Self-Adjointness and the Renormalization of Singular Potentials

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Abstract

Schrödinger operators with very singular potentials fail to produce reasonable spectra, because the usual boundary conditions are insufficient to make them self-adjoint. If one regularizes a singular potential at a length ϵ, the bound state energies diverge as $\epsilon \to 0$. A meaningful spectrum can be restored by picking a self-adjoint extension of the operator, by renormalizing the theory, or by allowing nonunitary time evolution. We show that renormalizations of the $1/r^2$ potential fall into two classes: those that are asymptotically equivalent to self-adjoint extensions, and those that reduce to treatments of delta functions. We also apply the apparatus of self-adjoint extensions and renormalization to clarify aspects of anomalous symmetry breaking, supersymmetric quantum mechanics, and one-dimensional quantum mechanics.

Lines composed upon reading a thesis abstract by S. Gopalakrishnan

Think a moment, dear reader, of that long-legged fly,
The sprung meniscus underfoot,
And what asymptotes invisible to well-trained eyes
Still break the surface at its root.

How a singular potential picks tight-bounded energy
Apart till it no longer recognizes
Its own mirrored face, its extensions, or symmetry;
Unless one cautiously renormalizes.

You have tried in these pensive pages to show the stuff
Such theory's made of, its quiddity
When logic is applied to the diamond rough,
And quantum notes ring purely.

May Apollo's clarity pierce through your reasoning
And self-adjointed truth and fact
Elevate your thought to that sense so pleasing
When truth recovers nature's pact.

Jesse McCarthy

Acknowledgments

First, I would like to thank my advisor, Professor Loinaz, for suggesting an interesting topic, guiding me through the literature, ploughing through quantities of papers that had nothing to do with his research, contributing his insight and his sharp nose for problems, catching several errors in drafts, and always being there—*literally* there, in his office—when I needed his advice. I would also like to thank him for the long, entertaining, and often instructive conversations we have had every week this year.

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Sarang Gopalakrishnan

Contents

Introduction

This thesis is concerned with the quantum mechanics of singular potentials in general. By a singular potential I mean anything that blows up at a single point, which is chosen to be the origin. Such potentials have several curious features, which can be summarized as follows:

1. Conditions such as square-integrability at 0 and ∞ do not unambiguously pick an orthonormal set of eigenfunctions. This is the failure of **self-adjointness**.

2. Sometimes, even imposing the requirement that $\psi(0) = 0$ fails to pick an orthonormal set. This is usually due to the failure of **boundedness**.

3. If you perturb Schrödinger Hamiltonians with singular potentials and tune the perturbation to zero, you might not recover the initial spectrum. This is known as the **Klauder phenomenon** [17], and is related to the failure of **analyticity**.

4. Two of these potentials, the two-dimensional delta function and the $1/r^2$ potential, are classically invariant under dilation, but acquire an intrinsic length scale upon quantization. This is known as the **anomaly**, and is a failure of **symmetry**.

Despite these failures, one can say rather a lot about singular potentials. Singular potentials cause trouble by their behavior at the origin, and disciplining them there by smoothing out the singularity (at, say, a short distance ϵ) gets rid of most of the problems. This doesn't quite do the trick on its own, though, because in the $\epsilon \to 0$ limit quantities such as bound state energies diverge. One way to remove these divergences is **renormalization**. The idea behind this is that since we don't know how physics works at very short distances from the singularity (or, equivalently, very high energies), we can access the form of the potential only down to certain distances. We have to deduce its behavior beneath these distances, assuming that such behavior

is finite and sensible, from some experimentally observed quantity like a bound state or a scattering phase shift. Of course, given a bound state energy and a description of long-distance behavior, there are infinitely many possible theories of short-distance physics. The remarkable thing about renormalization is that all the theories that have a bound state energy at E give the same values for all other low-energy observables. That is, with the addition of one arbitrary experimental parameter, we can predict all low-energy properties exactly.

There is an entirely different way to go about making these theories sensible, which is to fix the failure of self-adjointness. In practice, this works by specifying a bound state and deducing the rest of the spectrum from the requirement that all other eigenstates be orthogonal to it. For low-energy observables this technique produces exactly the same results as renormalization, and is mathematically more rigorous. The trouble with renormalization is that it's hard to prove something must be true of *all* imaginable short-distance physics; however, requiring that the renormalized theory should coincide with a self-adjoint extension fixes this, because we have a much better handle on the self-adjoint extensions of a Hamiltonian. We consider the relation between renormalization and self-adjoint extensions in the context of singular potentials—mostly delta functions and $1/r^2$ potentials—in the first five chapters. Chapter 1 is about delta functions, Chapter 2 introduces self-adjoint extensions, Chapter 3 introduces singular potentials and treats them with the apparatus of Chapter 2, and Chapter 4 introduces various renormalization schemes. Chapter 5 discusses the **renormalization group**, a powerful way to study the behavior of physical theories at various length scales.

The reason we like self-adjoint extensions—that they conserve probability—is sometimes a limitation. Suppose we are looking at a system where a particle moving in a singular potential falls into the singularity and gets absorbed: what then? This question is of particular importance because a recent experiment [23] with cold atoms moving in a $1/r^2$ potential noticed that some of the atoms were absorbed. Chapter 6 discusses nonunitary extensions of quantum mechanics that deal with such situations.

Chapter 7 is somewhat heterogeneous; it is about Klauder phenomena, non-analyticity, and resonance phenomena. The link between resonance and Klauder phenomena is that they are both **universal**. Klauder phenomena are independent of what the original perturbation was, and resonant interactions in quantum mechanics are the same for all potentials. Singular potentials are connected to resonance phe-

nomena by the **Efimov effect** [27]. In a system of three identical bodies for which all the two-body interactions are tuned to resonance, the three-body Schrödinger equation obeys a $1/r^2$ force law, and has infinitely many three-body bound states. This effect too has recently been observed experimentally [39].

Chapter 8 discusses the one-dimensional hydrogen atom and other issues in one-dimensional quantum mechanics that arise from the fact that $\mathbb{R}-\{0\}$ is disconnected. Chapter 9 discusses the symmetry structures, broken and otherwise, of the $1/r^2$ problem. Chapter 10 summarizes everything and briefly discusses physical applications of singular potentials.

Who Did What

Most of the key ideas in the first six chapters are not mine. The exception is the explanation of the relationship between the very different spectra of the renormalization schemes of Chapter 4 and Chapter 5. The treatment of self-adjoint extensions for singular potentials is, however, more explicit and detailed than elsewhere in the literature, and as far as I know this is the first detailed treatment of scattering observables in terms of self-adjoint extensions, and the first explicit treatment of nonunitary extensions as complex boundary conditions within the deficiency subspace framework.

I'm not aware of any previous work on the universality of Klauder phenomena; the idea isn't a deep one, but it is relevant to the renormalization schemes studied in Chapter 4. There have been several previous treatments of the one-dimensional hydrogen atom, but as far as I know, mine is the first to apply ideas from renormalization to the problem, or to characterize the family of extensions in terms of δ and δ' counterterms. My treatment of the two-parameter family was developed independently of Ref. [95], but they had the key idea before I did. (On the other hand, my treatment of the $x^2 + 1/x^2$ potential follows theirs quite closely.) The approach to the anomaly in terms of self-adjointness and finite dilations is, again, relatively obvious, but it hasn't been done in the literature. My approach to the $SO(2,1)$ algebra was different from Jackiw's [41]; for consistency with the rest of this thesis, I tried to reduce it to a time-independent symmetry, but was unable to get very far.

History of Previous Literature

There are, roughly speaking, three classes of singular potentials: mildly singular (solvable with regular QM), singular (problematic, but with ground states), and very singular (without a ground state). As the literature is considerable and I discuss most of the important ideas later, I have left my history skeletal, to avoid overwhelming the sequence of discoveries with irrelevant detail. For the most part, I have ignored exclusively pedagogical articles. I have left the history of the one-dimensional Coulomb problem, which is somewhat disjoint from this sequence, to the chapter on it.

Early Work

The first important paper on singular potentials was K.M. Case's treatment in 1950 [1]. Previously, the nonsingular—repulsive or weakly attractive—regimes had been treated by Mott and Massey (1933)[3] and by Titchmarsh (1946)[2]. The operator theory behind quantum mechanics had been developed in the 1930s by John von Neumann [4], Marshall Stone, and various others; Stone's monograph, *Linear Transformations in Hilbert Space* (1932) [5], is a standard reference in the literature. The strongly attractive (very singular) regime of the $1/r^2$ potential is dismissed as unphysical by the early writers; however, as Case notes, the Klein-Gordon and Dirac equations for the hydrogen atom have similar singularities.

Case shows that the strongly singular regime of the $1/r^2$ potential, treated naively, has a continuum of bound states. This implies that the operator is not Hermitian, but Case restricts the domain of definition of H to restore Hermeticity, and finds a point spectrum of bound states going all the way down to $-\infty$. These restrictions are Hermitian, but depend on an arbitrary phase parameter. He also shows that potentials more singular than $1/r^2$ have similar properties. A more specific early treatment of the $1/r^2$ case is due to Meetz (1964) [6], who discusses self-adjoint extensions explicitly (though the idea was implicit in Case's work). Meetz notes that there is a singular regime to this potential in addition to the very singular regime; this corresponds to the failure of self-adjointness for weakly repulsive and weakly attractive $1/r^2$ potentials. Narnhofer (1974) [7] gives a detailed expository treatment of this problem, and suggests that contraction semigroups might be helpful. She shows that the "natural" continuation of the "natural" self-adjoint extension into the very singular regime is nonunitary.

Vogt and Wannier (1954) [8] give a nonunitary solution to the $1/r^4$ problem, and preen themselves (rather ironically) about having avoided Case's "involved" mathematics. Nelson (1963) [9] arrives at a nonunitary result for the $1/r^2$ case by analytically continuing the functional integral; he basically hits the same nonanalyticity that Narnhofer does fifteen years later.

The 1967 review article by Frank, Land, and Spector [11] summarizes much of the early work on these potentials, and also discusses applications of very singular potentials. A lot of this work is on approximation schemes and applications. Spector's (1964) [12] analytic solution of the $1/r^4$ potential is an exception; unfortunately, it is not a very easy solution to use. A particularly important application is the Calogero-Sutherland model (1969) [13], which describes N bosons interacting with pairwise inverse-square potentials.

Self-Adjointness of Singular Potentials

The failure of self-adjointness at $\lambda < \frac{3}{4}$ seems to have already been familiar to mathematicians as an example of Weyl's limit-point/limit-circle theorem (1910); it is referred to quite casually in Simon's 1974 paper on self-adjointness [14]. The strictly mathematical literature on when Schrödinger operators are self-adjoint is huge, but Simon's "Review of Schrödinger operators in the 20th Century" (2000) [15] is a helpful guide, as is Vol. 2 of Reed and Simon's book on *Methods of Modern Mathematical Physics* [75]. Of more recent work, the most relevant papers are two papers by Tsutsui et al [95], [96] on one-dimensional quantum mechanics, and Falomir's discussion [92] of supersymmetry and singular potentials. An independent source of mathematical interest was Klauder's (1973) study of Klauder phenomena [17].

Nonunitary Solutions

The term **fall to the center** was first applied to singular potentials by Landau and Lifschitz in their quantum mechanics text (1958) [18], where the strong-coupling regime is compared with the classical situation, for which the particle's trajectory is defined only for a finite time. This comparison between classical completeness (i.e. having a solution for all time) and self-adjointness is explored rigorously in Reed and Simon vol. II [75], and makes its way into the pedagogical literature with an AJP article by Zhu and Klauder [19] on the "Classical Symptoms of Quantum Illnesses" (1993).

Non-self-adjoint extensions of singular potentials are explored in some more detail by Perelomov and Popov (1970) [20] and by Alliluev (1971) [21], using methods that are equivalent to Nelson's. The mathematical side of the semigroup theory had been worked out previously by Hille, Yosida, Kato, Trotter, etc.; a classic text is *Functional Analysis and Semigroups* by Hille and Phillips [10]. In 1979, Radin [22] observed that Nelson's nonunitary time-evolution operator could be written as an average over the unitary operators corresponding to all the self-adjoint extensions. (This is not especially shocking, since e.g. $e^{i\theta}$ and $e^{-i\theta}$, which are unitary, average to $\cos\theta$, which is not.)

This work found some physical application in 1998, when Denschlag et al experimentally realized an attractive $1/r^2$ potential by scattering cold neutral atoms off a charged wire [23], and found that the atoms were absorbed. This result was treated variously by Audretsch et al (1999) [24] and by Bawin and Coon (2001) [25], who use Radin's result to "justify" the cross-section.

A related, and intriguing, result is Bawin's proof (1977) [26] that spectra very different from Case's could be obtained by redefining the inner product.

Effective Field Theories

In his famous paper of 1971 [27], Vitaly Efimov noted that in certain regimes, the three-body problem reduces to that of particles moving in an effective $1/r^2$ potential, and this produces a large number of bound states. (There is a huge literature on the Efimov effect, which we will not attempt to cover.) Efimov's result made it desirable to apply ideas from the effective field theory (EFT) program to the $1/r^2$ potential, and thus prompted the treatments of Bedaque, Hammer, and Van Kolck (1999) [29], and of Beane et al (2001) [30]. The treatment in [29] uses field theoretic methods, while [30] constructs an effective theory of the interaction by cutting off the potential at short distances by a square well. In their paper, Beane et al find that the **renormalization group flow** equations of the $1/r^2$ potential have two sorts of solutions—continuous paths that don't go all the way to the origin, and log-periodic paths that represent **limit cycles**. Beane et al treat singular potentials quite generally; more specific treatments of the $1/r^2$ case are done by Bawin and Coon (2003) [31], who solve the RG flow equations analytically, and Braaten and Phillips (2004) [32], who discovered that using a δ-function ring cutoff instead of a square well cutoff forces one to choose the limit cycle. The idea of limit cycles in this context,

and a lot of the conceptual basis for this work, is due to Kenneth Wilson's (1971) work on the renormalization group [34].[1] The specific method that these authors use was suggested by Lepage(1997) [33]. Recently, Alberg, Bawin, and Brau (2005) [36] used a similar approach to treat the $1/r^4$ potential; however, they did not consider δ-function regularizations.

After decades of strenuous effort, the Efimov effect was finally demonstrated in the laboratory this year with cold atoms [39]. Another recent milestone in that area was the long review article on universality by Braaten and Hammer [40], which uses the same language as above-mentioned papers.

In general, solutions found by these methods are unitary and involve spectra with arbitrarily many bound states.

Algebraic Structures

Anomalies are cases where a classical symmetry is broken by quantization. They are pervasive and very important in quantum field theory. It has been known for some time that the $1/r^2$ and $\delta^2(r)$ potentials are examples of the anomaly in nonrelativistic quantum mechanics. Jackiw [41] looks at the broken SO(2,1) algebra associated with both potentials in his 1991 paper on delta function potentials; this is taken up in more detail by Camblong and Ordonez (2003, 2005) [44], [43], who also discuss various applications of conformal QM. A somewhat different algebraic treatment is given by Birmingham, Gupta, and Sen (2001) [42], who study the representation theory of the Virasoro algebra underlying this problem.

Renormalizing the Coupling

Gupta and Rajeev (1993) [52] renormalized the long-distance coupling of the very singular $1/r^2$ potential, and got a renormalized spectrum with just one bound state, which looked essentially the same as that of the δ^2 potential. Their result was worked out in just one dimension, but it was later generalized by Camblong et al (2000) [45], who also got the same answer by dimensional regularization [47], [48]. Camblong's result was reworked in an AJP article by Coon and Holstein (2002) [46], and later by Essin and Griffiths (2006) [51]. This approach to the potential also constituted the bulk of Essin's undergraduate thesis (2003).

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[1]Limit cycles were, however, borrowed from dynamics, where they actually make sense.

Notes to the Reader

Sequence

This thesis was written to be read in sequence, but it needn't be. The first three chapters are essential context for chapters 4-7 and 9. Chapter 5 uses the results of Chapter 4 but not the details. Chapter 6 is independent of Chapters 4 and 5, and may be skipped without loss of continuity. Chapter 7 deals with issues raised in Chapters 4 and 5, so it should be read after them. Chapter 8 uses the entire apparatus developed thus far, but is independent of Chapters 3 and 4. Chapter 9 is independent of Chapters 4-8. In later chapters I sometimes use the terms "Chapter 4" and "Chapter 5" renormalization to refer, respectively, to schemes that renormalize the long-distance coupling and schemes that don't.

The bulk of original work is in the later sections of Chapters 3 and 5, and all of Chapters 7 and 8.

Units, Dimensions, Notation

I have set $\hbar = 2m = 1$. Since the first term in Schrödinger's equation is then just $-\nabla^2\psi$, which has dimensions $[length]^{-2}[\psi]$, consistency requires that V and E have dimensions of $[length]^{-2}$. This turns out to be an immense convenience, though it might take some getting used to.

More irritatingly, I suppose, I have freely used the identity $\log kr = \log k + \log r$ even if k and r have dimensions. The departure from dimensional consistency might make the equations harder to check, but is standard in the literature and makes several equations a lot tidier. The reader is requested to imagine, should s/he wish, that there are ghostly η's and η^{-1}'s hovering by the dimensional quantities and just canceling them out.

References of the form AS 1.1.1 are to identities in Abramowitz and Stegun [58].

Finally, I should comment on my inner products, which are always (ψ_1, ψ_2) and never $\langle\psi_1|\psi_2\rangle$. In Dirac notation, one is used to thinking that a Hermitian operator A in the middle of a bracket

$$\langle\psi|A|\phi\rangle$$

might be acting either to its left or to its right, depending solely on the reader's whim. When dealing with issues of self-adjointness, it is extremely important to know

whether one is operating on the bra or the ket, and the mathematicians' notation, which forces us to pick either $(A\psi, \phi)$ or $(\psi, A\phi)$, has the merit of being entirely unambiguous about this.

Chapter 1

Delta Functions

Potentials shaped like Dirac delta functions are useful in the study of singular potentials for several reasons, most of which will be left to subsequent chapters. There are two general strands to the answer; the first is that delta functions are easy to solve, and the second is that they are conceptually important to the effective field theory (EFT) program, which I'll discuss now. The two dimensional delta function is independently interesting because it lacks an explicit scale; along with the $1/r^2$ potential, it is an example of the "anomaly" in quantum mechanics.

1.1   Effective Field Theories

The idea behind effective field theories is that you can describe the low-energy, long-distance behavior of a theory very powerfully by an "effective theory" without knowing much about its high-energy, short-distance behavior. This generally requires **renormalization**, which casts our effective theory entirely in terms of low-energy experimental observables; renormalization becomes necessary when our effective theory has divergences due to high-energy behavior (where the approximation breaks down), but isn't always required. In the case of the hydrogen atom, for instance, the effective model of a $1/r$ potential is not valid to arbitrarily short distances, but the eigenvalues still converge, and so we needn't worry about short-distance behavior at all. On the other hand, some theories *cannot* be renormalized because their behavior *at all energies* is strongly affected by the details of high-energy processes—so different parameterizations of high-energy behavior lead to radically different theories.

Delta function potentials are frequently used in effective theories as a simple char-

acterization of high-energy physics, because their action is entirely local, and they are relatively easy to do calculations with—especially in momentum space, where they are constant. They also provide particularly simple and instructive examples of renormalization, which we shall see in the following sections. A detailed introduction to EFT ideas is given in Ref. [33].

1.2 $\delta(x)$ in One Dimension

This is a classic problem discussed in introductory QM textbooks [53]. There are two standard treatments, of which the quicker one is perilously glib. The idea is that if you integrate the time-independent Schrödinger equation with $\hbar = 2m = 1$:

$$\left[-\frac{d^2}{dx^2} + g\delta(x)\right]\psi = E\psi \tag{1.1}$$

from small $-\epsilon$ to ϵ, you get

$$-\left[\frac{d\psi}{dx}\right]_{-\epsilon}^{\epsilon} + g\psi(0) = \int_{-\epsilon}^{\epsilon} E\psi dx \approx 0 \tag{1.2}$$

because ψ is required to be continuous and you can pull E out of the integral. Note, however, that this logic *assumes* that E is finite, which turns out not to be the case for the naive $\delta^2(x, y)$ potential. Anyhow, it works here, and gives

$$\psi'(\epsilon) - \psi'(-\epsilon) = g\psi(0). \tag{1.3}$$

We're looking for a bound state, with $E = -k^2 < 0$. We know what it should look like on both sides of the delta function, because there $V = 0$ and so

$$-\frac{d^2\psi}{dx^2} = -k^2\psi$$

which has the familiar solutions

$$\psi = Ae^{kx} + Be^{-kx}. \tag{1.4}$$

Since a bound state must be normalizable, we can throw out the positive exponent on $x > 0$ and the negative exponent on $x < 0$. Plugging into (1.3) we get

$$-2k = g \Rightarrow E = g^2/4. \tag{1.5}$$

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The wavefunction goes smoothly to its limiting form.
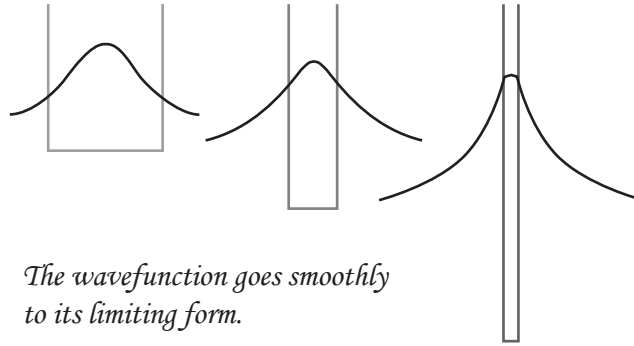
Figure 1.1: Delta Function as Limit of Wells

Note that g must be negative for (1.5) to be consistent. This is as one would expect, since a positive potential would be a barrier rather than a well.

The other—in some sense more obvious—way to do this problem is to treat the delta function as the limit of narrower and deeper square wells. We'll parameterize these as follows:

$$V_n(x) = \begin{cases} V_n = gn/2 & |x| < 1/n \\ 0 & |x| > 1/n \end{cases} \tag{1.6}$$

The square well is known to have only one bound state for sufficiently small $|Va^2|$, where a is the well width (see [54], 10.3). Since

$$|V_n a_n^2| = \frac{g}{2n} \overset{n\to\infty}{\to} 0, \; a_n = 1/n,$$

this holds in our limit, and we needn't worry about excited states. As for the bound state, by even symmetry about the origin we need only to match at a_n. The solutions are:

$$\psi_{in} = A\cos(qx), \psi_{out} = Ae^{-kx}$$

where $q = \sqrt{|V_n| - k^2}$, $k = \sqrt{|E_n|}$. Matching the wavefunctions and their derivatives, we get the equation

$$q\tan(qa_n) = k. \tag{1.7}$$

Since $0 \leq k^2 < |V_n|$, $qx \leq \sqrt{|V_n a_n^2|} \to 0$ and we can use the small angle approximation

$$q^2 a_n = k \Rightarrow \frac{g}{2} - k_n^2 a_n = k_n \tag{1.8}$$

where I've added subscripts to emphasize that the energy depends on n. Now this can be rewritten as

$$\frac{g}{2} = k_n(1 + k_n a_n)$$

and since $k_n a_n \leq q_n a_n \to 0$, we get (1.5) again.

Scattering

We can apply a similar analysis to the scattering sector—that is, positive-energy states—instead of the bound state sector. Recall that in one-dimensional scattering our usual "observable" is the asymptotic phase shift we get if we send in the wave e^{-ikx}. It's convenient for later purposes to send in a rather unconventional waveform that's symmetric about the origin: so that there's a wave Ae^{ikx} coming in from the left, and a wave Ae^{ikx} from the right. This makes the problem symmetric about the origin, so that we can reduce it to a problem on a half-line. From our previous analysis we know that the boundary condition at the origin is

$$\frac{g}{2}\psi(0) = \psi'(0^+). \tag{1.9}$$

The general form of the wavefunction (including the reflected wave) is $Ae^{-ikx} + Be^{ikx}$ on the right half-line, and imposing the boundary condition on this we get

$$-i\frac{2k}{g} = \frac{A+B}{A-B} \tag{1.10}$$

Now we can replace g by $2k_b$ where k_b is the bound state energy[1], because of our previous calculation. (In the case of the δ function it's just a renaming, but one could also think of it as a trivial example of renormalization, as the short-distance coupling has been replaced by a long-distance observable in the theory.) Rearranging this expression, we get

$$\frac{B}{A} = \frac{k - ik_b}{k + ik_b} \tag{1.11}$$

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[1]Strictly, $E_b = k_b^2$ is the bound state energy, but since k_b is much more useful, we will freely refer to it as an energy.

B/A has magnitude one; the phase angle δ is what's generally considered the most useful scattering observable, since the asymptotic behavior of the wavefunction is $A(e^{-ikx} + e^{i\delta}e^{ikx})$.

$$\tan\delta = \frac{-2kk_b}{k^2 - k_b^2}. \tag{1.12}$$

A feature of particular interest is the singularity in $\tan\delta$ at $k = k_b$; this is an instance of a general result known as Levinson's theorem [62], which we will discuss later (see Chapter 7).

We could also have sent in a more conventional waveform e^{-ikx} from the right, and solved the problem without assuming symmetry. In this case we would have arrived at the equation

$$i\frac{k}{k_b} = \frac{A + B}{B}.$$

This can be rearranged as

$$\frac{B}{A} = \frac{k_b}{ik - k_b},$$

and evidently the magnitude *isn't* always one. The phase shift is a less complete description for this problem, but it also has a simpler form:

$$\tan\delta = \frac{k}{k_b}.$$

Now let's add a dimension.

1.3   The 2D Schrödinger Equation

Separating variables in polar coordinates in the two-dimensional Schrödinger equation [60] gives us the equations

$$\frac{d^2\Theta}{d\theta^2} + m^2\Theta = 0 \tag{1.13}$$

and

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \left(k^2 - \frac{m^2}{r^2} - V\right) = 0 \tag{1.14}$$

where m is a constant introduced in the separation of variables, and must be an integer in order to have $\Theta(\theta)$ be single-valued. (1.14) can often be rewritten in the sometimes more useful form

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \left(k^2 - \frac{m^2}{r^2} - V\right)R = 0. \tag{1.15}$$

In free space, this reduces to Bessel's equation [56]

$$r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + (k^2r^2 - m^2)R = 0 \tag{1.16}$$

to which the two solutions are the functions $J_m(kr)$ and $N_m(kr)$ (a.k.a. Y_m), called respectively the Bessel and Neumann functions of order m. (Note that a constant potential would add on to k^2r^2 and thus change the argument of the Bessel functions to qr, just as we do with trig functions.) In fact, Bessel functions bear several resemblances to sines and cosines, as we'll have occasion to see. Bessel's equation does not require m to be an integer, and in fact there are even Bessel functions of complex order. But we'll come to those as we need them. Figs 1.2 and 1.3 show the behavior of the first few J_m and N_m.
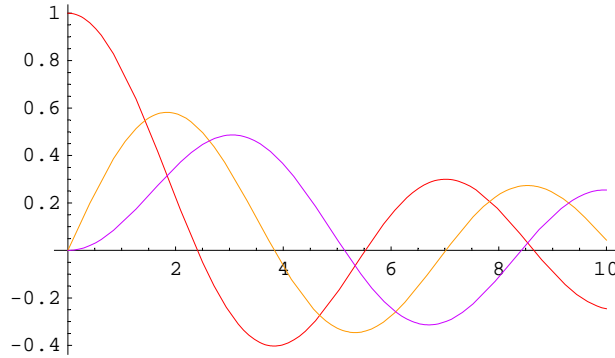
Figure 1.2: $J_0(x)$ (red), $J_1(x)$ (orange), $J_2(x)$ (purple)

These are the eigenfunctions for positive energy. Negative energy states generate the following equation:

$$r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} - (k^2r^2 + m^2)R = 0 \tag{1.17}$$

This is called the modified Bessel equation, and its solutions are $I_m(kr)$ and $K_m(kr)$, which look vaguely like growing and decaying exponentials respectively.
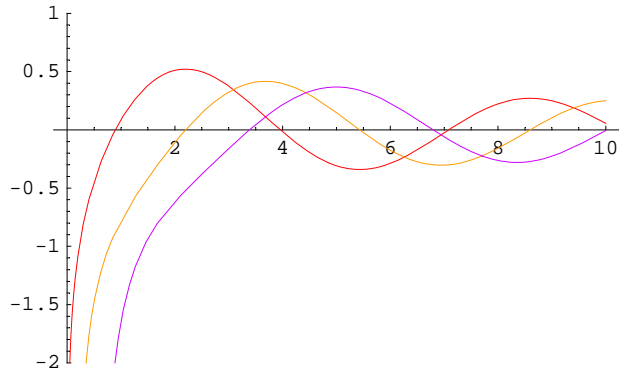
Figure 1.3: $N_0(x)$ (red), $N_1(x)$ (orange), $N_2(x)$ (purple)
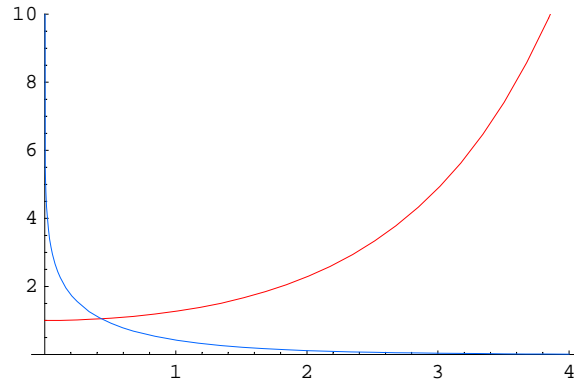
Figure 1.4: I_0 (red), K_0 (blue)

A peculiarity of N_m and K_m is that they blow up at the origin; this is unacceptable with finite potentials, and therefore (as in three dimensions) the requirement that the wavefunction be finite at the origin picks out a solution [79].

1.4 The 2D Delta Function

Now let's try to mimic the procedure of Section 1.2 with cylindrical wells. To ensure that the **volume** of the well stays constant, we use the sequence

$$V_n = -\frac{gn^2}{\pi}, a_n = \frac{1}{n}. \tag{1.18}$$

Note that there's only one interior eigenvalue for any m, since the Neumann functions are unacceptable at the origin *for a potential without singularities*. For the ground state $(m = 0)$ the solutions are

$$\psi_{in} = AJ_0(qr), \psi_{out} = BK_0(kr). \qquad (1.19)$$

Matching the wavefunctions and their derivatives at a_n gives us

$$q\frac{J_0'(qa)}{J_0(qa)} = k\frac{K_0'(ka)}{K_0(ka)}, \qquad (1.20)$$

which we would like to simplify, but can't, because

$$(q_n a_n)^2 \rightarrow \frac{gn^2 - k^2}{n^2}.$$

We have no justification, at this time, for assuming that the arguments are either small or large, so we're stuck. To see what's going wrong here, let's look at the unseparated Schrödinger's equation

$$-(\nabla^2 + g\delta^2(r))\psi = -k^2\psi. \qquad (1.21)$$

We are looking for a ground state, so we can restrict ourselves to $m = 0$, which implies cylindrical symmetry. Since any solution must be a free-space solution except at the origin, our eigenfunction must be of the form $K_0(kr)$ where $-k^2$ is the bound state energy. Suppose $k < \infty$. Then the rhs vanishes if you integrate the equation over a small disc centered at the origin. The first term is $\nabla^2(\log r)$ near the origin. Since $\log r$ is the Green's function for Laplace's equation in two dimensions [56] (it's parallel to $1/r$ in three dimensions), the volume integral returns a finite quantity (the "enclosed charge"). However, K_0 blows up at the origin and the second term is infinite, so the lhs cannot add up to zero. Therefore there are no finite energy bound states. However, since it's the case that arbitrarily weak 2D square wells have bound states, we would like the attractive delta function to have one. We can do this by renormalizing the delta function.

1.5 Renormalizing the 2D Delta Function

Our theory diverges because the "real" short distance behavior isn't accurately characterized by our delta function. The first step is to **regularize** our theory by using
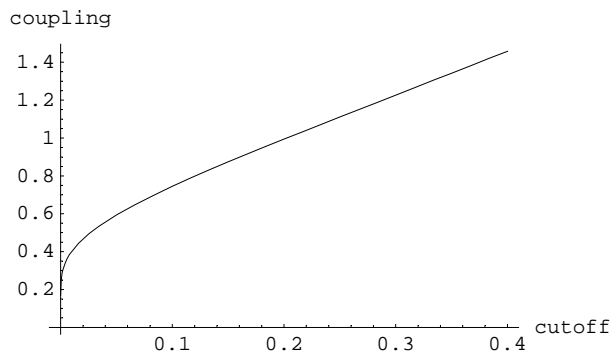
Figure 1.5: Renormalization Group Flow for $\delta^2(r)$

some sort of regular approximation to it (say a square well of width a, where a is called the *cutoff*). Since the theory is still problematic in the limit $a \to 0$, we need to **renormalize** it as described previously, by replacing the coupling constant with an experimental observable. (For the reasoning behind this procedure, see the Introduction.) We choose the bound state energy to fix, because it's most convenient, but we could have chosen the more physical scattering amplitude as well. Anyway, here's how renormalization works if we fix the bound state. Let's say we've measured its energy to be E_0, so we need a theory that gives us this answer. Recall the boundary condition

$$q\frac{J_0'(qa)}{J_0(qa)} = k\frac{K_0'(ka)}{K_0(ka)}$$

Substituting

$$q^2 = |V| - k^2 = \frac{g}{\pi a^2} - k^2 \tag{1.22}$$

we have an equation that's entirely in terms of g, a and k. Fixing k reduces this to an expression connecting g and a, which we can plot on Mathematica (Fig 1.5).

(Incidentally, a plot of this kind is called a **renormalization group flow**, and a line of constant k_b is referred to as a line of constant physics. We shall see more of these later.) Our eventual goal is to take a to zero, and it's clear from the picture that as we do this $g \to 0$ as well no matter what k might be. Our decision to fix k means we can make ka as small as we like. By (1.22) and the figure, $(qa)^2 = g - (ka)^2$ also becomes as small as we like, and we can use the standard relations

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$$J_0'(x) = -J_1(x), K_0'(x) = -K_1(x) \tag{1.23}$$

and the small argument approximations

$$J_0(x) \approx 1, J_1(x) \approx x/2, K_0(x) \approx -\log x, K_1(x) \approx 1/x \tag{1.24}$$

to simplify the boundary condition to the form

$$q(-qa/2) = k\frac{-1/ka}{-\log(ka)}, \tag{1.25}$$

which simplifies to

$$-q^2 a^2 = \frac{2}{\log(ka)}. \tag{1.26}$$

Using (1.22) and dropping the term that's second order in a, we get

$$\log(k_{bs}a) = -2\pi/g, \tag{1.27}$$

which can be rearranged to make $E = k^2$ the subject:

$$E_{bs} = \frac{1}{a^2}e^{-4\pi/g}. \tag{1.28}$$

Now we use this relation to calculate other quantities in terms of the BS energy. Let's consider the scattering problem. Lapidus [59] works out the $m = 0$ scattering phase shift for a square well to be

$$\tan(\delta_0) = \frac{kJ_0'(ka)J_0(qa) - qJ_0'(qa)J_0(ka)}{kN_0'(ka)J_0(qa) - qJ_0'(qa)N_0(ka)} \tag{1.29}$$

by the usual procedure of matching wavefunctions and their derivatives at the boundaries. Since k is fixed independently (by the incoming wave), for small a we can use (1.22), leaving out the second order (in ka) terms, to get

$$qa = \sqrt{g} = -1/\sqrt{\log(k_{bs}a)}. \tag{1.30}$$

Since our renormalization scheme has $g \to 0$, we can use small-argument approximations for all the Bessel functions. The leading terms are:

$$J_0(x) \approx 1, J_1(x) \approx x/2, N_0(x) \approx (2/\pi)\log x, N_1(x) \approx (2/\pi x)$$

Plugging in the expansions and dropping second-order terms, we get

$$\tan \delta_0 = \frac{\frac{\pi}{\log(k_{bs}a)}}{2 - 2\frac{\log(ka)}{\log(k_{bs}a)}} \tag{1.31}$$

which simplifies to

$$\tan \delta_0 = -\frac{\pi}{2\log(k_{bs}/k)}. \tag{1.32}$$

The important thing about this result is that our final answer is independent of the value of a, so the $a \to 0$ limit is simple. This is the hallmark of a correctly renormalized theory.

Refs. [55] and [46] prove the renormalizability of the scattering problem using the Born approximation and Fourier transform methods.

1.6 Scale Invariance and the Anomaly

An interesting thing about the Schrödinger equation with $\hbar = 2m = 1$ is that all dimensions can be expressed in terms of lengths. One can see from the form of the equation

$$-\nabla^2 \psi + V\psi = E\psi$$

that (if the energy terms are to be dimensionally consistent with the first term) energy must have dimensions $[length]^{-2}$. Mass has no dimensions, by construction, and the dimensions of time can be seen from the uncertainty relation

$$\Delta E \Delta t = \frac{1}{2}$$

to be $[length]^2$. With most normal potentials, one can use dimensional analysis [47] to predict the bound state energy (to within a multiplicative constant) from the scales intrinsic to the problem. Two examples:

- **The Harmonic Oscillator**. The scale is set by the constant in ax^2, which has dimensions $[length]^{-4}$. So if we want to construct a bound state energy it must be of the form $\sqrt{a}$ up to a multiplicative constant. a is normally written as ω^2, which gives $E = \omega$, as we expect.

