mathcal{L}(2)$ and $\mathcal{D}(S_+)$ in some detail. As it turns out, it is more convenient to work on $C(2) \cong \mathbb{R} \times S^2$, the universal covering space of $\mathcal{L}(2)$. Thus, for a fixed $E$, we lift the flow on $C(2)$, under the surjection $C(2) \to \mathcal{L}(2)$, which is uniquely defined upto a choice of an end point. Similarly, $\tilde{\mathcal{D}}(S_\alpha)$ is the lift of $\mathcal{D}(S_\alpha)$, which is a set of double cones in $C(2)$. In the rest of this chapter, we derive an explicit parametrization of the Dirac equation in terms of the parametrization of $C(2)$.

### 4.3 An explicit parametrization

Let $\psi = (u,v)^T$ be a solution of the Dirac equation satisfying the zero current condition and let the corresponding curve in $\mathcal{L}(2)$ be $\psi = \text{span} \{ \mathcal{R}(\psi), \mathcal{R}(i\psi) \}$. For the sake of notational clarity, we have suppressed the explicit dependence on $x$ wherever it is unambiguous. We use the sequence of maps in eq. (A.18) to compute

$$\tilde{\Psi} = \begin{pmatrix} u^* \\ v \end{pmatrix} \implies U = \frac{1}{|u|^2 + |v|^2} \begin{pmatrix} u^* & -iv^* \\ v & iv \end{pmatrix},$$

so that

$$S = UU^T = \frac{2u^*v}{|u|^2 + |v|^2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = e^{-2i\theta} \sigma^1,$$

where $\theta(x)$ is the Prüfer angle variable. Using the parametrization of $S$ from eq. (A.17) as

$$S(\alpha, \beta, \chi) = e^{i\chi} \left[ \cos \alpha \mathbb{1} + \sin \alpha \cos \beta (i\sigma_3) + \sin \alpha \sin \beta (i\sigma_1) \right],$$

where $\chi \in \mathbb{R}$ and $(\alpha, \beta)$ parametrize a 2-sphere, we read off

$$\chi(x) = -2 \left( \theta(x) + \frac{\pi}{4} \right), \quad \alpha(x) = \frac{\pi}{2}, \quad \beta(x) = \frac{\pi}{2}.$$
This is the trajectory on $C(2) \cong \mathbb{R} \times S^2$, where we have chosen a left endpoint such that $\alpha = \beta = \pi/2$. A convenient way to visualize $C(2)$ is to plot each 2-sphere as a disk, with the edge identified to a point, so that the total space becomes a cylinder (see Appendix A, esp Fig A.1 for details). This representation is of course not unique, as we are free to choose the center of the disk as any point on $S^2$, with its antipodal point being identified to the boundary of the disk. A convenient choice here is the point corresponding to $(\alpha, \beta) = (\pi/2, \pi/2)$, in which case, the trajectory $\chi(x)$ is restricted to the axis of the cylinder $C(2)$.

Under the same map, the stable and unstable subspaces from eq. (4.20) and eq. (4.19) correspond to the unitary matrices

$$U_u^a = \frac{1}{\sqrt{2}} \begin{pmatrix} \lambda_a - i \xi_a & \xi_a + i \lambda_a \\ i & 1 \end{pmatrix}, \quad U_s^a = \frac{1}{\sqrt{2}} \begin{pmatrix} -i & -1 \\ \lambda_a + i \xi_a & -\xi_a + i \lambda_a \end{pmatrix},$$

which further correspond to the symmetric unitary matrices $M_a = U_a U_a^T$, as

$$M_u^a = (\xi_a + i \lambda_a)\sigma^1 = e^{2i\text{sgn}(\mu_a)\gamma_a}\sigma^1,$$

$$M_s^a = (\xi_a - i \lambda_a)\sigma^1 = e^{-2i\text{sgn}(\mu_a)\gamma_a}\sigma^1, \quad \gamma_a = \frac{1}{2} \cos^{-1} \xi_a,$$

which can be identified with points on the axis of $C(2)$, i.e, with $\alpha = \beta = \pi/2$, with

$$\chi_u^a = \left(2n - \frac{1}{2}\right)\pi + 2\gamma_a\text{sgn}(\mu_a),$$

$$\chi_s^a = \left(2n - \frac{1}{2}\right)\pi - 2\gamma_a\text{sgn}(\mu_a); \quad n \in \mathbb{Z}.$$  

(4.42)

Thus, for $\xi_a \neq \pm 1 \implies E \neq \pm \mu_a$, the stable and unstable subspaces correspond to a set of alternating points on the axis of $C(2)$.

Next, we derive the explicit equation for $\mathcal{D}(S_+) = \mathcal{D}(e^{-2i\gamma+}\sigma^1)$, using the definition of of $S_+$ from eq. (4.20) as well as the condition from eq. (A.25) as

$$-\frac{1}{1 - \xi_+^2} (\lambda_+ \cos \chi + \xi_+ \sin \chi + \sin \alpha \sin \beta) = 0,$$

(4.43)

which can be rewritten for $\xi_+ \neq \pm 1$ as

$$\sin(\chi + 2\gamma_+\text{sgn}(\mu_+)) + \sin \alpha \sin \beta = 0.$$

(4.44)

For a fixed $\chi$, this is an equation of the form $\sin \alpha \sin \beta = C$, where $C$ is a constant. But $(\alpha, \beta)$ are the polar
coordinates on a 2-sphere, for which the Cartesian coordinates are

\[ x = \sin \alpha \cos \beta, \quad y = \sin \alpha \sin \beta, \quad z = \cos \alpha. \]  \hfill (4.45)

Hence, the condition for the train simply corresponds to the condition \( y = C \), which is a circle on \( S^2 \). In our representation of \( C(2) \), for a constant \( \chi \) slice, the \( S^2 \) correspond to a disc, and the \( y = C \) circles correspond to circles centered at the center of the disk. Thus, \( D(S_+) \) corresponds to a set of double cones, whose vertices are given by

\[ \alpha = \beta = \frac{\pi}{2} \implies \chi = \left( 2n - \frac{1}{2} \right) \pi - 2\gamma_+ \text{sgn}(\mu_+); \quad n \in \mathbb{Z}. \]  \hfill (4.46)

These are simply points in \( C(2) \) corresponding to \( S_+ \).

**Remark 4.3.** The calculations of this section imply that for the Dirac equation with a scalar potential, all trajectories of interest in \( C(2) \) lie on the axis, so that the problem is essentially reduced to a 1-dimensional problem, which is equivalent to the Prüfer formulation of the problem. We shall show this explicitly in Lemma 5.3. However, this construction is much more general than the Prüfer representation, which hinges on the form of Hamiltonian as well as the zero current condition.

### 4.3.1 The \( E = 0 \) solution

We finally demonstrate the machinery developed in this chapter and Appendix A by working out all the maps for the exact solution for an instanton potential with \( E = 0 \), as discussed in §2.1.2:

\[ \psi(x) = \zeta_0 \exp \left\{ - \int_0^x m(x') dx' \right\} \left( \begin{array}{c} 1 \\ -i \end{array} \right), \]  \hfill (4.47)

where we took \( \mu_\pm = \pm \mu, \mu > 0 \). We can solve for the same state using the Prüfer angle equation,

\[ \theta'(x) = -m(x) \cos 2\theta(x) \implies \theta(x) = \pm \frac{\pi}{4}, \]  \hfill (4.48)

where we choose the former to ensure that

\[ \zeta(x) = \zeta(x_0) \exp \left\{ - \int_{x_0}^x m(x') \sin 2\theta(x') dx' \right\} = \zeta_0 \exp \left\{ - \int_0^x m(x') dx' \right\} \]  \hfill (4.49)

has a finite \( L_2 \) norm. Thus, the solution from Prüfer equations is identical to the direct solution, up to a phase of \( \pi/4 \).
The corresponding trajectory on $\mathbb{R}^4 \times [-1, 1]$ is given by

$$
\Psi(x) = \exp \left\{ -\int_0^x m(x')dx' \right\} (1, 0, 0, -1)^T, \quad \tau(x) = \tanh(\kappa(x - x_0)).
$$

(4.50)

Next, $\eta_a = 0$ and $\delta_a = \text{sgn}(\mu_a) = \pm 1$, so that the relevant stable/unstable subspaces in the invariant planes become

$$
S_+ = \text{span} \left\{ (0, 1, -1, 0)^T, (-1, 0, 0, 1)^T \right\},
$$

$$
U_- = \text{span} \left\{ (1, 0, 0, -1)^T, (0, -1, 1, 0)^T \right\}.
$$

(4.51)

As only the magnitude of $\psi(x)$ depends on $x$, we get the corresponding subspace $\psi(x) = S_+ = U_- \in G_{2,4}$. Furthermore, we can compute $\mathcal{D}(S_+)$ using eq. (4.44) with $\gamma_+ = \pi/4$ as

$$
\mathcal{D}(S_+) = \{ (\chi, \alpha, \beta) | \cos \chi + \sin \alpha \sin \beta = 0 \}.
$$

(4.52)

In $\mathcal{L}(2)$, the $E = 0$ solution corresponds to a single point with coordinates $\chi = -\pi$, $\alpha = \beta = \pi/2$, which clearly lies on $\mathcal{D}(S_+)$, as expected for a bound state.
5 Bound States

In this chapter, we finally put together the results from the last two chapters to derive conditions for the existence bound states of the Dirac equation with instanton or potential wells. We demonstrate the usefulness of these conditions by computing the bound states analytically and numerically, in some cases with much less effort than the corresponding direct computation in typical Quantum Mechanics 101 fashion in Chapter 3. Finally, we use the condition so derived to obtain an upper bound on the number of bound states as a function of the potential.

