

# Anomalies in Quantum Mechanics

Owen Edward Marschall

April 17, 2015

Submitted to the  
Department of Physics and Astronomy  
of Amherst College  
in partial fulfillment of the requirements  
for the degree of  
Bachelor of Arts with honors

Faculty Advisor: Professor William Loinaz

Copyright © 2015 Owen Edward Marschall

# Abstract

The scale-symmetric  $1/r^2$ , Dirac delta in two dimensions, and Dirac delta prime potentials are solved using various techniques of regularization and self-adjoint extensions, in order to study the effect of anomalous scale symmetry breaking. All of the methods used qualitatively agree for the two-dimensional delta potential. Those used on the one-dimensional delta prime potential do not all agree, but it is found that the Griffiths approach and momentum-space regularization produce the exact same, symmetry-preserving bound-state and scattering sectors. It is reaffirmed that the two-dimensional delta potential is anomalous, but it is posited that the delta prime potential may not be. It is discussed whether anomalous symmetry breaking happens due to regularization schemes or quantization.

# Acknowledgements

I am deeply indebted to my advisor William Loinaz for investing so much of his time and energy into this project, both over the summer and over this past academic year. He was always willing and eager to talk about the minutiae of this topic for hours on end, week after week, despite his primary field of research being largely unrelated. Moreover, he was a great mentor to me, encouraging and empowering me to confidently reason through these tricky concepts on my own without deferring to authorities in the literature. I also must thank him for dedicating several hours of his week (and several pieces of his prized imported chalk) to a special topics class with me on applications of abstract algebra to problems in physics during my sophomore year, which needless to say was invaluable experience to have for writing a thesis in theoretical physics.

Thanks to Sarang Gopalakrishnan '06 for writing such an excellent senior thesis to base my work on. Whenever I was hung up on some concept or detail, my first thought would be "Let's see what Sarang thinks about this." Sections of his thesis were often way clearer than published textbooks about the same topic, in particular when it came to the theory of self-adjoint extensions.

I want to give a shout out to the math and physics faculty for their excellent teaching, in particular Professors David Hanneke, Rob Benedetto, and Michael Ching, from whom I took multiple courses and/or had research experiences with. Without the excellent training I received in mathematics and physics over four years from the brilliant, dedicated teachers at this college, writing a thesis on this topic would not have been possible.

Lastly, I want to thank my family for being so supportive and my friends for being such fun distractions during this extremely busy year. Thanks to my parents for always being willing to listen to my ramblings about my thesis, and for their love and encouragement.

Thanks to Nicole Chi for her endless supply of coffee, snacks, and laughs; and to the Homie Patrol for their constant vigilance.

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Anomalies . . . . .	1
1.2	A Guide to the Reader . . . . .	4
1.3	Who Did What . . . . .	4
<b>2</b>	<b>Theory of Anomalies</b>	<b>7</b>
<b>3</b>	<b>Self-Adjoint Extensions</b>	<b>16</b>
3.1	Domains and Adjoints . . . . .	17
3.2	Finding Self-Adjoint Extensions “By Hand” . . . . .	21
3.3	Deficiency Subspace Method . . . . .	22
3.3.1	Summary . . . . .	24
<b>4</b>	<b>The Algebra of Scale Symmetry</b>	<b>26</b>
4.1	Continuum of Eigenstates . . . . .	27
4.2	Scale Invariance in Classical Mechanics . . . . .	28
4.3	Scale Invariance in Quantum Mechanics . . . . .	30
4.4	SO(2,1) Algebra . . . . .	32
<b>5</b>	<b>The <math>1/r^2</math> Potential</b>	<b>34</b>
5.1	Solving the Schrödinger Equation . . . . .	34
5.2	Self-Adjoint Extensions . . . . .	36
<b>6</b>	<b>The 2D <math>\delta</math> Potential</b>	<b>39</b>
6.1	Position-Space Regularization . . . . .	39