- **The Infinite Well**. The only intrinsic parameter is the width L. To construct an energy out of this we clearly need L^{-2}.

It should be noted that this reasoning sometimes breaks down. A good example is the case of singular potentials $1/r^n, n > 2$, where the bound state energies depend on scales set by the short-distance physics, rather than the intrinsic scales of our effective theory.

A particularly interesting situation arises with the δ^2 and $1/r^2$ potentials, since the coupling constant is dimensionless and so there is no intrinsic scale to the problems. The Hamiltonians are *scale invariant*, i.e. they are invariant under a dilation $r \to \lambda r$. This is obvious in the case of the inverse square potential in 1D:

$$H_x = -\frac{d^2}{dx^2} + \frac{g}{x^2}, \, H_{\lambda x} = -\frac{d^2}{d(\lambda x)^2} + \frac{g}{(\lambda x)^2} = \frac{1}{\lambda^2} H_x \qquad (1.33)$$

Since $H_{\lambda x}\psi(\lambda x)$ has the same eigenvalues as $H_x\psi(x)$ (it's just a relabeling of variables), it follows from our result that

$$H_x\psi(x) = E\psi(x) \Rightarrow H_x\psi(\lambda x) = \lambda^2 E\psi(\lambda x) \qquad (1.34)$$

Therefore, if E is an eigenvalue then so is $\lambda^2 E$, and if there are any (finite energy) bound states then all negative energy states are bound states. This is impossible because it violates the requirement that eigenfunctions be orthogonal[2] (which is related to self-adjointness), so a scale invariant QM potential can have no bound states except at $-\infty$. The proof for $\delta^2(x)$ is similar, but depends on the well-known fact that

$$\delta^n(ax) = \frac{1}{a^n}\delta^n(x)$$

(to compensate for the Jacobian).

This is what happens with the naive $\delta^2(x)$ potential. What renormalization does is to introduce a scale—the renormalized bound state energy—into this problem by hand, thus *breaking* the scale invariance of the classical potential. This phenomenon is known as the **anomaly** in quantum mechanics, and is an example of a common occurrence in field theory known as **dimensional transmutation**, which is said to occur when a dimensionless quantity (the coupling) is traded in for a quantity with dimensions (the bound state energy).

---

[2]Intuitively, the eigenvectors corresponding to infinitesimally separated eigenvalues should look exactly alike, in which case they certainly can't be orthogonal.

1.7 The 2D Delta Function as Limit of Rings

This is the method used by [55]. The "regular" approximate potential is a ring of 1D delta functions of radius ϵ:

$$V = \frac{g\delta(r - \epsilon)}{2\pi\epsilon} \tag{1.35}$$

(The denominator is clearly needed to have g be dimensionless, and it's also intuitive that the 1-D delta functions must get stronger as their "density" decreases.) We're looking for a bound state with $m = 0$, which implies spherical symmetry. We can move to momentum space, where the ∇'s turn to p's, and our equation has the following form:

$$-p^2\phi(p) + g\psi(\epsilon) = k^2\phi(p) \tag{1.36}$$

We can solve this for $\phi(p)$:

$$\phi(p) = g\psi(\epsilon)\left(\frac{1}{p^2 + k^2}\right) \tag{1.37}$$

We can transform this back into position space. The inverse Fourier transform of the quantity in parentheses is known (see [56]) to be $K_0(kr)/2\pi$, so we get

$$\psi(r) = g\psi(\epsilon)K_0(kr)/2\pi \tag{1.38}$$

Plugging in $r = \epsilon$ and cancelling out the ψ's[3], we get the condition

$$2\pi = gK_0(k\epsilon) \tag{1.39}$$

Since K_0 is logarithmic at the origin, we can rearrange this expression as

$$k = \frac{1}{\epsilon}e^{-2\pi/g}$$

which is of the same form as (1.27). The rest of the renormalization proceeds just as it did with the square well, and we won't go into the details.

---

[3]This requires $\psi(\epsilon) \neq 0$, but otherwise our wavefunction would be trivial.

1.8   The 3D Delta Function

Again, we might want to solve this potential as a limit of spherical wells, of the form

$$V = -\frac{g}{\frac{4}{3}\pi a^3} \tag{1.40}$$

The radial Schrödinger equation with $l = 0$ looks exactly like its 1D counterpart in terms of $u = \psi/r$. The difference is that in order to ensure that ψ stays regular at the origin we require $u(0) = 0$. This means that the ground state is a sine and not a cosine—and that for sufficiently weak coupling there is no ground state. Matching equations and derivatives at the boundaries, we get

$$q \cot qa = k \Rightarrow \sqrt{\frac{g}{a^3} - k} = k \tan\left(\sqrt{\frac{g}{a^3} - k}a\right) \tag{1.41}$$

There are three possibilities. One is that $q \to 0$ slower than a, in which case the argument of $\tan qa$ gets very big, and we know that x intersects $\tan x$ infinitely often, so the equations don't flow anywhere in particular. The second is that $g \to 0$ fast enough, so that we're in the small argument regime. In this case, we can expand $\cot qa \approx 1/qa$, so $q \cot qa \to 1/a$, and we can't renormalize because the coupling has disappeared from the equations. The third possibility is that g falls off at exactly the same rate as a, but this is not a helpful regime for analytic work. In fact this approach is problematic for several reasons, one of which is that the regular solutions all obey $\psi(0) = 0$ and the "real" solution doesn't. It turns out that one **can** regularize the problem with a square well, but needs to parameterize the wells in a non-obvious way to have the limit work out [64]. The easiest solution is by means of self-adjoint extensions (see Chapter 2); however, delta function shells also do the trick. If we solve the equation by Fourier transformation as before, and recall that the appropriate 3D Green's function is e^{-kr}/r, our consistency criterion becomes

$$1 = -\frac{g e^{-k_b a}}{2\pi a}. \tag{1.42}$$

We can use this to solve the scattering problem in the usual way, remembering that the derivative jumps at the delta function:

$$C \sin(ka) = A e^{ika} + B e^{-ika} \tag{1.43}$$

$$kC \cos(ka) + \frac{gC \sin(ka)}{2\pi a^2} = ik(A e^{ika} - B e^{-ika}). \tag{1.44}$$

And so

$$k \cot(ka) + \frac{g}{2\pi a^2} = ik \left[\frac{Ae^{ika} - Be^{-ika}}{Ae^{ika} + Be^{-ika}} \right]. \tag{1.45}$$

The rhs simplifies considerably if we drop all higher-order terms. Substituting for γ from (1.39) we get

$$\cot(ka) - \frac{1}{kae^{-k_b a}} = i \left[\frac{A - B}{A + B} \right] \tag{1.46}$$

Expanding the lhs and keeping terms of up to zeroth order in a, we get the singular terms to cancel out and leave us with

$$i\frac{k_b}{k} = \left[\frac{A - B}{A + B} \right] \tag{1.47}$$

from which we can derive an expression for the phase shift that is consistent with self-adjoint extensions (Chapter 2).

1.9   More Dimensions, etc.

Since most of this thesis takes place in three or fewer dimensions, the properties of higher-dimensional delta functions are not that relevant. In five or more dimensions all cutoff regularizations give a trivial result, though the popular (in QFT) technique of dimensional regularization sometimes allows bound states. (See [68] for more details.) Which of these regulation schemes do we trust, and to what extent are these effects scheme-independent? We will look at these issues again in later chapters, in the richer context of power-law potentials.

1.10   The $\delta'(x)$ Potential

The delta function and its derivatives are less unfamiliar in momentum space than in position space. We know that the Fourier transform of $\delta(x)$ is

$$\int \delta(x)\psi(x)e^{-ipx}dx = \psi(0),$$

a constant. Now $\delta'(x)$ is a little more interesting.

$$\int \delta'(x)\psi(x)e^{-ipx}dx = -\int \delta(x)[\psi'(x) - ip\psi(x)]e^{-ipx}dx = ip\psi(0) - \psi'(0),$$

so $\delta'(x)$ is basically dual to the entirely mundane operation of multiplication by p in momentum space. That a function appears in a certain context in quantum mechanics does not make it useful as a potential, but it sometimes appears as a short-distance "counterterm" in renormalization. (We'll see what this means in Ch. 5.)

The 1D delta function derivative is particularly nice because, along with the 2D delta function, it possesses the mysterious property of scale invariance. ($\delta'(x)$ has dimensions of length^{-2}.) If you integrate the Schrödinger equation around zero,

$$- \left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} + g \int_{-\epsilon}^{\epsilon} \delta'(x)\psi(x) = k^2 \int_{-\epsilon}^{\epsilon} \psi(x)$$

the potential term can be integrated by parts to give

$$-g \int_{-\epsilon}^{\epsilon} \delta(x)\psi'(x) = -g\psi'(0)$$

For this to be meaningful the derivative must be continuous at zero, so we can throw out the derivative terms. But if we do so the result is bound to be trivial *for finite energies*, since ψ is regular and its integral vanishes. However, a bound state with infinite energy is still a possibility. Its integral in a region right around the origins would go roughly as $\psi(0)a$ for tiny a. (It turns out that integrating from $-\epsilon$ to ϵ doesn't work, because the function we're looking for is odd.)

It might seem silly to force this problem to have a bound state. However, we do have a bound state in mind, and it's an odd version of the delta function's bound state:

$$\psi = sgn(x)e^{-k|x|}$$

Our desire for a bound state is motivated partly by Simon's theorem (see Chapter 3), which states that there should be one for any short-range not-too-pathological odd potential.

The situation is symmetric to the delta function; there we had a discontinuity in the derivative proportional to $\psi(0)$; here we have a discontinuity in the function proportional to $\psi'(0)$, but the derivative is continuous. The fact that the wavefunction is discontinuous is enough to irritate most people with the $\delta'(x)$ potential, and maybe its physical applications are limited. However, if you think of wavefunctions as waves on a string, it is possible to make sense of this potential. First, notice that the delta function is a cusp, of the sort that would correspond to having a bead at the origin (or a spring pulling down). The "mass" is proportional to the derivative at the origin,

and hence to g. Now, suppose that instead of a bead you had a spring of the sort in Fig 1.6.
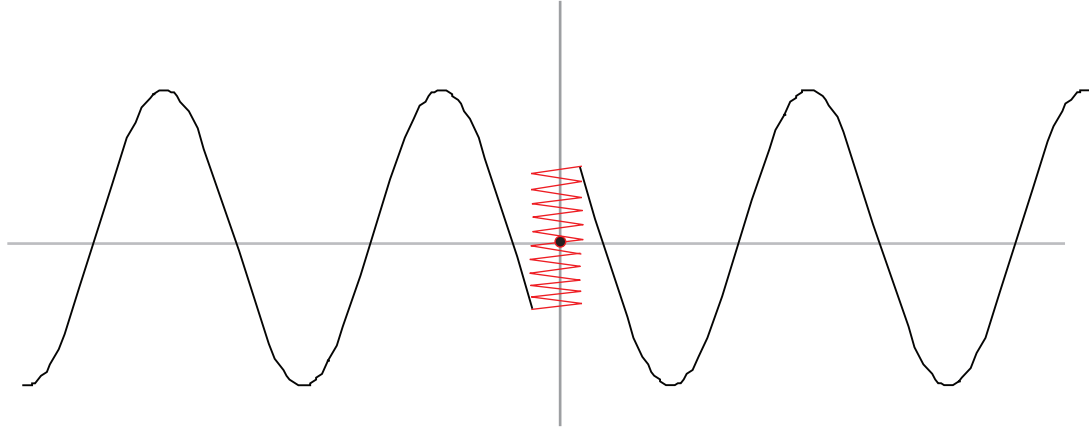
Figure 1.6: The $\delta'(x)$ potential. When you stretch one side of the spring the other side stretches in the opposite direction. Assume the spring can move only vertically, so that we can ignore torques.

This boundary condition is identical to a $\delta'(x)$ potential. However, like the 2D delta function, it is pathological and needs to be renormalized. In a way their problems are exact opposites. The trouble with $\delta^2(r)$ is that for any finite value of k the ground state blows up. With $\delta'(x)$, if you make k finite then ka vanishes and the state becomes trivial. This potential is surprisingly hard to renormalize, and was successfully treated only rather recently in Ref. [97]; they discovered that they were forced to take the coupling to ∞. The $\delta'(x)$ potential is one of the cases where the machinery of self-adjoint extensions (see Chapter 8) is much simpler than any other.

As far as scattering goes this potential is much like $\delta(x)$; in fact, it's basically just an odd-parity version of $\delta(x)$. The main difference is that the boundary condition must be expressed in terms of the bound state energy, because the potential needs renormalization.

We will see more of $\delta'(x)$ in later chapters. Higher derivatives of $\delta(x)$ are less interesting because they all produce the same spectra. This was to be expected; when the e^{-kx} function is continuous then so is its second derivative and its fourth derivative and so on—and if $f'(x)$ is continuous then so are $f^{(3,5,7\ldots)}(x)$. There are

two distinct δ function like interactions in one dimension; even this is anomalously rich, as in two or three dimensions all point interactions are delta functions, and in $d \geq 4$ there are no point interactions at all [68].

Chapter 2

Self-Adjoint Extensions

The first three sections are meant to be a hurried and heuristic introduction to some ideas from functional analysis. Formal proofs have been avoided wherever possible; they can be found in Refs. [71], VIII-X; [69], 11-14; and [75], X.

2.1 Hilbert Space

Operators are "functions" that act on functions, which is to say, they take functions to other functions. So, if we're talking about functions of a single real variable x, $f \to f^2$ is an operator, and so is $f \to \frac{df}{dx}$. Now, we want to distinguish operators that behave sensibly from operators that don't; and part of this is determining whether they act similarly on similar functions, e.g. we'd worry about an operator that sent x^2 to x^4 and $x^2 + \epsilon x^3$ (arbitrarily small ϵ) to zero. A useful approach is to treat functions as "points" in an abstract space, and to introduce a concept of distance between two functions. This is the basic idea behind Hilbert spaces.

Of course, we aren't interested in *all* functions but only in those that are relatively well-behaved. As a first guess we might want to restrict our attention to continuous functions. However, many of the properties of our space depend on its "completeness" (the existence of limits, *in the space*, to convergent sequences in the space) and it's easy to create sequences of continuous functions that have discontinuous limits, so that won't quite do.

It turns out that achieving completeness is pretty difficult. The details are highly technical and irrelevant to our purposes, so we'll just state the definitions and request the reader not to look at them too closely.
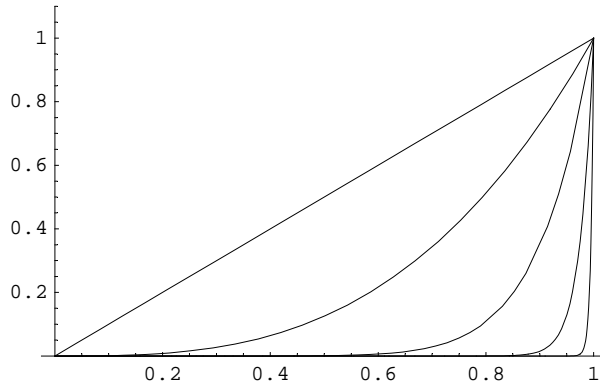
Figure 2.1: x^n on $[0, 1]$

Definition 1 *The space $L^2([a, b])$ consists of all functions $f : [a, b] \to \mathbb{C}$ (resp. $\mathbb{R}$) with the property that*

$$\int_a^b |f(x)|^2 dx < \infty$$

One could think of this as the space of all normalizable wavefunctions. (Henceforth, unless otherwise stated, all the underlying spaces are either finite intervals or $\mathbb{R}$, and all integrals are over the whole underlying space.)

Definition 2 *L^2 has an inner product (f, g) defined by*

$$(f, g) = \int \overline{f(x)} g(x) dx$$

and (correspondingly) a norm given by $\|f\| = (f, f)$, and a distance function $d(f, g) = \|f - g\|$.

*If $(f, g) = 0$ then we say f and g are **orthogonal**.*

Prop 1 (Lots of Little Results) *The space $L^2([a, b])$ is a vector space over $\mathbb{C}$, i.e. for all $f, g \in L^2, z \in \mathbb{C}, f + g, zf \in L^2$.*

The inner product (f, g) has the following properties:

1. *$(f, f) \geq 0$, equality iff $f = 0$*

2. *$(f, g) = \overline{(g, f)}$ (complex conjugation)*

3. *$(f, \lambda g) = \lambda(f, g)$*

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4. $(f, g + h) = (f, g) + (f, h)$

The norm has the following properties:

1. $\|f\| \geq 0$, *equality iff* $f = 0$

2. $|(f, g)| \leq \|f\|\|g\|$ *(Cauchy-Schwarz inequality)*

3. $\|f + g\| \leq \|f\| + \|g\|$ *(the triangle inequality)*

There are some subtleties about $f = g$. Because point discontinuities don't affect the integral, two functions that differ at isolated points are considered the same (i.e. we think of them as the same point in our function space). There's a more general form of this equivalence, called "equality almost everywhere," but that need not concern us.

The upshot is that for many (though not all) purposes, L^2 behaves like $\mathbb{R}^n$, if you think of the inner product as a dot product.

An important difference between L^2 and physical space is that L^2 is *infinite-dimensional*, i.e. you can't write all functions as a finite sum of basis functions. This is clear enough, since there are so many different types of functions. It is a remarkable property of $L^2([a, b])$ that it does have a *countably infinite* basis, because every function in it can be written as the sum of its Fourier series. As is usual with infinite series, there are issues involving convergence. Our definition of convergence is as follows:

Definition 3 *We say* $f_k \to f$ *if* $\|f - f_k\|$ *gets arbitrarily small for large k, i.e. if*

$$\int |f - f_k|^2 \to 0$$

This definition is quite different from *pointwise convergence*, which implies that the function converges to its limit at every point. (i.e. $|f(x) - f_k(x)|$ gets arbitrarily small for each x with sufficiently large k). It's possible for either form of convergence to hold without the other, as shown by the two examples below. (The first is a standard example in analysis textbooks; the second is a variant of a standard example.)

Example 1

Consider the sequence of triangles f_k (Fig 2.2) with one leg fixed at zero and the other moving towards zero so as to leave the area fixed.

$\{f_k\}$ converges pointwise to zero everywhere, but not in area, since $\|f_k - 0\| = 1$.
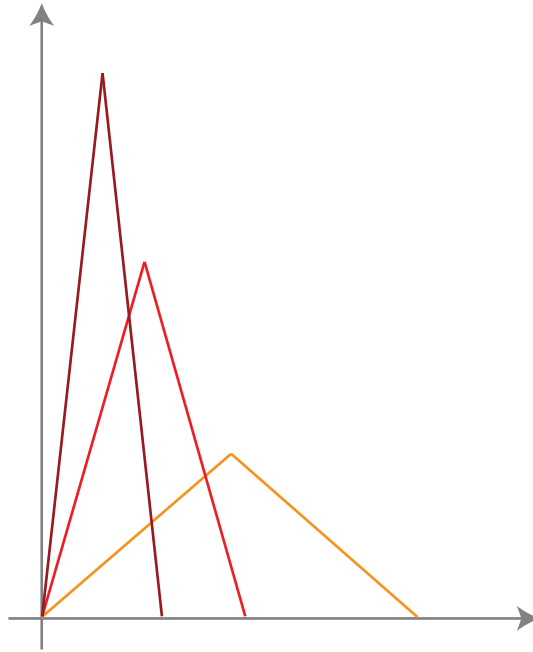
Figure 2.2: The Vanishing Triangles

Example 2

This example is slightly more involved, but the nice thing about it is that f_k does not converge pointwise *anywhere*. f_k is the unit square with increasingly thin slivers of the same depth but diminishing width cut out of it (Fig 2.3). $f_1 = \frac{1}{2}$ on $(\frac{1}{2}, 1)$, $f_2 = \frac{1}{2}$ on $(0, \frac{1}{2})$, $f_3 = \frac{1}{2}$ on $(\frac{3}{4}, 1)$, $f_4 = \frac{1}{2}$ on $(\frac{1}{2}, \frac{3}{4})$, and so on. This sequence clearly converges in norm to the whole unit square; however, it doesn't converge at any point because any x will always be in a pit for f_k further down the line, and so $|f(x) - f_k(x)| = \frac{1}{2}$ very far into the sequence, and convergence doesn't hold.

(There's a classic theorem of Dirichlet that establishes pointwise convergence of Fourier series under certain additional assumptions, but that's way off topic.)

We need two more basic definitions:

Definition 4 *A function f in a Hilbert space $\mathcal{H}$ is said to be orthogonal to a set $\mathcal{A} \subseteq \mathcal{H}$ if it is orthogonal to all functions in $\mathcal{A}$.*

Definition 5 *A set $\mathcal{A} \subseteq \mathcal{H}$ is said to be **dense** if every point in $\mathcal{H}$ is the limit of a sequence in $\mathcal{A}$. (For example, $\mathbb{Q}$ is dense in $\mathbb{R}$.)*
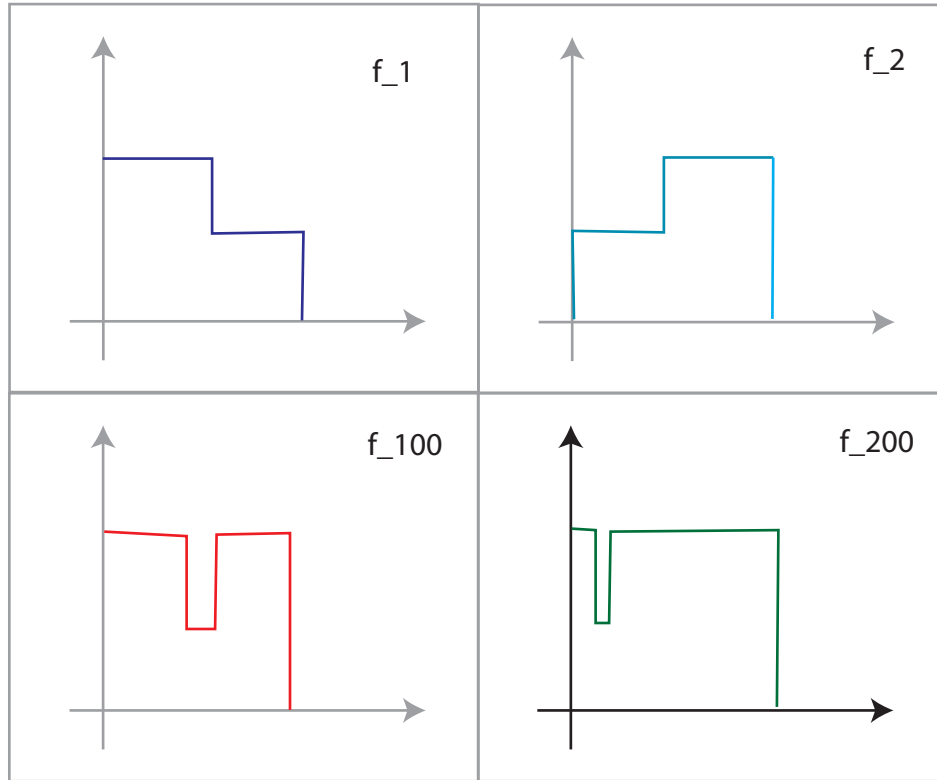
Figure 2.3: The Disappearing Gash

(So, for instance, the space consisting of all functions

$$f(x) = \sum_{n=1}^{k} a_n e^{inx} \tag{2.1}$$

is dense in $L^2([-\pi, \pi])$ by virtue of the convergence of Fourier series.)

The following proposition will be useful later.

Prop 2 *If $\mathcal{A}$ is dense in $\mathcal{H}$ and f is orthogonal to $\mathcal{A}$, then $f = 0$.*

Proof. Suppose $f \perp \mathcal{A}, f \neq 0$. Pick a sequence $f_k \in \mathcal{A}$ that converges to f.

$$(f, f) = (f, f) - (f, f_k) = (f, f - f_k)$$

since $(f, f_k) = 0$ by hypothesis. Now we can use the Cauchy-Schwarz inequality:

$$\|f\|^2 = |(f, f)| = |(f, f - f_k)| \leq \|f\| \|f - f_k\|$$

and since $f \neq 0$ we get

$$\|f\| \le \|f - f_k\|$$

which is impossible because $f \ne 0$ but $f - f_k$ gets arbitrarily small.

And we'll close this section with a major result in real analysis that will be useful to us:

Theorem 1 (Stone-Weierstrass Approximation Theorem) *$C_0^\infty(I)$, the set of all bounded, infinitely differentiable functions on I, is dense in $L^2(I)$, where $I \subseteq \mathbb{R}$ is a finite or infinite interval.*

This means that every function can be approximated arbitrarily well by a very well-behaved function. For finite intervals, this result follows since all finite Fourier series sums are members of C_0^∞. In practice we normally need just $C^2[\supseteq C_0^\infty]$ with maybe a few pointwise conditions (say, "everything and its derivative must vanish at the origin") and the issue of density is rarely relevant. We generally assume that all sets we are working with are dense.

2.2 Linear Operators and their Domains

A linear operator $L : D \subseteq H \to H$ acts linearly on the *function space*, so $L(af+bg) = aLf+bLg$ (and $L(0) = 0$). $\frac{d^n}{dx^n}$ is a linear operator, as is multiplication by a constant or a function in the space. For many purposes linear operators are just infinite matrices, and the familiar equation

$$H\psi = E\psi$$

is called an eigenvalue equation because of that analogy. However, the analogy sometimes breaks down, and a good example of how this happens is the issue of domains. For example, the function $f(x) = x^{-0.1}$ is a respectable member of $L^2([0, 1])$, but its derivative is not. What can be said about domains generally is stated in the following proposition:

Prop 3 *The domain of an operator A will be denoted as $D(A)$.*

1. $D(\lambda A) = D(A)$, $\lambda \in \mathbb{C}$

2. $D(A + B) = D(A) \cap D(B)$

3. $D(AB) = D(A) \cap R(B)$, where $R(B)$ is the range of B

Definition 6 *An operator A is said to be bounded if there's a number λ such that $\|Af\| \le \lambda\|f\|$ for all functions in $D(A)$.*

The importance of operator domains is suggested by the following theorem:

Theorem 2 (Hellinger-Toeplitz) *A Hermitian operator defined everywhere is bounded.*

As luck would have it, Schrödinger operators are virtually never bounded.

Hermitian Operators and Adjoints

A Hermitian operator H has the property that, for all $f, g \in D(H), (f, Hg) = (Hf, g)$. Hermitian operators always have real eigenvalues and orthogonal eigenfunctions. However, the following commonly assumed properties are **not** generally true of Hermitian operators:

1. They always generate unitary time evolution.

2. They always have well-defined adjoints.

3. Their adjoints are Hermitian.

4. They always have a complete set of eigenfunctions.

The rest of this section will be dedicated to discussing these points. First, the issue of adjoints. The action of an adjoint $H^\dagger$ is defined by $(Hf, g) = (f, H^\dagger g)$, so of course $D(H^\dagger) \supseteq D(H)$, but the adjoint might be well-defined outside of $D(H)$. Here's a simple example involving the 1-D infinite well (taken from Ref. [77]):

The Frailty of Hermeticity

This example, from [77], illustrates what can happen if we don't think about operator domains. The Hamiltonian for this system is

$$H = -\frac{\hbar}{2m}\frac{d^2}{dx^2}, |x| < L/2$$

Now consider the (not normalized) wavefunction

$$\psi = -\sqrt{\frac{30}{L^5}}\left[x^2 - \frac{L^2}{4}\right]$$

Evidently

$$H\psi = \frac{\hbar^2}{m}\sqrt{\frac{30}{L^5}}, \langle E \rangle = (\psi, H\psi) = \frac{5\hbar^2}{mL^2}$$

This is also what we get if we write ψ in terms of the infinite well eigenvalues and calculate

$$\langle E \rangle = \sum_n |(\psi, \phi_n)|^2 E_n$$

The paradox is that these two methods give wildly inconsistent results for E^2.

$$\sum_n |(\psi, \phi_n)|^2 E_n^2 = \frac{30\hbar^4}{m^2 L^4}$$

but

$$(\psi, H^2\psi) = (\psi, 0) = 0$$

since $H\psi$ is a constant. The latter result is clearly wrong (e.g. it implies an imaginary ΔE), but this is a little surprising, because

$$
\begin{aligned}
\langle E^2 \rangle_\psi &= \sum_n |(\psi, \phi_n)|^2 E_n^2 \\
&= \sum_n E_n(\phi_n, \psi)(\psi, \phi_n)E_n \\
&= \sum_n (E_n\phi_n, \psi)(\psi, E_n\phi_n) \\
&= \sum_n (H\phi_n, \psi)(\psi, H\phi_n) \\
&= \sum_n (\phi_n, H\psi)(H\psi, \phi_n) \\
&= (H\psi, H\psi) \\
&= (\psi, H^\dagger H\psi) \neq (\psi, H^2\psi)
\end{aligned}
$$

The answer is that $H\psi$ is in the domain of $H^\dagger$ (since $(H\phi, H\psi)$ is perfectly well defined) but not in the domain of H, since it doesn't vanish at the ends of the square well.

The domain of the adjoint is every ϕ such that $(H\psi, \phi)$ makes sense for all $\psi \in D(H)$.

All of this assumes that the action of $H^\dagger$ is uniquely defined. Let's see if that works. Suppose we have an operator A, with two adjoints B_1 and B_2. Given $x \in D(A), y \in D(B_1) \cap D(B_2)$, it follows that

$$(x, (B_1 - B_2)y) = (x, B_1 y) - (x, B_2 y) = (Ax, y) - (Ax, y) = 0.$$

This implies that $(B_1 - B_2)y \perp D(A)$. In general it's impossible to improve on this, but if D(A) is dense, it follows from prop 1.1.2 that $(B_1 - B_2)y = 0$, and since this is true for all y we have uniqueness of the adjoint.

For the rest of this chapter we assume that all our operators are densely defined.

Definition 7 *A self-adjoint operator is a Hermitian operator that has the same domain as its adjoint. (Equivalently: a Hermitian operator with a Hermitian adjoint.)*

It turns out that only self-adjoint operators generate unitary time evolution; therefore it's important for our Hamiltonians to be self-adjoint. Since $D(H) \subseteq D(H^\dagger)$ generally, one must extend a non-self-adjoint operator to make it self-adjoint. From the definition of $D(H^\dagger)$, as $D(H)$ grows each $f \in D(H^\dagger)$ needs to have well-defined inner products with more vectors—it needs to make more sense, so to speak—so extending the operator domain involves *constraining* the adjoint domain... and, indeed, failures of self-adjointness manifest themselves in physics mostly through ill-defined boundary conditions.

Our next goal is to see how to construct self-adjoint extensions of a Hamiltonian.

2.3   Self-Adjoint Extensions

I recognize that this section is unpleasantly technical, but the central result sounds pretty mysterious without justification. The idea is that $H^\dagger$, being potentially non-Hermitian, might have complex eigenvalues, and you can restrict it to a Hermitian operator by allowing only some combinations of the corresponding eigenvectors in the domain. (The freedom you have in choosing this is normally indicative of additional physics, which must be imposed by means of a boundary condition.) The key objects in this process are

Definition 8 *The **positive (resp. negative) deficiency subspace**, $N_{\pm}$, of H is the eigenspace of $H^{\dagger}$ corresponding to eigenvalues $\pm i$. The **deficiency indices** $n_{\pm}$ are the dimensions of $N_{\pm}$.*

It turns out that any $\chi \in D(H^{\dagger})$ can be written uniquely as follows:

$$\chi = a\phi + b\Psi_{+} + c\Psi_{-} \tag{2.2}$$

where

$$\phi \in D(H), \Psi_{\pm} \in N_{\pm}$$

In other words, $D(H)$, N_{+}, and N_{-} are linearly independent. Be warned, however, that the three spaces are **not** mutually orthogonal, since nothing is orthogonal to $D(H)$. If $n_{+} = n_{-}$, we can define an "extension" H_{θ} to have the same action as $H^{\dagger}$ and be defined on $D(H_{\theta}) = \{\phi + A(\Psi_{+} - U_{\theta}\Psi_{+}) : \phi \in D(H), \Psi_{+} \in N_{+}\}$, where $\Psi_{\pm}$ are vectors, A is a matrix, $U_{\theta} : N_{+} \to N_{-}$ is a unitary (strictly speaking, "norm-preserving") operator that characterizes the particular extension chosen. By definition of $N_{\pm}$,

$$H_{\theta}\chi = H\phi + i\sum_{k=1}^{n_{+}} \lambda_{k}(\Psi_{+,k} + U_{\theta,kj}\Psi_{+,j}) \tag{2.3}$$

for all $\chi \in D(H_{\theta})$. For deficiency indices $(1,1)$, this is a subspace of $D(H^{\dagger})$ with b/c fixed at a phase angle. A schematic and unfaithful representation of what's going on is given in the figure below.[1]

(We will typically use the characterization:

$$D(H_{\theta}) = \{\phi + B(\Psi_{+} + V_{\theta}\Psi_{-})\} \tag{2.4}$$

(V_{θ} unitary) which is equivalent because all vectors in N_{-} are equivalent to Ψ_{-} under a unitary transformation.)

It's straightforward to show that H_{θ} is symmetric. The importance of these extensions is that they are self-adjoint because of the following theorem:

Theorem 3 *If $n_{+} = n_{-} = 0$, H is self-adjoint or has a unique self-adjoint extension.*

---

[1] Among other things that are wrong with the picture, the subspaces are not supposed to be orthogonal, the angle is supposed to be a phase between vectors of equal magnitude, and $D(H)$ is infinite dimensional.
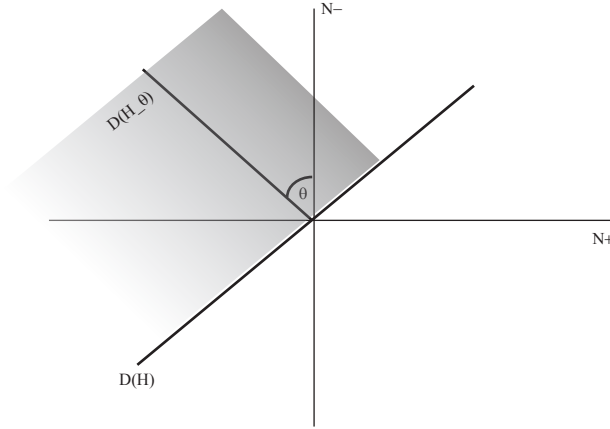
Figure 2.4: "Artist's Impression" of $D(H^\dagger)$

Our deficiency indices are in fact zero, by the following logic. We know that $H_\theta^\dagger$ is a restriction of $H^\dagger$ because H_θ extends H. Suppose $n_+ \neq 0$, then that's got to be because some members of the positive deficiency subspace are still in $D(H_\theta^\dagger)$. Let one of them be ζ. Now,

$$\zeta + U_\theta \zeta \in D(H_\theta) \subseteq D(H_\theta^\dagger)$$

Either $U_\theta \zeta \in D(H_\theta)$ or $U_\theta \zeta \in N_-$. Both cases lead to an immediate contradiction with (2.9), since you can write $\zeta + U_\theta \zeta$ as an element of $D(H_\theta)$ and as a linear combination of terms in $N_\pm$, which contradicts linear independence. And once we've established that the deficiency subspaces are trivial, it follows by (2.9) that $D(H_\theta^\dagger) = D(H_\theta)$ so H is self-adjoint.

For completeness, note that the converse of our result is also true. (We will not prove this.)

Theorem 4 *If $n_+ \neq n_-$ then H has no self-adjoint extensions.*

These results are very helpful, because they reduce the difficult question, "Where does the adjoint make sense?" to the relatively simple one of whether the equation $H\phi = \pm i\phi$ has normalizable solutions.

The following list suggests how tricky self-adjointness can be:

- The free-particle Hamiltonian on all of $\mathbb{R}$ is self-adjoint.

- The free Hamiltonian on $[-L, L]$ has deficiency indices (2,2). One of its self-adjoint extensions corresponds to the particle in a box.

- The Hamiltonian with Coulomb potential in three dimensions is self-adjoint, but the radial equation is not.

- The Hamiltonian with a/r^2 potential is self-adjoint for $a > 3/4$ but has deficiency indices (1,1) below that.

- Hamiltonians with $-x^n$ potentials in one dimension (bottomless hills) are self-adjoint for $0 < n \leq 2$ but need extensions for $n > 2$.

- The momentum operator on $\mathbb{R}^+$ has deficiency indices (0,1) and can't be made self-adjoint.