5.1 Existence

We begin by describing two equivalent conditions for the existence of a bound state solution and showing their equivalence. The first is based on the computation by Jones, while the second one is based on a direct stability analysis of the Prüfer equation.

5.1.1 Shooting argument

In the last chapter, we described the interpretation of a solution of the Dirac equation as a flow on $L(2) \times [-1,1]$ and interpreted the global stable/unstable manifolds $W$ as trajectories under these flows. In Lemma 4.4, the condition for for the existence of a bound state is reduced to the condition that the overlap between $W^u_+$ and $W^u_-$ is nontrivial. We now derive the equivalent condition on the trajectories in $L(2)$.

Consider, then, the trajectory defined by

$$
\psi(E,x) = P(W^u_+(E) \cup \{\tau = \tau(x)\}), \quad \psi : (-\mu_0, \mu_0) \times \mathbb{R} \to L(2),
$$

(5.1)

where $P : L(2) \times [-1,1] \to L(2)$ is the natural projection that forgets $\tau$. This corresponds to shooting from the “unstable” subspace at $\tau = -1$ with the parameter $E$. For a given $E$, we “hit the target” if $\psi(E,x) \to \mathcal{D}(S_+)$, as $x \to \infty$, since $\mathcal{D}(S_+)$ is defined as the set of subspaces that have a nontrivial overlap with $S_+$. More formally,
Lemma 5.1. A trajectory $\psi(x)$ on $\mathcal{L}(2)$ corresponds to a bound state iff

$$\alpha(\psi(E, x), \tau(x)) \subset (U_-(E), -1),$$

$$\omega(\psi(E, x), \tau(x)) \cap \mathcal{D}(S_+(E)) \times \{+1\} \neq \emptyset. \quad (5.2)$$

Remark 5.1. As $\mathcal{D}(S_+)$ is a repeller to the flow in $\mathcal{L}(2)$ (Lemma 4.8), any trajectory that ends up not exactly on $\mathcal{D}(S_+)$ ends up far from it as $x \to \infty$. Thus, in the shooting method, the trajectory must end up exactly on $\mathcal{D}(S_+)$, which explains the fine-tuned nature of the bound states.

5.1.2 Stability analysis of Prüfer equation

Consider the Prüfer equation for large $|x|$, with $m(x) = \mu_a; a = \pm$, which is an autonomous nonlinear equation in $\theta(x)$:

$$\theta' = E - \mu_a \cos 2\theta. \quad (5.3)$$

This equation has fixed points (§2.2.1) at $\cos(2\theta_a^*) = E/\mu_a$, which can be solved for $E \in (-|\mu_a|, |\mu_a|)$ as

$$\theta_a^*(x) = n\pi \pm \gamma_a, \quad \gamma_a = \frac{1}{2} \cos^{-1}\left(\frac{E}{\mu_a}\right) \in \left[0, \frac{\pi}{2}\right]. \quad (5.4)$$

The linearized equation near $\theta = \theta_a^*$ is given by

$$\varphi'(x) = 2\mu_a \sin(2\theta_a^*) \varphi(x). \quad (5.5)$$

As $\sin(2\gamma_a) > 0$ by definition, a fixed point $\theta_a^*$ is

stable if $\mu_a \sin(2\theta_a^*) < 0 \implies S_a = \{n\pi - \gamma_a \text{ sgn } (\mu_a), n \in \mathbb{Z}\}$

unstable if $\mu_a \sin(2\theta_a^*) > 0 \implies U_a = \{n\pi + \gamma_a \text{ sgn } (\mu_a), n \in \mathbb{Z}\}, \quad (5.6)$

where we have defined $S_a$ and $U_a$ as the set of attractors and repellers on $\mathbb{R}$. From Theorem 2.1, the nonautonomous system (with a nonconstant $m(x)$) also tends to one of these fixed points as $x \to \pm \infty$. Thus, define the asymptotic value of $\theta$ as

$$\theta_-^* \equiv \lim_{x \to -\infty} \theta(x) \in \alpha(\theta(x)), \quad \theta_+^* \equiv \lim_{x \to \infty} \theta(x) \in \omega(\theta(x)), \quad (5.7)$$

where for a given trajectory, the $\alpha$ and $\omega$ limit sets are singleton.
The Prüfer amplitude is given by

\[ \zeta(x) = \zeta(x_0) \exp \left\{ - \int_{x_0}^x m(x') \sin 2\theta(x') dx' \right\}, \]

so that asymptotically, \( \zeta(x) \sim e^{-k \pm x} \), where \( k_\pm = \mu \pm \sin(2\theta^* \pm) \). For a solution that decays to zero as \( x \to \pm \infty \), we demand that

\[
\begin{align*}
\mu_- \sin(2\theta^*_-) &< 0 \implies \theta^*_- = -\gamma_- \sgn(\mu_-) \in S_- , \\
\mu_+ \sin(2\theta^*_+) &> 0 \implies \theta^*_+ = n\pi + \gamma_+ \sgn(\mu_+) \in U_+, \quad n \in \mathbb{Z} ,
\end{align*}
\]

where we have used Remark 2.6 to note that the solutions of the Dirac equation are invariant under the shift \( \theta \to \theta + \ell \pi, \ell \in \mathbb{Z} \), so that we can set \( \theta(-a) = -\gamma_- \sgn(\mu_-) \) without loss of generality. Thus,

**Lemma 5.2.** A solution \( \theta(x) \) of the Prüfer equation corresponds to a bound state iff

\[ \alpha(\theta(x)) \subset S_-, \quad \omega(\theta(x)) \subset U_+. \]

**Remark 5.2.** As all solutions to the Prüfer equation must tend to a fixed point for \( x \to \pm \infty \), the solution that do not correspond to a bound state, hereafter termed a “generic” solution, tend to a stable fixed point as \( x \to \infty \) and an unstable fixed point as \( x \to -\infty \), i.e., \( \theta^*_- \in U_- \) and \( \theta^*_+ \in S_+ \), which is the exact opposite of the condition for a bound state. This is the case for all initial conditions in the basin of attraction of a given fixed point, so that we have a bound state only when the initial condition falls at the boundary such consecutive basins. Hence, the bound states need a finely tuned \( E \).

### 5.1.3 Equivalence

We prove the following lemma:

**Lemma 5.3.** The conditions for a bound state obtained in Lemma 5.1 and Lemma 5.2 are equivalent.

**Proof.** The proof essentially follows from the parametrization of \( C(2) \cong \mathbb{R} \times S^2 \) as \( (\chi, \alpha, \beta) \), under which (eq. (4.39))

\[ \chi(x) = -2 \left( \theta(x) + \frac{\pi}{4} \right), \quad \alpha(x) = \frac{\pi}{2}, \quad \beta(x) = \frac{\pi}{2} . \]

Thus, the trajectory is confined to the line \( \alpha = \beta = \pi/2 \). Lemma 5.1 demands that a trajectory \( \chi(x) \) tend
to $\chi_u^-$ as $x \to -\infty$ and to $\chi_s^+$ as $x \to \infty$, where (eq. (4.42))

$$
\chi_u^- = (2\ell_1 - \frac{1}{2}) \pi + 2\gamma_+ \text{sgn}(\mu_+) \implies \theta_u^- = -\ell_1 \pi - \gamma_- \text{sgn}(\mu_-),
$$

$$
\chi_s^+ = (2\ell_2 - \frac{1}{2}) \pi - 2\gamma_+ \text{sgn}(\mu_+) \implies \theta_s^+ = -\ell_2 \pi + \gamma_+ \text{sgn}(\mu_+).
$$

Comparing this to eq. (5.9) with $\ell_i = -n_i$, $i = 1, 2$, we conclude that

$$
\theta_u^- = \lim_{x \to -\infty} \theta(x) \in S_-, \quad \theta_s^+ = \lim_{x \to \infty} \theta(x) \in U_+,
$$

which is the condition in Lemma 5.2.

**Remark 5.3.** We note that the notion of “stable” and “unstable” are the exact opposites for the case of the Prüfer angle, $\theta$ and amplitude, $\zeta$. As $S_a, U_a$ are defined for $\theta(x)$ while $S_a, U_a$ are defined for the growth/decay of the solution in magnitude, i.e, $\zeta(x)$, we notice that they are opposites, in the sense that $\theta_s^* \in U_a$ and $\theta_u^* \in S_a$. This essentially follows from the fact that a stable fixed point for $\theta$ implies an exponentially growing (i.e, “unstable”) solution for $\zeta$, and vice versa.

### 5.2 Computation

In this section, we further develop the bound state conditions obtained in the previous section and use them for explicit computations. Define a **winding**, $\Delta \theta(E)$, associated with a solution $\theta(x)$ as:

$$
\Delta \theta(E) = \theta(\infty) - \theta(-\infty) = \int_{-\infty}^{\infty} dx \left( E - m(x) \cos(2\theta(x)) \right).
$$

Then, there is a bound state with energy $E$ iff

1) $\theta(-a) = \gamma_- \text{sgn}(\mu_-)$, and

2) $\Delta \theta(E) - \gamma_- \text{sgn}(\mu_-) - \gamma_+ \text{sgn}(\mu_+) = n\pi$.