6.2	Momentum-Space Regularization . . . . .	45
6.2.1	1D $\delta$ Potential . . . . .	46
6.2.2	2D $\delta$ Potential . . . . .	50
6.3	Self-Adjoint Extensions Method . . . . .	53
6.3.1	Free Particle on the Unpunctured Plane . . . . .	54
6.3.2	Free Particle on the Punctured Plane . . . . .	57
6.4	Dimensional Regularization . . . . .	58
6.5	Path-Integral Approach . . . . .	61
6.6	The Classical Problem . . . . .	63
6.7	Interpretation as Anomaly . . . . .	65
<b>7</b>	<b>The 1D <math>\delta'</math> Potential</b>	<b>68</b>
7.1	Position-Space Regularization . . . . .	69
7.2	Momentum-Space Regularization . . . . .	72
7.3	Griffiths Method . . . . .	77
7.4	Self-Adjoint Extensions . . . . .	80
7.4.1	Self-Adjointness of 1D $\delta$ . . . . .	81
7.4.2	Self-Adjointness of 1D $\delta'$ . . . . .	82
7.4.3	Deficiency Subspaces . . . . .	83
7.5	Interpretation . . . . .	84
<b>8</b>	<b>Applications and Conclusion</b>	<b>85</b>
8.1	Theoretical Applications . . . . .	85
8.2	Experimental Applications . . . . .	86
8.3	Conclusion . . . . .	87
8.4	Future Work . . . . .	88
<b>A</b>	<b>1D <math>\delta'</math> Calculation Details</b>	<b>90</b>
<b>B</b>	<b>Self-Adjoint Extensions On <math>\mathbb{R} \setminus \{0\}</math></b>	<b>95</b>
	<b>Bibliography</b>	<b>98</b>

# Chapter 1

## Introduction

### 1.1 Anomalies

An anomaly is the breaking of a classical symmetry that occurs in the corresponding quantum theory. Anomalies occur frequently in the context of quantum field theory and often have consequences for a theory such as the non-conservation of currents, the emergence of new types of particles, or the introduction of a mass scale [47]. Anomalies in quantum field theory have been studied for decades and are relatively well-understood [31].

But there has more recently been a surge of interest in quantum *mechanical* anomalies, for a number of reasons. One reason is strictly pedagogical: given how important anomalies are in quantum field theory but how inaccessible this subject is to undergraduates, many authors have taken to finding examples in ordinary quantum mechanics that can help build students' intuition for the concept in a simpler context [30].

The more important reason, however, is that ordinary quantum mechanics has been found to be useful as a simplifying approximation to quantum field theories [44]; this is the central idea behind the *effective field theory* program. Quantum mechanics itself can be thought of as a 0+1-dimensional field theory, and the Fock Space formalism of QFT, which is used to allow for indefinite numbers of particles, is built up from quantum mechanical Hilbert spaces [49]. Therefore phenomena in quantum field theory ought to have analogues in quantum mechanics.

As a part of the effective field theory program, many tools and ideas from quantum field theory such as regularization, renormalization, and dimensional transmutation are being

applied to singular potentials in ordinary quantum mechanics [21]. These processes usually involve getting rid of some unwanted infinity—even if it appears very naturally in a calculation—or inserting dimensions into an originally dimensionless parameter. It is assumed that the infinity is unphysical and that it instead represents some inadequacy of the theory that needs to be fixed. Since these techniques are responsible for the creation of anomalies in quantum field theory, it is not surprising that bringing them into quantum mechanics would also bring about anomalous symmetry breaking. These quantum mechanical anomalies have become interesting objects of study in their own right.

The only classical symmetry that has found to be broken in quantum mechanics is *scale symmetry*, which is essentially the property of a potential having only dimensionless couplings. A consequence is that there is no dimensional parameter available to set the energy scale of, say, a bound state or energy dependence in a scattering phase shift. Therefore, this symmetry can be shown to be broken through what is called the anomalous emergence of a bound state—and this bound-state energy can be a reference for the anomalous energy dependence of scattering observables, too. These ideas will be more fully fleshed out in Chapter 4.