Generally, Hamiltonians of the usual form $-\nabla^2 + V$, where V is reasonably well-behaved, do have self-adjoint extensions. This is a consequence of the following theorem:

Theorem 5 *If H commutes with complex conjugation, i.e. if $\overline{H\psi} \equiv H\overline{\psi}$ then H has equal deficiency indices.*

(For a proof, see [75].) Note that p does not commute with complex conjugation, but is often self-adjoint in any case.

2.4 The Physics of Self-Adjoint Extensions

There is generally some physical reason behind the failure of self-adjointness, most commonly an unspecified boundary condition. Our strategy will be as follows:

1. Find as small a domain as possible for the operator. How small we can make this is limited by the requirement that H be dense. However, we can normally restrict our original domain to C_0^2 with the pointwise constraints that all functions and their derivatives should vanish at boundaries, singularities, and other dubious points.

2. This leaves the adjoint domain as essentially L^2, so we don't need to worry about whether a particular normalizable solution is in the adjoint domain.

3. Calculate the deficiency indices and determine the corresponding eigenspaces.

4. Use $\Psi_\pm$ to determine the boundary conditions.

For all the examples below, we've assumed that the original operator is Hermitian, the domain of definition is C^2 vanishing at the boundaries (except as otherwise specified), and that the adjoint domain is sufficiently large. The examples considered below are all standard in the literature. A detailed treatment of how one finds the adjoint domain is given in Chapter 8 for the one-dimensional free particle.

First, we consider a case where the operator is **essentially self-adjoint**, i.e. where its deficiency indices are (0,0) but it still needs extension.

Momentum for Free Particle on the Real Line

Let our original domain be C_0^∞, which we know to be dense, and the operator be $i\frac{d}{dx}$, which we know to be Hermitian. Solving for deficiency indices

$$i\frac{d\psi}{dx} = \pm i\psi$$

we get $\Psi_\pm = e^{\pm x}$. Neither of these is normalizable; therefore there are no eigenfunctions for $\pm i$ in L^2 and our deficiency indices are (0,0). However, the adjoint domain is considerably larger than the original domain and includes just about anything in L^2, since the result

$$\int \overline{\psi}\frac{d\phi}{dx}dx = -\int \frac{d\overline{\psi}}{dx}\phi dx$$

certainly does not require $\psi \in H^\dagger$ to be infinitely differentiable. There's no new physics involved in finding a self-adjoint domain, however, so the distinction is not important to physicists. For our purposes an essentially self-adjoint operator is self-adjoint.

Free Particle on $x > 0$

This problem is underspecified; to see why, consider the corresponding problem with waves on a string. Since we want to conserve amplitudes *on our domain*, the wave must be reflected at the origin, but the reflector could be either fixed (a clamped end) or movable (a ring sliding on a rod). The reflection coefficient is one both ways, but the phase shifts are different, so the physics is *not* completely specified unless you know the exact boundary condition.

Now let's look at the quantum mechanical situation. Solving for imaginary eigen-values:

$$-\psi''(x) = i\psi(x) \Rightarrow \Psi_+ = Ae^{(1-i)x/\sqrt{2}} + Be^{-(1-i)x/\sqrt{2}} \tag{2.5}$$

The second solution, which decays exponentially, is normalizable; similarly we have a normalizable solution

$$\Psi_- = e^{-(1+i)x/\sqrt{2}}$$

for the negative case. A single function defines a one-dimensional subspace, so our deficiency indices are (1,1) and our extensions will be parameterized by $U(1)$. We would like to add the function $\Psi_+ + U_\theta \Psi_+$ to our domain. As we noted in the last section, $U_\theta \Psi_+$ is a normalized vector in N_-; since N_- is one dimensional the only such vectors are of the form $e^{-i\theta}\Psi_-$. So we add the function $\Psi_+ + e^{-i\theta}\Psi_-$ to our domain. Since all the functions in our original domain—and their derivatives—vanish at the origin, any behavior at the origin is determined by what the function we added does there.

$$\Psi_+ + e^{-i\theta}\Psi_- = e^{-x/\sqrt{2}}(e^{ix/\sqrt{2}} + e^{-ix/\sqrt{2}}e^{-i\theta})$$

This can be written a little more simply as

$$\Psi_+ + e^{-i\theta}\Psi_- = 2e^{-x/\sqrt{2}-i\theta/2}\cos\left(\frac{x}{\sqrt{2}} + \frac{\theta}{2}\right). \tag{2.6}$$

So θ is the phase at the origin, in agreement with our classical analysis. The solution corresponding to an infinite step is $\theta = \pi$. For our purposes it's useful to have a single condition relating $\psi(0)$ and $\psi'(0)$—the two quantities determined by the deficiency subspaces—to θ, and we can get this by calculating $\psi'(0)$ and dividing, to get

$$\frac{\psi'(0)}{\psi(0)} = -\frac{1}{\sqrt{2}}(1 + \tan(\theta/2)). \tag{2.7}$$

Since it doesn't matter very much *how* we parameterize our self-adjoint extensions, we can define the rhs of this equation to be α, to get the condition

$$\psi(0) + \alpha\psi'(0) = 0 \tag{2.8}$$

which must hold for all functions in the operator's domain. It's clear that for scattering solutions the boundary condition (2.8) determines the phase shift. A more

interesting feature of this potential, pointed out by Faraut et al [77], is that you can have bound states of the form

$$E = -\frac{1}{\alpha^2}, \psi = \sqrt{\frac{2}{|\alpha|}} e^{-x/|\alpha|} \tag{2.9}$$

as with the delta function. Here, again, one needs to remember that there could be all sorts of things at the origin that affect the behavior of the particle, including an attractive delta function. The only constraint is unitary time evolution *in the region*, which forbids situations—such as a porous barrier—that would allow probability to leak out of the system at the origin. Let's define $r = A/B$ for a wave $\psi = Ae^{-ikx} + Be^{ikx}$, and the reflection amplitude $R = |r|^2$. Then imposing (2.8) we get

$$r = -\frac{1 + i\alpha k}{1 - i\alpha k} \Rightarrow R = 1 \tag{2.10}$$

since α is real. Allowing α to be complex would let us deal with a wider range of situations, but our solutions would be *incomplete* because the time evolution of a particle that went through the origin would be entirely unspecified.

Free Particle in an Unspecified Box

Both solutions in (2.5) are normalizable in this case, leading to deficiency indices (2,2) which correspond (naively) to multiple boundary conditions and something of a mess. The details are in [77], and are best left there. The thing is, we don't know it's a box until we've specified the boundary conditions (and therefore the self-adjoint extension). It's clear from the previous example that there are at least two sets of boundary conditions, since either end of the "box" could be a fixed end, ($\psi(a) = 0$) a loose end ($\psi'(a) = 0$), or anything in between. But there's more to the story. Suppose we require that all wavefunctions have some parity (whether even or odd) about the middle of the box. Now the purpose of self-adjoint extensions is to come up with a complete orthogonal set of eigenfunctions, and even functions are orthogonal to odd functions no matter what, so the boundary conditions on even and odd functions are entirely independent. These two families are different, since most members of the first have boundary conditions without parity, and most members of the second have two distinct sets of boundary conditions at the same wall. In fact these are just two two-parameter subfamilies of the $U(2)$ family that have fairly obvious physical significance. A more detailed treatment of the spectra can be found in [77].

Delta Functions

The method of self-adjoint extensions is particularly important for studying delta functions because it is mathematically rigorous, and avoids the infinities and potentially dodgy reasoning of other renormalization schemes. The dread symbol $\delta(x)$ is avoided altogether; we will deal only with the extensions of free-particle Hamiltonians on $\mathbb{R}^n - \{0\}$. The full 1D case is relegated to Chapter 8; here we neglect some subtleties and identify the 1D delta function with the extensions on the half-line. If you pick one of the extensions with bound states, you can compare the bound state energy (2.9)

$$E = -\frac{1}{\alpha^2}$$

with our previous expression for the strength of the delta function

$$E = -\frac{g^2}{4}$$

to get a relation between the self-adjoint extension chosen and the strength of the delta function. It's not strictly correct to say that you can *solve* delta function potentials by the method of self-adjoint extensions; what you can do is show that our delta function Hamiltonian corresponds to a self-adjoint—i.e. physically sensible—operator. This might seem pedantic in the one-dimensional case, but it is reassuring in two dimensions, because it isn't *a priori* obvious that renormalization gives us a sensible theory.

The two dimensional radial Hamiltonian, with $m = 0$, is

$$\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}$$

so the deficiency index equations are

$$\frac{d^2\psi}{dr^2} + \frac{1}{r}\frac{d\psi}{dr} \mp i\psi = 0$$

These are modified Bessel equations, and have the solutions $I_0(\sqrt{\mp i}r)$ and $K_0(\sqrt{\mp i}r)$, of which only the K's are normalizable. Therefore our deficiency indices are (1,1) and we have a family of self-adjoint extensions characterized by the functions

$$\Psi = K_0(\sqrt{i}r) + e^{i\theta}K_0(\sqrt{-i}r)$$

It's somewhat harder to get a boundary condition out of this, since K_0 blows up at the origin. Remembering, however, that

$$K_0(x) \approx \log(x/2) + \gamma, \, K_0'(x) \approx 1/x$$

for small arguments, we can turn this expression into

$$\Psi = \log r + \gamma + \frac{\pi}{4} \tan \frac{\theta}{2} + \gamma \tag{2.11}$$

(γ being the Euler-Mascheroni constant.) And we can condense all the random stuff, as before, into a new parameter B, which gives us that

$$\Psi = \log(Br) \tag{2.12}$$

around the origin. This expression will be massaged further, but we can draw an important consequence immediately. Recall that the bound state wavefunction for this potential is $K_0(k_b r)$. Near the origin, it's going to have behave like $\log(Br)$ and that's only possible if $\frac{1}{2} k_b e^\gamma = B$. Therefore, our self-adjoint extension parameter picks a scale for this problem. Note that scale invariance can be preserved by setting $\theta = \pi$, in which case the log terms cancel out; this corresponds to a trivial delta function.

For scattering calculations it is useful to express (2.12) as a boundary condition on $\phi \in H_B$. It's easy to see that the condition

$$\lim_{r \to 0} \left[\phi - r \frac{d\phi}{dr} (\log k_b r + \gamma - \log 2) \right] = 0 \tag{2.13}$$

follows from the form of (2.12). Now let's solve the scattering problem using (2.13). The solution for the free particle Schrödinger equation is

$$A J_0(kr) + B N_0(kr)$$

and the s-wave phase shift is given by

$$\tan \delta_0 = -B/A.$$

Plugging the asymptotic form of our wavefunction into (2.13) and rearranging we find that

$$A - \frac{2B}{\pi} \log kr - \left[A \frac{(kr)^2}{2} - \frac{2B}{\pi} \right] \log k_b r \to 0 \tag{2.14}$$

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and if we drop the second order term this simplifies to

$$A\pi = 2B \log(k_b/k) \tag{2.15}$$

and our phase shift agrees with what we got previously. For $m > 0$ the free particle Hamiltonian is self-adjoint, as we'll see in the next chapter, so a delta function at the origin can have no impact. The centrifugal barrier shields the particle from seeing the delta function at all. For the delta function it's clear enough why this happens: as you take the cutoff to zero, the repulsive $1/r^2$ centrifugal potential—which integrates to ∞ around the origin—drowns out the delta function.

The 3D delta function, from the point of view of self-adjoint extensions, is the same as the particle on a half-line in the $l = 0$ channel, since it has the same differential equation and the same boundary conditions. (The solution using regularization methods is $\psi = e^{-kr}/r$, or $u(r) = e^{-kr}$.) The s-wave phase shift should therefore be the same as in the 1D case, and it is according to the regularization scheme of Chapter 1, so once again we're consistent.

As we will see in the next chapter, all delta functions are self-adjoint in the $l > 0$ channels.

Fall to the Center

Consider the classical two-body problem with $V(r) = \rho/r^2$. This potential just modifies the centrifugal barrier term, and when it is repulsive or weaker than the barrier term the problem is well-behaved. However, if it is strong enough to overcome the centrifugal barrier, the particle falls to the origin in a finite time, and its behavior after that point is not well-defined. The general equation of motion is (Thornton and Marion [82], 8.20)

$$\frac{d^2u}{d\theta^2} + u = -\frac{\mu}{l^2u^2}F(1/u) \tag{2.16}$$

where $u = 1/r$. As Thornton shows (Example 8.1), an inverse square potential (equivalently an inverse cube force) leads to solutions of the form

$$r = Ae^{-k\theta} + Be^{k\theta} \tag{2.17}$$

for some constant k. Evidently, there are no periodic combinations of these solutions, so the particle must spiral in or out. The solution that spirals outwards is not interesting; the important thing about the inward spiral is that as the particle approaches

the origin, its velocity must be infinite to conserve angular momentum. We can see this directly from Thornton's expression for the radial velocity:

$$\dot{r} = \sqrt{E - U - \frac{l^2}{r^2}}. \tag{2.18}$$

In our case, this is

$$\dot{r} = \sqrt{E + \frac{\lambda_{eff}}{r^2}}.$$

As the particle approaches the origin this expression blows up. If we separate the equation and integrate, we see that

$$t_f - t_i = \int_0^R \frac{dr}{\sqrt{E + \frac{\lambda_{eff}}{r^2}}} \propto \sqrt{1 + R^2} \tag{2.19}$$

so any particle reaches the origin with an infinite velocity in a finite time. This phenomenon is known as fall to the center. The equations of motion cease to be well-defined when the particle reaches the origin, and therefore our solution doesn't work for all time. Solutions of this type are called **classically incomplete**. On quantizing the theory this turns into a failure of unitary time evolution, and therefore of self-adjointness. However, as Ref. [19] points out, one could make the classical theory well-defined for all time by requiring that the particle be reflected whenever it gets to the origin—i.e. running our time evolution forwards and backwards endlessly. This corresponds, in the quantum problem, to picking a self-adjoint extension.

Note that there's a slight subtlety here. Mildly singular quantum mechanical problems are regular even in the $l = 0$ channel, whereas classically they collide with the origin after a finite time. In general, the "centrifugal potential" (the l term) in quantum mechanics works quite differently from its classical counterpart; this is why it's misleading to think of the critical value of the $1/r^2$ potential (see Chapter 3) as the point at which the particle overcomes the centrifugal barrier.

Because of the importance of singular potentials, I will leave the quantum mechanical treatment to a later chapter, noting only that the deficiency indices are (1,1) as we'd expect (one boundary condition at the origin).

Fall to Infinity

Consider the classical 1D Hamiltonian

$$H = \frac{p^2}{2} - q^4. \tag{2.20}$$

By Hamilton's equations,

$$\dot{q} = \frac{\partial H}{\partial p} = 2p.$$

Since the total energy $E = H$ is conserved, we can rewrite this as the relation

$$E = \dot{q}^2 - q^4 \tag{2.21}$$

which can be rearranged to give

$$\frac{dq}{dt} = \sqrt{E + q^4}. \tag{2.22}$$

Solving this equation for t, we find that

$$t_f - t_i = \int_{q_i}^{q_f} \frac{dq}{\sqrt{E + q^4}}. \tag{2.23}$$

For a particle with $E > 0$ this integral converges from $-\infty$ to ∞, so any particle reaches infinity in a bounded time, and the solution is not complete. In fact, we need to add two boundary conditions—reflection at ∞ and at $-\infty$—to make the solution complete.

One might expect the same result to hold for the upside down oscillator:

$$H = p^2 - q^2. \tag{2.24}$$

However, the integral in this case,

$$t_f - t_i = \int_{q_i}^{q_f} \frac{dq}{\sqrt{E + q^2}} = \sinh^{-1} q_f/\sqrt{E} - \sinh^{-1} q_i/\sqrt{E} \tag{2.25}$$

does not converge, and we have a complete classical solution.

As you might expect, these potentials have deficiency indices (2,2) and (0,0) respectively. In general, **power-law** potentials are classically complete if and only if they are quantum mechanically complete. However, this is not generally true of quantum mechanical potentials. There are exceptions to this rule both ways, given in [75]. An interesting one is the following potential, a bottomless hill with increasingly tall and narrow spikes at integer values of x:

$$V(x) = -x^4 + g(x)$$

$$g(x) = |N|, |x - N| < 1/N.$$

This is classically complete, since a particle of any energy eventually runs into a sufficiently tall barrier. However, the quantum mechanical problem is still pathological, because a particle can tunnel through all the barriers. Similarly, the delta function is classically well-behaved since it has zero range and nothing scatters off it; however, wavefunctions are spread-out so it has a nontrivial quantum mechanical scattering range, which needs to be specified by picking a self-adjoint extension.

A useful general result due to Weyl is the following:

Theorem 6 (Weyl) *A Hamiltonian of the form*

$$H = -\frac{d^2}{dx^2} + V(x)$$

is essentially self-adjoint on $(0, \infty)$ iff the equation $H\psi = i\psi$ has at least one solution that fails to be square integrable near zero, and at least one solution (possibly the same one) that fails to be square integrable near infinity.

The forward direction is trivial from the definitions; the reverse is proved in Reed and Simon (X.7). This result makes life a little simpler in some cases because we can treat short-range and long-range singularities as independent. If there's only one solution at 0 (∞), the potential is said to be **limit point** at 0 (∞); otherwise it's said to be **limit circle**. The terms are basically conventional.

2.5 Boundedness and the Friedrichs Extension

An **upper semi-bounded** operator A has the property that for functions in its domain, $(\phi, A\phi) \geq c\|\phi\|$, where $c \in \mathbb{R}$ is a fixed number. Most operators that we deal with in physics have this property; it is basically the same thing as requiring that the system have a ground state. Most operators are not bounded above; for instance the harmonic oscillator has arbitrarily high bound states, and so does any operator with a scattering sector. On the other hand, we have seen two instances of operators that are bounded neither above nor below—attractive singular potentials and upside down

polynomials. These operators are fundamentally unbounded, in that the Hamiltonian itself has no lower bound. On the other hand, in cases like the 2D delta function, it is only the adjoint that is unbounded from below, and picking a self-adjoint extension bounds the operator.

Most of quantum mechanics is done with the assumption of semiboundedness, however, and the particular extension that is typically picked out is the **Friedrichs extension**. A rough and ready way to obtain the Friedrichs extension on a domain D is by imposing the boundary condition $\psi(x) = 0$ on all $x \in \partial D$. This is the correct boundary condition for most cases that we are interested in: the particle in a box, the 3D Coulomb problem, and so on. But sometimes, as with $\delta(x)$, there might be a specific motivation for choosing a non-Friedrichs extension, and sometimes— e.g. one-dimensional quantum mechanics, discussed later—the Friedrichs extension is blatantly unphysical, and leads to strange spectra.

There are two subtleties with the Friedrichs extension that show up in later chapters. The first has to do with the free-particle Hamiltonian in two dimensions, for which neither solution vanishes at the origin, and the second, with the weakly attractive $1/r^2$ problem in one dimension, for which both solutions vanish at the origin. In the second case, if one substitutes $v(r) = u(r)/\sqrt{r}$, one gets a new differential equation for which only one of the solutions vanishes. The Friedrichs extension of the substituted differential equation is also the Friedrichs extension of the original differential equation. However, in general, even when the Friedrichs extension doesn't set all boundary conditions to zero, it is the extension that corresponds to throwing out the more singular solution.

Friedrichs extensions are defined only for semibounded Hamiltonians; if the original Hamiltonian is unbounded from below, then so are all self-adjoint extensions, and there is no Friedrichs extension.

2.6   Rigged Hilbert Space Formalism

(The introductory material follows Refs. [79] and [83].) To understand the need[2] for a rigged Hilbert space, consider an operator like x. This is a self-adjoint operator, and we are used to saying that a self-adjoint operator has a complete set of eigenvalues, but x in fact has *no* eigenvalues, since the formal solutions $\delta(x - \lambda)$ are not in the

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[2]Or what some consider the need.

Hilbert space. Similarly, a Schrödinger operator with a continuous spectrum, such as $H = -\nabla^2$, has no eigenvalues in the Hilbert space, and the square well has only a few. The rest of the spectrum is normally accounted for by means of projection operators and the spectral theorem ([71]). The rigged Hilbert space is an expanded Hilbert space that includes several non-normalizable solutions.

The rigged space is constructed as follows. We first construct a **nuclear** space Ω, which is a subset of the Hilbert space. Recall that the Hilbert space contains all convergent sums of Fourier series. Now Ω includes only those sums that have the property that for all positive m,

$$\sum_n |c_n|^2 n^m < \infty.$$

A continuous version of this might be

$$\int_0^\infty |\psi|^2 x^m dx < \infty$$

and in fact de la Madrid [83] derives the nuclear space from the requirement that wavefunctions in it should be in the domain of the operators x^m and p^m for all m.

The space we are really interested in is Ω^D, the dual space of Ω, or the space of all linear functionals $f : \Omega \to \mathbb{C}$. The correct way to think of a dual space is as a one-sided inner product: Ω^D consists of all the bras that are well-behaved with respect to the kets in Ω. The stronger the restrictions on the kets, the more bras we are likely to find that work, so one would expect $\Omega^D \supseteq H \supseteq \Omega$. H is special in that $H = H^D$.

In fact, because wavefunctions in Ω are required to vanish so much more rapidly than in H, the continuous spectrum is normally in Ω^D. This is the basis of the generalized spectral theorem, which is the key to interest in rigged Hilbert spaces:

Theorem 7 (Generalized Spectral Theorem) *A self-adjoint operator has a complete set of eigenfunctions in the rigged Hilbert space.*

The theory just outlined raises a few questions about our understanding of self-adjoint extensions. For instance, if, as de la Madrid claims, the nuclear space Ω is the *physical* sector of the Hilbert space, it follows that self-adjoint extensions introduce new physics only if they have some impact on members of Ω. But this implies that Ω should never be a subset of a non-self-adjoint original domain D_H. If this is true, then

(since self-adjoint extensions affect a domain by throwing out several states in the adjoint domain) there must be vectors in Ω that didn't make it to D_{H_θ}. Therefore, Ω consists of more than just physically meaningful states, since functions outside D_{H_θ} are physically irrelevant.

Besides, this raises the question of what happens if the momentum operator fails to be self-adjoint: can one still define a rigged Hilbert space from the physicality requirement? We have not had the time to address these questions, but they seem relevant if the nuclear space is to be interpreted in physical terms.

Chapter 3

Singular Potentials

Singular potentials are poorly behaved in classical mechanics too, as we saw in the previous chapter, but at least one has a fairly good physical idea of what is going on there. In quantum mechanics, this is somewhat harder to obtain. In some ways the cleanest way to look at singular potentials is through the formal apparatus of Chapter 2, so that's what we'll do first. We focus on the inverse square potential, not because it's the most typical case (it isn't), but because it is exactly solvable.

3.1 The Inverse Square Potential

The 3D radial Schrödinger equation looks like this:

$$-\frac{d^2u}{dr^2} + \frac{\lambda}{r^2}u + \frac{l(l+1)}{r^2}u = k^2u \tag{3.1}$$

in terms of $u(r) = \psi/r$. This substitution is convenient because it makes the 3D problem look like a 1D problem. It's especially convenient that the space of functions $u : (0, \infty) \to \mathbb{C}$ corresponding to $\psi \in L^2(\mathbb{R}^3)$ is almost exactly $L^2(0, \infty)$ because the $1/r$'s cancel the spherical Jacobian. The additional constraint [79] is that usually we enforce $u(0) = 0$ to have the wavefunction be regular at the origin. This constraint leads to some of the important differences between 3D and 1D quantum mechanics, e.g. the fact that 3D square wells do not always have bound states; however, we shall sometimes have reason to relax it.

With an inverse square potential, the "one-dimensional" Hamiltonian becomes

$$H = -\frac{d^2}{dr^2} + \frac{\lambda}{r^2} + \frac{l(l+1)}{r^2} = -\frac{d^2}{dr^2} + \frac{\lambda_{eff}}{r^2} \tag{3.2}$$

Since—as investigators of EFTs—we are most interested in low-energy aspects of this problem we shall normally have $l = 0$, and for simplicity we shall generally write λ_{eff} as λ. The eigenfunctions of (3.2) can be expressed in terms of Bessel functions as follows:

$$\sqrt{r} Z_{\zeta+1/2}(kr)$$

where

$$\zeta(\zeta + 1) = \lambda. \tag{3.3}$$

Now we'd like to use Weyl's result to check for self-adjointness. The eigenfunctions corresponding to i are $\sqrt{r} I_{\zeta+1/2}(\sqrt{i}r)$ and $\sqrt{r} K_{\zeta+1/2}(\sqrt{i}r)$. As $r \to \infty$, we can see from the asymptotic expansions

$$I_\nu(z) \sim \frac{e^z}{\sqrt{z}} \Rightarrow |I_\nu(x + iy)| \sim \frac{e^x}{\sqrt{x}}$$

$$K_\nu(z) \sim \frac{e^{-z}}{\sqrt{z}} \Rightarrow |K_\nu(x + iy)| \sim \frac{e^{-x}}{\sqrt{x}}$$

that for any ζ, we always have exactly one integrable solution at ∞. At zero, however, the expansions are:

$$I_\nu(z) \sim z^\nu; K_\nu(z) \sim z^{-\nu}.$$

Depending on ζ, we could have three different situations. The boundary between the first two is based on integrability of bound state wavefunctions; the more drastic change in behavior takes place when the discriminant of (3.3) changes sign and ζ becomes complex.

3.2 Strongly Repulsive Regime ($\lambda \geq \frac{3}{4}, \zeta \geq \frac{1}{2}$)

$$K_{\zeta+1/2}(\sqrt{i}r) \sim r^{-(\zeta+1/2)} \tag{3.4}$$

The solution with K fails to be square integrable at the origin because

$$|r^{1/2} K_{\zeta+1/2}(\sqrt{i}r)|^2 \sim r^{-2\zeta} \tag{3.5}$$

which is more singular than $1/r$ at the origin. Therefore, by Weyl's theorem, the Hamiltonian is self-adjoint.

3.3 Weak Regime $\left(-\frac{1}{4} < \lambda < \frac{3}{4}, |\zeta| < \frac{1}{2}\right)$

Both solutions are square integrable at the origin, though their leading behavior is different, so we have deficiency indices of $(1,1)$. The fact that one of the solutions is K_ν is suggestive of the presence of a bound state, and (as we will see shortly) most of the self-adjoint extensions permit one. In fact, we already knew this was going to happen, at least for the case $\lambda = 0$, the free particle Hamiltonian on $\mathbb{R}^3$, which we extended while solving for the 3D delta function.

In the weakly repulsive case $(0 < \lambda < \frac{3}{4})$ the plain $1/r^2$ potential ought to have no bound states; the trouble is that a sufficiently strong attractive singularity at the origin might overcome the repulsive barrier. We can make this problem regular by the simple expedient of enforcing the $u(0) = 0$ boundary condition, but this needs some justification. First, we show that there *is* a self-adjoint extension with $u(0) = 0$.

Self-Adjoint Extensions

The deficiency index calculation gives us the following function to add to our domain:

$$\Psi = \sqrt{r}\left[K_{\zeta+1/2}(e^{i\pi/2}r) + e^{-i\theta}K_{\zeta+1/2}(e^{-i\pi/2}r)\right] \tag{3.6}$$

We are interested in its asymptotic behavior near the origin. Using the small argument forms from [58], this is

$$\Psi \rightarrow \sqrt{r}\left[\frac{\Gamma(\zeta+1/2)}{2}\left(\frac{e^{i\pi/4}r}{2}\right)^{-\zeta-1/2} + e^{-i\theta}\frac{\Gamma(\zeta+1/2)}{2}\left(\frac{e^{-i\pi/4}r}{2}\right)^{-\zeta-1/2}\right].$$

We can simplify this to the form

$$\Psi \rightarrow \frac{\Gamma(\zeta+1/2)}{\sqrt{2}}\left(\frac{r}{2}\right)^{-\zeta}\left[e^{i\pi\zeta/4} + e^{-i\theta-i\pi\zeta/4}\right]. \tag{3.7}$$

We can make the term in brackets vanish by picking $\theta = \theta_f \equiv \pi(1 - \zeta/2)$. We are free to do this because ζ is fixed. Since our original domain, as usual, included only functions that vanished at the origin, so does the extended domain. A particularly important feature of θ_f is that it's the only extension that retains scale invariance; the others all introduce bound states. Scale invariance is generally not preserved under self-adjoint extensions, but sometimes there are specific extensions that preserve it. We will discuss these issues in Chapter 9.
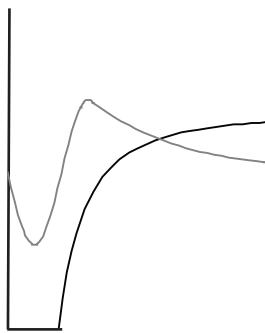
Figure 3.1: Regularized Inverse Square Potential

Naive regularization schemes automatically pick this extension, as we shall see. In the repulsive case we don't really need this reassurance; however, it's not obvious that the weakly attractive $(-\frac{1}{4} < \lambda < 0)$ inverse square potential should have no bound states.

Regularization

We regularize the singularity with a square well, following [6]. We replace the λ/r^2 potential with a nonsingular understudy:

$$V_a(r) = \frac{\lambda}{a^2}\theta(a - r) + \frac{\lambda}{r^2}\theta(r - a) \tag{3.8}$$

where $\theta(x)$ is the Heaviside step function.

Since this potential is regular we can impose $u(0) = 0$. Let $v = \zeta + 1/2$. Suppose there were a bound state. Imposing the usual boundary conditions on our solutions and their derivatives we'd get:

$$A \sin qa = BK_v(ka)$$

$$qA \cos qa = kBK'_v(ka)$$

$$qa \cot qa = ka\frac{K'_v(ka)}{K_v(ka)}. \tag{3.9}$$

The quickest way forward is to make a small angle approximation; this might seem a little suspect, but

$$ka \leq qa \approx \sqrt{-\lambda - k^2a^2} \leq 1/2 \tag{3.10}$$

and while this might not seem like a sufficiently tight constraint, $1/2$ is actually a pretty small angle—sufficiently small that first-order terms dominate the behavior of the trig functions. Expanding out both sides,

$$1 = ka \frac{(-v/2)(ka/2)^{-v-1}}{(ka/2)^{-v}} \Rightarrow 1 = -v \tag{3.11}$$

and this is inconsistent, so there can be no bound states. This treatment might be somewhat sloppy, but it's valid for small λ at any rate, and is meant merely to provide a heuristic justification for picking the Friedrichs extension. A hand-wavy mathematical reason for picking the Friedrichs extension over this domain is as follows. The problem is analytic in λ on $(-\frac{1}{4}, 0)$, and there are no singularities or zeros of $\cot qa$, so we don't expect θ (or the number of bound states) to behave non-analytically in λ. Since $\theta = \theta_f$ on $(-e, 0) \subseteq (-\frac{1}{4}, 0)$ for some e, it should be constant for all e.

There's a tighter argument in Radin's paper [22]. Radin also observes that the regularized theory has singularities only in the $l = 0$ sector. One of the flaws of earlier treatments is that they regularize the centrifugal barrier term as well as the potential; Radin conscientiously avoids this.

The boundary between weak and strong regimes at $\lambda = -1/4$ is still weak, but has a slight calculational subtlety.

3.4   Critical Value $(\lambda = -\frac{1}{4})$

Since the treatments of the next chapter come down to solving this regime, it is of some historical importance. The solution of the weak regime isn't directly applicable here, because both solutions go as $\sqrt{r}$, and we're missing one independent solution. A way to see what's going on is to notice that the Schrödinger equation, under the transformation $v(r) = u(r)/\sqrt{r}$, is exactly the free Bessel equation in two dimensions. (This is no accident, see the definition of spherical Bessel functions in [56].) The independent solutions are therefore $\sqrt{kr}K_0(kr) \sim \sqrt{kr} \log kr$ and $\sqrt{kr}I_0(kr) \sim \sqrt{kr}$. We *could* take the Friedrichs extension, throw out the K_0 solution, and retain scale invariance, so we aren't yet in the strong regime.

3.5 Strongly Attractive Regime $(\lambda < -\frac{1}{4})$

Solving (3.3) for ζ, we get

$$\zeta = -\frac{1}{2} \pm \sqrt{\lambda + \frac{1}{4}}. \tag{3.12}$$

In this regime, the square root is imaginary; let's call it $i\Xi$. The solutions to Schrödinger's equation are now

$$\sqrt{kr}Z_{\pm i\Xi}(kr)$$

All Bessel functions of nonzero order have the behavior $Z_v(x) \sim x^{\pm v}$ at the origin. This means that that they either blow up or vanish at the origin as long as $\Re(v) \neq 0$, but when $\Re(v) = 0$,

$$x^{\pm iy} = e^{\pm iy \log x} = \cos(y \log x) \pm i \sin(y \log x)$$

The solutions differ from each other by a phase, but the phase isn't even well-defined at the origin, since both solutions are oscillating infinitely rapidly there. Since all solutions of this form are certainly *integrable* near the origin, we have deficiency indices (1,1), and a one-parameter family of self-adjoint extensions, which select the phase. We can pick the correct self-adjoint extension by the same method as before, and we do this a few sections down, but there is a simpler procedure due to Case [1].

Case's Way

The failure of self-adjointness manifests itself very dramatically in the fact that every negative energy has an eigenfunction. With most potentials the boundary conditions keep the bound state spectrum discrete by forbidding most energies. However, with our potential, $K_{i\Xi}$ is always sufficiently well-behaved at infinity and at the origin. Near the origin it goes like

$$\sqrt{r}\cos(\Xi \log(kr) + B),$$

where B is energy-independent. We can rewrite this, with our usual abuse of notation, as

$$\cos[\Xi \log r + (B + \Xi \log k)] = \cos(\log r + B') \tag{3.13}$$

and this behaves the same way for all energies at the origin, because $\log r$ blows up. Evidently, this violates orthogonality, since functions for infinitesimally separated k look alike and certainly are not orthogonal. However, we can restore orthogonality by hand, as Case does, by the following procedure. Consider the two Schrödinger equations

$$D^2\psi_1 + \left[\frac{\lambda}{r^2} - k_1^2\right]\psi_1 = 0$$

$$D^2\overline{\psi_2} + \left[\frac{\lambda}{r^2} - k_2^2\right]\overline{\psi_2} = 0.$$

(The derivative commutes with complex conjugation.) If we multiply the first equation by ψ_2 and the second by ψ_1, and then subtract, the inverse-square term cancels. This leaves us with the following equation

$$\psi_1\frac{d^2\overline{\psi_2}}{dr^2} - \frac{d^2\psi_1}{dr^2}\overline{\psi_2} = (k_1^2 - k_2^2)\psi_1\overline{\psi_2}. \tag{3.14}$$

If we integrate this over all space, the rhs becomes

$$(k_1^2 - k_2^2)\int_0^\infty \psi_1\overline{\psi_2}\,dx = (k_1^2 - k_2^2)(\psi_2, \psi_1).$$

To have orthogonality, therefore, the integral over all space of the lhs must be zero. Since

$$(fg')' = f'g' + fg''$$

we can simplify the integrand on the lhs to

$$(\psi_1\overline{\psi_2'})' - (\psi_1'\overline{\psi_2})'$$

and use the fundamental theorem of calculus to get the following condition:

$$\left[\psi_1\frac{d\overline{\psi_2}}{dr} - \overline{\psi_2}\frac{d\psi_1}{dr}\right]_0^\infty = 0. \tag{3.15}$$

Since everything vanishes at ∞ because of the exponential falloff of $K_{i\Xi}$, all we need is equality at zero. Plugging in the small-argument form (3.13) and simplifying, we find the constraint:

$$\sin(B_2' - B_1') = 0. \tag{3.16}$$

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In terms of the energy-dependent phase this equation implies

$$\Xi(\log k_a - \log k_b) = n\pi \tag{3.17}$$

and the bound state separation is given by

$$\frac{k_a}{k_b} = e^{n\pi/\Xi}. \tag{3.18}$$

Fixing any one of the bound state energies determines the entire spectrum, and—as we expect—specifies a self-adjoint extension of the Hamiltonian. The bizarre thing about this spectrum is that it is unbounded from below, since n can be either positive or negative; there are infinitely many bound states going all the way up to 0 and all the way down to $-\infty$. Case dismissed the potential as unphysical for this reason, but it might still be useful from an effective field theory point of view because deep bound states are not obviously low-energy observables. In fact, as Refs. [30], [32] show, if we regularize the potential with a square well or a delta function ring of radius a, we can take $a \to 0$ without affecting the shallow bound states at all. The accumulation of bound states at $E = 0$ is a result of the long-range nature of this potential, and can be avoided—as with the hydrogen atom—by cutting off the potential at large distances.

3.6   Singularity *vs.* Anomaly

The literature on the inverse square potential has two threads—one addresses its pathologies as a result of scale invariance, the other, as consequences of fall to the center. Pathologies like a continuum of bound states might seem characteristic of scale invariant potentials. However, let's look at the close-in behavior of potentials more singular than $1/r^2$.[1] These are generally not analytically solvable; however, we can still investigate the behavior near the origin, since, in the Schrödinger equation

$$u''(r) = \left(k^2 - \frac{\alpha}{r^n}\right)$$

the energy k^2 becomes negligible as $r \to 0$. So we solve the simpler equation

$$H\psi = 0. \tag{3.19}$$

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[1]With highly singular potentials there is no qualitative difference between the 1D and 3D problems, so I'll switch back and forth at will.