However, we shall often need only the second condition (hereafter “winding condition”), as per the following:

**Lemma 5.4.** The winding condition is sufficient for the existence of a bound state if

$$
\gamma_- \text{sgn}(\mu_-) + \gamma_+ \text{sgn}(\mu_+) \neq \frac{\ell \pi}{2}, \quad \ell \in \mathbb{Z}.
$$
Proof. For a generic and bound state solution, the winding satisfies

\[
\Delta \theta(E)_{\text{generic}} = \ell_1 \pi - (\gamma_- \text{sgn}(\mu_-) + \gamma_+ \text{sgn}(\mu_+)) , \\
\Delta \theta(E)_{\text{bound state}} = \ell_2 \pi + (\gamma_- \text{sgn}(\mu_-) + \gamma_+ \text{sgn}(\mu_+)).
\] (5.16)

As every solution must satisfy one of these two, the winding condition is not sufficient for the existence of a bound state only if \( \exists \ell_1, \ell_2 \in \mathbb{Z} \) such that

\[
\Delta \theta(E)_{\text{generic}} = \Delta \theta(E)_{\text{bound state}}.
\] (5.17)

Substituting the expression and defining \( \ell = (\ell_1 - \ell_2) \in \mathbb{Z} \) completes the proof.

We begin by considering potentials which are unknown only over a finite domain \((-a, a)\), where, at the end of the day, we may take \(a \to \infty\). In the following, \(h : \mathbb{R} \to (0, 1)\) is a piecewise \(C^1\) function supported over \((-a, a) \subset \mathbb{R}, a > 0\). The expression for the winding reduces to

\[
\Delta \theta(E) = \theta(\infty) - \theta(-\infty) = \theta(a) - \theta(-a).
\] (5.18)

This is because since \(m(x)\) is constant for \(x \notin (-a, a)\), the only way \(\theta(x)\) tends to an unstable fixed point \(\theta^*_+\) for \(x \to \infty\) is if \(\theta(a) = \theta^*_+\), so that \(\theta(x) = \theta(a) \forall x > a\) (as otherwise the system flows to a stable fixed point), and similarly for \(x \to -\infty\). We consider two specific cases:

1) Potential well : Consider the potential

\[
m(x) = \mu(1 - h(x)), \quad \mu > 0,
\] (5.19)

so that \(\mu_\pm = \mu\) and hence \(\gamma_\pm = \gamma\). Thus, the Prüfer equation has the same set of stable and unstable fixed points for \(x \to \pm \infty\), i.e, \(U_- = U_+\) and \(S_- = S_+\). The condition from Lemma 5.2 reduces to

\[
\theta(-a) = -\gamma, \quad \theta(a) = n\pi + \gamma.
\] (5.20)

The bound state condition can also be written as

\[
- \cot \theta(-a) = \cot \theta(a) = \cot \gamma.
\] (5.21)
In terms of the winding, the bound state condition becomes the transcendental equation

\[ 2\gamma = \Delta \theta(E) + n\pi \implies E = \pm \mu \cos(\Delta \theta(E)). \]  
(5.22)

From Lemma 5.4, this condition is sufficient if

\[ 2\gamma \neq \frac{\ell \pi}{2} \implies E \neq \mu \cos(2\gamma) = 0, \pm \mu. \]  
(5.23)

2) **Instanton**: Consider the potential

\[ m(x) = \mu(1 - h(x)) \text{sgn}(x), \quad \mu > 0, \]  
(5.24)

so that \( \mu_\pm = \pm \mu \) and

\[ \gamma_+ = \gamma, \quad \gamma_- = \frac{\pi}{2} - \gamma; \quad \gamma = \frac{1}{2} \cos^{-1}\left(\frac{E}{\mu}\right). \]

The condition from Lemma 5.2 reduces to

\[ \theta(-a) = \gamma - \frac{\pi}{2}, \quad \theta(a) = n\pi + \gamma. \]  
(5.25)

In terms of the winding, the bound state condition becomes the transcendental equation

\[ 2\gamma = \Delta \theta(E) + \left(n + \frac{1}{2}\right)\pi \implies E = \pm \mu \sin(\Delta \theta(E)), \]  
(5.26)

which is again sufficient if

\[ 2\gamma \neq \frac{\ell \pi}{2} \implies E \neq \mu \cos(2\gamma) = 0, \pm \mu. \]  
(5.27)

**Remark 5.4.** The latter expressions in eq. (5.22) and eq. (5.26) are more convenient to solve numerically, but they have twice as many solutions as the former, so that one needs to consider only the relevant solutions.

**Remark 5.5.** In the following, the winding condition is always taken to be sufficient, as typically we are not interested in the \( E = \pm \mu \) solutions, as these do not decay for \( x \to \pm \infty \), and we can solve the system exactly for \( E = 0 \), (§2.1.2), so that we only seek the solutions for \( E \neq 0 \).

**Remark 5.6.** The discrete symmetries of the Dirac equation may, in some cases, lead to a doubling of the bound state spectrum. However, as this is independent of the bound state condition obtained above, we shall restrict ourselves to computing only the values of bound state energies, and not their multiplicities.
5.2.1 Example: “Particle in a box”

We demonstrate the bound state condition derived above by computing the spectrum analytically for the square well, often termed as the “particle in a box”:

\[
m(x) = \mu \begin{cases} 
b, & x \in (-a, a) \\
1, & \text{otherwise},
\end{cases}
\]

(5.28)

where

\[
a \in (0, \infty), \quad b \in (-1, 1), \quad \mu > 0.
\]

We simply need to solve

\[
\theta'(x) = E - b\mu \cos 2\theta(x), \quad x \in (-a, a).
\]

(5.29)

Consider \( b = 0 \) first, in which case \( \theta(x) = Ex \implies \Delta \theta(E) = 2aE \), so that we have a bound state when

\[
2\gamma = 2Ea + n\pi \implies E = \mu \cos(2\gamma) = \pm \mu \cos(2Ea).
\]

(5.30)

We obtain the same transcendental equation by a direct calculation in eq. (3.37). As

\[
\sin(2\theta_\ast) = \sin(2n\pi + 2\gamma) = \sin(2\gamma) = \sin \cos^{-1} \left( \frac{E}{\mu} \right) = \frac{1}{\mu} \sqrt{\mu^2 - E^2},
\]

the normalized Prüfer amplitude is

\[
\zeta(x) = A \begin{cases} 
1, & |x| \leq a \\
e^{-\sqrt{\mu^2 - E^2}|x-a|/\mu}, & \text{otherwise},
\end{cases}
A = \frac{1}{\sqrt{2}} \left( a + \mu e^{-a\sqrt{\mu^2 - E^2}/\mu} \right)^{-\frac{1}{2}}.
\]

(5.31)

We plot the first three states, along with the corresponding numerical computation, in Fig 5.1.

For \( b \neq 0 \), we can use the alternative representation of the Prüfer equation from eq. (2.42), using the fact that \( m'(x) = 0 \), to get

\[
\phi' = \sqrt{E^2 - (b\mu)^2} \equiv k, \quad \cot \theta = \sqrt{\frac{E + b\mu}{E - b\mu}} \cot \phi \equiv \lambda \cot \varphi.
\]

(5.32)

The solution is simply \( \phi(x) = kx + C \). To obtain the bound state condition, it is more convenient to use eq. (5.22), which becomes

\[
-\cot \phi(-a) = \cot \phi(a) = \frac{1}{\lambda} \cot \gamma.
\]

(5.33)
The first equality leads to
\[ \cot(ka - C) = \cot(ka + C) \implies C = \frac{n\pi}{2}, \quad (5.34) \]
and the second equality leads to
\[ \lambda \tan \gamma = \tan \left( ka + \frac{n\pi}{2} \right), \]
which is precisely the condition obtained from a direct calculation in eq. (3.35).

### 5.2.2 Numerics

We can also compute the bound state energies by numerically integrating the Prüfer equation to compute the winding, and then search for the energy that satisfies the bound state condition in eq. (5.22). For instance, consider the potential in eq. (5.28), with \( a = 5, \ b = 0 \), and numerically integrate the Prüfer equation on the domain \((-20, 20)\). The LHS of the bound state condition, \( \Delta \theta(E) - \cos^{-1} E \) as a function of \( E \) are plotted in Fig 5.2. In order to solve for the energies numerically, we note that the system is quite badly conditioned, as evident from the steepness of the curve in Fig 5.2 near its points of intersection with \( n\pi \). In this case, a simple but robust binary search was used to solve for the energies\(^1\), employing the fact that \( \Delta \theta(E) - \cos^{-1} E = n\pi \), the LHS is monotonically increasing and thus has only one solution. Clearly, there are 4 bound states for \( b = 0 \), corresponding to intersection with \( n\pi, \ n = 1, 2, 3, 4 \).