The solutions to this equation are called **zero-energy wavefunctions**, and are very helpful in the study of singular potentials. In general the two independent solutions to the zero-energy equation

$$\frac{d^2u}{dr^2} + \frac{\alpha}{r^n}u(r) = 0 \tag{3.20}$$

can be written as follows:

$$u(0,r) \sim \sqrt{r}\left[(AJ_{1/(n-2)}\left(r^{(2-n)/2}\right) + BJ_{-1/(n-2)}\left(r^{(2-n)/2}\right)\right]. \tag{3.21}$$

There is a particularly nice solution for $n = 4$:

$$u(0,r) = x\cos\left(\frac{\sqrt{\alpha}}{r} + B\right). \tag{3.22}$$

(3.21) oscillates wildly near the origin for $n < -2$, and all solutions of form (3.22) behave the same way at the origin because the phase is negligible compared with the singularity in r. So, once again, we have a failure of self-adjointness and a continuum of bound states. The fix *a la Case* is the same as before, since the derivation in the previous section holds for basically arbitrary $f(x)$ in place of $\sin(\log x)$. However, we get less information out of the condition on B than we formerly did. In particular, without a solution to the actual Schrödinger equation, we can't get much information about the eigenvalues and their spacing. For $E \to -\infty$, Perelomov [20] uses the quasiclassical approximation to obtain

$$\frac{E_k}{E_0} = k^{2N/(N-2)} \tag{3.23}$$

for the $1/r^N$ potential. However, this is not the sector we are interested in. The case $N = 4$ is slightly better than others because Schrödinger's equation is exactly solvable in terms of Mathieu functions [12]. The asymptotic form of the solution near the origin is

$$\phi(r) \to r\cos\left(\frac{\sqrt{\alpha}}{r} - \frac{\nu\pi}{2} + \chi\right) \tag{3.24}$$

where ν is (in the words of Ref. [12]) a "very complicated function" with a less than straightforward dependence on k. The presence of energy-dependent phases was expected; however, the relation is sufficiently unpleasant that we have no hope of getting a simple general expression for the energy level spacing. An interesting feature of this problem is the way both short-distance and long-distance length scales enter

into the treatment—the levels are determined by ν, which depends on k, therefore on the self-adjoint extension, and finally on the short-distance physics; however, the frequency of oscillation near the origin is determined by the "intrinsic scale" of α. This is an example of when dimensional analysis breaks down, since there are two entirely different scales that influence both long-distance and short-distance behavior.

That multiple scales are necessary can be seen from the following dimensional argument. The coupling of the g/r^n potential is a positive power of inverse length (i.e. an energy) for $n < 2$, but a positive power of length for $n > 2$. Suppose $n > 2$, and g is the only scale. Then the **magnitude** B of the ground state energy must scale with g. Since g is a length and B is an inverse length, it follows that B must decrease as the coupling increases; that is, the ground state must get shallower as the potential well becomes deeper. This doesn't make physical sense, and the only way to rescue the situation is to put the ground state at $-\infty$, or to introduce a new scale using self-adjoint extensions or renormalization.

With weakly singular potentials like $1/r$, the coupling is an energy, so the ground state energy scales as it should. However, the scattering length is an inverse energy, so it should *decrease* as the coupling increases. Again, this makes no sense, and the only way out is for the scattering length to be infinite.

Something that Newton [62] considered terminally weird about the $1/r^4$ and more singular attractive potentials, is that for these the full 3D Schrödinger equation has no solutions at all. The pathology is essentially the same as that of the point source in electrostatics.

$$\nabla^2(1/r) = -4\pi\delta^3(r) \neq 0.$$

It has been shown in the literature ([62],[11]) that the correct radial part of the Hamiltonian in this case is

$$\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \delta(r)\frac{\partial}{\partial r}$$

so that our correct radial Schrödinger equation has an extra term, which looks like a δ' potential. Newton used this as an excuse to dismiss the potential as unphysical; however, to our EFT-indoctrinated minds, all this shows is that some form of renormalization is essential.

We'll consider the $1/r^4$ potential again, in the context of limit cycles, but the point of this detour was to point out that at least some of the features of the $1/r^2$ potential are shared with potentials that are not scale-invariant.

3.7 Non-Friedrichs Extensions of the $1/r^2$ Potential

Case's method is quite broadly applicable as a way of doing self-adjoint extensions. For example, we could use it to solve the two-dimensional delta function. Suppose we fix a bound state k_b. Because the particle is free except at the origin, this would have to have the wavefunction $K_0(k_b r)$. Suppose there were another ($m = 0$) bound state, k_s. It would also have to have the wavefunction $K_0(k_s r)$ almost everywhere. Both wavefunctions are nodeless and always positive, so

$$\int_0^\infty K_0(k_b r) K_0(k_s r) \geq 0$$

and the states cannot be orthogonal, so the operator cannot be self-adjoint. This tells us that there's at most one bound state with arbitrary energy.

However, a limitation of Case's method is that it doesn't tell us about the Friedrichs extension, or about extensions without bound states. In particular, it does not tell us a very important thing about the $1/r^2$ potential, which is that the Friedrichs extension ceases to exist for $\lambda < -1/4$. This is important because it shows that—unlike the "2D delta function," which has an anomaly only because it's defined as an extension with an anomaly—anomalous symmetry breaking is inevitable for a strong $1/r^2$ potential.

This section treats the inverse square potential using the apparatus of self-adjoint extensions that we developed in the previous chapter. The expressions obtained here are used in later chapters; however, the algebra is unpleasant and not dissimilar to what we did in Chapter 2.

3.7.1 One Dimension

In the regime $-1/4 < \lambda < 3/4$, both solutions to the Schrödinger equation are square-integrable at the origin, so probability conservation is no longer adequate to distinguish between them. Let $\lambda = \zeta(\zeta+1)$; then the regular and less regular solutions go as $x^{\zeta+1}$ and $x^{-\zeta}$ near the origin respectively. As λ decreases and becomes negative, the regularity gap between the two solutions closes; for $\lambda < 0$ both functions vanish at the origin. For $\lambda = 0$ the irregular solution is a constant, like e^{-kx} or $\cos kx$; this is the case of $\delta(x)$. For $\lambda = -1/4$ the irregular solution is $\sqrt{kx}K_0(kx)$, which goes as $\sqrt{x}\log x$; the regular solution is $\sqrt{x}$.

The attractive region is weird because neither of the solutions behaves as one would expect: for both solutions, $\psi(0) = 0$ and the derivative has an infinite discontinuity. (The latter feature is shared with the one-dimensional Coulomb potential, see Chapter 8.)

Energies and Extensions

To a better approximation than (3.3), the small-argument form of (3.6) is

$$\psi \sim x^{1+\zeta} f(\zeta) \left[e^{i\pi\zeta/4} + e^{i(\theta - \pi\zeta/4)} \right] + x^{-\zeta} g(\zeta) \left[e^{i(\theta + \pi\zeta/4)} + e^{-i\pi\zeta/4} \right]. \tag{3.25}$$

If we rewrite this as

$$\psi \sim A r^{1+\zeta} + B r^{-\zeta}$$

we can rearrange it to read

$$\frac{\zeta\psi + x\psi'}{(1+\zeta)\psi - x\psi'} = \frac{A}{B} x^{1+2\zeta}. \tag{3.26}$$

The effective length scale is set by A/B, which has dimensions $k^{1+2\zeta}$ and is a function of θ. We could work this out explicitly with gamma-function identities, but it's simpler in this case to point out that, by tweaking θ, we can have $A = 0, B \neq 0$ and vice versa. Absorbing the θ-dependence into our length scale, we get a boundary condition of the form

$$\frac{\zeta\psi + r\psi'}{(1+\zeta)\psi - r\psi'} = F(\zeta)(\kappa r)^{1+2\zeta} \tag{3.27}$$

where β is an arbitrary constant, and $|\kappa| \in (0, \infty)$ parameterizes the extension chosen. If we plug in a bound state of the form $\sqrt{k_b x} K_{\zeta+1/2}(k_b x)$, we swiftly discover that

$$F(\zeta) = \frac{\Gamma(-\zeta - 1/2)}{\Gamma(\zeta + 1/2)}$$

so the bound state energy is proportional to κ, as we expect, and our final boundary condition is

$$\frac{\zeta\psi + x\psi'}{(1+\zeta)\psi - x\psi'} = \frac{\Gamma(-\zeta - 1/2)}{\Gamma(\zeta + 1/2)}(k_b x)^{1+2\zeta}. \tag{3.28}$$

This is a useful form for the boundary condition, because it's cast solely in terms of observables and the long-distance coupling. We can derive the s-wave phase shift by applying the boundary condition to a scattering state, $\sqrt{kx}(AJ_{\zeta+1/2}(kr)+BN_{\zeta+1/2}(kr))$. The leading behavior of scattering states is

$$J_\nu \sim \left(\frac{kr}{2}\right)^\nu \frac{1}{\Gamma(1+\nu)}$$

$$N_\nu \sim \frac{1}{\pi}\Gamma(\nu)\left(\frac{kr}{2}\right)^{-\nu} + \frac{\cos\pi\nu}{\pi}\Gamma(-\nu).\left(\frac{kr}{2}\right)^\nu$$

Applying the boundary condition to this gives

$$\frac{A\pi + B\cos[\pi(\zeta+1/2)]\Gamma(-\zeta-1/2)\Gamma(\zeta+3/2)}{B\Gamma(\zeta+1/2)\Gamma(\zeta+3/2)}\left(\frac{kr}{2}\right)^{1+2\zeta} = \frac{\Gamma(-\zeta-1/2)}{\Gamma(\zeta+1/2)}\left(\frac{k_b r}{2}\right)^{1+2\zeta} \tag{3.29}$$

which looks slightly less unpleasant rearranged:

$$\frac{B}{A} = \frac{\pi}{\Gamma(\zeta+3/2)\Gamma(-\zeta-1/2)}\frac{1}{\cos[\pi(\zeta+1/2)] - (k/k_b)^{1+2\zeta}}. \tag{3.30}$$

(Let's write $\nu = \zeta + 1/2$.) One further simplification comes from the reflection formula $\Gamma(\frac{1}{2}+z)\Gamma(\frac{1}{2}-z) = \pi\sec\pi z$. For us, $z = \nu + 1/2$, we get the expression down to

$$\frac{B}{A} = \frac{\cos[\pi(\nu+1/2)]}{\cos\pi\nu - (k/k_b)^{2\nu}}. \tag{3.31}$$

Now B/A is a quantity related to the $l = 0$ phase shift; its dependence on k breaks scale invariance, and we have (once again) an anomaly.

The scattering phase shifts of the $1/x^2$ potential are a little tricky because, like the Coulomb potential, it's a long-range interaction and the asymptotic forms are $\sqrt{kx}Z_{\zeta+1/2}(kx)$ rather than e^{ikx}. It's slightly easier because the Bessel functions are just phase-shifted sines and cosines (AS 9.2.3). (Henceforth we're going to write $\zeta + 1/2 = \nu$.)

$$\sqrt{kx}J_\nu(kx) = \cos\left(kx - \frac{\pi\nu}{2} - \frac{\pi}{4}\right)$$

$$\sqrt{kx}N_\nu(kx) = \sin\left(kx - \frac{\pi\nu}{2} - \frac{\pi}{4}\right).$$

And one can check that

$$A\sqrt{kx}J_\nu(kx) + B\sqrt{kx}N_\nu(kx) \sim C\cos\left(kx - \frac{\pi\nu}{2} - \frac{\pi}{4} - \tan^{-1}\frac{B}{A}\right). \tag{3.32}$$

Because of Levinson's theorem [62], which we discuss later, we expect the phase shift at $k = k_b$ to be $\pi/2$. Let's check this. 3.31 simplifies to

$$\frac{B}{A} = \frac{\cos[\pi(\nu + 1/2)]}{\cos\pi\nu - 1}. \tag{3.33}$$

With the help of two well-known trig identities one can get this down to

$$\frac{B}{A} = -\cot(\pi\nu/2)$$

which means that

$$\tan\frac{B}{A} = \frac{\pi\nu}{2} - \frac{\pi}{2}.$$

Putting this back into 3.32 we see that

$$\sqrt{kx}(AJ_\nu(kx) + BN_\nu(kx)) \sim C\cos\left(kx + \frac{\pi}{4}\right). \tag{3.34}$$

This is not quite what we expect from a normal potential. However, if we look at the behavior of 3.31 at very high energies, $B/A = 0$, and the phase shift is $-(\frac{\pi\nu}{2} + \frac{\pi}{4})$ rather than 0, as we have been bred to expect.

3.7.2 Two Dimensions

In two dimensions with $m = 0$, the bound-states Schrödinger equation with a $1/r^2$ potential is

$$r^2\frac{d^2\psi}{dr^2} + r\frac{d\psi}{dr} \pm k^2r^2 + \lambda\psi = 0 \tag{3.35}$$

and the solutions to this are simply the relevant Bessel functions $Z_\nu(kr)$, where $\nu = \sqrt{\lambda}$. So everything goes pretty much as in the 1D and 3D cases, except for the clutter of $\sqrt{kr}$ terms. The self-adjointness calculation is more straightforward in two dimensions, but the details are similar enough to be beneath repetition.

$$\frac{\nu\psi + r\psi'}{\nu\psi - r\psi'} = \left(\frac{\beta r}{2}\right)^{2\nu} \tag{3.36}$$

where β is a parameter related to the self-adjoint extension and the bound state energy. This sets us up to calculate an energy dependent scattering phase shift, as we did in one dimension. We can replace β with a bound state energy as we did before, and get

$$\frac{\nu\psi + r\psi'}{\nu\psi - r\psi'} = \frac{\Gamma(-\nu)}{\Gamma(\nu)}\left(\frac{k_b r}{2}\right)^{2\nu}. \tag{3.37}$$

Plugging in the general scattering solution, which is $AJ_\nu(kr) + BN_\nu(kr)$, we get 3.31 once again. The treatment of scattering works identically, *except* that in 2D scattering [60] we don't subtract the $\pi/4$, since it's built into the asymptotic forms of the Bessel functions. Therefore the phase shift at $k = k_b$ is $\pi/2$, which is consistent with Levinson's theorem.

Now let's do the same calculation in the strong regime. First of all, the equivalent of 3.25 is

$$\psi \sim x^{i\nu} f(\nu)\left[e^{-\pi\nu/4} + e^{i(\theta - i\pi\nu/4)}\right] + x^{-i\nu} g(\nu)\left[e^{i(\theta + i\pi\nu/4)} + e^{\pi\nu/4}\right] \tag{3.38}$$

Since $x^{\pm i\nu}$ look the same at the origin, there isn't a preferred extension. Setting a phase between the two solutions means introducing arbitrary new physics, but that'd be true in some sense even if there were a Friedrichs extension: the special thing about the Friedrichs extension is that by throwing out one of the states altogether, we can escape the anomaly. We would avoid the anomaly, even here, if we could arbitrarily throw out one of the solutions. However, if we look at the ratio of the coefficients in this case (leaving out stuff independent of θ), it is

$$\frac{\Pi_1}{\Pi_2} = \frac{e^{-i\theta/2}e^{-\pi\nu/4} + e^{i\theta/2}e^{\pi\nu/4}}{e^{i\theta/2}e^{-\pi\nu/4} + e^{-i\theta/2}e^{\pi\nu/4}}$$

and since the numerator and denominator are conjugates, $|\Pi_1/\Pi_2| = 1$ and the solution with vanishing $x^{\pm i\nu}$ is not a self-adjoint extension, so there is absolutely no way to preserve scale invariance.

The rest of the self-adjointness calculation goes the same way it did before,

$$\frac{i\nu\psi + r\psi'}{i\nu\psi - r\psi'} = \left(\frac{\beta r}{2}\right)^{2i\nu} = e^{2i\nu \log Br} \tag{3.39}$$

or, in terms of a bound state energy,

$$\frac{i\nu\psi + r\psi'}{i\nu\psi - r\psi'} = e^{2i\{\nu \log(k_b r/2) - \arg[\Gamma(i\nu)]\}} \tag{3.40}$$

Having emphasized the modulus-one-ness of everything, we revert to our previous notation. None of the identities we used previously depended on $\nu \in \mathbb{R}$ so we can skip the details. Sending in $AJ_{i\nu}(kr) + BN_{i\nu}(kr)$ we get an expression parallel to 3.31:

$$\frac{B}{A} = \frac{\cos[\pi(\nu + 1/2)]}{\cos \pi\nu - (k/k_b)^{2\nu}} \tag{3.41}$$

In the $k = k_b$ case one can whittle this down, as usual, to

$$\frac{B}{A} = -\cot i\pi\nu/2,$$

which gives a net phase shift of $\pi/2$ in this case, just as it did before. The difference between this result and the previous ones is that $(k/k_b)^{2i\nu}$ is log-periodic, so $(k/k_b)^{2i\nu} = 1$ has infinitely many solutions, and the scattering sector notices infinitely many bound states. This is more an internal consistency check than a new statement, but all the same it is comforting to know.

3.7.3 Three Dimensions

The calculations are identical to the 1D case. An interesting contrast between this problem and the Coulomb problem is that here the Friedrichs extension *is* in fact a choice on our part. Consider the full Schrödinger equation:

$$-\nabla^2\psi + \frac{\lambda}{r^2}\psi = k^2\psi.$$

If we integrate this over a tiny ball around the origin, assuming that ψ is spherically symmetric, we get the form

$$-\int \nabla^2\psi dV + 4\pi\lambda \int \psi dr = k^2 \int \psi r^2 dr$$

Normalizability forbids ψ from blowing up more rapidly than $r^{-3/2}$, but that leaves open the possibility that ψ falls off faster than $1/r$. The only way to throw out the non-Friedrichs extensions is to use a regularization scheme such as Meetz's.

3.8 Infinite Well with an Inverse Square Term

The boundary condition (Case's phase) is not influenced by long-distance physics, so it's the same in all cases where you have a nonsingular potential plus an inverse square potential. This is because there are arbitrarily deep and localized bound states, and whether one is orthogonal to these can have nothing to do with one's long-distance behavior.

We're interested in states with $E > 0$, $E \gg 0$ if we must. The wavefunctions are of the form $\sqrt{kx}(AJ_{i\nu}(kx) + BN_{i\nu}(kx))$ inside the region. We need two boundary conditions to get a quantization condition; Case's phase gives one, and the other is the requirement that the wavefunctions vanish at R, the well radius. The latter condition can be written as

$$AJ_{i\nu}(kR) + BN_{i\nu}(kR) = 0$$

and so

$$-\frac{B}{A} = \frac{J_{i\nu}(kR)}{N_{i\nu}(kR)} \approx \cot(kR - i\pi\nu/2 - \pi/4).$$

We can plug this value into our boundary condition 3.31 with imaginary ν to get

$$-\cot(kR - i\pi\nu/2 - \pi/4) = \frac{\cos[\pi(i\nu + 1/2)]}{\cosh \pi\nu - (k/k_b)^{2i\nu}}, \tag{3.42}$$

which is the eigenvalue equation. The long-distance boundary condition here might be a little more complicated than in the simple $1/r^2$ potential, but there is a long-distance boundary condition there too—square integrability, which throws out the I solution and makes it so that all contributions to the phase shift come from the energy. We can plot this on Mathematica (see figure), but unfortunately this transcendental equation cannot be solved analytically.

In this limit $\nu \to 0$ we have the following behavior:

$$-\cot(kR - \pi/4) = \frac{\cos(\pi/2 + i\pi\nu)}{1 - e^{2i\nu \log(k/k_b)}}$$

So for the most part the rhs vanishes and we have bound states at

$$k = \frac{\pi + 4\pi n}{4R}$$

so basically the dependence on ν disappears. However, near the resonance $k = k_b$, the rhs is a 0/0 limit and the boundary condition becomes (with some expanding and simplifying)
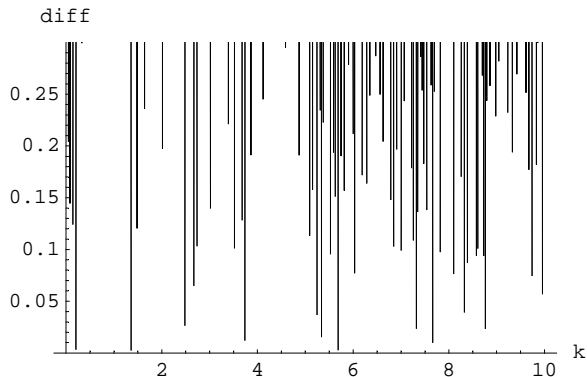
Figure 3.2: Magnitude of boundary condition. Intercepts are bound states.

$$\cot(kR - \pi/4) = -\frac{\pi}{2\log k/k_b}.$$

This is the characteristic Klauder phenomenon of the $-1/4r^2$ Hamiltonian, and it leads to a bound state at $-\pi/4R$ if the boundary conditions match up.

3.9 The Classical Limit

The behavior of the classical $1/r^2$ potential has been discussed in Chapter 2. Note that the classical Hamiltonian $p^2 + q^{-2}$ is scale-invariant like the quantum Hamiltonian, for exactly the same reasons. (Therefore, the coupling is dimensionless in the appropriate units.) Classical scattering in a $1/r^2$ potential is worked out in [62]; the cross-section is derived to be

$$\frac{d\sigma}{d\Omega} = \frac{\lambda}{2\pi} \frac{1 - y}{Ey^2(2 - y)^2 \sin \pi y} \tag{3.43}$$

where $\pi y = \theta$, the classical scattering angle [62], which depends only on the angular momentum of the incoming particle:

$$y = 1 - \frac{L}{\sqrt{L^2 + m\lambda}}.$$

One of the conditions for scattering to be classical (i.e. for the quantum mechanical uncertainties to be small) is derived in [18] and cited by [81]:

$$L_{cl}\theta_{cl} \gg \hbar.$$

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Kayser uses this to deduce that $m\lambda \gg \hbar^2$—and therefore, in our units, $\lambda \gg 1$. Therefore, Kayser [81] argues, a classical *repulsive* $1/r^2$ potential is strongly repulsive. (In fact, it is known [62] that the classical limit is the strong-coupling limit even for attractive coupling.) For a sufficiently attractive potential, we've seen that the classical solution is incomplete [75]: the particle collides with the center of the field at a finite time t_0 and after that the motion isn't well-defined. However, as Zhu and Klauder [19] point out, one can have the origin reflect everything back exactly the way it came in, and so the scale symmetry isn't obviously broken.

We observe that Case's spectrum approaches continuity in the limit $|\Xi| \to \infty$, since the level spacing $k_n/k_m = e^{(n-m)/\Xi} \to 1$ as $\Xi \to \infty$. Consider two self-adjoint extensions, one with a bound state at k_a and another with a bound state at k_b. Clearly, for any Ξ there is an m such that $k_a e^{m\pi/\Xi} \leq k_b \leq k_a e^{(m+1)\pi/\Xi}$. As $\Xi \to \infty$, therefore, k_b gets sandwiched arbitrarily closely between two wavefunctions of the extension k_a, and the self-adjoint extensions corresponding to a and b become indistinguishable. This establishes[2] that the anomaly disappears in the classical limit, which makes its existence a little less disturbing.

There is only one "unitary" (non-dissipative) classical solution, since the phase is irrelevant, and therefore the disappearance of phase differences is not undesired.

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[2]Well, maybe not. k, l and λ are all large in the classical limit. However, as long as k doesn't grow exponentially faster than λ we're safe.

Chapter 4

Global Renormalization

Now that all the expressions, and the naive formal solution, have been presented, let us consider more physical approaches to the strongly attractive potential. There are three questions involved: (1) do we really need self-adjointness? (2) is the coupling constant determined by long-distance physics? (3) how many bound states should the system have? This determines the different choices of regularization scheme, and the different spectra, deduced by Refs. [45], [30], [86], and [22]. In this chapter, I'll merely introduce the schemes; their physical implications will be discussed in later chapters.

4.1 Hardcore Cutoff

This method is due to [52] and is followed by [45] and [46]. One replaces the potential at a short distance a with an infinite repulsive barrier. This forces the wavefunction to vanish at that point, so that

$$K_{i\Xi}(ka) = 0.$$

Now there are two regimes of $K_{i\Xi}(x)$, the small x regime where it oscillates wildly, and the big x regime where it is a decaying exponential with no roots. It has a largest zero at some x_n. By making k sufficiently large we can cram all the small x behavior into $(0, a)$ and set $a = k/x_n$, so the function vanishes as we require it to, *and* looks like a ground state. As it happens, x_n is still a "small argument," and we can say to good accuracy that the expression

$$K_{i\Xi}(ka) \sim \sin\left[\Xi \log\left(\frac{ka}{2}\right) - \arg[\Gamma(1 + i\Xi)]\right]$$

is valid. So, if we require it to vanish,

$$\Xi \log(ka) - \Xi \log 2 - \arg[\Gamma(1 + i\Xi)] = n\pi. \tag{4.1}$$

This might look a little like our previous result; the key difference is that our cutoff allows us to pick a lowest-energy allowed state (since the boundary condition rules out $k' > k$ whose first zero is too close in). Our goal is to fix the energy of this state as our parameter of "constant physics," and scale the coupling appropriately as the cutoff goes to zero. Since the first term can't be allowed to blow up, we know $\Xi \to 0$. To get its exact scaling behavior we need to simplify the third term a little, with the identity (AS 6.1.24):

$$\arg[\Gamma(1 + z)] = \arg \Gamma(z) + \tan^{-1}(y/x).$$

In our case, the second term is $\pi/2$, and the first is given by the series expansion

$$\Gamma(i\Xi) \sim -\frac{i}{\Xi} - \gamma$$

where γ is the Euler-Mascheroni constant. This is approximately along the $-y$ axis, so its argument can be expanded about $-\pi/2$ to give

$$\arg[\Gamma(i\Xi)] \sim -\frac{\pi}{2} - \gamma\Xi$$

and putting it all together for small Ξ, we get

$$\arg[\Gamma(1 + i\Xi)] \approx -\gamma\Xi.$$

Now we can put this back in (4.1) to get the scaling behavior

$$\log(ka) = \log 2 + \gamma + \frac{n\pi}{\Xi}. \tag{4.2}$$

For fixed k and $a \to 0$ the lhs is negative, so $n < 0$ for $\Xi > 0$. We choose $n = -1$ because that happens to correspond to the rightmost zero of the Bessel function. [1] The ground state energy is

$$E_{gs} = \left(\frac{e^\gamma}{a}\right)^2 e^{-\pi/\Xi}. \tag{4.3}$$

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[1] One could use, say, $n = -5$; it would just change the scaling properties of Ξ.
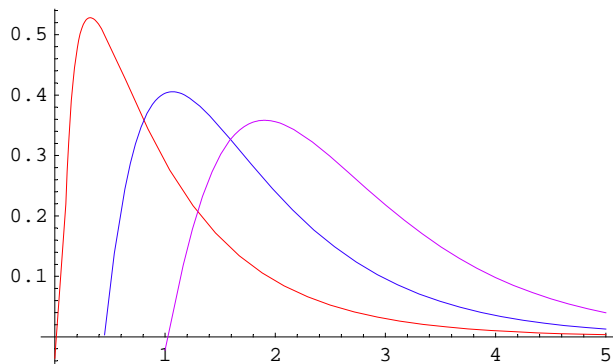
Figure 4.1: Evolution of $u(r)$ as $a \to 0$

An important feature of this method is the existence of a unique bound state. For $l > 0$ we're no longer in the strong regime, so there are no bound states; for $n > 1$ we can see from (4.2) that

$$\frac{E_n}{E_{gs}} = e^{(n+1)\pi/\Xi}$$

so $E_n \to 0$ as $\Xi \to 0$, and $n < 0$ because our regularization scheme rules out the other cases by construction.

4.2   Square Well Cutoff

We could follow the same cutoff procedure with an attractive square well instead of an infinite barrier. The 3D square well has issues as a calculational scheme because it doesn't always have bound states, so let's work in one dimension.

$$V = \begin{cases} \lambda/x^2 & x > a \\ \lambda/a^2 & x < a \end{cases}$$

The ground state wavefunction will be

$$u_{in}(x) = A\cos(qx)$$

$$u_{out}(x) = B\sqrt{kx}K_{i\Xi}(kx)$$

$$q = \sqrt{\frac{\lambda}{a^2} - k^2}.$$

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If we choose to work in the small-coupling regime, we can use the usual asymptotic form for u_{out} near the origin:

$$u_{out} \sim B\sqrt{kx}\sin(\Xi\log(kx) + \delta).$$

Matching wavefunctions and their derivatives at a, we get

$$-qa\tan(qa) = \frac{1}{2} + \Xi\cot(\Xi\log(ka) + \delta). \tag{4.4}$$

Dropping all terms in $(ka)^2$ and rearranging,

$$-\frac{\lambda - \frac{1}{2}}{\Xi} = \cot(\Xi\log(ka) + \delta). \tag{4.5}$$

In the $\Xi \to 0$ limit, $\lambda \to 1/4$ and the LHS blows up, so

$$\Xi\log(ka) = n\pi + \delta \tag{4.6}$$

as we had earlier, and we can follow through with the same logic. We will always have a *ground state* this way too, since the regularized theory always has one, and 4.6 forces all the excited states to zero.

4.3 Dimensional Regularization

In [48], Camblong renormalizes the inverse square potential by means of dimensional regularization (DR), a popular method in QFT. The idea behind DR is that problems are sometimes better-behaved in complex dimensions, and their bad behavior shows up as a pole at $d = 3$, which we can renormalize away. So instead of a cutoff, we scale the coupling against ϵ, if our regularized theory lives in $d \pm \epsilon$ dimensions. This procedure involves a lot of machinery that we don't need for anything else, so I'll leave out the details; however, the point of the technique is to continue the potential analytically in a way that does not leave it scale invariant. In our case, this means making it a $1/r^{2-\epsilon}$ potential in $3 - \epsilon$ dimensions. This is equivalent to the next— conceptually simpler—method we consider.

4.4 Schwartz's Way

In his 1977 paper, Schwartz [86] solved potentials of the class

$$V = \frac{\lambda}{r^2}\left(\frac{r}{r_0}\right)^\epsilon.$$

These are not exactly solvable in general, but there's a trick for small ϵ. It has been well-known for centuries [89] that negative power-law potentials have dual positive power-law potentials, with the remarkable property that equations of motion for one are equivalent to those for the other under a change of variable. For example, the Kepler and harmonic oscillator problems are equivalent under the change of variables

$$r_{kep} = r_{sho}^2.$$

This result was first discovered by Newton. Generally, as [48], [90], and [89] show, dual power-law potentials obey the relation

$$(N+2)(N'+2) = 4$$

which is a 1-1 correspondence between $(-2,0)$ and $(0,\infty)$. This correspondence carries over into quantum mechanics. The important consequence, for us, is that $N \to -2$ is dual to $N' \to \infty$, which looks like an infinite square well. We can use this duality to solve almost singular potentials; however, let's first look at the square well as a limit of r^n potentials.

Particle in a Box, Revisited

Consider the potential

$$V(r) = \frac{\lambda}{r_0^2}\left(\frac{r}{r_0}\right)^n \tag{4.7}$$

where λ is dimensionless, and n very large. We know there are basically two regimes: one with $r \ll r_0$, where V is essentially zero; and one with $r > r_0$, where $V \gg E$. Inside, our solution is the free particle wavefunction for a particle of angular momentum l:

$$u_{in}(r) = A\sqrt{kr}\,J_{l+1/2}(kr) \tag{4.8}$$

whereas outside the "well" it's the zero-energy solution to the potential since $E \ll V$ (we needn't worry about l since the centrifugal term is negligible outside the well). For normalizability we choose the exponentially decaying solution (let $p = n + 2$):

$$u_{out}(r) = B\sqrt{kr}K_{1/p}\left[\frac{\sqrt{\lambda}}{p}\left(\frac{r}{r_0}\right)^{p/2}\right]. \tag{4.9}$$

In our limit it's a pretty good approximation to say that *everything*[2] is in one of these regimes, so we can guess that our full wavefunction has the form

$$u(r) = kr J_{l+1/2}(kr)K_{1/p}\left[\frac{\sqrt{\lambda}}{p}\left(\frac{r}{r_0}\right)^{p/2}\right]. \tag{4.10}$$

It's clear that this vanishes outside the well in the limit; the "inside" behavior of the decaying part is a little more interesting. We use the asymptotic form

$$K_{1/p}(x) = 2^{\frac{1}{p}-1}\left(\frac{1}{p}-1\right)!x^{-1/p}.$$

Plugging our argument in, we see that the decaying part goes as

$$\lambda^{-2/p}\left(\frac{r}{r_0}\right)^{-1/2}.$$

Now, k is approximately $n\pi/r_0$, which is its value for the square well, so the factor of $\sqrt{r/r_0}$ cancels a $\sqrt{kr}$ in the prefactor and leaves us with

$$u_{in} = \sqrt{kr}J_{l+1/2}(kr)$$

as we wanted. An interesting feature of this derivation is the parallel between how λ becomes less important for $n \to \infty$ and how the same thing happens to r_0 as $n \to -2$. In fact, there's something very like dimensional transmutation about this duality transformation near the limit, since the square well has a dimensional scale but no coupling, and the inverse-square potential has a coupling but no dimensional scale. The correspondence isn't as simple as it looks, though, because the duality transformation works in a rather odd way that's easier to demonstrate than to explain.

Back in the Inverse Square

Schwartz implements the duality transformation by the following change of variables:

$$r = \frac{y^{2/\epsilon}}{2k}; u_l(r) = y^{-(\frac{1}{\epsilon}+\frac{1}{2})}v(y). \tag{4.11}$$

Upon these substitutions, the Schrödinger equation

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[2]Except $r = r_0$, of course.

$$-\frac{d^2u}{dr^2} + \frac{l(l+1)}{r^2}u - \frac{\lambda}{r^2}\left(\frac{r}{r_0}\right)^\epsilon u = -k^2u$$

becomes

$$\left[-\frac{d^2}{dy^2} + \frac{[(2l+1)/\epsilon]^2 - \frac{1}{4}}{y^2} + \frac{y^{4/(\epsilon-2)}}{\epsilon^2}\right]v = \Lambda v \tag{4.12}$$

where

$$\Lambda = \frac{4\lambda}{\epsilon^2}(2kr_0)^{-\epsilon}$$

(The details of this procedure are worked out in Appendix A.) For sufficiently small ϵ, this is basically the Schrödinger equation for a state of very high angular momentum in a square well. Therefore, the appropriate solution is of the form

$$v(y) = \sqrt{\sqrt{\Lambda}y}J_\nu(\sqrt{\Lambda}y) \tag{4.13}$$

for $y < 1$, where

$$\nu \approx \frac{2l+1}{\epsilon}$$

and by (4.10) otherwise. We can match the functions and their derivatives at $y = 1$; this is done in [48], but it turns out that we get essentially the same result if we just require $v(1) = 0$, which happens if $J_\nu(\sqrt{\Lambda}) = 0$. Schwartz quotes the following formula for Bessel functions of very large order:

$$Z_n = \nu + C_n\nu^{1/3}$$

where Z_n is the nth zero, and C_n is basically independent of ν. So if we require that

$$\sqrt{\Lambda} = \nu + C_n\nu^{1/3} \tag{4.14}$$

and write everything out in terms of the original variables, we see that

$$\sqrt{\frac{4\lambda}{\epsilon^2}(2r_0k)^{-\epsilon}} = \frac{2l+1}{\epsilon} + C_n\left(\frac{2l+1}{\epsilon}\right)^{1/3}. \tag{4.15}$$

This can be rearranged in the form

$$\log(2kr_0) = -\frac{2}{\epsilon}\log\left[\frac{2l+1}{2\sqrt{\lambda}} + \frac{C_n\epsilon^{2/3}(2l+1)^{1/3}}{2\sqrt{\lambda}}\right] \tag{4.16}$$

where the second term in the argument of the logarithm is small relative to the first, and can be expanded to first order using $\log(1 + x) \sim x$ to give us

$$\log(2kr_0) = -\frac{2}{\epsilon} \left[\log \left(\frac{l + 1/2}{\sqrt{\lambda}} \right) + \frac{C_n \epsilon^{2/3}}{(2l + 1)^{2/3}} \right]. \tag{4.17}$$

Exponentiating this gives us Schwartz's final form

$$E_n = -\frac{1}{4r_0^2} \exp \left[\frac{2}{\epsilon} \log \frac{\lambda}{(l + 1/2)^2} \right] \exp \left[-\frac{4C_n}{\epsilon^{1/3}(2l + 1)^{2/3}} \right]. \tag{4.18}$$

In particular, for $l = 0$ states this is

$$E_n = -\frac{1}{4r_0^2} (4\lambda)^{2/\epsilon} e^{4C_n/\epsilon^{1/3}}. \tag{4.19}$$

What our energy states look like in the limit depends on whether $\lambda > 1/4$; if so, all the energies go to $-\infty$, otherwise they all go to zero. We could regularize this scheme by fixing E_n and scaling λ with ϵ, just as in our two previous schemes, and it works in essentially the same way. The strangest consequence, though, is that

$$\frac{E_n}{E_m} = \exp \left[-\frac{4(C_n - C_m)}{\epsilon^{1/3}} \right] \tag{4.20}$$

which always blows up. The C_n increase with n, so any higher-level energy state vanishes relative to the ground state as $\epsilon \to 0$. What's strange about this result is that it is *independent* of the coupling. This means that the bare, unregularized limit of this theory looks very different from what we derived in chapter 3 from the Schrödinger equation—there is neither a continuum of states nor a tower.

As Schwartz's approach and dimensional regularization turn out to be inconsistent with those we consider next, we should point out some of the reasons they might be inappropriate. First, there's no reason to suppose that the limit is unique, since we have an essential singularity in ϵ. In fact, we have good reason to believe it isn't, since things don't look the same at all for $r^{2+\epsilon}$ potentials. Suppose 4.20 held for complex ϵ; we would have wildly oscillatory behavior rather than what we see.

Another way to think about it is as follows. All the bound states associated with the Schwartz family—which all have finite numbers of nodes by construction—go down to $-\infty$, but a new family of bound states, each with infinitely many nodes and finite energies, appears at the transition. (These are shallower than the previous states, so their appearance isn't too mysterious.) The former statement follows from the fact that

$$E_n = -\frac{1}{4r_0^2} (4\lambda)^{2/\epsilon} e^{4C_n/\epsilon^{1/3}}$$

and as $\epsilon \to 0$ keeping everything else fixed, the behavior is dominated for all n by the exploding first term.

A further strike against dimensional regularization in quantum mechanics is the fact [68] that it gives nontrivial scattering phase shifts for the d-dimensional delta function whenever d is odd. Cutoff regularization gives trivial scattering phase shifts for $d \geq 4$, as [68] shows. This is supported by Simon's result [14], which says that the Hamiltonian $-\nabla^2 + V$ is self-adjoint in d dimensions if

$$V \geq -\frac{(d-1)(d-3) - 3}{4r^2}.$$

If $d \geq 4$, the free-particle Hamiltonian meets this criterion; therefore the free-particle Hamiltonian is self-adjoint. Since delta functions are self-adjoint extensions of the free-particle Hamiltonian, delta functions cannot exist in $d \geq 4$.

4.5   Summary

We have looked at three different ways of renormalizing the $1/r^2$ potential, all of which involve renormalizing the global coupling. All of these ways give us a renormalized spectrum with one bound state, in which the coupling goes to a critical value ($-\frac{1}{4}$ in one and three dimensions) as we take the renormalization parameter to zero. This disagrees with both Chapter 3 and Chapter 5. We show in Chapters 5 and 7 that the results of this chapter are a *limit*, and not a very useful one, of the more general treatments of Chapters 3 and 5.

Chapter 5

Limit Cycles

A feature common to the methods we looked at in Chapter 4 is that they all involve renormalizing the coupling. This might go against our original conception of renormalization as modifying only short-distance behavior, since the coupling also affects the long-distance behavior of our theory. For instance, we saw in Chapter 3 that the potential had many shallow bound states; even if bound states are not treated as observables, the scattering poles associated with them certainly count as low-energy observables. But if the coupling is fixed, what parameter are we to trade in for our energy? A scheme to do this was implemented in Ref. [30], and later by Refs. [31], [36], and [32]. The technique was first laid out by Lepage in Ref. [33] in a more general context.

5.1   Running Square Well

We regularize with the following potential:

$$V_a = -\frac{\lambda}{r^2}\theta(r - a) - \frac{\rho}{a^2}\theta(a - r) \tag{5.1}$$

The important difference between this scheme and that in Section 4.2 is that ρ is variable, so that the potential is discontinuous at $r = a$. (This is just a finite discontinuity, though, and we see its like in the finite well every day.) The parameter ρ gives us something to trade in for our "energy," and has the advantage of describing exclusively short-distance interactions. Now our question becomes how to alter ρ as $a \to 0$ to keep the "physics" fixed. But what is the physics?

Before we answer this, let's generate a renormalization group flow for this scheme.

As usual, we use the square well matching relation for small a

$$qa \cot qa = \frac{1}{2} + \Xi \cot(\Xi \log ka + \delta).$$

Since $q \approx \sqrt{V}$, we can write this—defining $\chi \equiv \sqrt{\rho}$, and combining the logarithmic terms into $-\log a_0$—as

$$\chi(a) \cot \chi(a) = \frac{1}{2} + \Xi \cot\left(\Xi \log \frac{a}{a_0}\right). \tag{5.2}$$
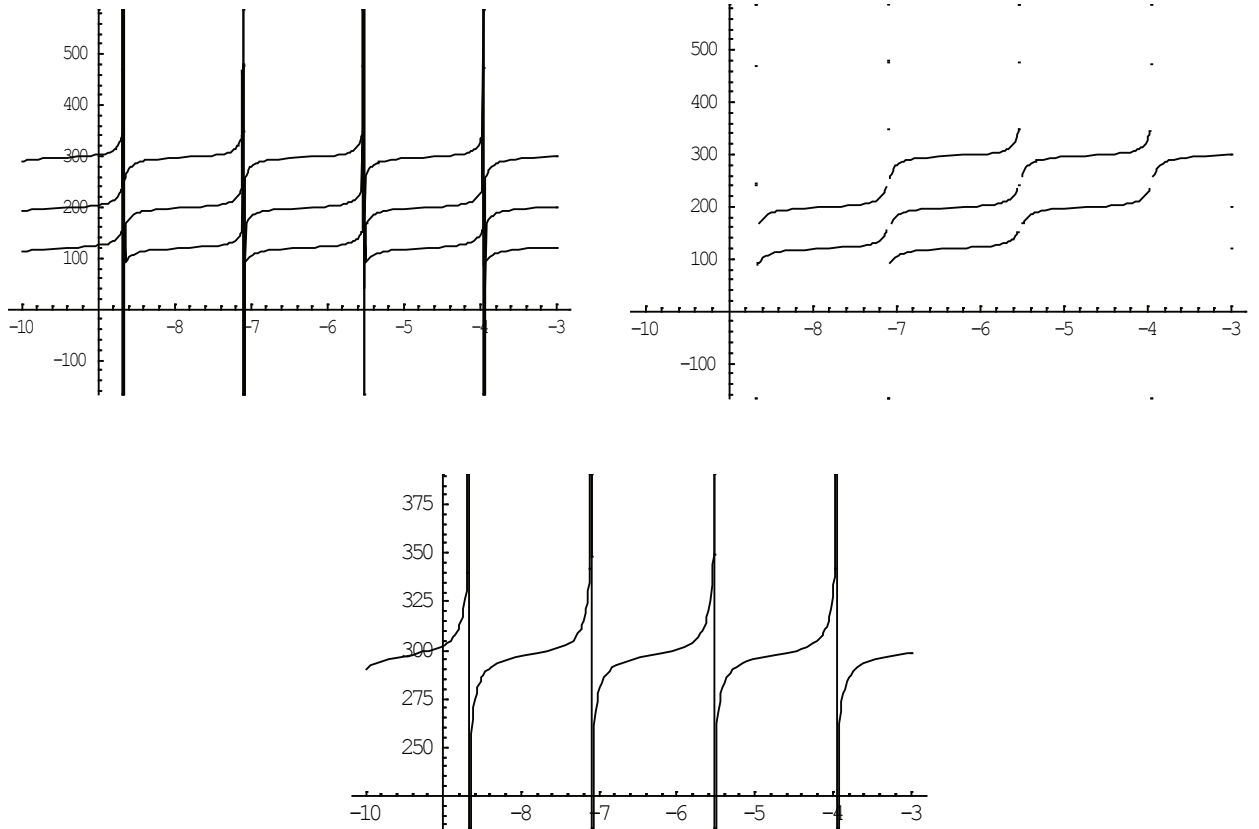
Figure 5.1: Multivalued solution, continuous path, log-periodic path. χ vs $\log ka$

What the cutoff at a does is separate our domain into a region of high-energy/short-distance physics and one of low-energy/long-distance physics. As we take a to 0, the shallow bound states (i.e. those with $a_0 \gg a$) have hardly any of their probability in the region of high-energy physics, so their *form* is mostly unaffected by the nature of the interaction there. This means, for instance, that they basically regain the discrete

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scale symmetry. Of course, if we kept χ fixed as $a \to 0$, a_0 (and therefore the bound state energy) would have to scale with a for the boundary conditions to match, so the lines would cease to represent constant physics.

The situation is different with deep bound states ($a_0 < a$), since much of their probability is in the high-energy region, and they are affected by the details of high-energy behavior. The flip side is that their wavefunctions are so localized that we need very high resolution to observe them—i.e. we need to scatter high-energy states off the potential, by $E = h\nu$. Therefore these bound states are not low-energy observables, and we need not require them to be invariant under renormalization.

The most intuitive paths through the RG flow are given by the continuous lines in the figure, which one gets by picking a bound state, fixing it, and changing χ continuously and monotonically. χ decreases as $a \to 0$—i.e. becomes weaker and then repulsive. A heuristic way to understand what's happening is as follows: let's think of the state index as the number of nodes in the the wavefunction, as we do in nonsingular cases. (Since our theory is regularized, this is finite to start with.) As we move a closer in, the inverse-square sector of our wavefunction gains wiggles rapidly, and so the high-energy sector must lose them correspondingly, which it does by increasing the potential. *Even if* the inside were a hard core, as we've seen in Section 4.1, the wavefunction would have arbitrarily many wiggles as a got smaller—and after that we would have no way to keep the state index. There is, therefore, a minimal length ϵ down to which our effective theory is valid for a given a_0. If we had higher resolution, we could pick a lower a_0—i.e. a deeper bound state—to treat as a low-energy observable, so this isn't necessarily a strike against the procedure. However, if we want a procedure that gives us bound states all the way down, we must use the so-called limit cycle (Fig 5.1).

This scheme is based on the fact that the regularized potential has infinitely many shallow bound states with a discrete scaling symmetry. (The infinitely many shallow bound states exist because of the slow falloff of the potential.) In the asymptotic region, fixing *any* bound state to be at a certain energy gives you the same self-adjoint extension and the same physics. (This corresponds to the picture of Chapter 3, where none of the wavefunctions has an index because they're all at ∞.) The log-periodic path exploits this fact by jumping discontinuously from fixing one bound state to fixing the one just deeper than it every time the wavefunction grows another node in the low-energy region.
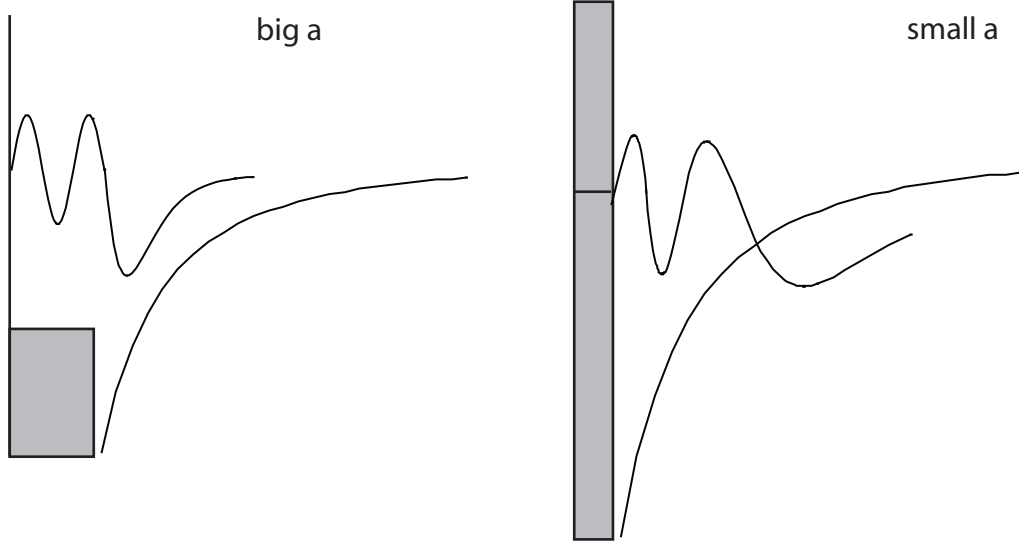
Figure 5.2: Where the Wiggles Go

This gets us all the way to the origin on any given path, but it doesn't give us a coupling corresponding to $a \to 0$, since our flow oscillates wildly near that point.

5.2   Flows, Revisited

We have already seen a couple of RG flows. The point of these diagrams is to give us an idea of how the lines of constant physics behave as $a \to 0$. The nomenclature comes from Wilson's analogy [34] with nonlinear dynamics. In nonlinear dynamics we are interested in what a system evolves to as $t \to \infty$. This is often dependent on initial conditions, e.g. for a free particle. However, it is often possible to make statements that hold for most initial conditions. For instance, a damped pendulum goes to the origin as $t \to \infty$ no matter what the initial conditions were. A feature like this is called an **attractor**. Another simple possibility is the limit cycle, which means that the system settles down into some sort of periodic behavior. This is the case, for instance, with the damped driven oscillator, which ends up moving at the driving frequency no matter what the initial conditions are. The natural properties of the oscillator show up only as a phase shift, analogous to Case's phase. These ideas can be mapped onto renormalization group flows by having $-\log ka = \log(a_0/a)$ correspond to t. In the RG, one thinks of short-distance behavior as a transient, and
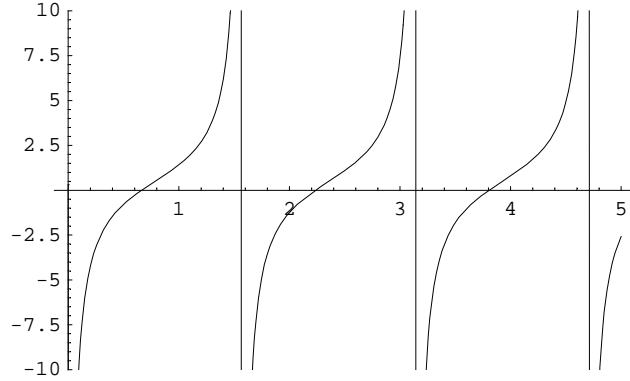
Figure 5.3: Delta Ring Cutoff, χ vs. $\log ka$

therefore not an important part of the asymptotic description of the system. We are eventually interested in the $ka \to 0$ sector, which is the $\log(a_0/a) \to \infty$ sector (which corresponds to $t \to \infty$ sector)—that is, energies that are arbitrarily weak relative to the cutoff.

5.3 Running δ-function

Instead of a square well, we could regularize the theory using a δ-function ring at radius a. This would give us the regularized potential

$$V(r) = -\frac{\lambda}{r^2}\,\theta(r-a) - \frac{\chi^2}{a^2}\,\delta(r-a)\,\theta(a-r) \tag{5.3}$$

We know how the 1D δ-function behaves, and we can use our matching strategy to obtain the RG flow equation:

$$\chi(a) = \frac{1}{2} - \Xi \cot\left(\Xi \log \frac{a}{a_0}\right) \tag{5.4}$$

This is a very different equation from that governing our previous flow, since χ isn't multivalued. This flow is plotted in Fig 5.3.

A limit cycle is our only solution. Intuitively the difference between this scheme and the previous one is that this time we don't have direct control over the number of wiggles inside the shell—or, therefore, on the total number of wiggles. The delta function cutoff is equivalent to sticking in a phase shift by hand. The dependence of deeper bound states on a under this scheme is explored in Ref. [32].

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Renormalization theory is interested with properties that are independent of the cutoff potential chosen; this makes the limit cycle a more appealing solution. (It might seem glib to infer universality from multiplicity, but limit cycle behavior is related to the discrete scale symmetry of the spectra.) Still, the difference is not terribly important in any particular case because both states produce the same asymptotic spectra.

5.4   The $1/r^4$ Potential

This was worked out in [36]. Most of our observations still hold; an important difference is that the zero energy wavefunction is

$$\psi(0; r) \sim r \sin\left(\frac{\lambda}{r}\right).$$

(Let's ignore the phase for a moment.) This oscillates rapidly at the origin, as we have learned to expect, but in the infrared regime it has no nodes for $r > \lambda/\pi$—as opposed to the $1/r^2$ potential, which has infinitely many nodes both ways. So if you impose an ultraviolet cutoff, $\psi(0; r)$ has only finitely many nodes, and—since it is the shallowest bound state—$\psi(-E; r)$ has as many or fewer. Therefore, the regularized solution has only finitely many bound states, and the continuous path preserves the number of bound states.

As before, we can regulate the potential with a square well cutoff or a ring cutoff. The procedure is a little harder than before because we lack usable analytic expressions for anything but the zero energy solution. However, the state we are fixing is a shallow state, so for a short-distance cutoff it's reasonable to take $|E| \ll |V|$ and use the zero energy outside solution. With this, our wavefunction is

$$\psi(0; r) = \begin{cases} A \sin qr & r < a \\ Br \cos\left(\frac{\lambda}{r} + \phi\right) & r > a \end{cases} \tag{5.5}$$

ϕ is a phase shift between the cosine and sine exterior solutions. The boundary condition one gets by imposing continuity at $r = a$ is

$$q \cot qa = \frac{1}{a} + \frac{\lambda}{a^2} \tan\left(\frac{\lambda}{a} + \phi\right),$$

which we can rewrite as

$$qa \cot qa = 1 + \frac{\lambda}{a} \tan\left(\frac{\lambda}{a} + \phi\right). \tag{5.6}$$

Now qa is just the inside coupling, which we can call α_{in}, and we can write λ/a as α_{out}. (λ is fixed for our purposes, so this is an inverse cutoff radius.) This gives us the final flow equations:

$$\alpha_{in} \cot \alpha_{in} = 1 + \alpha_{out} \tan(\alpha_{out} + \phi).$$

Evidently there is a branch that's periodic in α_{out}, but this doesn't correspond to any particularly nice symmetry.
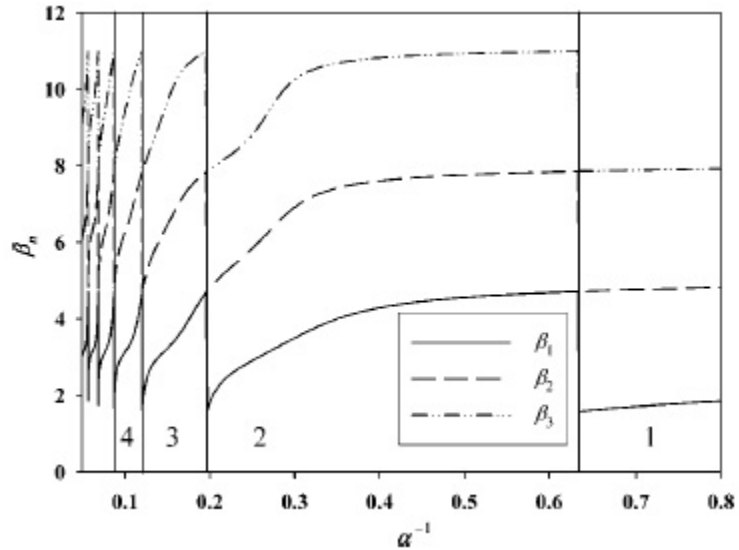
Figure 5.4: RG Flow for $1/r^4$ potential. Reproduced from [36].

Following what Braaten and Phillips do, we might try regularizing with a δ-function ring. The internal zero-energy solution is $Ar+B$, and the boundary condition at the δ-function at a is

$$\psi'(a^+) - \psi'(a^-) = \frac{1}{a}\gamma\psi(a).$$

where the delta-function ring has strength γ/a^2 since we're working in three dimensions. Dividing through by $\psi(a)$ and plugging in the functions, we get

$$1 + \alpha_{out} \tan(\alpha_{out} + \phi) = \gamma(a)\left[+\frac{A}{B}a\right], \tag{5.7}$$

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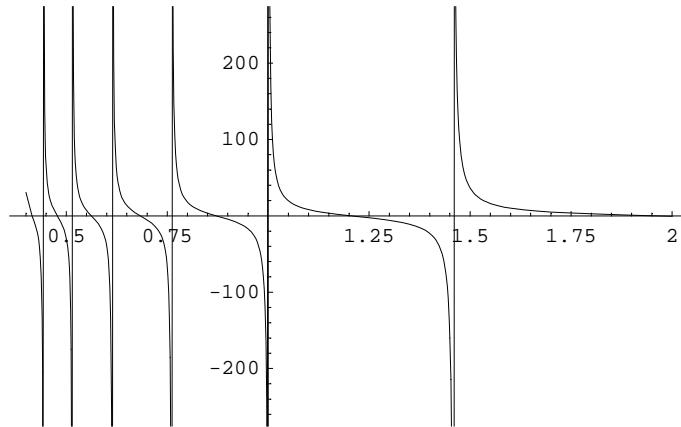
Figure 5.5: χ vs. α^{-1}

and the last term can be dropped for small a. Similarly to the $1/r^2$ case, this cutoff scheme gives us only limit cycle-like behavior.

Note that as $a \to 0$, the lhs goes through infinity repeatedly, as you'd expect, so there are *no* fixed points of the flow.

5.5   Scaling Properties

Refs. [37] and [38] use a somewhat different way of looking at renormalization group flows. The idea behind their work is to replace the potential with a boundary condition at some length scale, and investigate how the boundary condition behaves at different length scales. As their paper is fairly detailed, we merely present an outline of the strategy.

To specify a solution to a Schrödinger equation on (a, ∞) it suffices to give the logarithmic derivative $g(r) = r\psi'(r)/\psi(r)$ for all energies at $r = a$. The purpose of their work is to see how g scales with a. This is one of the general aims of renormalization theory, which is concerned with the separation of energy scales that makes renormalization possible. It's helpful to recast the Schrödinger equation in terms of dimensionless variables $x = r/a$, $\kappa = ka$, $U = Va^2$, so that our boundary condition is applied at $x = 1$:

$$\left[-\frac{d^2}{dx^2} + U(x) \right] \psi(x) = \kappa^2 \psi(x)$$

$$x \frac{\psi'(x)}{\psi(x)} \bigg|_{x=1} = g(1, \kappa)$$

(We use a slightly nonstandard form of the logarithmic derivative in order to make g dimensionless.) Of course, we could impose the boundary condition at any other value of x, say $x = \lambda$. It would be useful to have the new equation be as close to the form of the old ones for comparison, so we might want to express the boundary condition as $x/\lambda = 1$. What we really want to do is rescale the Schrödinger equation so that the boundary condition is of the form $x = 1$ (we will see the benefit of this when we are done); this is done by dilating the Schrödinger equation, as we did in ch. 1, but since we are not necessarily working with scale invariant potentials we have to be careful. The first step is to dilate the wavefunction:

$$\psi_\lambda(x) = \psi(\lambda x)$$

So when you differentiate it with respect to x a factor of λ pops out, and for the Schrödinger equation to retain its form the potential must scale appropriately, so that

$$U_\lambda(x) = \lambda^2 U(\lambda x)$$

and

$$\kappa_\lambda = \lambda^2 \kappa.$$

The boundary condition scales as it should:

$$g_\lambda(x, \kappa_\lambda) = g(\lambda x, \kappa).$$

In terms of these variables our scaled equations look like our original equations:

$$\left[-\frac{d^2}{dx^2} + U_\lambda(x) \right] \psi_\lambda(x) = \kappa_\lambda^2 \psi_\lambda(x)$$

$$x \frac{\psi'_\lambda(x)}{\psi_\lambda(x)} \bigg|_{x=1} = g_\lambda(1, \kappa_\lambda)$$

We can write formal expressions for how U_λ and g_λ depend on λ. We are interested in two cases, the $\lambda \to 0$ limit, which corresponds to probing the system at short distances and is related to our cutoff schemes, and the $\lambda \to \infty$ limit, since that corresponds to asymptotic low-energy properties.[1] It's possible to get a fair amount

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[1] Mueller and Ho [37] are interested mostly in the $\lambda \to \infty$ properties.

of information out of the problem from the form of U_λ. For a potential that falls off slower than $1/r^2$, U_λ tends to become very large as $\lambda \to \infty$, and for one that falls off faster it tends to vanish. Scale invariant potentials don't do anything at all. This is linked to the fact that some potentials are more "active" in some regimes; for instance, the $1/r$ potential has infinitely many shallow bound states, while the $1/r^4$ potential has infinitely many deep bound states.

The relation for the boundary condition is derived from the following form of the Schrödinger equation in terms of logarithmic derivatives:

$$x\frac{\partial g}{\partial x} = x^2(U(x) - E) + g(x) - g(x)^2$$

If we plug in all the scaling factors and do out the algebra, the scaled version of this is

$$\lambda\partial_\lambda g_\lambda(x, \kappa_\lambda) = x^2(U_\lambda(x) - E_\lambda) + g_\lambda(x, \kappa_\lambda) - g_\lambda^2(x, \kappa_\lambda) \tag{5.8}$$

We are not interested in the dependence of g_λ on x, since we only ever evaluate it at $x = 1$, so we can write it as $g_\lambda(\kappa_\lambda)$, and expand out in powers of κ. We are most interested in low-energy solutions, so we can drop all powers of κ and investigate leading behavior. (At least, it's worth a try.) For the case of the inverse-square potential, since U doesn't flow, we find that the equation is

$$C + g - g^2 = 0. \tag{5.9}$$

For $C > -1/4$, this equation has two real roots; otherwise, it has complex roots, which do not correspond to a self-adjoint boundary condition. (For more on this, see ch. 6.) This shows that there isn't a single asymptotic solution for the boundary condition. These properties are the same at both the infrared and ultraviolet ends, which is expected since the $1/r^2$ potential done by the method of self-adjoint extensions has an exact limit cycle at all levels.

The scaling method also gives us a pleasing duality between the behavior of long-range forces like $1/r$ in the infrared and shorter-range forces like $1/r^4$ in the ultraviolet. (We are thinking of the attractive behavior; the repulsive potentials always have a fixed point at the Friedrichs extension.) The fixed point, as $\lambda \to 0$ or $\lambda \to \infty$, is $U \to -\infty$ in this case. Ref. [37] works out the infrared case; we do the ultraviolet, which is more relevant to our purposes. By construction of our boundary condition, $x = 1$ always, so for a low energy state,

$$\lambda \partial_\lambda g_\lambda = -U(1)\frac{1}{\lambda^m} + g_\lambda - g_\lambda^2 \tag{5.10}$$

where $m = -n + 2$ for an x^n potential. Since the only dependence is on λ, we can rewrite the partial derivatives as total derivatives, and consider

$$\lambda \frac{dg}{d\lambda} - g + g^2 = -\frac{a^2}{\lambda^m}$$

which can be solved in terms of Bessel functions of argument $1/x^{m/2}$. For the particular case of the $1/r^4$ potential, Mathematica yields

$$g(\lambda) = \frac{(-\lambda + aA)\cos\left(\frac{a}{\lambda}\right) - (a + A\lambda)\sin\left(\frac{a}{\lambda}\right)}{\lambda\left[\cos\left(\frac{a}{\lambda}\right) + A\sin\left(\frac{a}{\lambda}\right)\right]}$$

Asymptotically this is

$$g(\lambda) \sim \frac{a}{\lambda}\frac{A\cos\left(\frac{a}{\lambda}\right) - \sin\left(\frac{a}{\lambda}\right)}{\cos\left(\frac{a}{\lambda}\right) + A\sin\left(\frac{a}{\lambda}\right)}.$$

The form of boundary condition that we've used earlier is $\lambda g(\lambda)$, so this is consistent. The condition is periodic in $1/\lambda$, as we found by our previous methods. One can escape the periodicity only by allowing λ to take on complex values in order to turn the trig functions into hyperbolic functions. Doing this corresponds to the complex boundary conditions that we discuss in the next chapter. Interestingly, the flow behavior of long-range potentials as $\lambda \to \infty$ is very similar to this (for details, see [37]).

The $\lambda \to \infty$ limit of this potential is also interesting because it actually has a fixed point. In this case, $U \to 0$ for the $1/r^4$ potential, and therefore (for the zero-energy solution) the equation becomes:

$$\lambda \frac{dg}{d\lambda} = g - g^2$$

The solution to this is

$$g(\lambda) = \frac{\lambda}{-C + \lambda}$$

which flows to 1 as $\lambda \to \infty$. This is a manifestation of the fact that the potential has no infrared pathologies because it falls off sufficiently fast. However, the short distance physics still affects our low-energy observables, and renormalization of the ultraviolet spectrum is still required; for example, the zero-energy phase shift is determined by Case's phase/a regularization scheme:

$$\psi(0, r) = Br \cos\left(\frac{\lambda}{r} + \phi\right)$$

and therefore the scattering length a is given by

$$a = \lambda \cot \phi.$$

The scaling technique is equivalent to the δ-function ring cutoff in the ultraviolet, since both in effect specify the logarithmic derivative of the function at the boundary point. The difference is one of interpretation. In one case, you squeeze the function in and out of the $r = 1$ area by stretching and contracting the coordinate variable and find out how the logarithmic derivative evolves; in the other, you counteract the changes of the outside region by adding a term to the logarithmic derivative that's big enough to cancel it out.

5.6   Consistency with Chapter 4

We now have two different pictures of the $1/r^2$ potential—one with a single bound state and another with infinitely many. The cutoff methods and self-adjoint extensions both give the (asymptotic) relation

$$\frac{E_n}{E_m} = e^{2(n-m)\pi/\Xi}.$$

As $\Xi \to 0$, if we fix an arbitrarily chosen bound state E_m at k, both methods agree in sending all others with $n < m$ to zero. However, the method of self-adjoint extensions sends a whole family of states $m < n$ to $-\infty$, whereas the cutoff schemes of Ch. 4 do not have these states at all. Don't the deep states matter? The answer is that they don't, from our EFT perspective, because they are highly localized, and therefore cannot be probed unless we have arbitrarily good resolution—in which case we know the theory exactly at all energies and renormalization is unnecessary.

For example, one of the ways to detect a bound state is to look for poles in the scattering length or, equivalently, in $\tan \delta_0$. Levinson's theorem (see Chapter 7 or [62]) says that the scattering phase shift goes through $N\pi$ as k is increased from 0 to ∞, where N is the number of bound states. (We require that it be a monotonic function of k, which is why it goes through π instead of going back to zero.) However,

to detect a bound state with energy k_b you need to be able to send in a beam of energy k_b, and this ensures the privacy of deep bound states.

From what we've seen so far it seems that RG flows asymptotically produce the same behavior as self-adjoint extensions. This is not too surprising if you think of self-adjoint extensions as corresponding to the possibilities for point interactions at the origin. The renormalization techniques we have used in this chapter work by adding smeared-out point interactions, and self-adjoint extensions are the limiting forms as $ka \to 0$. This would explain, for example, why the self-adjoint extensions of the $1/r^2$ potential have a limit cycle going all the way down. This is also why self-adjoint extensions are not a complete treatment of any physical problem; at some energy level we enter the regime of transient (high-energy) physics, where the true potential differs from its asymptotic form.

Spectra Unbounded from Below

Strongly attractive power-law potentials have very often been rejected as unphysical because they have spectra unbounded from below. But as our treatment in this chapter has shown, as far as the two-body self-adjoint problem is concerned the unboundedness is not an issue, and in fact it's impossible even to tell—except with infinite energy resolution—whether a given potential is unbounded from below. No doubt there are several physical situations where such a potential would be entirely unacceptable; however, as we see in the context of the Efimov effect [27], there are some where it gives a powerful description of the physics.

The fact that the asymptotic solution is unbounded also gives us a way of classifying renormalization schemes. We saw earlier in this chapter that the continuous paths would not go all the way down, and mentioned that this was due to unboundedness. This connection is important, so let's go over it more carefully. Given a regularization scheme Σ of the λ/r^2 potential, we denote the regularized potential by $V(\Sigma, a, x)$ and the lower bound (see Chapter 2) of the Hamiltonian by $B(\Sigma, a)$. For $|x| > a$, $V(\Sigma, a, x) \equiv V(x)$ for all regularization schemes. Clearly, if $V(\Sigma, a, x) \leq V(\Sigma', a, x)$ at all $x \in \mathbb{R}^n$, then $B(\Sigma) \leq B(\Sigma')$. Therefore, for all cutoff regularization schemes, $B(\Sigma, a) \leq B(\Sigma_0, a)$, where Σ_0 is an infinite barrier for $|x| < a$. Since $B(\Sigma_0, a) \to -\infty$ as $a \to 0$ (new wiggles, and new states, keep appearing at a log-periodic rate), $B(\Sigma, a) \to -\infty$ too.

Now suppose we want to fix a bound state of index j. This is the same as fixing

the ground state (or bounding the ground state energy from below), and is therefore equivalent to fixing $B(\Sigma, a)$ as we take $a \to 0$. We know we can't do this because $B(\Sigma, a) \to -\infty$ as we just proved. This shows us that *no* regularization scheme that keeps the long-distance physics fixed can also fix the bound state with j nodes; thus the suggestion in [31] that the unbounded spectrum might result from using the wrong point interaction is invalidated. For the $1/r^4$ potential, it shows that there is no way to renormalize the system to arbitrary distances so that it has a fixed number of bound states. On the other hand, it also shows that any renormalization scheme that maintains the lower bound of the spectrum must force the coupling up to the critical value, where it becomes a Klauder phenomenon, as discussed in Chapter 7.

This argument is harder to make rigorous for schemes like Schwartz's, but clearly the basic idea carries through. The bound of the regularized theory goes smoothly to $-\infty$, and if you fix it the only way to keep the bound is to change the theory continuously so that in the limit you get a bounded theory. This clearly can't still be very singular, so one has to push it up to the critical point where the theory becomes bounded. For the $1/r^2$ potential this is at $\lambda = -\frac{1}{4}$; for more singular potentials it's at zero coupling (the renormalized theory is a delta function).

5.7   RG Treatment of Weak Coupling

Let's return to the non-Friedrichs extensions we discussed in chapter 3 with our new apparatus, which allows us to talk about the extensions of the $1/r^2$ potential from a more physical point of view.

5.7.1   What Sort of Physics?

A curious feature of these extensions is that a potential that appears to be everywhere positive has states of negative energy. It has been suggested ([20],[51]) that this is due to δ-function interactions. It is certainly true that *all* short-distance physics is due to delta function-like operators from an EFT point of view; however, it turns out not to be true that

$$V = \frac{\lambda}{x^2}\theta(x - a) - \frac{\beta}{a}\theta(a - x)$$

produces one of these extensions as $a \to 0$. From our usual boundary condition

$$qa \tan qa = \frac{1}{2} + ka \frac{K'_{\zeta+1/2}(ka)}{K_{\zeta+1/2}(ka)}$$

since $qa \sim \sqrt{\beta a} \to 0$, we can use the small-angle approximation, so that (letting $\xi \equiv (ka/2)$ and $\nu = \zeta + 1/2$)

$$\beta a = \frac{1}{2} + \nu \frac{\xi^\nu \Gamma(-\nu) - \xi^{-\nu} \Gamma(\nu)}{\xi^\nu \Gamma(-\nu) + \xi^{-\nu} \Gamma(\nu)} \tag{5.11}$$

There are two easily solved cases. The first is when ν is sufficiently big that we can drop the x^ν terms; the other is when $\nu \to 0$. In the first case, the equation reduces to

$$0 \approx \beta a = \frac{1}{2} - \nu \Rightarrow \nu = 1/2 \Rightarrow \lambda = 0 \tag{5.12}$$

so the only solution is our old acquaintance the delta function. When $\nu \ll 1$ we can use $\Gamma(\nu) \sim 1/\nu$ to get

$$0 = \frac{1}{2} - \nu \frac{\xi^\nu + \xi^{-\nu}}{\xi^\nu - \xi^{-\nu}}$$

and the rhs is recognizably hyperbolic:

$$\frac{1}{2} = \nu \coth(\nu \log \xi) \Rightarrow \nu \leq \frac{1}{2} \Rightarrow \lambda \leq 0 \tag{5.13}$$

and therefore the potential must be attractive for bound states to exist. This is telling us less than we assumed, since anything in the $\nu \approx 0$ regime is attractive.

So what sort of attractive point potential would work? The following theorem, due to Simon [85], is suggestive:

Theorem 8 (Simon, 1975) *Given a (not wildly pathological) 1D function $V(x)$ such that*

$$\int_{-\infty}^{\infty} (1 + x^2) |V(x)| dx < \infty,$$

the Hamiltonian with potential λV has a bound state for small $\lambda > 0$ iff

$$\int_{-\infty}^{\infty} V \, dx \leq 0,$$

and if the integral is zero, then the potential has a bound state for all $\lambda > 0$.

As it happens our inverse square potential doesn't fit Simon's hypotheses because of its long-range character, but if we cut it off at a suitable $R \gg 1/k$ the theorem becomes applicable. Consider the potential

$$V = \frac{\lambda}{x^2}\theta(R-x)\theta(x-a) - \frac{\beta}{a^2}\theta(a-x)$$

If $\beta > \lambda > 0$ then this potential supports a bound state for arbitrarily large R. Of course, the bound state energy might depend on R—though this is unlikely, since the state is much more localized than the potential. Anyway, Simon's theorem motivates us to see if this potential works. We are forced to choose the weak *interior* coupling regime to expand out $\tan qa = \sqrt{\beta}$. The boundary condition permits nontrivial results this time: $\beta = -\lambda$ for biggish λ, and $\beta < -\lambda$ for small λ. However, the limit is problematic, and you can see this directly from the fact that the only dimensional parameter in the problem is a.