\(^1\)The bound state energies are very finely tuned; even an error of \( 10^{-8} \) would make the state exponentially growing as opposed to exponentially decaying.
We also set up a symmetric finite difference calculation by discretizing $x \in (-a,a)$ in steps of $\epsilon = 2a/N$, where $N$ is the number of “sites”, to set up the Dirac eigenvalue problem as a recursion relation

$$
\mathcal{H}\psi_n = \frac{1}{2i\epsilon}\sigma^3(\psi_{n+1} - \psi_{n-1}) + m(n\epsilon)\sigma^1\psi_n = E\psi_n; \quad \psi_n \equiv \psi(n\epsilon) \in \mathbb{C}^2.
$$

Thus, the Hamiltonian can be written as a Hermitian matrix and diagonalized numerically. We compare the energies obtained by the three methods in Table 5.1.

<table>
<thead>
<tr>
<th>#</th>
<th>Exact solution</th>
<th>Numerical integration</th>
<th>Finite difference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Square well potential</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1)</td>
<td>0.142755177876</td>
<td>0.142755178273</td>
<td>0.14259 ± 0.00113</td>
</tr>
<tr>
<td>2)</td>
<td>0.427109533763</td>
<td>0.427109533688</td>
<td>0.42662 ± 0.00112</td>
</tr>
<tr>
<td>3)</td>
<td>0.706889123734</td>
<td>0.706889123736</td>
<td>0.70610 ± 0.00109</td>
</tr>
<tr>
<td>4)</td>
<td>0.967888401848</td>
<td>0.967888401821</td>
<td>0.96700 ± 0.00090</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Tanh instanton potential</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1)</td>
<td>0</td>
<td>0.000000032398</td>
<td>($-3.19 \pm 0.81$) $\times 10^{-14}$</td>
</tr>
<tr>
<td>2)</td>
<td>0.6</td>
<td>0.600000033808</td>
<td>0.59998 ± 5 $\times 10^{-12}$</td>
</tr>
<tr>
<td>3)</td>
<td>0.8</td>
<td>0.799999993083</td>
<td>0.79997 ± 9 $\times 10^{-9}$</td>
</tr>
<tr>
<td>4)</td>
<td>0.916515138991</td>
<td>0.916518020729</td>
<td>0.91648 ± 5 $\times 10^{-6}$</td>
</tr>
</tbody>
</table>

Table 5.1: The energies of the bound states computed using various methods.
We immediately note that the energy eigenvalues obtained from a direct solution of \( E = \cos(2Ea) \) match extremely well with those obtained from a numerical integration of Prüfer equation, up to 8 decimal places. The eigenvalues from finite difference were computed for \( N = 6400 \), but are not very accurate for this case.

Next, consider the case of \( b = 0.5 \). The profiles of the (normalized) bound states, along with their energies, are plotted in Fig 5.3. We immediately notice a few salient features of the bound states: they decay for large \( |x| \), and have \( N \) maxima and \( N - 1 \) minima corresponding to the \( N^{th} \) bound state (in contrast to the flat features\(^{42}\) for the case of \( b = 0 \)), reminiscent\(^{43}\) of the Sturm oscillation for the eigenstates of the Schrödinger operator.

In Fig 5.4, we plot the bound states for the potential

\[
m(x) = \begin{cases} \frac{(x)^2}{a}, & x \in (-a, a) \\ 1, & \text{otherwise} \end{cases}
\]  

(5.37)

The central part of this potential is similar to the harmonic oscillator potential for the Schrödinger equation. For \( a = 5 \), we again see behavior in terms of decay and oscillation characteristics similar to the square well.

Finally, we consider an instanton potential, for which we explicitly computed the bound state for \( E = 0 \), but there are possibly other bound states that we can compute using the bound state condition. Consider the potential given by

\[
m(x) = \tanh \left( \frac{x}{a} \right).
\]  

(5.38)

The spectrum for this potential was obtained analytically in Chapter 5, eq. (3.45) as

\[
E = \pm \sqrt{1 - \left( 1 - \frac{a}{a} \right)^2}.
\]  

(5.39)

We can again compare the spectrum obtained from a direct calculation, the numerical solution as well as the finite difference method. In this case, the finite difference method works quite well, even with \( N = 1000 \) sites, as shown in Table 5.1. Finally, the wavefunctions, which can analytically be expressed in terms of the associated Legendre functions, are plotted in Fig 5.5.
Figure 5.3: Bound states for the piecewise-linear potential well of eq. (5.28) with $\mu = 1$, $a = 5$ and $b = 0.5$. The corresponding energies are (a) $E = 0.5525804930$, (b) $E = 0.6914366837$ and (c) $E = 0.8762735076$.

Figure 5.4: Bound states for the quadratic potential well ($m(x) = \left( \frac{x}{a} \right)^2$, $x \in (-a,a)$ and 1 otherwise), with $a = 5$ and energies (a) $E = 0.2561342343$, (b) $E = 0.6556617429$ and (c) $E = 0.9092070819$.

Figure 5.5: Bound states for the tanh instanton ($m(x) = \tanh \left( \frac{x}{a} \right)$), with $a = 5$ and energies (a) $E = 0$, (b) $E = 0.6$ and (c) $E = 0.8$. 

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5.3 Estimates and bounds

We seek to derive an upper bound on the number of bound states with \( E \in (0, \mu) \) for the 1+1 dimensional Dirac equation for a given scalar potential. Following Jones, we put together the flows parametrized by \( E \) to generate a flow on \( C(2) \times [-1, 1] \times (E_1, E_2) \). As this involves lifting the uniquely defined flows on \( L(2) \) under the covering map \( C(2) \to L(2) \), which are defined only up to a choice of initial point, we demand that this choice, and hence the lifts, be continuous in \( E \). For the Dirac equation, we have a tremendous simplification, as the trajectory lies only on the axis of \( C(2) \), so that we only need the submanifold \( \mathbb{R} \times [-1, 1] \times (E_1, E_2) \) parametrized by \( (\chi, \tau, E) \), on which \( D(S^+) \) is simply the set of points corresponding to \( S^+ \). Explicitly, the flow on \( \mathbb{R} \times [-1, 1] \times (E_1, E_2) \) is given by the autonomous system

\[
\chi' = -2(E + \tilde{m}(\tau) \sin \chi), \quad \tau' = \lambda (1 - \tau^2), \quad E' = 0. \tag{5.40}
\]

For one, as \( E \) remains constant under the flow, we are only concerned with the flows parallel to the \( E \)-axis. Furthermore, as the \( \tau \) equation is independent of \( E \) and \( \chi \), the flow along \( \tau \) is trivial.

From Lemma 4.8, \( \mathcal{D}(S^+) \) is a repeller in \( C(2) \). Furthermore, it is a set of points in \( \mathbb{R} \), the axis of \( C(2) \), which divides the space into an infinite number of disjoint open sets. Thus, consider the set

\[
\mathcal{A} = \bigcup_{E \in (E_1, E_2)} (\mathcal{A}(E), 1, E), \tag{5.41}
\]

which consists of an infinite number of disjoint components. We can choose one of these disjoint components as

\[
\mathcal{A} = \bigcup_{E \in (E_1, E_2)} (\mathcal{A}(E), 1, E). \tag{5.42}
\]

Consider the trajectories \( \chi(E, x) \) in the \( \tau = +1 \) plane that tend to \( U_- \) as \( x \to -\infty \). Then, the trajectory for a bound state at \( E = E_0 \) implies that the corresponding \( \omega \)-limit set intersects with \( \hat{\mathcal{D}}(S^+) = \partial \mathcal{A} \). Using Jones’ lemma 3.1, if we can find \( E_1 \) and \( E_2 \) such that

\[
\omega(\chi(E_1, x)) \cap \mathcal{A} \neq \emptyset, \quad \omega(\chi(E_2, x)) \cap (\mathbb{R} \times (E_1, E_2)) \setminus \bar{\mathcal{A}} \neq \emptyset, \tag{5.43}
\]

where \( \bar{\mathcal{A}} \) is the closure of \( \mathcal{A} \), then \( \exists E_0 \in (E_1, E_2) \) such that \( \omega(\chi(E_0, x)) \cap \partial \mathcal{A} \neq \emptyset \), i.e., there is a bound state for \( E = E_0 \). We can generalize this in a straightforward fashion by considering a set of components \( \mathcal{A} \), so that the number of bound states in \( (E_1, E_2) \) is equal to the number of such components crossed by \( \omega(\chi(E_2, x)) \).

As the spectrum is symmetric about \( E = 0 \), let us take \( E_1 = 0 \) and \( E_2 = \mu \). Then,
Figure 5.6: The set of fixed points on the $E - \chi$ plane for a potential well. The black dashed lines denote the repeller $S_+$ and the red solid lines the attractors $U_-$. The blue shaded region denotes $\mathcal{A}$, a component of the set $\mathcal{A}$ which is the complement of $S_+$ in $\mathbb{R} \times (-\mu, \mu)$. All trajectories in this picture are horizontal lines starting at $U_-$, with the one at $E = 0$ staying in $\mathcal{A}$ while the one for $E = \mu$ intersecting a component of $S_+$ at least $N_B$ times, where $N_B$ is the number of bound states with $E \in (0, \mu)$.

**Lemma 5.5.** The number of bound states with eigenvalues $E \in (0, \mu)$ (ignoring degeneracies) is given by

$$N_B = \left\lfloor \frac{1}{2\pi} \lim_{R \to \infty} |\chi(R) - \chi(-R)| \right\rfloor,$$

where $\chi_0(x)$ solves $\chi' = -2(\mu + m(x) \sin \chi)$.

**Proof.** For $E = 0$, we have a constant solution, as $U_-$ does not evolve under $x$, so that $\omega(\chi(0, x)) \subset \mathcal{A}$. We also know that every time $\chi_0(x)$ crosses a branch of $\mathcal{D}(S_+)$, we get a bound state. Thus, the number of bound states is simply the distance traversed by $\chi_0(x)$ as $x$ varies from $-\infty$ to $\infty$. $\square$

We can derive an identical condition for the Prüfer phase variable:

**Lemma 5.6.** The number of bound states $N_B$ with $E \in (0, \mu)$ satisfies

$$N_B = \left\lfloor \frac{1}{\pi} |\Delta \theta(\mu)| \right\rfloor.$$

**Proof.** The proof essentially follows from the fact that $\Delta \theta(E)$ is piecewise constant on the basins of the stable fixed points, which are spaced apart by $\pi$. Thus, given $E_1, E_2 \in (0, 1)$ with $|\Delta \theta(E_2) - \Delta \theta(E_1)| = \pi$, there is at least one $E_0 \in [E_1, E_2]$ for which the system does not tend to a stable fixed point, and thus tends to an unstable one, which corresponds to a bound state. Thus, there is exactly one bound state for each such jump of $\pi$ in $\Delta \theta(E)$ as a function of $E$, so that the total number of bound states for $E \in (0, 1)$ is given simply by $\left\lfloor \frac{1}{\pi} |\Delta \theta(\mu) - \Delta \theta(0)| \right\rfloor$. But for $E = 0$, the Prüfer phase equation admits a constant solution $\theta = (2n + 1)\pi/4$, so that $\Delta \theta(0) = 0$, which completes the proof. $\square$
Note that the two are identical, as $\Delta \chi = 2 \Delta \theta$. We prove the following Calogero-like bound:

**Theorem 5.1.** The number of bound states $N_B$ with $E \in (0, \mu)$ satisfies the upper bound

$$N_B \leq N_0 + \frac{1}{\pi} \int_{-\infty}^{\infty} dx \sqrt{\mu^2 - m^2(x)},$$

(5.46)

where $N_0$ is the number of isolated zeros of $m'(x)$.

**Proof.** The proof is based on the proof of the Calogero bound for the bound states for Schrödinger equation in Reed and Simon, vol IV [9]. To use Lemma 5.6 we need to estimate $\Delta \theta(\mu)$. Set $E = \mu$, and consider the Riccati-Prüfer equation

$$y' = (\mu + m(x)) + y^2(\mu - m(x)), \quad y = -\cot \theta,$$

(5.47)

whose RHS is always positive as $-\mu \leq m(x) \leq \mu$, so that $y(x)$ is an increasing function of $x$ over $\mathbb{R}$. Denote the zeros of $y(x)$ by $z_n$ and the poles by $p_n$, which form a pair of interleaving sequence (i.e., $\ldots < z_n < p_n < z_{n+1} < \ldots$). Thus, $\Delta \theta(\mu) \leq \pi N(\mathbb{R})$, where $N(D)$ denotes number of poles $p_n \in D \subset \mathbb{R}$.

The Riccati equation can also be expressed as (eq. (2.42))

$$\varphi' = \sqrt{\mu^2 - m^2(x)} + \frac{m'(x)}{\mu^2 - m^2(x)} \sin^2 \varphi \cot \varphi, \quad \cot \theta = \sqrt{\frac{\mu + m(x)}{\mu - m(x)}} \cot \varphi,$$

(5.48)

so that

$$\theta(p_n) = \varphi(p_n) = n\pi, \quad \theta(z_n) = \varphi(z_n) = \left(n - \frac{1}{2}\right)\pi.$$  

(5.49)

Thus, $\Delta \theta(\mu) < \Delta \varphi \equiv \varphi(\infty) - \varphi(-\infty) + \frac{\pi}{2}$, so that for estimating the number of bound states, we can simply take $\Delta \theta = \Delta \varphi$.

Consider a domain $D \subset \mathbb{R}$ such that $m'(x) \geq 0 \forall x \in D$, and containing at least one pair $z_n, p_n \in D$. As $\cot \varphi(x) < 0$ for $x \in (z_n, p_n)$, we get the inequality

$$\varphi' = \sqrt{\mu^2 - m^2(x)} - \frac{|m'(x)|}{\mu^2 - m^2(x)} \sin^2 \varphi |\cot \varphi| \leq \sqrt{\mu^2 - m^2(x)}.$$

(5.50)

Integrating from $z_n$ to $p_n$,

$$1 = \frac{2}{\pi} \int_{z_n}^{p_n} dx \varphi'(x) \leq \frac{2}{\pi} \int_{z_n}^{p_n} dx \sqrt{\mu^2 - m^2(x)}.$$

(5.51)
If there are multiple zeros and poles in $D$, then summing over all such $(z_n, p_n)$, we get

$$N(D) \leq \sum_n \frac{2}{\pi} \int_{z_n}^{p_n} dx \sqrt{\mu^2 - m^2(x)} \leq \frac{2}{\pi} \int_D dx \sqrt{\mu^2 - m^2(x)}. \quad (5.52)$$

For the region $R \setminus D$ where $m'(x) < 0$, we can instead take the intervals $(p_n, z_{n+1})$, where $\cot \varphi(x) > 0$. A similar calculation leads to

$$N(R \setminus D) \leq \frac{2}{\pi} \int_{R \setminus D} dx \sqrt{\mu^2 - m^2(x)}. \quad (5.53)$$

We might be missing one set of zeros and poles for each boundary between $D$ and $R \setminus D$, i.e., for each isolated zero of $m'(x)$, so that

$$N_B \leq \frac{1}{\pi} \Delta \theta(1) \leq N_0 + \frac{2}{\pi} \int_{-\infty}^{\infty} dx \sqrt{\mu^2 - m^2(x)}, \quad (5.54)$$

where $N_0$ is the number of isolated zeros of $m'(x)$ on $\mathbb{R}$.

**Corollary 5.6.1.** The bound is saturated by the tanh instanton potential.

**Proof.** Given $m(x) = \tanh \left( \frac{x}{a} \right)$, $a > 0$. Clearly, $\mu_{\pm} = \pm 1 \implies \mu = 1$ and $m(x)$ is monotonically increasing, so that $m'(x)$ has no zeros, and hence $N_0 = 0$. Thus,

$$N_B \leq \frac{1}{\pi} \int_{-\infty}^{\infty} dx \sqrt{1 - \tanh^2 \left( \frac{x}{a} \right)} = a. \quad (5.55)$$

where we integrate by substituting $v = e^{x/a}$ as

$$\int_{-\infty}^{\infty} dx \text{sech} \left( \frac{x}{a} \right) = 2 \int_{-\infty}^{\infty} \frac{e^{x/a} dx}{1 + e^{2x/a}} = 2a \int_{0}^{\infty} \frac{dv}{1 + v^2} = 2a \tan^{-1} v \bigg|_{0}^{\infty} = \pi a. \quad (5.56)$$

But using the spectrum, we get the number of bound states in $(0, 1)$ as $\lfloor a \rfloor$. \hfill \Box
Conclusions and Discussions

In this work, we have analyzed the bound state spectrum for a 1+1 dimensional Dirac equation in presence of a scalar potential \( m(x) \), alternatively thought of as a space-dependent “mass”, which approaches a constant value exponentially as \( x \to \pm \infty \). Thinking of the Dirac eigenvalue problem as a flow on \( \mathbb{C}^2 \) under the position coordinate \( x \), we have used the tools from ODEs and dynamical systems to reformulate the problem of existence of a bound state in terms of the asymptotic behavior of a flow. We have consider two distinct approaches, which we have shown to be equivalent for the problem at hand.

The first approach is the derivation of a Prüfer-like representation, well known from the theory of Sturm-Liouville equation, for the Dirac equation. As the 1+1 dimensional Dirac equation has 4 real degrees of freedom (corresponding to \( \mathbb{C}^2 \)), we make two additional assumptions to reduce it to the 2 real degrees of freedom (the “amplitude” and the “phase”) for the standard Prüfer analysis. The first quite general assumption is that the generator of the flows is real, which we arrange by making a suitable choice of the Dirac matrices. This reality condition implies a symmetry of the flow on \( \mathbb{C}^2 \), which we exploit to ensure that the solutions are eigenfunctions of that symmetry operator. The second, and much stronger, assumption is that the current vanish everywhere, which sounds reasonable for a bound state, but there may possibly be bound state solutions that do not satisfy this condition.