So we have an irregular theory, and some kind of renormalization is called for. What we need to do is run either β or λ against k and see if the theory can be renormalized. Simon's theorem might suggest that somehow one should try and keep the integral fixed; this entails fixing a relationship between β and λ. This is a bad idea, since one will have to force the external coupling to zero as $a \to 0$, and this will give us back the delta function.[2] So we run the coupling of the short-distance term against the cutoff radius a. (For the moment let's assume $\nu \approx 0$.) The flow equation is similar to that in Beane's case:

$$-\chi(a)\tan\chi(a) = \frac{1}{2} - \nu\coth(\nu\log(a/a_0))$$

where we've used the previous approximation. But the flow looks like this:

Unexpectedly, χ blows up at a_0, which means that β blows up at a_0. There are infinitely many choices of path for smaller values of χ, but all of them flow to $\chi = 1/2$ or some bigger χ. Using a delta function regulator forces χ to flow to $1/2$. Both solutions correspond to a counterterm of the form $\delta(x)/x$, but it's unclear why the square well regularization gives you so much freedom.

Looking at the wavefunctions makes it evident that the potential is pathological in one dimension, at least in the attractive case, since both solutions $x^{1-\zeta}$ and x^{ζ} vanish at the origin. For one dimensional potentials a ground state that vanishes at the origin is abnormal, and has been conjectured [98] to imply an impenetrable barrier at the origin.

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[2]We're assuming a result from Chapter 7.
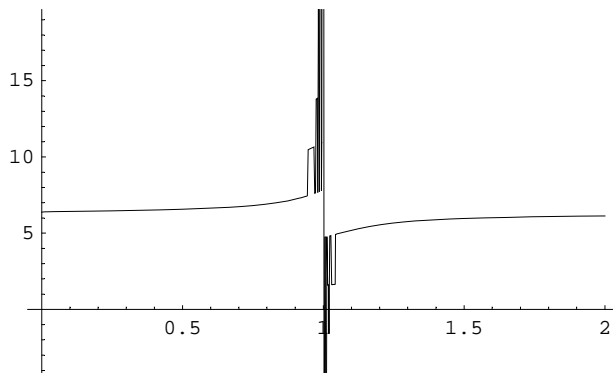
Figure 5.6: RG Flow for Weak 1D Case. χ vs. a

Now let's consider the weakly repulsive regime; in this case the boundary condition (using a delta function regulator) is

$$-\chi(a) = \frac{1}{2} - \nu \left[1 - 2\frac{\Gamma(-\nu)}{\Gamma(\nu)} \left(\frac{ka}{2} \right)^{2\nu} \right] \tag{5.14}$$

where $\nu > 1/2$. This time it's evident that as $a \to 0$,

$$\chi(a) = \frac{1}{2} - \nu$$

so χ flows to $\frac{1}{2} - \nu = -\zeta$, and once again the result is a function of the form $\delta(x)/x$. This is independent of k, so it's a fixed point (attractor) of the RG flow.

5.7.2 Critical Coupling

We know how to renormalize this problem in two different ways. The first, more intelligible, method is to transform it into the 2D free particle equation as suggested in Chapter 3 (i.e. by the transformation $v(x) = \psi(x)/\sqrt{x}$), and renormalize it with square wells as in Chapter 1; the second is to use any of the regularization schemes of Chapter 4. The results are the same; one gets a bound state with wavefunction $\sqrt{kr}K_0(kr)$. (And the same s-wave phase shift too, see Chapter 7.) One should point out, though, that the ground state wavefunction is pathological in one-dimensional QM, since it vanishes at the origin and has an infinite derivative there.

5.7.3 Two Dimensions

(Recall that in two dimensions the weak regime is for $0 \le \lambda < 1$.) Suppose we try regular 2D delta functions: the matching condition for $\nu \ll 1$ is

$$\beta = \nu \coth(\nu \log(ka/2)). \tag{5.15}$$

If long-distance physics is fixed then $\beta \to -\nu$ as $a \to 0$, independent of k. (We approximated out the Bessel function; For small ν consistency demands small β.) Here, again, we have a fixed point in the flow, and it corresponds to an *unregularized* 2D delta function. Amusingly, this equation explains "why" the 2D delta function needs to be renormalized, since $\nu = 0$ requires $\beta = 0$ too. For less weak coupling the expression is not as compact, but the result is pretty similar:

$$\sqrt{\beta}\frac{J_0'(\sqrt{\beta})}{J_0'(\sqrt{\beta})} = -\nu$$

5.7.4 Conclusions

In two dimensions it's reasonably clear what's going on. There's a delta function interaction at the origin that just overcomes the repulsive enveloping potential; it flows to a fixed point under renormalization, because a finite-strength delta function is too strong in two dimensions (see Chapter 1). The three-dimensional problem, too, is relatively sensible; we used Meetz's regularization scheme [6] in Chapter 3 to argue for the Friedrichs extension. With the one dimensional repulsive case, too, one can argue for the Friedrichs extension from the positivity of the potential. However, as Simon's theorem proves, a regularized 1D attractive potential does have a bound state.

The wavefunction is pathological at the origin, but this doesn't affect low-energy physics. Once we know that there are (a) self-adjoint extensions and (b) reasonable renormalization schemes, our work as physicists is done. It's entertaining to speculate about the "true causes" of pathologies, but a good answer isn't necessary, which makes one feel better about not having one.

Chapter 6

Fall to the Center

In the classical two-body problem, **fall to the center** happens if the particles collide at a finite time. For the $l \neq 0$ case—which is the interesting one, classically—the centrifugal barrier must be overcome, and a class of potentials that does this is the attractive $1/r^n, n \geq 2$ potentials. Under these potentials, the two bodies are moving infinitely fast towards each other as they collide, so the boundary conditions for the collision are ill-defined. If the collision is elastic, they bounce back in a way that keeps the solution time-reversal invariant, moving with infinite velocity at first. If we had a bound state (total $E < 0$) to begin with, this motion is repeated endlessly. The total energy of the system is conserved; this corresponds to the quantum mechanical problem as we have been doing it, in which a bound state evolves without dissipating energy. Classically the collision might also be inelastic; the particles might stick together after they collide. The energy has got to go somewhere, even in the classical view, but if we aren't interested in the details it's easy to treat the energy as just being dissipated. The self-adjoint operator formalism of quantum mechanics does not permit this general sort of dissipation, however, since the (unitary) time evolution of a state is given by $\psi(t) = e^{-iEt}\psi(0)$ for an eigenstate, and evidently[1]

$$\langle H \rangle_{\psi(t)} = \langle \psi(t) \,|H|\, \psi(t) \rangle = e^{-iEt}e^{iEt} \langle \psi(0) \,|H|\, \psi(0) \rangle = \langle H \rangle_{\psi(0)}$$

and energy is conserved for eigenstates. Since any Hermitian operator has a complete set of eigenstates, it has at least some nontrivial eigenstates (bound or not); but in the classical picture with an inelastic collision, there simply can't be any energy eigenstates.

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[1] I have used Dirac notation this once because the ideas are so familiar.

The quantum theory of inelastic collisions [62] deals with this problem by introducing the so-called multiple-channel method, where energy and probability are allowed to slosh back and forth among the "channels" corresponding to interactions of the subsystems. Energy is conserved for the whole system, but not in any particular channel; therefore, projections of the Hamiltonian to a particular channel are not necessarily self-adjoint operators. Note, however, that as the Hamiltonian is not time-dependent, neither are its projections.[2]

A special case of this idea is when incoming particles are absorbed at the origin; this leads to probability loss, as well as energy loss, from the system. Clearly, one way to get this would be if we had complex eigenvalues of the form $E_x - iE_y$, since this would lead to time evolution given by

$$\langle \psi(t) | \psi(t) \rangle = e^{-2E_y t}$$

and the probability of finding the particle anywhere would decay exponentially.

6.1   Contraction Semigroups

The time evolution operators $U(t) \equiv e^{iHt}$ form a group under composition, since $U(t)U(t') = U(t+t')$, and each element has the inverse $U(-t)$, which is also unitary. Probability-dissipating operators $V(t)$ have the same additive property, but their inverses create probability—so the group splits into two parts, called semigroups. The semigroup that dissipates probability is called a **contraction semigroup**; these structures are common in mathematical physics, especially in the study of the heat equation. The generator of a contraction semigroup is called a **dissipative** operator. The theory of semigroups has been extensively developed, and most results are too technical to be directly helpful; in practice one typically just assumes that complex phase shifts work because they seem to. This is the attitude, for instance, of Schiff [61]. The exception is the relation linking semigroups and the machinery of self-adjoint extensions, which we will now discuss.

Recall from Chapter 2 that a densely defined Hermitian operator generates unique unitary time evolution iff its deficiency indices are $(0,0)$. For deficiency indices $(1,1)$

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[2]This is the Schrödinger picture, in which wavefunctions carry the time dependence. If one were particularly interested in energy loss one might prefer the equivalent Heisenberg picture, in which the operators (dynamical variables) of the theory carry the time dependence.

we saw that the self-adjoint extensions were parameterized by $U(1)$, a one-parameter family of boundary conditions. One way to represent $U(1)$ is as $e^{i\theta}$. One is motivated by mindless curiosity, as usual, to ask what happens if θ is permitted to be complex. Since $|e^{a+ib}| = e^a$, this is the same as asking what happens if, instead of extending our domain by functions of the form

$$\Psi_+ + e^{i\theta}\Psi_-,$$

we allow

$$\Psi_+ + Ae^{i\theta}\Psi_-$$

for some fixed $A \in \mathbb{R}^+$ (or as $\Psi_+ + z\Psi_-$ for $z \in \mathbb{C}$). (This isn't all that unreasonable, since many of the examples of Chapter 2 make sense with complex boundary conditions.) Now suppose we wanted to prove that our self-adjoint extension G was in fact self-adjoint: one way to do this would be to check for complex eigenvalues of the form $c = a + ib$ by solving $(G - c)\psi = 0$, or $(\psi, (G - c)\psi) = 0$ for an arbitrary $\psi \in D_G$. ψ can be written as $\phi + \lambda(\Psi_+ + e^{i\theta}\Psi_-)$, so that

$$
\begin{aligned}
0 &= (\psi, H\psi) \\
&= (\phi, H\phi) + \lambda(\phi, H(\Psi_+ + e^{i\theta}\Psi_-)) + \overline{\lambda}((\Psi_+ + e^{i\theta}\Psi_-), H\phi) \\
&\quad + |\lambda|^2(\Psi_+ + e^{i\theta}\Psi_-, H(\Psi_+ + e^{i\theta}\Psi_-)).
\end{aligned}
$$

Of these the first term is the expectation value of a Hermitian operator in its domain, so it must be real. Because $\phi \in D_H$, the domain of the original symmetric operator, we can rewrite the second pair of terms as

$$\lambda(H\phi, \Psi_+ + e^{i\theta}\Psi_-) + \overline{\lambda}(\Psi_+ + e^{i\theta}\Psi_-, H\phi).$$

These terms are conjugates, so their sum is real. Note that this only uses the fact that Ψ_+ and Ψ_- are in the adjoint domain. Similarly, the last term can be rewritten as

$$|\lambda|^2\left[i - i + ie^{i\theta}(\Psi_+, \Psi_-) - ie^{-i\theta}(\Psi_-, \Psi_+)\right] \tag{6.1}$$

and since the last two terms are just conjugates this vanishes. Therefore,

$$\Im[(\psi, (H - c)\psi)] = \Im[(\psi, H\psi)] + \Im[(\psi, -c\psi)] = \Im[-c(\psi, \psi)] = -b \neq 0.$$

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A fortiori, $(H - c)\psi \neq 0$ and c is not an eigenvalue. Now suppose that $\psi = \phi + p\Psi_+ + q\Psi_-$, which is a more general boundary condition. The first two terms would still cancel out, and the third term would be

$$|\lambda|^2 \left[i|p|^2 - i|q|^2 + i\bar{p}q e^{i\theta}(\Psi_+, \Psi_-) - ip\bar{q}e^{-i\theta}(\Psi_-, \Psi_+) \right] \tag{6.2}$$

The cross terms are still conjugates and add up to give a real value, but that leaves us with the certainly imaginary quantity

$$i|\lambda|^2(|p|^2 - |q|^2).$$

For a complex eigenvalue to have any chance of working, the condition is that

$$|\lambda|^2(|p|^2 - |q|^2) = b.$$

Since p and q are determined by our choice of self-adjoint extension, b is fixed by the boundary condition, and in particular, is always going to have the same sign. This gives us an important result:

Theorem 9 *All the eigenvalues of extensions of a symmetric H are in the same closed half-plane.*

(Our discussion of this result has followed Ref. [7].) The boundary condition is either entirely a source or entirely a sink, that is, probability is either only created or only lost. This might seem trivial, but it isn't; we could have had eigenvalues in both half-planes, in which case we would have a mixture of source and sink behavior for different states.

In the rest of our treatment we will assume that permitting complex θ is equivalent to permitting complex numbers instead of real numbers in our boundary conditions. These complex eigenvalues are about the furthest meaningful generalization we can make. Suppose we try to use the whole adjoint as our nonunitary Hamiltonian, and send in a scattering state along the half-line. When it gets to the origin, it doesn't know what to do because there's no boundary condition there, and we cease to have a well-defined problem.

6.2   Dissipative Particle on Half-Line

In Chapter 2, we had derived the boundary condition for a particle on the half-line to be

$$\psi(0) = \alpha\psi'(0)$$

Let $\alpha = ia$. Suppose we send in a scattering state $Ae^{-ikx} + Be^{ikx}$. The boundary condition enforces $A + B = ka(A - B)$. For $a = 0$, the boundary condition is $A = -B$, which is self-adjoint. (This is the Friedrichs extension.) As we increase a,

$$B = \frac{1 - ka}{1 + ka}A$$

so the amplitude of the reflected wave diminishes until at $ka = 1$ it vanishes altogether. However, as we increase k further we get back some reflection, and B/A asymptotically approaches 1 again. The vanishing of the reflected wave for certain values of k is familiar from wave mechanics.

One might interpret the absorptive solution as saying that there's no outgoing wave and the particle has been absorbed at the origin—or, more mundanely, just transmitted through the origin. This is a good example of how complex phase shifts work; we can replace all information about the negative half-line with a boundary condition. It cannot be emphasized enough that using a dissipative Hamiltonian on a subspace does not necessarily imply pathological behavior on the whole space or in the physical problem.

The boundary condition $\alpha = ia$ does not permit any bound states. But letting $\alpha = -(1-i)a$ gives us a normalizable eigenfunction of energy $-\left(\frac{1}{a-ai}\right)^2$, which decays exponentially with time.

6.3   Absorption by a $1/r^2$ potential

The first treatment of absorption by singular potentials is by Vogt and Wannier (1954) [8], who worked the scattering problem for $1/r^4$ potentials. Perelomov and Popov (1970) [20] treated absorption by a $1/r^2$ potential in some detail, and Alliluev (1971) [21] proved that the set of eigenfunctions was complete. The solution of greatest interest corresponds to complete absorption. The interest in this solution is chiefly due to three features: its similarity to the classical limit *with absorption*, its analytic relation to the weakly attractive problem, and its connection with the experimental realization of $1/r^2$ potentials by scattering neutral atoms off a charged wire [23]. In addition to these, it is the only extension for which scale invariance holds.

To keep the problem as simple as possible—and also to relate it directly to experiment—we will work in two dimensions. We saw previously how a boundary condition can be derived from the method of self-adjoint extensions for this potential; here we will merely cite the result:

$$\frac{i\nu\psi + r\psi'}{i\nu\psi - r\psi'} = \frac{\Gamma(-i\nu)}{\Gamma(i\nu)}\left(\frac{k_b r}{2}\right)^{2i\nu} \tag{6.3}$$

Self-adjoint extensions correspond to real choices of k_b, for which the rhs has magnitude one; allowing k_b to be complex relaxes this restriction. In particular, it allows us to pick a sort of "Friedrichs extension," in which the solution corresponding to $J_{-i\nu}$ vanishes.

It's easiest to work the scattering problem by requiring that $\psi \sim (kr)^{-i\nu}$ near the origin. If the form we send in is $AJ_{i\nu} + BN_{i\nu}$, this means that

$$\frac{B}{\pi}\Gamma(-i\nu)\cosh(\pi\nu) = \frac{A}{\Gamma(1 + i\nu)} \tag{6.4}$$

which means that

$$\frac{B}{A} = \frac{\pi}{\Gamma(-i\nu)\Gamma(1 + i\nu)\cosh(\pi\nu)}. \tag{6.5}$$

This can be simplified, using the reflection formula for gamma functions, to

$$\frac{B}{A} = \frac{-\sin(i\pi\nu)}{\cos(i\pi\nu)} = -\tan(i\pi\nu). \tag{6.6}$$

So asymptotically the function goes as

$$\sqrt{\frac{1}{kr}}A\cos(kr - i\pi\nu/2 + i\pi\nu - \pi/4) = A\cos(kr + i\pi\nu/2 - \pi/4)$$

and the phase shift is purely imaginary.

Perelomov [20] adapts Case's method to get the same result. Suppose you require all wavefunctions to satisfy the boundary condition

$$\psi \sim \cos(\nu \log r + B)$$

for complex B. For simplicity let's suppose $B = i\beta$. Then the wavefunction goes as $\cos(\nu \log r)\cosh\beta - i\sin(\nu \log r)\sinh\beta$. For the special case $B = +i\infty$, $\cosh\beta = \sinh\beta$; therefore the wave goes as $r^{-i\nu}$ and we have complete absorption.

Complex phase shifts make perfect sense since you can deduce the asymptotic forms from them; we also avoid the existence of bound states, and therefore the

anomaly. A further part of the appeal of the absorptive solution is that it's a natural continuation of the Friedrichs extension into the strong-coupling regime [7]; it might seem conceptually suspect to think of θ and ν as having an analytic dependence, but Nelson shows that analytic continuation of the functional integral into strong coupling produces the absorptive result.

Radin's Result

Radin [22] relates Nelson's extension to self-adjoint extensions by the following result:

Theorem 10 *Let the purely dissipative time-evolution operator (i.e. Nelson's operator) be denoted U_d, and the evolution operators generated by the self-adjoint extensions be denoted U_θ. Then*

$$U_d \psi = \frac{1}{2\pi} \int_0^{2\pi} U_\theta \psi \, \frac{d\chi}{d\theta} \, d\theta. \tag{6.7}$$

In other words, the dissipative solution is an average over all unitary solutions, weighted by some probability measure. It's not surprising that unitary solutions average out to a dissipative solution; for instance, $e^{i\theta}$ and $e^{-i\theta}$ are both unitary, but their average is $\cos\theta$, which is not.

The probability measure is the phase of the $(kr/2)^{-i\nu}$ solution relative to the $(kr/2)^{i\nu}$ solution. Recall from Chapter 3 that this was given by

$$\frac{\Pi_1}{\Pi_2} = \frac{e^{-i\theta/2}e^{-\pi\nu/4} + e^{i\theta/2}e^{\pi\nu/4}}{e^{i\theta/2}e^{-\pi\nu/4} + e^{-i\theta/2}e^{\pi\nu/4}} = e^{-i\theta}\frac{e^{i\theta} + e^{\pi\nu/2}}{e^{-i\theta} + e^{\pi\nu/2}}. \tag{6.8}$$

Radin calls this term $L(\theta)$, and observes that $\chi(\theta) = \arg[L(\theta)]$ does the trick. It's a fairly equitable average, as one can see from Figs 6.1 and 6.2.

This makes an interesting comparison with the less singular case, where Π_1/Π_2 behaves as in Fig 6.3.

The physical implications of this result aren't discussed by Radin. It's hard to see what exactly one is to make of them; there is something akin to the spirit of path integration in the procedure of integrating over a phase, and there are cases in statistical mechanics when one averages over a degree of freedom, but the connection isn't obvious. One might suppose that the particle sees all possible boundary conditions and evolves according to all of them somehow, but this leaves the issue of probability loss somewhat mysterious (energy doesn't leak into the self-adjoint extensions), and doesn't fit in with our EFT understanding of the problem: it doesn't make sense to
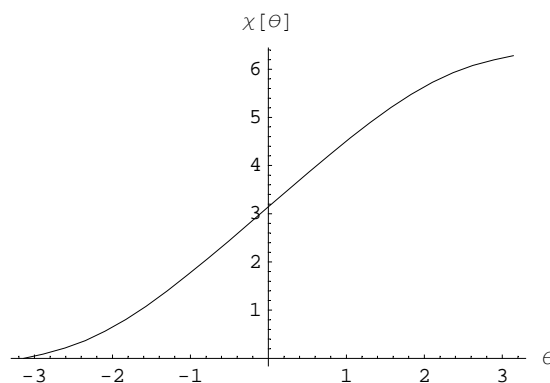
Figure 6.1: Graph of $\chi(\theta)$ vs. θ
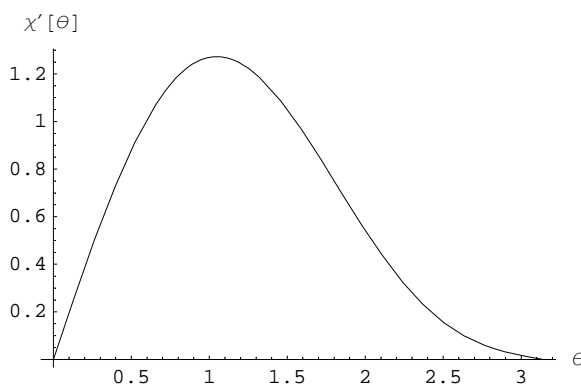
Figure 6.2: Graph of $\frac{d\chi}{d\theta}$ vs. θ

talk of a particle seeing all imaginable short-distance physics, since in fact there is only one type of short-distance physics, and we would know what it was if we had sufficiently good resolution. We feel that the claim by Bawin and Coon [25] that this result explains absorption with more "rigorous mathematics" than the complex phase shifts is unjustified, even if one defines rigorous as difficult.

This result, or an analogue, ought to apply for potentials more singular than $1/r^2$; unfortunately, they're not analytically solvable so it's hard to prove this. The general idea is that if there is no preferred self-adjoint extension—and there isn't for any of the strongly singular potentials—the only preferred solutions are those that correspond to complete absorption and complete emission.
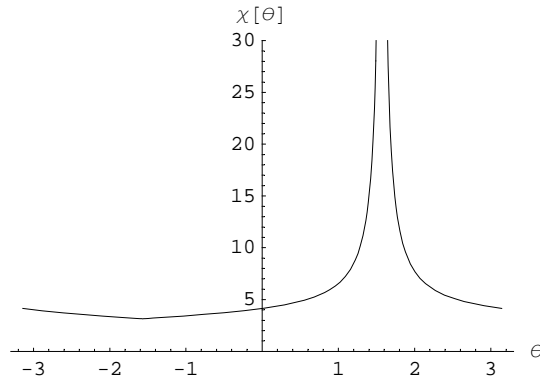
Figure 6.3: Graph of (alleged) χ vs. θ in the weak regime

6.4   Experimental Realization

In 1998, Denschlag et al [23] realized a (basically quantum) 2D inverse square potential experimentally. They studied the behavior of cold lithium atoms in a cylindrical magnetic-optical trap (MOT), through the middle of which there was a thin wire. They observed the number of atoms in the trap to decay exponentially, consistent with the classical limit and also with the contraction semigroup treatment of the problem. The important thing conceptually about this experiment is that it reminds us of the diversity of boundary conditions that can be realized—there is nothing strange about atoms being absorbed by a charged wire—and the corresponding breadth of sensible solutions to a problem like the $1/r^2$ potential.

Chapter 7

Klauder Phenomena and Universality

Klauder phenomena are cases where a perturbed Hamiltonian $H_0 + \lambda V$ does not go smoothly to H_0 as $\lambda \to 0$, i.e. the spectra don't converge to their limiting value. This clearly requires V to be singular somewhere, but on the other hand not all singular potentials have associated Klauder phenomena. The origin of Klauder phenomena isn't too surprising. For instance, consider the one-dimensional repulsive potential $\lambda|x|^{-N}$ for very large N. This is an infinite barrier between the half-lines for arbitrarily weak λ. For $\lambda = 0$, however, $V = 0$. Cases like this arise all the time in one-dimensional quantum mechanics (see Chapter 8), but this chapter deals mostly with similar phenomena on the half-line and for $d > 1$.

7.1 Self-Adjoint Extensions and Klauder Phenomena

Generally, for self-adjoint extensions of a Hamiltonian, the bound state energy k_b is related to the coupling λ and the self-adjoint extension parameter θ. We can draw contours of constant $k_b(\lambda, \theta)$, and the intersections of these contours with the $\nu = 0$ axis can be thought of as representing a particular Klauder phenomenon. For singular potentials (at least, in more than one dimension), $\nu = 0$ corresponds to a delta function at the origin. (This is not saying very much, since δ-function potentials are *defined* in terms of self-adjoint extensions.) There isn't anything particularly suspect about this, since as one tunes an interaction one doesn't normally leave its

short-distance parts unchanged, but expects them to vary smoothly.

Assuming that potentials are continuous in the extended $\lambda - \theta$ plane, the limit as $\lambda \to 0$ of any perturbation should be a δ-function. The physical reason for this is that as you tune the coupling to zero the potential becomes very weak almost everywhere, and since the wavefunctions are almost never within the central region of the potential they are very slightly affected by the details of the interaction. (This is the same logic we use a few sections down, while discussing universality in resonance phenomena.) If this were true then all Klauder phenomena *of the free Hamiltonian* should be δ functions. This would have severe consequences for any attempt to renormalize, say, the $1/r^2$ potential by running the bound state against the global coupling. We know from the treatment of Chapter 5 that, at least asymptotically, a regularized theory reproduces the behavior of a self-adjoint extension. Therefore, taking the λ of a regularized theory to zero with the energy kept constant *is the same* as following a $k_b(\lambda, \theta)$ contour, and should take you to a delta-function perturbation of H_0 as you take the coupling to zero. That is, for any of the regularization schemes of Chapter 4:

$$ a \to 0 \Rightarrow \nu \to 0 \Rightarrow \theta \to \theta_0 $$

for constant k_b. This suggests that any such renormalization eventually reproduces a point interaction—which is consistent with the fact that the bound state wavefunction and the s-wave phase shift for the 2D "renormalized" inverse square potential are the same as for the 2D delta function. This obviates the need for a renormalization procedure, as well as calling its validity into question. We work out the $1/r^2$ example again, and also demonstrate that the $1/x^2$ potential reproduces the 1D delta function if you perform Chapter 4 renormalization on it. We also explicitly work the former problem in the (λ, θ) plane.

Another application of these relations is to avoid Klauder phenomena by following lines that pass through $k_b(0, \theta_0) = 0$, which corresponds to no Klauder phenomenon. The paths are generally not unique, but (as we shall see) a sensible parameterization of short-distance physics picks one.

7.2 Examples

7.2.1 $1/r^2$ in the Plane

Except for the factor of $\sqrt{kr}$ this is the same as the 1D/3D case, so that

$$\psi(r) = K_{i\nu}(kr)$$

and under ch. 4 type renormalization the ground state wavefunction becomes

$$K_0(k_b r).$$

We can work out the s-wave phase shift as usual, by looking at the boundary conditions for $AJ_{i\nu} + BN_{i\nu}$. Since at the end we're going to take $\nu \to 0$, the quantity $-B/A$ will, as usual, serve as $\tan\delta$. Using the hardcore cutoff scheme from Ch. 4,

$$AJ_{i\nu}(ka) + BN_{i\nu}(ka) = 0$$

so that

$$-\frac{B}{A} = \frac{J_{i\nu}(ka)}{N_{i\nu}(ka)} = \frac{\pi(ka)^{i\nu}/\Gamma(1+i\nu)}{(ka)^{i\nu}\Gamma(-i\nu) - (ka)^{-i\nu}\Gamma(i\nu)}.$$

With the assumption that $\Gamma(1+i\nu) \approx 1$ and a small-argument approximation, this becomes

$$-\frac{i\pi\nu}{1 - (ka)^{-2i\nu}}$$

and, plugging in our renormalization rule $\nu = \pi/\log k_b a$, this is

$$\frac{i\pi^2}{\log k_b a - \log k_b a e^{-2\pi i \log ka/\log k_b a}}.$$

The last of these expressions looks a little forbidding, but we know that as $a \to 0$,

$$\frac{\log ka}{\log k_b a} \approx \frac{\log a}{\log a} \approx 1$$

we can do a series expansion in the small quantity $1 - \log ka/\log k_b a$. We can write the argument of the exponential as

$$1 - \left(1 - \frac{\log ka}{\log k_b a}\right)$$

in which case a first order Taylor expansion about $e^{-2\pi i}$ is

$$e^{-2\pi i} - 2\pi i \left(1 - \frac{\log ka}{\log k_b a}\right)$$

and putting it all together,

$$-\frac{B}{A} = \frac{\pi}{2 \log k_b/k}$$

$$\tan \delta_0 = \pi/2 \log(k_b/k),$$

which is, of course, the same as with $\delta^2(r)$.

7.2.2 $1/x^2$ on the Half-Line

The primary difference between the 1D and 3D ($l = 0$) Schrödinger equations is the boundary condition that requires $u(0) = 0$ in three dimensions. A consequence is that in one dimension an (even remotely well-behaved) attractive potential always has a bound state, while in three dimensions that need not be the case. A more mathematical way of stating the distinction is that one normally picks the Friedrichs extension on $\mathbb{R}^+ - 0$ when one is doing 3D quantum mechanics, but in one dimension this extension is usually inappropriate for attractive potentials.

Suppose we regularize the potential with a square well at radius a. It is well-known that a one-dimensional always attractive potential always has a bound state, and since the only dimensional parameter is a, dimensional analysis suggests that the bound state energy must go as $1/a^2$. To keep it fixed as $a \to 0$ we have to scale λ accordingly, so that we can take $\zeta = \nu - \frac{1}{2}$ small for our purposes. The boundary condition is

$$-qa \tan qa = \frac{1}{2} + ka\frac{K_\nu'(ka)}{K_\nu(ka)}$$

which simplifies, with the usual approximations (see Chapter 3), to

$$-\lambda = \frac{1}{2} - \nu \left[1 - 2\frac{\Gamma(-\nu)}{\Gamma(\nu)}\left(\frac{ka}{2}\right)^{2\nu}\right].$$

Keep terms only to first order in ν we can reduce this expression to

$$-\lambda = 4\nu(ka/2)^{2\nu}$$

which simplifies further to

$$k_b = \frac{\lambda}{a}.$$

The bound state wavefunction flows to e^{-kx} as $\nu \to 1/2$.

Now let's consider the scattering states. The outside form of the wavefunction is $AH_\nu^{(1)}(ka) - BH_\nu^{(2)}(ka)$ in terms of the Hankel functions, which we will refer to as H_1 and H_2. The inside wavefunction is a cosine because we're working on the half-line and we assume the problem is symmetric. Once again, the boundary condition is

$$(qa)^2 = \frac{1}{2} + k \frac{AH_1' - BH_2'}{AH_1 - BH_2}$$

and, if we write the Hankel functions in terms of Bessel functions and take the $\nu \to 0$ limit, this becomes

$$\lambda = \frac{1}{2} + \frac{1}{2} \frac{(ka)^{3/2}}{i(A+B)} \left[(A-B) \left(\frac{ka}{2} \right)^{-1/2} - i(A+B) \left(\frac{ka}{2} \right)^{-3/2} \right],$$

which is a nice form because two of the terms cancel out and what's left is

$$-i\frac{k_b}{k} = \frac{A-B}{A+B}$$

which is the result we expect for the 1D delta function. Therefore, the renormalization procedure of Chapter 4 has left us once again with a point interaction.

There are infinitely many other ways to calculate the delta function in principle, but most singular potentials are not exactly solvable so we won't bother.

7.2.3 Self-Adjoint Extensions

It suffices to show that one can vary the coupling continuously from the strong regime to the weak regime without losing self-adjointness at any stage, and without having a discontinuity in the boundary condition. We know that there's always an extension in the weak regime, the critical regime, and the strong regime with a given bound state energy $k_b \neq 0$. So we can tune down the coupling and keep picking the appropriate extensions. Our boundary conditions (in two dimensions) have the form

$$\frac{\nu\psi + r\psi'}{\nu\psi - r\psi'} = \frac{\Gamma(-\nu)}{\Gamma(\nu)} \left(\frac{k_b r}{2} \right)^{2\nu}$$

For $\nu \to 0$ this simplifies to

$$\frac{\nu\psi + r\psi'}{\nu\psi - r\psi'} = -\left(\frac{k_b r}{2}\right)^{2\nu}$$

and unless $k_b = 0$ both sides approach the same limit. The boundary condition is vacuous in the limit; however, since the limit exists from both sides and ψ is analytic in ν at zero, one can think about this as a removable discontinuity, and plug in the appropriate value of k_b. Under a Chapter 4-type renormalization a strong $1/r^2$ potential flows up the k_b contour to the critical value under renormalization; however, we could just as well have done the critical problem directly. One might also point out again that the critical problem isn't in fact *anomalous*, if by that we mean that there are no scale invariant boundary conditions. We would always choose the one case for which the discontinuity is not removable is $k_b = 0$.

This is also the only case for which the boundary condition isn't vacuous in the limit; it goes to $r\psi'(0) = 0$, which is equivalent to throwing out the K_0 solution.

How does one explain the disappearance of the Friedrichs extension in RG terms? Suppose you have a potential with a running square well or delta function ring, and turn up the coupling slightly past its critical value. The ground state does nothing strange, because the rightmost zero of $K_{i\nu}(x)$ is at about π/ν, which is within our regularized core. However, the very shallow states—whose rightmost zeros are at $n\pi/\nu$ for arbitrarily large n, and which are therefore relatively unaffected by interior behavior—appear near the threshold at this point. Of course, in practice there's an infrared cutoff too, so not quite. There will be regimes in any physical (no ultraviolet or infrared divergencies) potential where the $1/r^2$ interaction is above critical strength but there are no bound states.

A notable thing about the strong inverse square potential in two dimensions is that it's impossible to avoid a Klauder phenomenon, since you can't get smoothly to the Friedrichs extension by tuning the coupling to zero. Therefore any way of tuning the coupling to zero leaves a bound state in the problem. Presumably this is generic to strongly singular potentials, since the *reason* we can't access the Friedrichs extension has to do with the loss of the boundary condition. With singularities stronger than $1/r^2$ it's also the case that one can't get at any non-Friedrichs extensions from the repulsive side, since the operators are self-adjoint and the wavefunctions vanish at the origin; the critical value at $\lambda = 0$ is therefore highly nonanalytic. It's physically more evident in these cases that the Klauder phenomena must be generic, since as you tune down the potential strength you also tune down its range, so that the bound

state finds itself less and less within the range of the interaction, and therefore less and less sensitive to its details.

Finally, one should note that there can be no Klauder phenomena in $l \neq 0$ channels, because the limit as perturbation strength $\lambda \to 0$ is self-adjoint. This fact establishes Klauder phenomena as distinctively quantum mechanical, since the classical limit usually corresponds to $l \gg 1$.

7.3   Nonanalyticity

Suppose you're tuning up the depth of a square well: at the critical coupling just before a new shallow bound state appears, there's a zero-energy scattering resonance. In contrast, there's no such resonance in the critical $1/r^2$ interaction. This is an example of the non-analytic dependence of some parts of the theory on coupling strength. This non-analyticity is also characteristic of the 3D hydrogen atom, which has infinitely many bound states when it's attractive but no resonance at zero coupling. In both cases the non-analyticity takes place because we didn't regularize the infrared properties; however, the α/r^4 potential [20], which has no infrared problems, has a similar non-analyticity in its scattering length at $\alpha = 0$.

An important thing about Klauder phenomena is that they are an example of "non-analytic" (by which we mostly mean non-smooth) dependence of the spectra on coupling at zero. A square well, in contrast, exemplifies "analytic" dependence. With singular potentials we have drastic transitions at the points where they become attractive, where the number of bound states goes up suddenly from 0 to ∞, and the properties of the wavefunctions change drastically. Within a renormalization theory framework, however, these transitions are artefacts of our theory, and the regularized theory has no nonanalytic properties.

These nonanalyticities are a natural consequence of the universality of Klauder phenomena. All singular perturbations must go to a delta function in the $\lambda \to 0$ limit; however, most of them have infinitely many bound states for arbitrarily low coupling, and the nonanalyticity comes from the disappearance of all bound states but one to either $-\infty$ or 0.

7.4 Universality

The renormalization group gives us a way to think about the universal asymptotic features of a class of potentials, regardless of their short-distance structure. However, for the most part we have been dealing directly with motion in long-distance *potentials*. A more striking instance of universality is the resonances of short-range potentials. A standard result of scattering theory is that (in the s-wave channel) the scattering length $a \to \infty$ for a potential with a very shallow bound state. One would expect resonance phenomena to be generic for the same reason that one would expect Klauder phenomena to be generic: the scattering length (or the width of a bound state) is so much larger than the range of the potential that the effect could not possibly depend on the details of the interaction: most scattering particles go nowhere near the core. The resonance phenomena of the two-body problem are relatively straightforward [40]; however, a resonant three-body system exhibits the remarkable Efimov effect.