Having so derived the Prüfer equation, the bound state condition, or equivalently, the condition that the amplitude decay exponentially for \( x \to \pm \infty \), paradoxically ends up being completely determined by the Prüfer equation governing the “phase” of the solution. The phase equation is a nonlinear nonautonomous ODE, equivalent to a Riccati equation under a suitable transformation. As the nonautonomous behavior enters through the dependence on \( m(x) \), the equation becomes autonomous for large \( x \) when \( m(x) \) approaches a constant. Using dynamical systems techniques, we prove that for large \( x \), the asymptotic behavior of the nonautonomous system is same as the asymptotic behavior of the corresponding autonomous system. so that we simply need study the asymptotic behavior (fixed points and basins) of the corresponding autonomous equation. A bound state, in this picture, corresponds to a trajectory that tends to a stable fixed point for \( x \to -\infty \) and an unstable one as \( x \to \infty \). This is the exact opposite of what one expects from a generic trajectory, thereby leading to the fine-tuned nature of a bound state.
The second approach follows a construction by Chris Jones for the case of the nonlinear Schrödinger equation, which is essentially a shooting argument in the space of Lagrangian subspaces. The Dirac equation is mapped to a Hamiltonian flow on $\mathbb{R}^4$, which is rendered autonomous by defining a new variable $\tau = \tanh(\kappa x)$, which offers the added advantage of “compactifying” the system by bringing the $x \to \pm \infty$ behavior to $\tau = \pm 1$. The induced flow on $\mathcal{L}(2)$, the space of Lagrangian subspaces of $\mathbb{R}^4$, are studied. In case of our problem, owing to a $U(1)$ symmetry of the original Dirac equation, the trajectories under the induced flow are in one-to-one correspondence to the solutions of the original Dirac equation, with the condition for a subspace to be Lagrangian equivalent to the zero current condition. This correspondence is specific to our setup for the Dirac equation; however, the rest of the construction is rather general.

In this picture, the exponential decay of the solution as $x \to \pm \infty$ is studied by considering the dynamics on the invariant planes $\tau = \pm 1$, for which the system becomes a constant coefficient ODE, for which the stable/unstable subspace are computed explicitly. As both these subspaces are Lagrangian, the bound state simply corresponds to a trajectory that starts off at the “unstable” subspace, $\mathbf{U}_-$, for $x \to -\infty$ and approaches a “stable” subspace, $\mathbf{S}_+$, as $x \to \infty$. The shooting argument then involves studying the trajectories that start off at $\mathbf{U}_-$ for $x \to -\infty$, and looking for a condition that the trajectory hits $\mathbf{S}_+$ as $x \to \infty$. In practice, this is formulated by considering the set of all subspaces that overlap with $\mathbf{S}_+$, which is also termed the train of $\mathbf{S}_+$.

Using an explicit parametrization of $\mathcal{L}(2)$ (from Jones[12]), we were able to construct the flows explicitly, and thus show that they are identical to the Prüfer equation obtained earlier. As an aside, we note that the terminology “stable” and “unstable” is exactly opposite for the Prüfer equation and the real flow condition. This follows from the fact that the Prüfer phase approaching a stable fixed point corresponds to the amplitude growing exponentially, a state of affairs one would term “unstable” if one were studying the amplitude only.

Having derived the condition for a bound state, we first use it to numerically compute the bound state spectrum using Mathematica™ for cases where an analytic solution is known, either explicitly or implicitly as a solution of a transcendental equation, and the result agrees quite well with the spectrum obtained analytically. We also use it to compute the spectra as well as bound states for other potentials, and observe oscillations analogous to the Sturm oscillation for the bound states of Schrödinger equation. This method, as well as the corresponding Mathematica code, make looking for bound states in other potentials a really trivial task. Indeed, the author spent a great many hours playing with different (and increasingly crazier) potentials that did not make the final cut of this thesis.

Finally, we also obtain a Calogero-like upper bound on the number of bound states for the Dirac equation in 1+1 dimensions, which is essentially similar to the Calogero bound for the Schrödinger equation[9] as well
as a bound obtained for the 3+1 dimensional Dirac equation in Ref [19]. This bound is saturated by the tanh potential, which corresponds to the Pöschel-Teller reflectionless potential for the corresponding Klein-Gordon equation, and is thus not without precedent.

The future projection of this work offers a few interesting directions. For one, we also expect a Bargmann-like bound for the number of bound states for a potential well, possibly something along the lines of $N_B \leq \|1 - m(x)\|_1$. However, a derivation using the Riccati-Prüfer equation is not amenable to bounds as in case of the Schrödinger equation.

Another problem of interest would be to use this analysis, especially the “flow in $\mathcal{L}(2)$” picture of the Dirac equation, to study the spectrum of a Dirac system with periodic potentials. Of particular interest is a defect, which can have localized modes in the band-gap of the otherwise periodic system, similar in characteristics to the bound states studied here. In such a case, we do not need to compactify $x$ as a periodic potential can simply be interpreted as $x \in S^1$. The corresponding trajectories in $\mathbb{R}^4$ should then approach a limit cycle instead of a fixed point, so that one might need to set up a shooting argument with higher-dimensional objects instead of curves in $\mathcal{L}(2)$. Such a problem might be of interest for studying multilayers, for instance, the topological insulator – normal insulator multilayer structure that realizes a Weyl semimetal[44].

This thesis, in part, grew out of the author’s attempt to connect the relatively vague, and almost lorelike, treatment of the bound states of the Dirac equation, esp with a mass domain wall on which so much of the physics of topological phases hinges, in the contemporary condensed matter literature, to the more rigorous and sophisticated techniques standard in studying similar solutions in dynamical systems, as well as for the case of Schrödinger equation. The hope is that this work, despite its feeble, at best, claim at originality, would prove a good springboard more more rigorous and detailed analysis of the Dirac equation in the condensed matter context.

And finally, in lieu of the more commonplace conclusions, the author has chosen to given in to his urge to end this thesis by quoting Goethe’s Faust:

*Da stehe ich nun, ich armer Thor!*  
*Und bin so klug als wie zuvor.*
A Geometry

In this chapter, we describe some of the geometry associated with the subspaces of \( \mathbb{R}^{2n} \), esp with \( \mathbb{R}^4 \), that will be needed for our analysis of the Dirac equation. Much of this chapter is based on the details from the Jones’ paper.

A.1 Subspaces of \( \mathbb{R}^{2n} \)

We begin with the even dimensional real vector space \( \mathbb{R}^{2n} \). Consider \( \{ e^i \}, i = 1, \ldots, 2n \) as a basis of \( \mathbb{R}^{2n} \), so that \( v = v_i e^i \forall v \in \mathbb{R}^{2n} \). We have the following additional structure:

- A Euclidean inner product \( \langle \cdot, \cdot \rangle \), defined by \( \langle v, w \rangle = v^T w = \sum_{i=1}^{2n} v_i w_i \). This also induces the corresponding positive definite norm \( |v| = \langle v, v \rangle^{1/2} \).

- A symplectic form \( \Omega(\cdot, \cdot) \), which is an antisymmetric, nondegenerate 2-form defined by as
  \[
  \Omega(v, w) = \langle v, Jw \rangle, \quad J = \begin{pmatrix}
  0_{n \times n} & I_{n \times n} \\
  -I_{n \times n} & 0_{n \times n}
  \end{pmatrix}.
  \]
  (A.1)
  
  where we have taken \( J \) in its canonical (Darboux) form.

A given \( n \)-dimensional subspace \( \mathbb{R}^n \subset \mathbb{R}^{2n} \) is said to be spanned by \( n \) vectors \( \{ v_1, v_2, \ldots, v_n \} \) if any point in the subspace can be written as a unique linear combination of these vectors. Clearly, we need these vectors to be linearly independent.

Definition A.1. The space of all \( r \) dimensional subspaces \( \mathbb{R}^r \subset \mathbb{R}^{2n} \) is called the Grassmannian of \( \mathbb{R}^{2n} \), and denoted by \( G_{r,2n} \).

In the following, we shall be primarily interested in \( G_{n,2n} \). In order to define the Grassmannian formally, start off by defining the \( n \)th exterior power of \( \mathbb{R}^{2n} \):

\[
\Lambda^n(\mathbb{R}^{2n}) \equiv \text{span} \left\{ e^{i_1} \wedge e^{i_2} \wedge \cdots \wedge e^{i_n} \mid 1 \leq i_1 < i_2 < \ldots < i_n \leq 2n \right\}.
\]

(A.2)
The wedge product is antisymmetric, so that \( v_1 \wedge v_2 \wedge \cdots \wedge v_n = 0 \) if \( v_i \)'s are not linearly independent. Clearly, \( \Lambda^n(\mathbb{R}^n) \) forms a \( 2^n C_n \) dimensional vector space over \( \mathbb{R} \). Also, as \( v_i \)'s form a \( n \)-dimensional subspace of \( \mathbb{R}^{2n} \), we have a map from the set of \( Q \in \Lambda^n(\mathbb{R}^{2n}) \) which can be written as \( Q = v_1 \wedge v_2 \wedge \cdots \wedge v_n, v_i \in \mathbb{R}^{2n} \) to \( G_{n,2n} \). This map is surjective but not injective, as we have an element of \( \Lambda^n(\mathbb{R}^{2n}) \) corresponding to every subspace of \( \mathbb{R}^{2n} \), but the subspace spanned by \( \{v_i\} \) is same as that spanned by \( \{\lambda_i v_i\}, \lambda_i \in \mathbb{R} \), whereas they correspond to different points in \( \Lambda^n(\mathbb{R}^{2n}) \).