7.4.1 Review of 3D Scattering

A key hypothesis of the usual scattering theory is that the scattering potential, or **scatterer**, is spherically symmetric and localized. (This is not the case with Coulomb or $1/r^2$ interactions, which need special treatment.) Let's assume that this holds for now. If we send in a waveform $e^{ikz} = e^{ikr\cos\theta}$, the steady-state solution at large distances from the scatterer has two parts: the initial waveform and an outgoing wave from the scatterer, which need not be spherically symmetric.

The expression

$$\psi(r, \theta) = e^{ikr\cos\theta} + f(k, \theta)\frac{e^{ikr}}{r}$$

holds asymptotically. f is called the scattering amplitude. The radial term is merely a positive energy solution to the free particle Schrödinger equation, which holds when we're outside the range of the scatterer. The scattering cross section is the integral of f over solid angle, and the scattering length is the zero energy limit of f. The partial-wave analysis, which expands out the θ-dependence of z and f in terms of Legendre polynomials, is a separation of variables in the scattering problem; its merit is that it reduces the 3D problem to radial problems with angular momentum l. At low energies, only the $l = 0$ (s-wave) equation matters; this is equivalent to saying that at low resolution (long wavelength) everything looks spherically symmetric. Since,

in this case, the asymptotic behavior is governed by the free-particle Schrödinger equation, the one asymptotic property that depends on the scatterer is the **phase shift** of the e^{ikr} wave. The scattering amplitude for low-energy problems is related to the phase shift as follows:

$$f(k) = \frac{1}{k \cot \delta_0(k) - ik}.$$

$\delta_0(k)$ must blow up as $k \to 0$, to keep the scattering length finite; this is the case with most sensible scatterers, such as the square well.

7.4.2 Bound States and Resonances

Bound states affect the behavior of the scattering problem bizarrely. Suppose you tune the energy of your incoming s-wave for a fixed scatterer: $\tan \delta_0$ always blows up as the incoming energy approaches that of a bound state. This result is called Levinson's theorem, and is sometimes a useful way to count the bound states of a system. (One can check that Levinson's theorem holds for all the scattering problems we work out; see also our discussion in Chapter 5.) A particularly important case of Levinson's theorem is when the bound state is very shallow, since then $a \to -\infty$. The physical origin of this effect is not entirely obvious, but what one sees in the *time-dependent* picture is that the particle is almost trapped into a bound state, and takes a long time to leave. The fact that the scattering length diverges is due to the fact that bound states become less and less localized as their energy goes to zero, since the asymptotic wavefunction e^{-kr}/r falls away very slowly as $k \to 0$. In fact, at $k = 0$, the asymptotic wavefunction goes as $1/r$.

The low-energy properties of systems near a resonance depend very slightly on the nature of the internal attraction. In the bound state sector, this follows from the fact that most of the bound state wavefunction is outside the range of the scatterer, and the particle is hardly ever in the range of the forces. Of course, the system needs to be exactly tuned for this to happen; in most cases the scattering length can be obtained by dimensional analysis from the potential.

The scattering length is in some sense a measure of the spatial extent of the shallowest bound state. Normally this is determined by k, which is determined by the intrinsic scale of the potential; however, when $k \to 0$ the scattering length diverges. This connection is made carefully and explicitly in [40].

Note that this discussion is hopelessly invalid for the $1/r$ and $1/r^2$ potentials, which have infinitely many arbitrarily shallow bound states.

7.4.3 Three-Body Scattering

The problem of three-body scattering is more intricate because of the greater number of possible configurations. A two-body system is either bound or in the continuum; but in a system of three interacting particles (let's say particles 1, 2, and 3) there are many more possibilities: for instance, two of the particles could be bound tightly and separate from the third, or all three could be flying apart from each other, or all three could be bound. Besides, all sorts of transitions—capture of 3 by the 1-2 system, which gets excited in the process; or deexcitation of 1-2-3 by the emission of 3, and other ways of sloshing energy about between the particles—are possible. The problem is hard enough to think of in the time-*dependent* picture; in terms of the time-independent picture it becomes even harder.

However, the physical basis for resonances is more intuitive in the three-body problem. The idea is that a three-body bound state might be degenerate with a state in which two of the particles are bound and the third is free. The third particle gets held up by transition to the bound state, and takes a long time to leave the system. This time-delay is the basic phenomenon; in the time-independent theory it shows up—by means we will not discuss, but which can be found in textbooks [62]—as a large phase shift.

7.4.4 The Efimov Effect

In the resonant two-body problem, there are no bound states; this is good, because there would be no relevant length parameter in the theory to describe their spatial extent. However, Efimov [27] discovered in 1971 that there are infinitely many shallow three-body states in a system of three identical, pairwise resonant bosons. This is associated with the fact that the effective three-body potential for this situation is inverse-square—in terms of the three-body "hyperspherical" radius $R = \sqrt{r_{12}^2 + r_{23}^2 + r_{31}^2}$—and strongly attractive. Since its discovery the Efimov effect has been studied in great detail; a straightforward but long derivation is given in [40]. The surprising feature is that there are three-body bound states; the $1/r^2$ structure follows from scale invariance, which follows from the absence of relevant dimensional

parameters. The argument that there are bound states is hard, but its conclusion isn't too implausible: if the two particles were almost bound without the third, then their attractive interactions with the third particle ought to push them over the edge.

Once we know this much, we can use our treatment of the $1/r^2$ potential to deduce most of the other properties of Efimov states: the level spacing, the single-parameter dependence of the states, Efimov's radial law [28], etc. As Ref. [40] notes, this approach has a slight danger in that the separation of scales is not as clear in the three-body problem as in the two-body problem. The issue is this: our treatments (and Efimov's) of the radial behavior of the problem have assumed that any probability that goes into the inner region will come out again. This is not the case if deep two-body states exist, because there's a small chance that two of the particles will form a deep bound state, which vanishes from the low-energy sector. Using the terminology of Chapter 6, we can say that some of the probability is dissipated, and account for this with the machinery of Chapter 6.

7.4.5 Consequences and Experimental Realization

Kraemer et al [39] recently observed the Efimov effect in an ultracold gas of cesium atoms. The signature they detected was **giant recombination loss**, which had previously been predicted by [94], [40]. Suppose we have a three-body system with a shallow pairwise bound state (equivalently, a large scattering length). The recombination rate is the rate at which a three-body bound state transitions into the state consisting of a shallow two-body bound state and a free particle. At very low energies recombination happens at a constant rate α. It turns out that the discrete scaling symmetry of the problem manifests itself in log-periodic oscillations of the recombination rate in the Efimov regime. The recombination rate is pretty easy to measure from the rate of loss of atoms (because of combination into shallow molecules) and the temperature change due to the "anti-evaporation" [39] associated with the formation of a two-body bound state.

Chapter 8

The One-Dimensional Hydrogen Atom

There is some controversy as to what the phrases "hydrogen atom" and "Coulomb potential" ought to mean in one dimension; the only problem we consider is the following Hamiltonian:

$$H = -\frac{d^2}{dx^2} - \frac{\lambda}{|x|} \tag{8.1}$$

The spectrum of this Hamiltonian has been argued over at some length in the literature. Loudon (1959) [98] found a ground state at $E = -\infty$, and degenerate $n > 0$ states. Haines and Roberts (1969) [99] claimed that there were no degeneracies, but a continuous negative-energy spectrum. Andrews (1976) [101] got rid of the ground state by enforcing $\psi(0) = 0$, but his procedure reinforced the degeneracies. Hammer and Weber (1988) [102] claimed that Loudon's ground state was an "extraneous" solution. Meanwhile, Gostev et al (1989) [104] discussed the potential from the point of view of self-adjoint extensions. Gordeyev and Chhajlany (1997) [103] solved the problem with Laplace transforms and semiclassical arguments, and decided that there were neither degeneracies, nor a barrier, nor a ground state at $-\infty$, nor an unspecified boundary condition, but that the one-dimensional hydrogen atom had the same spectrum as the three-dimensional hydrogen atom. Tsutsui et al (2002) [95] worked the mathematical problem using a technique equivalent to ours, but did not discuss its physical interpretation.

We work the mathematical problem within a general discussion of the peculiarities of 1D quantum mechanics. As treatments before this have found, the mathematical

treatment does not obviously suggest a self-adjoint extension, so our choice of sensible self-adjoint extensions must be motivated by arguments from renormalization.

8.1   The Trouble with 1D Quantum Mechanics

The nature of the first three spectra suggests a failure of self-adjointness—we have already seen a continuous spectrum with the $1/r^2$ potential, and a ground state at $-\infty$ with the $\delta^2(r)$ potential. The matter of degeneracy is distinctive to one-dimensional quantum mechanics. One dimension is topologically special in that if you take away a point the line is no longer connected, so the two half-lines can be made independent. This is not the case in more dimensions, since you can always go around the origin. But in one dimension the problem of degeneracy arises as follows: if $\psi(x)$ is an eigenfunction of eigenvalue k, then so is $-\psi(x)$. The following function is clearly an eigenstate of energy k that's orthogonal to ψ:

$$\phi(x) = \begin{cases} \psi(x) & x \geq 0 \\ -\psi(x) & x < 0 \end{cases} \tag{8.2}$$

This degeneracy also limits the usefulness of Case's method in one dimension—for instance, take the two solutions

$$\phi_1(x) = e^{-k|x|}, \phi_2(x) = \frac{x}{|x|}e^{-k|x|} \tag{8.3}$$

to the free particle equation on $\mathbb{R} - \{0\}$. They are normally considered to be the bound states of different point potentials—$\delta(x)$ and $\delta'(x)$ respectively—but enforcing orthogonality does not tell you that they belong to different self-adjoint extensions. Case's method fails because one boundary condition isn't enough; the deficiency indices of the free particle Hamiltonian on $C_0^\infty(\mathbb{R}-\{0\})$ are (2,2) rather than (1,1). The problem bears more resemblance to the particle in a box than to the one-parameter problems we have otherwise been looking at.

To see how degeneracies arise in one-dimensional quantum mechanics, let's consider a particle in a box on $(-L, L)$ with an infinite barrier of width $(-\epsilon, \epsilon)$ at the origin. Clearly, in this situation, the two states in Fig 8.1

are degenerate. Now suppose that, instead of an infinite barrier, we have a high finite barrier. Then the probability of tunneling is nonzero, and the wavefunction doesn't vanish in the shaded region. We no longer expect the wavefunctions to be
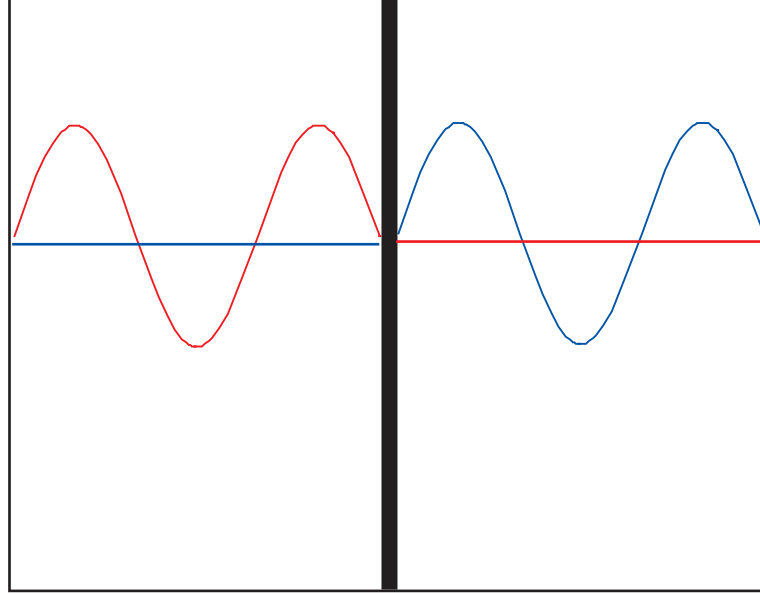
Figure 8.1: Degeneracy in the Square Well

degenerate, since they look qualitatively different in the shaded region—and in fact the odd function is at a slightly higher energy.

Allowing degeneracies between the left and right half-plane is equivalent to saying that they are independent, or separated by an impenetrable barrier, since these are the only things that would prevent tunneling. This is what Loudon [98] and Andrews [101] suggest. Their solution has no irregular ground states; however, it does have a Klauder phenomenon, as Gostev [104] notes. Suppose we perturb a one-dimensional square well with a Coulomb potential λ/r and tune λ to zero. If we followed the "disconnected half-lines" prescription for the Coulomb potential we would not recover the square well in this limit, or lose the degeneracies, because the half-lines would still be impenetrable in the limit.

8.2   Free Particle on $\mathbb{R} - \{0\}$

8.2.1   The General Solution

We choose as our initial domain

$$D_H = \left\{ f \in C^2(\mathbb{R} - \{0\}) | f(0) = f'(0) = f''(0) = 0 \right\},$$

which is dense in $L^2(\mathbb{R} - \{0\})$ because C^2 certainly is (by the Stone-Weierstrass

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Approximation Theorem) and pointwise constraints don't affect norm convergence (see Section 2.1). Now we find the adjoint by seeing for what functions $g \in L^2$ the expression $(Hg, f) = (g, Hf)$. This is equivalent to asking for what g

$$\int_{\mathbb{R}-\{0\}} \left(\frac{d^2\overline{g}}{dx^2} f(x) - \frac{d^2 f}{dx^2} \overline{g}(x) \right) dx = 0.$$

We must split up this integral into one over the positive half-line and one over the negative; in each case, if we assume that $g \in L^2_{ac}(\mathbb{R} - \{0\})$, the absolutely continuous functions (basically, those that can be integrated by parts) we can integrate by parts:

$$\int_0^\infty \frac{d^2\overline{g}}{dx^2} f(x) dx = \frac{d\overline{g}}{dx} f(x) \Big|_0^\infty - \int_0^\infty \frac{d\overline{g}}{dx} \frac{df}{dx} dx$$

and the second rhs term cancels with that in the $\overline{g}f''$ integral, so that we're left with the restriction

$$\left[\frac{d\overline{g}}{dx} f(x) - \overline{g}(x) \frac{df}{dx} \right]_{0+}^\infty .$$

Normalizable functions vanish at ∞ *and* f and f' vanish at 0, so there are no boundary conditions on $g \to 0^+$. Similarly, there are no boundary conditions as $g \to 0^-$, and we may assume that the adjoint domain is all of $L^2_{ac}(\mathbb{R} - \{0\})$. This allows us two solutions to each deficiency index calculation:

$$\Psi_i^1 = e^{-\sqrt{i}x} \theta(x)$$

$$\Psi_i^2 = e^{-\sqrt{i}|x|} \theta(-x)$$

and similarly with Ψ_{-i}. The most general way to characterize a particular self-adjoint extension is as a vector:

$$\begin{pmatrix} \Psi_i^1 \\ \Psi_i^2 \end{pmatrix} + U \begin{pmatrix} \Psi_i^1 \\ \Psi_i^2 \end{pmatrix}$$

where the choice depends on four complex parameters with a few restrictions coming from the unitarity of U. The general treatment isn't particularly enlightening; we consider only the most interesting special cases, corresponding to two-parameter families.

8.2.2 The Disconnected Family

This family of solutions corresponds to diagonal U, in which case Ψ_1 and Ψ_2 decouple, and the the functions we add to our domain are as follows:

$$\Psi_i^1 + e^{i\theta}\Psi_{-i}^1$$

$$\Psi_i^2 + e^{i\phi}\Psi_{-i}^2.$$

Since $\Psi_i^1(\Psi_i^2)$ is confined to the right (left) half-plane, we have two decoupled problems, each of the sort we described in Section 2.4. Depending on the extension we pick we could elect to have a bound state on either half-plane, both, or neither. The generic situation with this system is that we have two bound states,

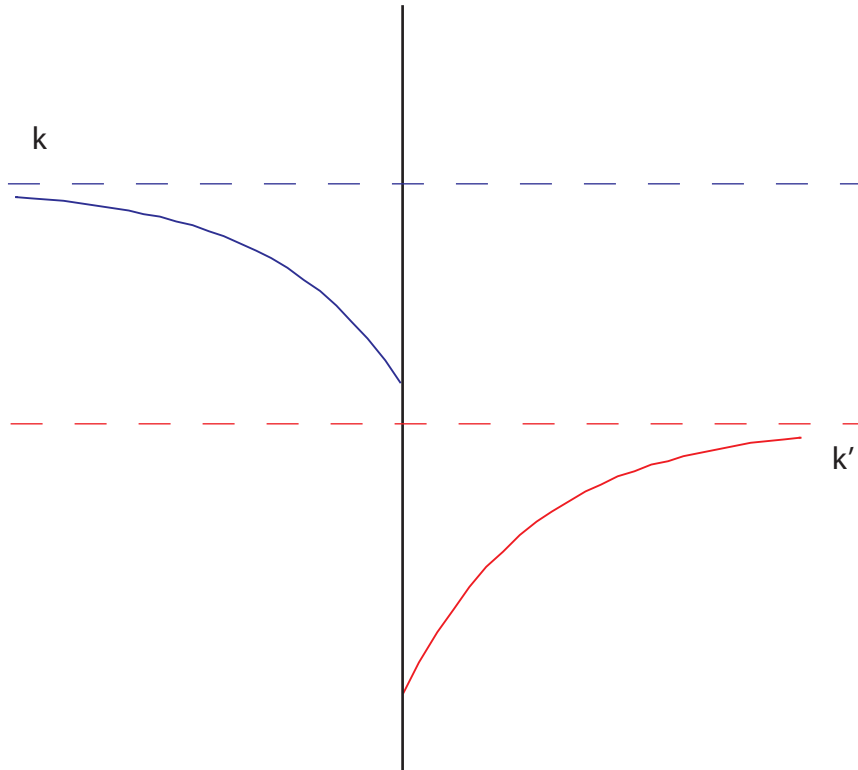$$\psi_1 = e^{-kx}\theta(x)$$

$$\psi_2 = e^{kx}\theta(-x)$$

Figure 8.2: Spectrum of disconnected family, with two bound states

The Friedrichs extension corresponds to requiring that the wavefunction vanish at 0^+ and 0^-. If we choose the same nontrivial boundary condition on both sides, the bound states we get are degenerate.

8.2.3 The Bipolar Family

Suppose we change our reference basis to

$$\Phi_i^1 = e^{-\sqrt{i}|x|}$$

$$\Phi_i^2 = e^{-\sqrt{i}|x|}(\theta(x) - \theta(-x))$$

and pick the new diagonal family. This gives us two decoupled boundary conditions once again, one applying to odd solutions and the other to even. The interesting cases are the limits where we pick the Friedrichs extension in the odd channel, which gives us $\delta(x)$, or the extension with $\psi'(0) = 0$ in the even channel, which gives us $\delta'(x)$. Recall that the domains of these operators are given by

$$D_\delta = \{\psi \in L^2_{ac}(\mathbb{R} - \{0\})|\psi'(0^+) - \psi'(0^-) = g\psi(0)\}$$

$$D_{\delta'} = \{\psi \in L^2_{ac}(\mathbb{R} - \{0\})|\psi(0^+) - \psi(0^-) = g\psi'(0)\}$$

The bipolar basis is a natural one to use for studying one-dimensional problems, because we're mostly interested in the solutions that correspond to point interactions, which must be either odd or even. A well-known feature of the interactions δ and δ' is that a smooth odd function ($\psi(0) = 0$) would not see a delta function, while a smooth even function ($\psi'(0) = 0$) would not see a δ' at the origin. This follows very naturally from our setup.

8.2.4 The Degenerate Family

If we choose degenerate boundary conditions with the disconnected reference basis, we get a two-dimensional eigenspace spanned by $e^{kx}\theta(-x)$ and $e^{-kx}\theta(x)$. The degenerate extensions are special in that the bound state wavefunctions don't depend on the basis we chose initially. The Friedrichs extension is the most famous member of this family.

One might wonder how much there is in common between the two-parameter families that correspond to various choices of basis; a general result relating the families is given in Ref. [95]:
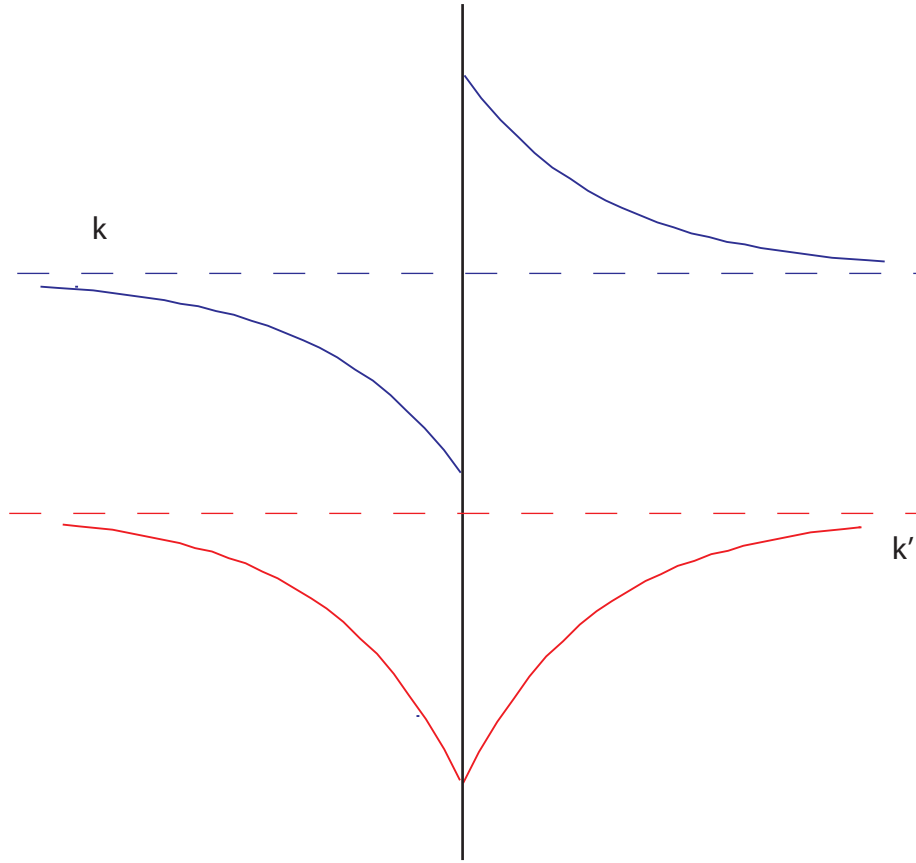
Figure 8.3: Spectrum of the bipolar family

Theorem 11 *If the potential on $\mathbb{R} - 0$ is even, and only one solution is regular at ∞—i.e. if the boundary condition at ∞ is determined—the spectrum of eigenvalues of a self-adjoint extension with characteristic matrix U is uniquely determined by the eigenvalues of U.*

For the simple case we are considering, this says nothing more than that the bound state energies we pick are the bound state energies; however, with spectra like that of the 1D hydrogen atom, there's somewhat more content to this statement.

8.2.5   The 1D Delta Function, Done Differently

(This treatment follows [74] and [76].) The one-parameter family corresponding to $\delta(x)$ can be derived more directly by making the original domain more restrictive. Suppose we are looking for extensions of the free Hamiltonian on the domain

$$D_H = \{\psi \in C^\infty(\mathbb{R}) | \psi(0) = 0\}.$$

As before, we can find the adjoint domain by integrating the inner product and looking at the expression

$$\left[\frac{d\overline{g}}{dx} f(x) - \overline{g}(x) \frac{df}{dx}\right]_{0^+}^\infty + \left[\frac{d\overline{g}}{dx} f(x) - \overline{g}(x) \frac{df}{dx}\right]_{-\infty}^{0^-}.$$

The first term vanishes because $f(0) = 0$, but since we have made no assumptions about $f'(0)$, we can't assume that the second term vanishes at zero. That is, the requirement of symmetry gives us nontrivial information about g in this instance. Our initial assumption of smoothness means that f' is continuous at zero, so the expression reduces to

$$f'(0)[\overline{g}(0^+) - \overline{g}(0^-)] = 0$$

and since $f'(0)$ is arbitrary, this constitutes a requirement that the wavefunction g be continuous at the origin. So our adjoint domain could be written as

$$L^2_{ac}(\mathbb{R} - \{0\}) \cap \{f \in L^2(\mathbb{R}) | f(0^+) = f(0^-)\}.$$

Imposing this condition reduces the deficiency indices to $(1, 1)$, since the only solution that's continuous at the origin is $e^{-\sqrt{i}x}$, and the self-adjoint extensions yield the one-parameter family of solutions corresponding to a delta function at the origin.

8.3   The 1D Coulomb Potential

8.3.1   Why We Need the Whole Family

Since $\frac{1}{x}\psi \in L^2$ iff $\psi(0) = 0$, the domain of the original Hamiltonian must be limited to functions that vanish at the origin. However, for $\psi \in D_H$, $(\psi, H^\dagger \phi) = (H\psi, \phi)$ is certainly well-defined for ϕ that don't vanish at the origin, so clearly we need to think about self-adjoint extensions. As we shall see shortly, some of the extended domains do *not* require wavefunctions to vanish at the origin. This illustrates an important feature of self-adjoint extensions, which is that the extended operator does not always do quite the same thing as you would expect of the original operator, at least at singularities.

8.3.2 Solving the Equation

If we substitute $z = 2kx$ into the Schrödinger equation on the positive half-plane:

$$-\left(\frac{d^2}{dx^2} + \frac{\lambda}{x}\right)\psi = -k^2\psi \tag{8.4}$$

it becomes

$$\frac{d^2\psi}{dx^2} + \frac{\lambda}{2kz}\psi - \frac{1}{4}\psi = 0 \tag{8.5}$$

which is a special case of Whittaker's equation (AS 13.1.31). The solutions to this equation are expressible in terms of confluent hypergeometric functions; the following are a linearly independent pair:

$$\Psi_1 \equiv M_{\kappa,1/2}(z) = ze^{-z/2}M(1 - \kappa, 2, z) \tag{8.6}$$

$$\Psi_2 \equiv W_{\kappa,-1/2}(z) = e^{-z/2}U(-\kappa, 0, z) \tag{8.7}$$

($\kappa = \lambda/2k$) Both functions are normalizable when κ is an integer, because the hypergeometrics are polynomials in this case. (For these values, both solutions are also linearly dependent). Otherwise, (AS 13.1.4)

$$\Psi_1 \sim e^{z/2}z^{-\kappa-1}$$

for large arguments. However,

$$\Psi_2 \sim e^{-z/2}z^{\kappa} \tag{8.8}$$

which always decays fast enough to be normalizable. So we have a normalizable solution on the half-plane for *every* negative energy; this is the continuum that Haines and Roberts find, and we recognize it to be a symptom of non-self-adjointness. The deficiency indices on the half-line are $(1, 1)$.

Since the derivative diverges at the origin, we can't do what we did with the 1D delta function. So we're forced to extend the potential on $\mathbb{R} - \{0\}$ and pick an appropriate family of extensions, as we did with the free particle. However, to understand what we're up against, we should first figure out how to extend the problem on the half-line.

8.3.3 The Boundary Condition

The self-adjoint extension on the half-line is determined by the factor θ, and the added wavefunction is

$$\psi = e^{-\sqrt{i}x}U(-\lambda\sqrt{-i}/2, 0, \sqrt{i}x) + e^{i\theta}e^{-\sqrt{-i}x}U(-\lambda\sqrt{i}/2, 0, \sqrt{-i}x). \qquad (8.9)$$

This is regular at the origin, since

$$U(a, 0, z) \approx \frac{1}{\Gamma(1+a)} + z\log z\frac{1}{\Gamma(a)} + \xi z$$

where $\xi = 2\gamma - 1 + \psi^0(1+a)$, and the names of the constants don't matter. On the other hand, $\psi'(x)$ is irregular at zero, and, to the crudest possible approximation,

$$\frac{\log(\sqrt{i}x)}{\Gamma(-\frac{\lambda}{2\sqrt{i}})} + e^{i\theta}\frac{\log(\sqrt{-i}x)}{\Gamma(-\frac{\lambda}{2\sqrt{-i}})} + \xi(\lambda, \theta)$$

If we divide the two forms near zero, we get that

$$\frac{U'(a, 0, z)}{U(a, 0, z)} = \frac{\Gamma(1+a)}{\Gamma(a)}\log z$$

What we want to do is, as usual, impose a condition on $\psi'(x)/\psi(x)$ as $x \to 0$. For notational convenience we introduce $-\lambda/2 = p$. This way, we get

$$\psi(0) = \frac{1}{\Gamma(1+\sqrt{i}p)} + e^{-i\theta}\frac{1}{\Gamma(1+\sqrt{-i}p)} = \frac{1}{p}\left(\frac{\sqrt{-i}}{\Gamma(\sqrt{i}p)} + \frac{e^{-i\theta}\sqrt{i}}{\Gamma(\sqrt{-i}p)}\right).$$

Now the other important thing is $\psi'(0)$, which is undefined, so we want to look at near-zero behavior. Note that a factor of $\sqrt{\pm i}$ gets pulled out while taking the derivative, so that

$$\psi'(x) \approx \log x\left[\frac{\sqrt{-i}}{\Gamma(\sqrt{i}p)} + \frac{e^{-i\theta}\sqrt{i}}{\Gamma(\sqrt{-i}p)}\right] + \xi$$

and, putting it all together, we see that

$$\frac{\psi'(x)}{\psi(x)} = 2p\log x + p\mu.$$

And this can be rewritten as the boundary condition

$$\frac{\psi'(x)}{\psi(x)} + \lambda\log x = \eta(\theta, \lambda) \qquad (8.10)$$

This expression is consistent with [104]. However, we can get some further details about the function η, which we need because it's unclear what its range should be for fixed λ. The basic form is

$$\eta(\theta, \lambda) = \xi(\theta, \lambda) \frac{\Gamma(1 + \sqrt{i}p)\Gamma(1 + \sqrt{-i}p)}{\Gamma(1 + \sqrt{-i}p) + e^{i\theta}\Gamma(1 + \sqrt{i}p)}.$$

Now we can write out ξ as

$$\xi(\theta, \lambda) = \sqrt{i} \frac{-1 + \gamma + \psi_0(1 + \sqrt{i}p)}{\Gamma(\sqrt{i}p)} + e^{i\theta}\sqrt{-i} \frac{-1 + \gamma + \psi_0(1 + \sqrt{-i}p)}{\Gamma(\sqrt{-i}p)}$$

The first part simplifies to $\lambda(-1 + \gamma)$; the second term looks messy, but all we need is its range, and Mathematica shows that it varies like this with θ:
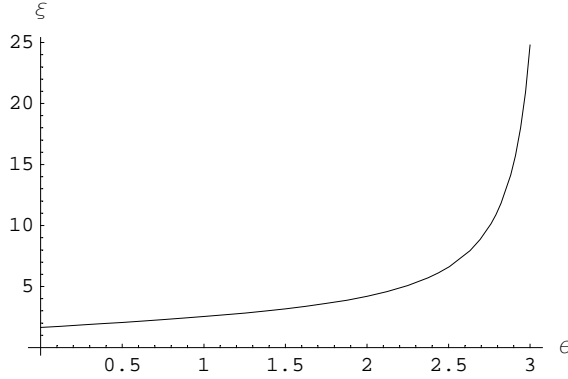
Figure 8.4: Variation of ξ with θ

The Friedrichs extension corresponds to picking $\theta = 2\tan^{-1} p$. For a bound state the ψ term would go as $ka \log kx + \xi$, which is $\frac{1}{2}(\lambda \log x + \lambda \log k) + \xi$, and this gives us the all-important "renormalized" boundary condition

$$\lambda \log k_b + \mu_\kappa = \eta(\theta, \lambda). \tag{8.11}$$

(μ_κ being some agglomeration of uninteresting terms.) We have two different boundary conditions to pick. In the odd sector, by analogy with the case we discussed above, the Friedrichs extension is appealing; it throws out the U solution altogether (since, as we know from the 3D case, the M's are a complete set) and makes the wavefunction vanish at the origin, which is exactly what we want. Now, this leaves us with a choice in the even sector—either we pick the Friedrichs extension again, at

the expense of introducing degeneracies and not having a ground state, or we pick a different extension. Which of the other extensions, though? The special one without a singular derivative sounds appealing, but is it really what we want? This is the point at which the formalism stops being determinative, and we need to look at regularization schemes.

8.4   Renormalization of the $1/|x|$ Potential

8.4.1   Loudon's Regularization

We regularize the potential as follows:

$$V_a(x) = \begin{cases} \frac{1}{|x|} & |x| > a \\ \frac{1}{a} & |x| \leq a \end{cases} \tag{8.12}$$

Matching at the boundary (and ignoring exponential falloff) gives

$$-qa \tan qa = 2ka \frac{U'(\kappa, 0, 2ka)}{U(\kappa, 0, 2ka)}.$$

We assume that k doesn't fall off faster than $1/a$ (we'll confirm this in the next section). Then the lhs can be small-angle-expanded and made to vanish, so that

$$\log ka + \xi = 0$$

and if this is to hold as $a \to 0$ then it's necessary that $k \to \infty$. Loudon concluded from this that the ground state went down to $-\infty$.

8.4.2   Chapter 5 Renormalization

Let's regularize the potential with a square well and see how that goes. The boundary condition is

$$-\chi(a) \tan \chi(a) = 2ka \frac{U'(-\kappa, 0, 2ka)}{U(-\kappa, 0, 2ka)}$$

where we've ignored the exponential falloff and the prime denotes differentiation w.r.t. $2kx$. The rhs goes as $ka \log ka \to 0$ near the origin, which means we can approximate the lhs. Using the fact that (by construction of the delta function), $\chi^2 = g(a)a$, this goes to

$$g(a) = -\frac{2}{k}\frac{U'(-\kappa, 0, 2ka)}{U(-\kappa, 0, 2ka)}. \tag{8.13}$$

The counterterm becomes logarithmic and repulsive as we take the cutoff to zero: in RG-speak, there's a fixed point at $g \to \infty$. However, in contrast with the continuous solutions for $1/r^2$, we can go down to arbitrarily high-energy cutoffs, so the theory might be considered renormalizable.

8.4.3 The Quantization Condition

What determines the even spectrum? In the odd case, where we throw out the U solution, the quantization condition is set by the fact that $M(-\kappa, b, z)$ blows up too rapidly at ∞ except when $\kappa = \lambda/2k$ is an integer. If we keep U solutions, which are always normalizable, we are forced to think of some other way to deal with this issue. As usual with renormalization, the choice of one of the states is arbitrary—this is why the physics does not uniquely pick an extension—and the determination of the rest of the even basis is a matter of finding the right orthogonal set. Unfortunately our boundary condition is a mess. Our problem comes down to finding all the solutions to

$$\lambda \log k + \mu_\kappa = \eta(\lambda, \theta)$$

where η is determined by our choice of self-adjoint extension. In this case, $\mu_\kappa = k\xi$ is

$$k\frac{-1 + \gamma + \Gamma'(1 - \lambda/2k)/\Gamma((1 - \lambda/2k))}{\Gamma(-\lambda/2k)}$$

and the last term oscillates wildly as $k \to 0$, so $\lambda \log k$ crosses it infinitely often.

The wavefunctions are irregular at the origin, but the spectrum is no longer degenerate. We know that the ground state can be taken arbitrarily near to $-\infty$, because for large k only the $\log k$ term matters, and ξ can be made arbitrarily large; also, we could follow Loudon's scheme until the energy hit our desired number $-K$, and then run the well strength in a manner that fixes K; therefore, we can always ensure that our deepest even state is the ground state of the theory.

8.4.4 Summary

We have presented a unified treatment of the $1/|x|$ potential, using both self-adjoint extensions and ideas from renormalization to pick a sensible solution—or, rather,
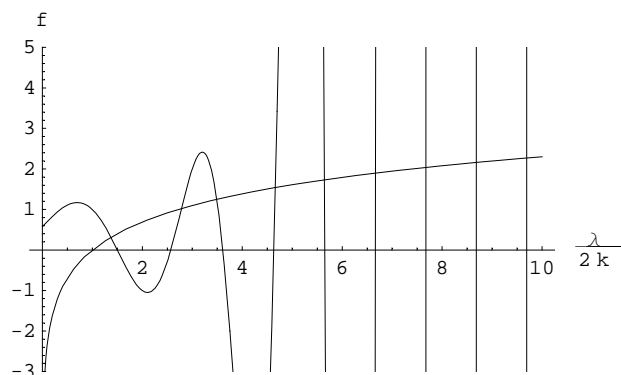
Figure 8.5: The Quantization Condition. Intersections denote bound states.

a family of sensible solutions corresponding to different values of the ground state energy. We have shown that in one-dimensional problems with parity where the boundary condition at the origin is unspecified, there are in fact two sets of boundary conditions to be applied: one for the even sector and another for the odd. We picked a boundary condition to return the "intuitive" feature that the system ought to have a ground state. The potential then behaves as if there were an added delta function at the origin. (Such a perturbation would, of course, have no impact on odd states.) The spectrum we found by this means was the same as that of Ref. [104].

Some previous authors (e.g. Gordeyev and Chhajlany [103]) rejected this spectrum by claiming that it solved a different problem from the $1/|x|$. However, we showed by an EFT-type renormalization of the potential that the delta function term can be derived from arguments identical to those that have been used quite widely to study singular potentials. We do not wish to claim that our solution is the only *intelligible* one—the widely accepted (Friedrichs) solution makes perfect sense if you assume that there's an impenetrable barrier at the origin. However, the logic that derives this solution from the behavior of the Schrödinger equation "at the origin" is inconsistent with a modern approach to singular potentials; from an EFT point of view, it is hubristic to suppose that you know anything about this sector of the theory. As long as the problem is strictly academic, one approach is no better than another, but to the extent that this problem is *physical* the EFT approach is the only sensible one, since we have no real knowledge of the short-distance physics involved.

8.5 Other 1D Potentials

8.5.1 The Strong $1/x^2$ Potential

In the strong regime this potential is pathological enough on the half-line; on the full line one finds that it's possible to have different sequences of boundary conditions (and therefore of energy levels) for the even and odd sets of states. In this case there's no physical difference between the behavior of even and odd states about the origin—they're both oscillating infinitely fast—so the sanest extensions appear to be the degenerate family.

8.5.2 Singular SUSY

For the potential

$$V(x) = \omega^2 x^2 + \frac{g}{x^2}$$

on the half-line, a pair of independent solutions is

$$\phi_1(x) = x^{\nu+1/2} e^{-\omega x^2/2} M\left(\frac{1}{2} + \frac{\nu}{4} - \frac{k^2}{\omega}, \frac{1+\nu}{2}, \omega x^2\right)$$

$$\phi_2(x) = x^{\nu+1/2} e^{-\omega x^2/2} U\left(-\frac{1}{2} - \frac{\nu}{4} + \frac{k^2}{\omega}, \frac{-1+\nu}{2}, \omega x^2\right).$$

We could play the usual self-adjointness game with these. But as Lathouwers [105] notes, there are two sets of orthogonal polynomials associated with the differential equation. These are the following:

$$\phi_1^n(x) = x^{1/2+\nu} e^{-\omega x^2/2} M\left(\frac{1}{2} + \frac{\nu}{4} - \frac{k_{1,n}^2}{\omega}, \frac{1+\nu}{2}, \omega x^2\right)$$

$$\phi_2^n(x) = x^{1/2-\nu} e^{-\omega x^2/2} M\left(\frac{1}{2} + \frac{\nu}{4} - \frac{k_{2,n}^2}{\omega}, \frac{1+\nu}{2}, \omega x^2\right)$$

Both sets are square integrable at the origin for $0 < \nu < 1$, and square integrable at ∞ because the M's are polynomials at the appropriate values, so there's a net exponential falloff. We have two sets of boundary conditions to pick, and we consider three possibilities. (A broader treatment is given in [95].)

The Friedrichs Extension

If we require that ϕ be "as regular as possible" at the origin, we must throw out ϕ_2. This gives us the Friedrichs extension, where the states are degenerate and the wavefunctions are odd and even extensions of $\phi_1^n(x)$. The energy of the states is given by $E_n = 4n+2+2\nu$. (As usual, the Friedrichs extension maintains the lower bound of the spectrum.) As we take the perturbation to zero, $\nu \to \frac{1}{2}$ and the original spectrum is not recovered: we find ourselves with only the odd states. The fact that the energy of all the states is increased by an *attractive* perturbation is a little surprising, as is the Klauder phenomenon.

The Anti-Friedrichs Extension

One could take the opposite tack and throw out all the ϕ_1's (I can't think of a physical motivation, but *someone* probably could.) The energy spectrum in this case is given by $E_n = 4n + 2 - 2\nu$, and as you tune the perturbation down you find that you've lost the odd eigenvalues.

The Perturbative Extension

Or, as we've tended to do in this chapter, one could pick one of these extensions for the even states and another for the odd. This has the generic advantage of lifting the degeneracy between even and odd states. The spectrum is then $4n + 2 - 2\nu$ for the even states, and $4n+2+2\nu$ for the odd. This choice is a particularly well-behaved one because, as we take $g \to 0$, the odd states go to $4n + 3$ and the even states to $4n + 1$, and we get back the spectrum of the original harmonic oscillator. The implications of these various choices for supersymmetry are discussed in the next chapter.

One of the nice things about this problem is that a naive analysis of the problem using perturbation theory [105] automatically reproduces the "correct" result from self-adjoint extensions. This might be tied to supersymmetry (see Chapter 9).

Chapter 9

Issues of Symmetry

The symmetries associated with the $1/r^2$ potential fall under two heads: scale invariance, which we saw a while ago, and supersymmetry. The latter applies only to the weak regime; however, it has a tendency to "break" under self-adjoint extensions. This is not entirely surprising since, as Ref. [77] notes, even such trivial symmetries as the parity invariance of the infinite well might break under self-adjoint extensions. However, it's interesting to see when and whether symmetries break under self-adjoint extensions of singular potentials, because gauging the robustness of symmetries is important in, say, field theory.

9.1   Anomaly Revisited

The operator O_a, defined as follows,

$$O_a f(x) = f(ax)$$

maps the domain of a scale-invariant Hamiltonian onto itself, since

$$H[O_a f(x)] = H f(ax) = \frac{1}{a^2} H_{ax} f(ax) = \frac{1}{a^2} H f,$$

and $f \in D(H)$ by hypothesis. Suppose we operate on the domain of the strongly attractive $1/r^2$ potential with O. Then

$$f(ax) \sim \cos(\Xi \log(ax) + B) = \cos(\Xi \log x + B'),$$

where $B' = \log a + B$ in general belongs to a different self-adjoint extension than $f(x)$. It follows that the domain of the self-adjoint Hamiltonian is necessarily **not**

scale invariant. Similar things can be said about the delta function and the weakly attractive $1/r^2$ potential; however, in those cases, we do have one extension that preserves scale invariance: the Friedrichs extension. (In the literature the delta function is treated as an anomaly but the weak $1/r^2$ potential is not, though the problems are in fact very similar. This is because the Friedrichs extension for a "delta function" corresponds to a zero strength delta function, which most authors take to be no delta function at all.)

We would expect very direct manifestations of the anomaly in the zero-energy wavefunction, since $H\psi = 0$ has absolutely no scale in it. For the Friedrichs extension of the inverse square potential with $\lambda > -\frac{1}{4}$,

$$\psi(0; r) = r^\nu$$

and this is a solution even if we scale the coordinates. However, for $\lambda < -\frac{1}{4}$, the zero energy wavefunction has the form

$$\psi(0; r) = \sin(\nu \log r + B).$$

Under scaling of coordinates this collects a phase shift and becomes part of a different self-adjoint extension, so we have lost scale invariance.

Once it has been shown that the domain of the Hamiltonian—and therefore the Hamiltonian—is not scale-invariant, it might seem overkill to work any harder to show that there is an anomaly. There is, however, an interesting algebra associated with scale invariance.

The Algebra of Scale Invariance

The $SO(2, 1)$ algebra associated with conformal invariance was first applied to this problem by Jackiw [41]. We start by deriving Jackiw's operator D.[1] The unitary operator that performs dilations, U_λ, is given by

$$U_\lambda \psi(x) = \frac{1}{1 + \lambda} \psi(x + \lambda x)$$

and if we suppose that U is generated by a dilation operator Λ, we can write infinitesimal dilations as

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[1] Our treatment, so far as it goes, is entirely different from Jackiw's. He treats the transformations as fundamentally acting on the time variable, whereas we work within the framework of the time-independent Schrödinger equation.

$$(1 + i\epsilon\Lambda)\psi(x) = \frac{1}{1+\epsilon}\psi((1+\epsilon)x).$$

Assuming ψ to be nonpathological we can expand it around x to first order and get

$$\psi(x) + i\epsilon\Lambda\psi(x) = \psi(x) + \epsilon x\psi'(x) - \epsilon\psi(x)$$

and this simplifies to

$$i\Lambda\psi(x) = x\psi'(x) - \epsilon\psi(x)$$

which is to say that

$$\Lambda \equiv -xp - 1.$$

(We can also write this in Jackiw's fashion as $-(xp + px)/2$, if we like.) Now we commute this with the Hamiltonian:

$$[H, xp] = [H, x]p + x[H, p]$$

$$[p^2 + V(x), x]p + x[p^2 + V(x), p]$$

This simplifies to

$$[p^2, x]p + x[V(x), p]$$

which can be evaluated to be

$$2ip^2 - ix\frac{dV}{dx}$$

using the position basis. Normally, $xV'(x)$ is not the same sort of thing as $-2V$, which is what we want; however, this *is* the case with the free particle (trivially), the $1/x^2$ potential, and the 2D delta function. So the commutator tidies up to

$$[\Lambda, H] = 2iH. \tag{9.1}$$

There is another operator associated with these, $\Omega = x^2$, whose commutator with H gives a quantity related to Λ:

$$[\Omega, H] = 4i\Lambda \tag{9.2}$$

Also,

$$[\Omega, \Lambda] = -2i\Omega. \tag{9.3}$$

The symmetry we expect to be associated with Ω is the conformal symmetry $x \to \frac{x}{1+ax}$. This transformation would send a state

$$\psi(x) \to (1 + ax)\psi\left(\frac{x}{1 + ax}\right),$$

where the prefactor maintains the norm, and applying the same procedure as we did for Λ we get

$$G = -ix + ix^2 p,$$

which is no good. So it seems that the conformal symmetry isn't a symmetry of the time-independent problem.

Now we move to the time-dependent picture, where we have immediate problems because the time-dependent Schrödinger equation says

$$\frac{d\Lambda}{dt} = [H, \Lambda] \neq 0,$$

Λ isn't a constant of the motion. A way to get around that problem is to add an explicit time dependence to Λ to cancel out the commutator. Doing this gives us Jackiw's operator D,

$$D = tH - \frac{(xp + px)}{4},$$

which *is* a constant of the motion. Similarly, the constant of motion associated with Ω is

$$K = -t^2 H + 2tD + \frac{1}{2}x^2,$$

which is called the **conformal generator**. The system closes under commutation:

$$i[D, H] = H, i[K, D] = K, i[H, K] = -2D.$$

This might look somewhat unfamiliar; however, if we make the following substitutions:

$$B = -D, A = \frac{H + K}{2}, C = \frac{H - K}{2}$$

we get the much more transparent symmetry group generated by the algebra

$$i[A, B] = C, -i[B, C] = A, i[C, A] = B$$

which is $SO(2, 1)$, the symmetry group associated with—among other things—Lorentz transformations in 2+1 dimensions. De Alfaro et al [107] point out that H and K correspond, in the standard basis, to rotations about lightlike axes.

These generators correspond directly to the symmetries of the time-dependent theory that Jackiw [106] notes:

$$\begin{aligned} H : t &\rightarrow t + \delta \\ D : t &\rightarrow t(1 + \delta) \\ K : t &\rightarrow \left(\frac{t}{1+t\delta}\right) \end{aligned} \qquad (9.4)$$

These are respectively invariance under time translation, time dilation, and special conformal transformations of the time variable. As Camblong [47] mentions, time has units of length squared in our dimensions, so a dilation of time is automatically a dilation of length.

The symmetry is broken because D ceases to correspond to a symmetry of the theory. This shows up in the fact that the commutator $i[D, H] = H$ (or, equivalently, $[\Lambda, H] = 2iH$) breaks. To see how this happens, consider a small finite transformation $U = 1 - i\epsilon\Lambda$. The commutator of this with H is $-i\epsilon[\Lambda, H]$. H acts on the undilated state and HU on the dilated state; since the transformation was infinitesimal rather than discrete, these states cannot be in the same self-adjoint extension of H. Therefore, the domain of $[U, H]$—and therefore of $[\Lambda, H]$—can include only those states that are in *all self-adjoint extensions* of H, and it is impossible to pick a self-adjoint H such that $[\Lambda, H] = 2iH$. This breaks the $SO(2, 1)$ algebra, and constitutes the anomaly discussed by Camblong et al [44].

9.2   A Ladder Operator?

The repulsive and $1/x^2$ potential have features in common with the harmonic oscillator, as we will discuss, and it's possible to define structures similar to ladder operators for them. As ladder operators these are fairly useless because there aren't any bound states. For $\lambda < -\frac{1}{4}$ we lose the operator structure, but we do have a tower of bound states. We know we can't define a *number operator* for this situation, because the

system has no ground state. However, in practice we know how the operators work; the raising operator takes a bound state $K_{i\Xi}(kx)$ to the state $K_{i\Xi}(e^{\pi/\Xi}kx)$. Therefore the raising and lowering operators are discrete dilation operators, of the form

$$A_\pm = e^{\pm i\Lambda(\Omega - 1)},$$

where $\Omega = \pi/\Xi$. We can deduce the commutators $[A_\pm, H]$ from their operation on an arbitrary state.

$$[H, A]\phi(x) = HA\phi - AH\phi = \frac{1}{\Omega}H\phi(\Omega x) - AH\phi(x)$$

We can do this explicitly for our scale invariant Hamiltonian by noting that $H\phi(x)$ is just some function $\Psi(x)$, so we can apply A to it by simply replacing all the x's with Ωx's.

$$\Omega HA\phi(x) = -\frac{d^2}{d(\Omega x)^2}\phi(\Omega x) + \frac{\lambda}{\Omega^2 x^2}\phi(\Omega x) = -\phi''(\Omega x) + \frac{1}{\Omega^2 x^2}\phi(x)$$

This is just $(\Omega^2 - 1)H\phi(\Omega x) = (\Omega^2 - 1)HA\phi(x)$, and it follows that

$$[H, A] = (\Omega^2 - 1)HA.$$

To see that A is a sort of lowering operator, consider its action on an eigenstate of energy E.

$$A\Psi = \frac{1}{E}AE\Psi = \frac{1}{E}AH\Psi = \frac{1}{\Omega^2 E}HA\Psi.$$

Therefore $A\Psi$ is an energy eigenstate of H with eigenvalue $E\Omega^2$.

9.3   Supersymmetry

(This treatment follows Das and Pernice [49] closely; I have tried to reinterpret their work in terms of self-adjoint extensions.)

The Hamiltonian for the simple harmonic oscillator can be written in dimensionless units as

$$H = \frac{\hbar\omega}{2}(P^2 + \omega^2 Q^2)$$

where $Q = x\sqrt{m\omega/\hbar}$ and $P = p/\sqrt{m\omega\hbar}$. If we write $A = Q + iP$ (in which case $A^\dagger = Q - iP$ since both operators are Hermitian) we can write the Hamiltonian as

$$H = \frac{\hbar\omega}{2}(AA^\dagger - 1) = \frac{\hbar\omega}{2}(A^\dagger A + 1)$$

and we'll call the prefactor 1. In these units the energy spacing is 2 and the ground state for the SHO is at 1. The product $A^{\dagger}A \equiv N$, the **number operator**, and the three operators have the following commutation relations:

$$[A, A^{\dagger}] = 1, [N, A] = -A, [N, A^{\dagger}] = A^{\dagger}$$

The first of these properties follows from $[x, p] = i\hbar$; the other two follow from the first. These properties make the oscillator very easy and elegant to solve. That's not all that it's good for; in fact, it's tremendously deep and important, though we won't do much more than graze the iceberg. Consider the two Hamiltonians

$$H_{+} = N + 1 = A^{\dagger}A$$

$$H_{-} = N - 1 = AA^{\dagger}$$

Evidently $H_{+} = H_{-} + 2$. So the spectrum of H_{+} is $\{2, 4, 6...\}$ and that of H_{-} is $\{0, 2, 4...\}$. That is, the spectra of H_{+} and H_{-} are identical except for a zero-energy ground state that H_{-} has and H_{+} does not. Potentials with this structure are said to be **supersymmetric (SUSY) partners**. Note that the degenerate states merely have the same energy; they do not look alike; in fact they're of opposite parity. The origin or point of this symmetry might seem obscure in quantum mechanics; however, it's an important symmetry in QFT and a familiar word to most physicists. The hope is that understanding the properties of SUSYQM—especially whether and how it is broken—might help us understand the same issues in field theory.

The almost-degeneracy of the spectrum is independent of what A and $A^{\dagger}$ are. Suppose

$$H_{-}\Psi = AA^{\dagger}\Psi = E\Psi$$

It follows that

$$H_{+}(A^{\dagger}\Psi) = A^{\dagger}AA^{\dagger}\Psi = A^{\dagger}E\Psi = E(A^{\dagger}\Psi)$$

i.e. we have an eigenstate of H_{+} with exactly the same eigenvalue. (We can run the same thing in reverse using Q.) The exception to this logic is if either A or $A^{\dagger}$ applied to a state ψ in the Hilbert space gives a trivial state. If we assume that $A = W + iP$, where $W(x)$ is some function of x called the **superpotential**, we give a quick and sloppy argument to show that it's impossible for both conditions to hold at once. Suppose $A\psi = 0$ and $A^{\dagger}\phi = 0$:

$$\frac{d\psi}{dx} = -W\psi \tag{9.5}$$

$$\frac{d\phi}{dx} = W\phi \tag{9.6}$$

$$\frac{d\psi}{\psi} = -\frac{d\phi}{\phi} \tag{9.7}$$

and therefore

$$\psi \sim \frac{1}{\phi}$$

so it's impossible for both of them to be normalizable.

Supersymmetry is said to hold when either of the solutions is normalizable; a mechanism that can potentially break supersymmetry is the imposition of boundary conditions that take the ground state out of the operator domain. This is how self-adjoint extensions come into the picture.

9.3.1 Supersymmetric Oscillator on the Half-Line

Suppose you take the harmonic oscillator on the half-line and put an infinite wall at the origin. This throws out the even states, so that the bound state for our harmonic oscillator is now at 3 and the spectrum is $\{3, 7, 11, ...\}$. For a supersymmetric pair, this would mean that the spectra were $\{4, 8, 12, ...\}$ and $\{2, 6, 10, ...\}$, and this is not a supersymmetric pair. Das and Pernice show that this is an artefact of our regularization scheme, which breaks supersymmetry between H_+ and H_-. They regularize the problem in a way that retains the symmetry; this leads to a supersymmetric spectrum, but adds delta function terms to the boundary. In terms of self-adjoint extensions, this means that the supersymmetric partners are not necessarily in the "same" self-adjoint extension. This is all right since $AA^\dagger$ and $A^\dagger A$ are not the same operator.

Supersymmetry is different from, say, scale invariance in that it's a spectral property; it makes sense to talk about the spectrum only after you've chosen a self-adjoint extension. However, the forms of the Hamiltonians are determined by the superpotential W, so it's reasonable to ask whether, for a supersymmetric pair, one is guaranteed that there will be at least *some* self-adjoint extension for which the spectra are supersymmetric. In the case of the half oscillator, there is; if we impose $\psi'(0) = 0$ on H_-

and $\psi(0) = 0$ on H_+, we get back a supersymmetric pair whose spectra are identical to those of the *full* oscillator restricted to the half-line.

The regularization scheme they choose works as follows. The superpotential is $W = x\theta(x)$ on the half-line, so they approximate it by $W_a = x\theta(x) + a\theta(-x)$ and take the limit as $a \to +\infty$. If we write $V_\pm$ as the potential terms of $H_\pm$, these work out to be

$$V_+ = x^2\theta(x) + a^2\theta(-x) - x\delta(x) - a\delta(x) - \theta(x)$$

$$V_- = x^2\theta(x) + a^2\theta(-x) + x\delta(x) + a\delta(x) + \theta(x)$$

and of course $x\delta(x)$ vanishes at the origin. As $a \to \infty$, the boundary conditions are set mostly by the δ-function terms, which become strongly repulsive for V_+—which acquires a Dirichlet boundary condition at the origin—and strongly attractive for V_-. In the limit, as Das and Pernice show, this system is supersymmetric.

The disadvantage of their scheme is that they implicitly assume that SUSY holds at all scales. Since we don't know that short-distance physics is supersymmetric, it seems overoptimistic to suppose that no explicit symmetry breaking occurs. However, within its limits the technique of Das and Pernice is robust, since a regularized superpotential will always generate supersymmetry, and this should hold in the limit as long as the potential isn't too pathological.

9.3.2 The $x^2 + 1/x^2$ Potential

Consider the superpotential $W(x) = \frac{g}{x} - x$. The operators associated with this are

$$A = \left(-\frac{d}{dx} + \frac{g}{x} - x\right)$$

$$A^\dagger = \left(\frac{d}{dx} + \frac{g}{x} - x\right).$$

The Hamiltonians can be calculated from this:

$$H_+ = A^\dagger A = -\frac{d^2}{dx^2} + \frac{g^2}{x^2} + x^2 - \frac{g}{x^2} - 2g - 1$$

$$H_- = AA^\dagger = -\frac{d^2}{dx^2} + \frac{g^2}{x^2} + x^2 + \frac{g}{x^2} - 2g + 1$$

The couplings of the inverse square terms are always in the weak regime; for $g(g \pm 1) < -1/4$ we must have g complex, but in that case A and $A^\dagger$ would fail to

be adjoints and all hell would break loose. In fact, this potential has issues even in the weak regime, since the Friedrichs extension is justifiable only for $\lambda > 0$,[2] and for any $\lambda < 0$ our choice of ground state is arbitrary. However, from the point of view of supersymmetry this is as much of an opportunity as a problem, since it means that we can put in a zero-energy ground state by hand. This is possible only if $\lambda < 3/4, |g| < 1/2$, which holds either for both Hamiltonians or for neither. The reason for this restriction is that if $\lambda > 3/4$ we have an impenetrable barrier at the origin; the only regular wavefunction is the one that vanishes. This gives us a twofold degenerate spectrum of bound states on the line, and supersymmetry is broken for the same reason as with the cutoff we discussed earlier.

However, for weak g one can use perturbation theory to solve the potential [105]. Let's assume, without loss of generality, that $g > 0$. As we have seen, a careful treatment using self-adjoint extensions gives a family of which a very small subset are consistent with perturbation theory; the method of Lathouwers picks one of these automatically. That the direct treatment works is a consequence of the theory of orthogonal polynomials, which Lathouwers uses. Anyway, the sensible/perturbative spectrum has two series of levels ($\alpha = \frac{1}{2}\sqrt{1 - 4\lambda}$):

$$E_n^\pm = 2(2n \pm \alpha + 1)$$

$$\phi_n^\alpha(x) = x^{\alpha+1/2} e^{-x^2/2} L_n^\alpha(x^2)$$

and the even (E_n^-) [resp. odd (E_n^+)] wavefunctions are even [odd] extensions of $\phi(x)$ to the negative half-plane.

There's also an algebraic solution to the problem, which Das and Pernice supply. One can look for a state of vanishing energy by solving $A\psi = 0$. As a first-order equation, this is relatively easy, and

$$\psi \approx x^g e^{-x^2/2}$$

so we have picked the self-adjoint extension that gives us a bound state at zero energy. Which extension does this correspond to? Regardless of which potential possesses this state, V_+ has been translated down from its canonical position, so what we're looking for is a ground state of the oscillator plus well system at $1 + 2g$. Since $2g < 1$ this is too low to be a bound state of the Friedrichs extension. By the method of Lathouwers

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[2]It's not required in any case; the barrier need not be impenetrable.

the bound state of the perturbative extension is $2(1 - \alpha) = 1 + 2g$, which is just what we wanted.

Does the rest of the spectrum line up? The first odd state goes to $2 + 2\alpha = 3 - 2g$. Translating it down takes it to $2 - 4g$. For V_- the first bound state using the Lathouwers extension is at $1 - 2g$ before translating; on translating by $1 - 2g$ it goes to $2 - 4g$ and lines up perfectly with the first excited state of V_+. The rest is left to the reader's imagination.

Of course, one should be careful about saying that SUSY is "preserved" under the Lathouwers extension. SUSY is, in quantum mechanics at least, basically a duality relationship; and a better phrasing might be that *one way* to make a formally SUSY pair of the $x^2 + 1/x^2$ type have supersymmetric spectra is to take the Lathouwers extension of both operators. One might speculate that the existence of a Lathouwers extension is related to the problem's being supersymmetric.

9.4   Virasoro Algebra of the $1/x^2$ Potential

We didn't need the harmonic oscillator term to make the $1/x^2$ potential factorizable. The relevant operators are

$$A = -\frac{d}{dx} + \frac{g}{x}, A^\dagger = \frac{d}{dx} + \frac{g}{x}.$$

These produce the Hamiltonians

$$H_+ = AA^\dagger = -\frac{d^2}{dx^2} + \frac{g(g+1)}{x^2}$$

$$H_- = A^\dagger A = -\frac{d^2}{dx^2} + \frac{g(g-1)}{x^2}$$

and commute as follows:

$$[A, A^\dagger] = \frac{2g}{x^2}$$

$$[A^\dagger, H] = \frac{-2g}{x^2} A^\dagger$$

$$[A, H] = \frac{2g}{x^2} A$$

So the Hamiltonian is *not* a number operator. None of this works for strong coupling, since that would require $g \in \mathbb{C}$, in which case the operators A and $A^\dagger$ would fail to

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be adjoints, and the product $AA^\ddagger$, where $A^\ddagger$ is the true adjoint of A, would not be a legitimate Schrödinger Hamiltonian.

As well as the generator of the $SO(2,1)$ group, this Hamiltonian has another algebra associated with it, called a **Virasoro algebra**, which Ref. [42] uses to discuss the scaling properties of black holes. Virasoro algebras are of great importance in string theory; we mention this one mainly for completeness. Let's suppose that $L_n = -x^{n+1}\frac{d}{dx}$ and $P_m = 1/x^m$. (It's easy to see that the Hamiltonian can be written as $AA^\dagger = (-L_{-1} + gP_1)(L_{-1} + gP_1)$. The generators L_m and P_n form the following algebra:

$$
\begin{aligned}
[P_m, P_n] &= 0 \\
[L_m, P_n] &= nP_{n-m} \\
[L_m, L_n] &= (m-n)L_{m+n} + \frac{c}{12}(m^3 - m)\delta_{m+n,0} \\
[P_m, H] &= m(m+1)P_{m+2} + 2mL_{-m-2} \\
[L_m, H] &= 2g(g-1)P_{2-m} - (m+1)(L_{-1}L_{m-1} + L_{m-1}L_{-1})
\end{aligned}
$$

are easy to establish, except for the last term in the third commutator, which is an "extension" of the algebra. Birmingham et al study the representations of this algebra, and possible extensions of it to the strong-coupling case; however, their main interest is in the weak sector. Their remarks on self-adjoint extensions are somewhat surprising; for example, they claim that the Hamiltonian with $\nu = -1/4$ (i.e. the 2D delta function) has infinitely many bound states with wavefunctions $\psi = \sqrt{x}K_0(k_n x)$. This is clearly inconsistent with the requirement that the operators be self-adjoint, since K_0 is nodeless and definitely cannot be made orthogonal to itself by dilation. (After all, $\delta^2(r)$ does **not** have infinitely many bound states.)

Chapter 10

Summary and Applications

Renormalization theory teaches us that deep down all singular potentials are normal and solvable, and that one doesn't need to know the details of their short-distance behavior to solve them. Suppose short-distance physics comes into play at a length scale ϵ. Then for particles with energy $k^2 \ll 1/\epsilon^2$, such physics manifests itself only as a boundary condition. The spectrum depends on the boundary condition, which has two implications—first, that we can't ignore it; and second, that we can determine the boundary condition by experimental observation of the spectrum.

So what we need is an effective theory that involves nothing more than the long-distance physics and the boundary condition (or the experimental observable), and gives accurate predictions for low-energy observables. There are two ways to do this. The more explicit one is renormalization, in which one picks a parameterization of short-distance physics (a square well, say) and explicitly replaces the details of the short-distance theory with a boundary condition. This is a procedure we have used in Chapter 5; we scale the short-distance physics as the long-distance physics goes to zero to keep the observable constant. The other way is to use the procedure of self-adjoint extensions, which involves applying the boundary condition directly to the operator's domain. These methods are equivalent because a square well in the limit $\epsilon \to 0$ is a smeared-out point interaction, and (as we have seen) point interactions can be written as self-adjoint extensions. One should note that self-adjoint extensions do not give an accurate description of the theory all the way down; their predictions are valid only to the extent that they coincide with renormalization, which is to say, for $k \ll 1/\epsilon$, where ϵ is the distance down to which we know what's going on.

Each of these methods has its limitations: self-adjoint extensions can be difficult

to calculate, and renormalization schemes might produce scheme-specific effects. (An example is the continuous paths of Chapter 5.) In addition, as we saw in the case of one-dimensional quantum mechanics, there are often self-adjoint extensions that do not correspond to a realistic parameterization of short-distance physics; renormalization is sometimes necessary to find the good extensions. In the one-dimensional problem, this might mean throwing out solutions with discontinuous wavefunctions.

The link between renormalization and self-adjoint extensions means that any symmetry in the self-adjoint extensions must manifest itself asymptotically in the renormalized theory. An example is the discrete scale symmetry of the strong $1/r^2$ potential. This symmetry also manifests itself in the log-periodic dependence of short-distance physics on the cutoff radius, which we call a **limit cycle**.

An interesting feature of very singular potentials is that no continuous scaling of short-distance physics with a works for arbitrarily small a. Physically this means that you can't keep, say, the ground state fixed under renormalization. This corresponds to the fact that the self-adjoint extensions have spectra unbounded from below, so as you take the cutoff to zero, bound states keep appearing near the bottom of your spectrum. What saves renormalization in this case is that a boundary condition is (asymptotically) fixed by requiring a bound state to be at a given energy, and it doesn't matter at all what the state number is. This is related to the notion of the privacy of deep bound states, which I have shown in the case of scattering observables—the presence of deep, localized bound states does not affect low-energy scattering at all. This is analogous to classical wave mechanics, where you need high frequency (high energy) waves to detect and resolve small features.

Another generic feature of singular potentials is the so-called Klauder phenomenon, where a potential V is sufficiently singular that $H_0 + \lambda V$ does not return the spectrum of H_0 as $\lambda \to 0$. We have explained Klauder phenomena—or at least the class associated with singular potentials—in terms of self-adjoint extensions of the free-particle Hamiltonian, and therefore in terms of delta functions. The origin of these phenomena becomes a lot clearer if one thinks of them in terms of the variation of boundary conditions as one alters the coupling. We argue (a) that Klauder phenomena are generic, and (b) that renormalizing the coupling of singular potentials—a technique quite widely used in the literature—produces a Klauder phenomenon, and therefore produces generic results that have nothing to do with the potential used.

We have worked mostly with exactly solvable potentials, because those are the

only cases for which self-adjoint extensions can be calculated exactly and compared with the results of various renormalization schemes.

10.1 Singular Potentials in Physics

This is a brief catalogue of some places where singular potentials and failures of self-adjointness are interesting, beyond the two-body Schrödinger equation. We omit the Efimov effect and the charged wire experiment, which have already been discussed.

10.1.1 The Relativistic Coulomb Problem

The Dirac equation for relativistic spin-1/2 particles in a Coulomb potential can be written as follows [1]:

$$\frac{du}{dr} - \chi \frac{u}{r} = \left(1 - E - \frac{\alpha Z}{r}\right) w(r)$$

$$\frac{dw}{dr} + \chi \frac{w}{r} = \left(1 + E + \frac{\alpha Z}{r}\right) u(r)$$

where (u, w) are the components of the spinor field, χ is a (half-integer) angular momentum quantum number, and αZ is the nuclear charge. We can already see the beginnings of trouble in the fact that the potential term scales with the derivative term. Case [1] rewrites this equation in terms of a new set of variables as follows:

$$\frac{d^2\psi}{d\rho^2} + \left(\frac{1}{\rho} - 1\right) \frac{d\psi}{d\rho} + \left(\frac{E\delta}{\rho} + \frac{\alpha^2 Z^2 - \chi^2}{\rho^2}\right) \psi = 0.$$

When $\alpha^2 Z^2 - \chi^2 > \frac{1}{4}$, i.e. if the nucleus is sufficiently highly charged, we have the usual pathologies of the inverse square potential.

Similarly, the Klein-Gordon equation for spin-0 particles can be rewritten as a Schrödinger equation:

$$\frac{d^2u}{dr^2} + \left(-(1 - E^2) + \frac{2E\alpha Z}{r} + \frac{\alpha^2 Z^2 - l(l+1)}{r^2}\right) u = 0$$

and this has the same features.

An early attempt to apply dimensional regularization to the pathologies of the relativistic Coulomb problem is in Ref. [87], but it has occasioned some controversy [88]. Another interesting paper is Ref. [26], which relates Case's method to absorptive solutions by changing the inner product relative to which self-adjointness is calculated.

10.1.2 Solvable Models with Singular Interactions

The most famous example is the **Kronig-Penney model**, which models an atomic lattice by a one-dimensional array of delta functions. This model, despite its simplicity, can reproduce the electronic band structure of crystals. For the details, see Ref. [53]. Two classes of one-dimensional models in condensed matter physics, the **Calogero-Sutherland models** [13] and the **Haldane-Shastry models** ([108],[109]), have inverse square interactions. A Calogero-Sutherland model was recently realized with ultracold Bose atoms [110]. In addition to these, several shape invariant and exactly solvable potentials, such as the **Pöschl-Teller** and **Rosen-Morse** potentials, have interactions that are inverse square at certain scales (for details see [91]).

10.1.3 Dipoles and Black Holes

These applications are discussed in Ref. [44]. A familiar fact from electrodynamics is that a point dipole produces a $1/r^2$ potential. One would expect to find a critical strength for the $1/r^2$ potential to have bound states. This has been verified experimentally for electrons and polar molecules. Another application is in the study of the near-horizon structure of black holes, which can be modeled by a $1/r^2$ potential in certain regimes [44],[42].

10.2 Executive Summary

We could have summed up the contents of this rather long thesis in the following equivalences:

- Self-Adjoint Extensions = Some Renormalization Schemes

- Other Renormalization Schemes = Delta Functions

- Boundary Conditions = Absolutely Anything

However, brevity $\neq$ intelligibility.

Appendix A

Deriving the Duality Transformation

Given the radial Schrodinger equation in its normal, unsubstituted form:

$$\left[-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{r^2} - \frac{g}{r^2}\left(\frac{r}{r_0}\right)^{\epsilon} + k^2\right]R(r) = 0 \qquad \text{(A.1)}$$

We make the substitutions

$$r = \frac{y^{2/\epsilon}}{2k} \qquad \text{(A.2)}$$

$$R(r) = y^{-\frac{1}{\epsilon}-\frac{1}{2}}v(y) \qquad \text{(A.3)}$$

Plugging (A.2) into (A.1) and collecting the r^2 terms gives us

$$4k^2 y^{-4/\epsilon}\left[-\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + l(l+1) - g\frac{y^2}{(2kr_0)^{\epsilon}} + k^2\right]u(r) = 0 \qquad \text{(A.4)}$$

If we left-multiply (order matters because of the differential operator) by $y^{4/\epsilon}$,

$$\left[4k^2\left(-\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + l(l+1) - \frac{gy^2}{(2kr_0)^{\epsilon}}\right) + k^2\frac{y^{4/\epsilon}}{4}\right]y^{-\frac{1}{\epsilon}-\frac{1}{2}}v(y) = 0 \qquad \text{(A.5)}$$

Now we're in a position to work out the derivative term. Plugging in the relation

$$dr = \frac{y^{\frac{2}{\epsilon}-1}k\epsilon}{d}y,$$

expanding, and simplifying, we get the form

$$\frac{d}{dr}\left(r^2\frac{d}{dr}\right) = \frac{\epsilon^2}{4}\left[y^{-\frac{1}{\epsilon}+\frac{3}{2}}\frac{d^2v}{dy^2} - \left(\frac{1}{\epsilon^2} - \frac{1}{4}\right)y^{-\frac{1}{\epsilon}-\frac{1}{2}}\right]. \tag{A.6}$$

Since we want the prefactor of the second-derivative term to be 1 we divide all of (A.5) by the appropriate term. Collecting similar terms gives us

$$-\frac{d^2v}{dy^2} + \left(\frac{1+4l(l+1)}{\epsilon^2} - \frac{1}{4}\right)\frac{v}{y^2} + \frac{1}{\epsilon^2}y^{\frac{4}{\epsilon}-2} = \frac{4g}{\epsilon^2}\frac{1}{(2kr_0)^\epsilon}v \tag{A.7}$$

This is recognizable as a Schrodinger equation with (as $\epsilon \to 0$) a very large centrifugal barrier term and a positive power-law potential shaped somewhat like an infinite square well. Our new energy term, denoted Λ,

$$\Lambda = \frac{4g}{\epsilon^2}\frac{1}{(2kr_0)^\epsilon}$$

is positive as we might expect, since a positive power-law potential has positive-energy bound states; a curious feature is that it has a vanishingly small dependence on the old energy term k, but is dependent on g. In fact, k hardly appears in this equation, and we recover it at the end of the problem only by performing the inverse transformation of (A.2) and (A.3).

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