In order to make this mapping unique, we can projectivize \( \Pi : \Lambda^n(\mathbb{R}^{2n}) \to \mathbb{P}\Lambda^n(\mathbb{R}^{2n}) \), in which we have a unique point corresponding to each point in \( G_{n,2n} \), and \( \Pi \) denotes the projection operator. This embedding of \( G_{n,2n} \) in \( \mathbb{P}\Lambda^n(\mathbb{R}^{2n}) \) is known as the Plücker embedding, and the corresponding coordinates on \( \mathbb{P}\Lambda^n(\mathbb{R}^{2n}) \) are known as Plücker coordinates. In the following, we describe the Plücker coordinates explicitly for the case of \( n = 2 \), as originally described by Julius Plücker. A 2-form \( Q \in \Lambda^2(\mathbb{R}^4) \) can be written as

\[
Q = \frac{1}{2} q_{ij} e^i \wedge e^j, \quad q_{ij} = \begin{vmatrix} v_i & v_j \\ w_i & w_j \end{vmatrix} \in \mathbb{R}, \quad i,j = 1,2,3,4. \tag{A.3}
\]

On the projection \( \Pi : \Lambda^2(\mathbb{R}^4) \cong \mathbb{R}^6 \to \mathbb{R}\mathbb{P}^5 \), \( \{q_{ij} \mid i < j\} \) are simply the projective coordinates. Then

**Lemma A.1.** The Grassmannian \( G_{2,4} \) forms an algebraic variety of codimension 1 inside \( \mathbb{P}\Lambda^2(\mathbb{R}^4) \), described by the equation

\[
q_{12}q_{34} - q_{13}q_{24} + q_{14}q_{23} = 0. \tag{A.4}
\]

**Proof.** A \( Q \in \mathbb{P}\Lambda^2(\mathbb{R}^4) \) corresponds to a 2-dimensional subspace of \( \mathbb{R}^4 \), i.e, a point in \( G_{2,4} \) iff

\[
0 = Q \wedge Q = \frac{1}{4} q_{ij} q_{kl} e^i \wedge e^j \wedge e^k \wedge e^l = \frac{1}{4} (\epsilon^{ijkl} q_{ij} q_{kl}) e^1 \wedge e^2 \wedge e^3 \wedge e^4, \tag{A.5}
\]

where \( \epsilon^{ijkl} \) is the totally antisymmetric tensor, and the indices are summed over. As \( q_{ij} \) is also antisymmetric, we have \( 4C_2/2 = 3 \) terms, writing which out completes the proof.

An important subspace of the Grassmannian is the space of Lagrangian planes of \( \mathbb{R}^{2n} \):

**Definition A.2.** A plane spanned by \( \{v_i\} \subset \mathbb{R}^{2n} \) is defined to be Lagrangian if \( \Omega(v_i, v_j) = 0 \forall i,j \). The space of all Lagrangian planes of \( \mathbb{R}^{2n} \) is denoted by \( \mathcal{L}(n) \). Clearly, \( \mathcal{L}(n) \subset G_{n,2n} \subset \mathbb{P}\Lambda^n(\mathbb{R}^{2n}) \).

**Lemma A.2.** The space of Lagrangian planes, \( \mathcal{L}(n) \), forms an algebraic variety of codimension 1 inside \( G_{2,4} \), described by the equation

\[
q_{13} + q_{24} = 0. \tag{A.6}
\]
Proof. Given \( Q = \frac{1}{2} q_{ij} e^i \wedge e^j = v \wedge w \), the space spanned by \( \{v, w\} \) is Lagrangian if

\[
0 = \Omega(v, w) = \langle v, Jw \rangle \\
= v_1 w_3 + v_2 w_4 - v_3 w_1 - v_4 w_2 \\
= (v_1 w_3 - v_3 w_1) + (v_2 w_4 - v_4 w_2) \\
= q_{13} + q_{24}.
\]

The space of Lagrangian planes forms a homogeneous space, as per the following theorem:

**Theorem A.1.** The space of Lagrangian subspaces, \( \mathcal{L}(n) \), is homeomorphic to the space of \( n \times n \) symmetric unitary matrices, i.e.,

\[
\mathcal{L}(n) \cong \text{SymU}(n) = \{ S | S \in U(n), S^T = S \}. \tag{A.7}
\]

**Proof.** We begin with a proof of the well-known result\[45, 46\] that \( \mathcal{L}(n) \cong U(n)/O(n) \). This isomorphism follows from the fact that the group \( U(n) \) acts on \( \mathcal{L}(n) \) transitively with the stationary subgroup \( O(n) \), which we shall show by an explicit construction.

We begin with a bijective map \( \mathbb{R}^{2n} \rightarrow \mathbb{C}^n \) defined as follows: Given \( v \in \mathbb{R}^{2n} \), define \( v = (v_R, v_I) \), s.t. \( v_R, v_I \in \mathbb{R}^{2n} \) and map \( v \mapsto \bar{v} = v_R + iv_I \in \mathbb{C}^n \). Given a Lagrangian plane \( \psi_v \subset \mathbb{R}^{2n} \) with an orthonormal basis \( \{v_1, v_2, \ldots v_n\} \),

1) \( \langle v_i, v_j \rangle = \delta_{ij} \quad \Rightarrow \quad v^T_{i,R} \cdot v_{j,R} + v^T_{i,I} \cdot v_{j,I} = \delta_{ij} \\
2) \langle v_i, Jv_j \rangle = 0 \quad \Rightarrow \quad v^T_{i,R} \cdot v_{j,I} - v^T_{i,I} \cdot v_{j,R} = 0
\]

For the standard inner product on \( \mathbb{C}^n \), we have

\[
\langle \bar{v}_i, \bar{v}_j \rangle_{\mathbb{C}} = (v_{i,R} + iv_{i,I})^\dagger \cdot (v_{j,R} + iv_{j,I}) \\
= (v_{i,R}^T \cdot v_{j,R} + v_{i,I}^T \cdot v_{j,I}) + i (v_{i,R}^T \cdot v_{j,I} - v_{i,I}^T \cdot v_{j,R}) \\
= \delta_{ij} \tag{A.8}
\]

Hence, \( \{\bar{v}_1, \ldots, \bar{v}_n\} \) form an orthonormal basis of \( \mathbb{C}^n \). Given \( \bar{e}^i \), \( (\bar{e}^i)^j = \delta^i_j \) as the canonical basis for \( \mathbb{C}^n \), we can define a unitary operator \( U_v = (\bar{v}_1, \bar{v}_2, \ldots, \bar{v}_n) \in U(n) \) such that \( \bar{v}_i = U_v \cdot \bar{e}_i \). This is essentially a complex rotation in \( \mathbb{C}^n \). Given any other Lagrangian plane \( \psi_w \subset \mathbb{R}^{2n} \) spanned by \( w_i \)'s, we can construct the corresponding unitary matrix \( U_w \) so that \( \bar{w}_i = U_w \cdot \bar{e}_i \iff \bar{e}_i = U_w^{-1} \cdot w_i \), which implies that \( \bar{v}_i = U_v \cdot U_w^{-1} \cdot \bar{w}_i \). But from the closure property of groups, \( U_v \cdot U_w^{-1} \in U(n) \). Hence, given any two
Let \( \mathbb{R}^{2n} \) be the \( n \)-dimensional Euclidean space, and let \( \mathcal{L}(n) \) be the set of \( 2 \times 2 \) matrices \( S = X + iY \in \text{SymU}(n) \), where \( X, Y \in \mathbb{R}^{n \times n} \). Then

\[
S^\dagger S = I \implies X^T Y = Y^T X, \quad X^T X + Y^T Y = I
\]

and

\[
S^T = S \implies X^T = X, \quad Y^T = Y,
\]

which imply that

\[
[X, Y] = 0, \quad X^2 + Y^2 = I.
\]

As \( X \) and \( Y \) commute, they can be simultaneously diagonalized by some \( O \in \text{O}(n) \) so that \( X = O^T \Theta_X O \) and \( Y = O^T \Theta_Y O \), where \( \Theta_X \) and \( \Theta_Y \) are \( 2 \times 2 \) diagonal matrices. The remaining condition becomes

\[
X^2 + Y^2 = I \implies \Theta_X^2 + \Theta_Y^2 = I.
\]

Take \( \Theta_X = \text{diag}\{\cos \theta, \cos \phi\} \) and \( \Theta_Y = \text{diag}\{\sin \theta, \sin \phi\} \), so that

\[
S = O^T (\Theta_X + i \Theta_Y) O = O^T \text{diag}\{e^{i\theta}, e^{i\phi}\} O, \quad \theta, \phi \in [0, 2\pi).
\]

Now, if \( O \) and \( O\Theta \) are two matrices in \( \text{O}(2) \), then they lead to the same \( S \) if \( \Theta \in \text{O}(2) \) is diagonal, i.e., if \( \Theta = \text{diag}\{1, -1\} \) or \( \Theta = \text{diag}\{-1, -1\} \). Hence, take \( O = \mathcal{R}(\beta/2) \), \( \beta \in [0, 2\pi) \), where \( \mathcal{R}(\alpha) \) is a rotation.
matrix. Explicitly,

\[ S(\beta, \alpha, \beta) = \left( \begin{array}{cc} \cos \frac{\beta}{2} & -\sin \frac{\beta}{2} \\ \sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{array} \right) \left( \begin{array}{cc} e^{i\theta} & 0 \\ 0 & e^{i\phi} \end{array} \right) \left( \begin{array}{cc} \cos \frac{\beta}{2} & \sin \frac{\beta}{2} \\ -\sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{array} \right). \] (A.15)

Define \( \theta = \chi + \alpha, \phi = \chi - \alpha \), so that

\[ S(\alpha, \beta, \chi) = e^{i\chi} \left( \begin{array}{cc} \cos \alpha + i \sin \alpha \cos \beta & i \sin \alpha \sin \beta \\ i \sin \alpha \sin \beta & \cos \alpha - i \sin \alpha \cos \beta \end{array} \right), \] (A.16)

which can be written in terms of Pauli matrices as

\[ S(\alpha, \beta, \chi) = e^{i\chi} \left[ \cos \alpha \mathbb{1} + \sin \alpha \cos \beta (i\sigma^3) + \sin \alpha \sin \beta (i\sigma^1) \right]. \] (A.17)

The coefficients of \((\mathbb{1}, i\sigma^3, i\sigma^1)\) are precisely a parametrization of \(S^2\) for \(\alpha \in [0, \pi], \beta \in [0, 2\pi]\), while \(\chi \in [0, 2\pi]\), identifying this parametrization with \(S^1 \times S^2\). However, we still have one remaining redundancy, viz. \(\chi, \alpha, \beta \sim (\chi + \pi, \pi - \alpha, \beta + \pi)\). The 2-spheres at \(\chi = 0\) and \(\chi = \pi\) are mapped by the antipodal map \(\alpha \mapsto \pi - \alpha, \beta \mapsto \beta + \pi\). Hence, geometrically, \(L(2)\) is a \(S^2\) fiber over \(S_1\), where the fiber is twisted by the antipodal map. We can also think of it as the orbifold \((S^1 \times S^2)/\mathbb{Z}_2\), where the \(\mathbb{Z}_2\) action on \(S^1 \times S^2\) is defined by \((\chi, \alpha, \beta, \chi) \mapsto (\chi + \pi, \pi - \alpha, \beta + \pi)\).

It is usually more convenient to work with the universal covering space, \(C(2)\), which simply corresponds to \(\mathbb{R} \times S^2\), parametrized by \(\chi \in \mathbb{R}, \alpha \in [0, \pi], \beta \in [0, 2\pi]\). As \(\pi_1(L(2)) \cong \pi_1(\text{SymU}(2)) \cong \mathbb{Z}\), the universal covering space contains an infinite number of copies of each point in \(L(2)\), with the covering map \(\mathbb{Z}\). Explicitly, the sequence of maps that map \(\psi\), a subspace of \(\mathbb{R}^4\) to the coordinates \((\chi, \alpha, \beta) \in \mathbb{R} \times S^2\) are

\[ \psi = \text{span}\{v, w\} \in L(2) \longrightarrow U = (\bar{v}, \bar{w}) \in U(2) \longrightarrow S = U^T U \in \text{SymU}(2). \] (A.18)

### A.2 Overlaps

**Definition A.3.** The overlap between two subspaces \(\psi \in G_r,2n, \phi \in G_{r'},2n\) is defined as the subspace \(\psi \cap \phi\). The overlap is termed nonzero if \(\psi \cap \phi \neq \{0\}\).

A related notion is that of a train of a subspace:

**Definition A.4.** The train of a subspace \(\psi \in G_r,2n\) is defined as

\[ \mathcal{D}(\psi) = \{\phi \in G_r,2n \mid \psi \cap \phi \neq \{0\}\}. \] (A.19)
Consider the trains in $G_{2,4}$. Given $\psi = \text{span}\{v_1, v_2\}$ and $\phi = \text{span}\{v_3, v_4\}$, the condition for $\phi$ to be in $\mathcal{D}(\psi)$ becomes

$$\phi \cap \psi \neq \{0\} \implies \exists \alpha_i \in \mathbb{R} \text{ s.t. } \alpha_1 v_1 + \alpha_2 v_2 = \alpha_3 v_3 + \alpha_4 v_4, \quad (A.20)$$

i.e., $v_i$'s are linearly dependent. This condition is equivalent to

$$\det (v_1, v_2, v_3, v_4) = 0. \quad (A.21)$$

Now, for simplicity, if we take $v_1 = e_1$ and $v_2 = e_2$, then this condition becomes

$$\begin{vmatrix}
1 & 0 & v_{3,1} & v_{4,1} \\
0 & 1 & v_{3,2} & v_{4,2} \\
0 & 0 & v_{3,3} & v_{4,3} \\
0 & 0 & v_{3,4} & v_{4,4}
\end{vmatrix} = 0 \implies \begin{vmatrix}
v_{3,3} & v_{4,3} \\
v_{3,4} & v_{4,4}
\end{vmatrix} = 0 \implies \phi_{34} = 0. \quad (A.22)$$

Hence, this is a hypersurface in $G_{2,4}$ of codimension 1.

We seek the geometric form of the train $\mathcal{D}(\psi)$ for a given $\psi \in \mathcal{L}(2)$ and the corresponding lift $\hat{\mathcal{D}}(\psi)$ under the covering map $C(2) \to \mathcal{L}(2)$. Given a parametrization of $\mathcal{L}(2)$ as in eq. (A.17), we can read the map in eq. (A.18) backwards to construct a basis of the subspace of $\mathbb{R}^4$ corresponding to the a given set of parameters $(\chi, \alpha, \beta)$. The first step is taking a “square root” of $S(\chi, \alpha, \beta)$, for which we note that as $S = U^T U$ is a linear combination of Pauli matrices and identity, so should be $U$. An explicit calculation shows that

$$U(\chi, \alpha, \beta) = e^{i\chi/2} \left[ \cos (\alpha/2) \mathbb{I} + i \sin (\alpha/2) \left( \cos \beta \sigma^3 + \sin \beta \sigma^1 \right) \right]. \quad (A.23)$$

Given $U = \left( \Phi_1, \Phi_2 \right)$ and $\phi = \text{span}\{\Phi_1, \Phi_2\}$, we can read off

$$\Phi_1 = \begin{pmatrix}
\cos \frac{\chi}{2} - \sin \frac{\chi}{2} \sin \frac{\alpha}{2} \cos \beta \\
-\sin \frac{\chi}{2} \sin \frac{\alpha}{2} \sin \beta \\
\sin \frac{\chi}{2} + \cos \frac{\chi}{2} \sin \frac{\alpha}{2} \cos \beta \\
\cos \frac{\chi}{2} \sin \frac{\alpha}{2} \sin \beta
\end{pmatrix}, \quad \Phi_2 = \begin{pmatrix}
-\sin \frac{\chi}{2} \sin \frac{\alpha}{2} \sin \beta \\
\cos \frac{\chi}{2} + \sin \frac{\chi}{2} \sin \frac{\alpha}{2} \cos \beta \\
\cos \frac{\chi}{2} \sin \frac{\alpha}{2} \sin \beta \\
\sin \frac{\chi}{2} - \cos \frac{\chi}{2} \sin \frac{\alpha}{2} \cos \beta
\end{pmatrix}. \quad (A.24)$$

Thus, given a subspace $\psi = \text{span}\{\Psi_1, \Psi_2\} \in G_{2,4}$, the corresponding train $\mathcal{D}(\psi)$ can be obtained by solving the condition

$$\det (\Psi_1, \Psi_2, \Phi_1(\chi, \alpha, \beta), \Phi_2(\chi, \alpha, \beta)) = 0, \quad (A.25)$$

to obtained a codimension 1 surface in $C(2)$.
Figure A.1: The train of a given subspace in $C(2)$. The light blue cylinder represents $C(2) \cong \mathbb{R} \times S^2$, so that each disc corresponding to a fixed $\chi$ has its edge identified to a point to form a 2-sphere. The set of double cones is the train $\mathcal{D}(\phi)$ of a $\phi \in \mathcal{L}(2)$, which is a submanifold of codimension 1.

Choose $\Psi_i = e_i$, so that $\psi = e_1 \wedge e_2 \in \mathcal{L}(2)$, so that the condition for $\mathcal{D}(\psi)$ becomes

$$0 = \left| \begin{array}{ccc} \Phi_1^1 & \Phi_1^2 \\ \Phi_2^1 & \Phi_2^2 \end{array} \right| = \left| \begin{array}{ccc} \sin \frac{\chi}{2} + \cos \frac{\chi}{2} \sin \frac{\alpha}{2} \cos \beta & \cos \frac{\chi}{2} \sin \frac{\alpha}{2} \sin \beta \\ \cos \frac{\chi}{2} \sin \frac{\alpha}{2} \sin \beta & \sin \frac{\chi}{2} - \cos \frac{\chi}{2} \sin \frac{\alpha}{2} \cos \beta \end{array} \right| , \quad (A.26)$$

which can be simplified to get

$$\sin^2 \frac{\alpha}{2} \cos^2 \frac{\chi}{2} = \cos^2 \frac{\alpha}{2} \sin^2 \frac{\chi}{2} \Rightarrow \frac{1 - \cos \alpha}{1 + \cos \alpha} = \frac{1 - \cos \chi}{1 + \cos \chi} \Rightarrow \cos \alpha = \cos \chi. \quad (A.27)$$

A convenient way to visualize $C(2)$ is to plot each 2-sphere as a disk, with the edge identified to a point, so that the total space becomes a cylinder. Thus, we embed $C(2)$ in $\mathbb{R}^3$ with $(\chi, \alpha, \beta)$ forming a cylindrical coordinate system, with $\alpha$ being the radial coordinate and $\beta$ being the azimuthal one, so that the edge of the disks corresponding to $\alpha = \pi$ are identified to make constant-$\chi$ slices into 2-spheres. Then, each $\chi$ slice corresponds to a circle in the disk, centered at the origin, and the train corresponds to a set of double cones, as shown in Fig. A.1.
References