On the first pass through calculating the spectrum of a scale symmetric potential, we usually find that there is no bound state sector, but we can sometimes force a bound state on the problem through techniques of regularization and renormalization, which are required for the problem to make well-defined physical predictions. This, in a nutshell, is the quantum mechanical anomaly. The Dirac delta potential in two dimensions and the  $1/r^2$  potential in any number of dimensions, both scale-symmetric potentials, have been presented in the literature as examples of the quantum mechanical anomaly [1], [9], [30], [33].

Invariably, the derivation of a quantum mechanical anomaly involves at some point in the calculation a kind of “fudging,” as one might call it, e.g. redefining certain limits in the middle of the problem, allowing a coupling constant to approach 0, or “cutting off” an integral’s bounds before infinity. Although it may seem shocking and distasteful to someone outside the field, such “fudging” can be well-motivated and sensible. In quantum field theory, techniques of regularization and renormalization are necessary to deal with the



artificial infinities that frequently arise due to the infinite degrees of freedom in the theory [37].

A simple example of renormalization is choosing, after the fact, to have a free-scalar-field Hamiltonian's eigenvalues correspond to energy density rather than energy, since space-time has infinite volume. Such a divergence is known as an infrared divergence, and it is fixed simply by dividing through by the volume of space  $V$  and taking the limit  $V \rightarrow \infty$  [37]. Another type of renormalization involves cutting off high-energy, short-distance oscillation modes in the field theory, because we assume that at some energy/length scale, the field theory breaks down. This is called an ultraviolet divergence, which arose because we presumed the field theory to be valid for all length scales [37].

This same mindset of trying to eliminate all unwanted infinities at all cost has been adopted into quantum mechanics. Therefore, it should not be surprising that we would encounter the anomalous breaking of scale-symmetry, since the lack of a bound state often results from the bound-state energy blowing up to  $-\infty$  during a regularization procedure that respects the scale symmetry. If we decide that such an infinity is unacceptable, then of course a bound state will emerge.

So on the one hand, these quantum mechanical anomalies result from the application of well-respected and well-understood techniques of renormalization borrowed from quantum field theory, used to deal with the artificial problem of having infinitely many degrees of freedom. But on the other, there's this troubling feeling that such an approach would necessitate an anomaly in any case, regardless of the particulars of the problem. If we were going to get rid of any infinity we encountered all along, then how would we *not* break scale symmetry? What would it mean for a scale-symmetric potential to not have an anomaly?

These are the kinds of questions we will attempt to answer. How should we view these examples of anomalies in quantum mechanics? Are they truly outliers, as the terminology "anomaly" suggests, or did theorists find them only because they were determined to find them?

As a side question, we will also consider the one-dimensional delta prime potential—that is, the derivative of the delta potential, whatever that means—which is scale symmetric but hasn't yet been entered into the literature's canon of quantum mechanical anomalies. By

performing similar calculations on this potential, we can gain more insight into whether it is due to characteristics of the potentials themselves that they are susceptible to anomalous symmetry breaking or simply a consequence of using field theory tools to calculate their spectra and scattering observables.

## 1.2 A Guide to the Reader

Chapter 3 is necessary to do a lot of the calculations that appear in Chapters 5-7 if one is not already familiar with self-adjoint extensions. Unfortunately, Chapter 3 is also necessary to understand one small detail of Chapter 2, but we have kept the order this way because Chapter 2 is still mostly introductory material. Chapter 4 presents in detail the consequences of scale and conformal symmetry in classical and quantum mechanics, using Noether's theorem. Chapters 5-7 present various approaches to solving three singular, scale-symmetric potentials, and there is no preferred order. Chapter 8 discusses the theoretical and experimental relevance to studying both anomalies in general and these specific scale-symmetric potentials in particular.

## 1.3 Who Did What

In the spirit of Sarang Gopalakrishnan '06, whose thesis work this project builds on, we include a brief note to explicitly cite the origins of the calculations we present. It is still made clear throughout the text when another source is being referenced, but it is not as apparent when an original calculation is being presented. There are three broad categories for the problems solved in this thesis:

1. Calculations done by the author that, to the author's knowledge of the literature, are original:
  - Double- $\delta$  regularization of 1D  $\delta'$ , bound-state problem and scattering problem including renormalization.
  - Finite-well approach to the classical 2D  $\delta$ .

- Momentum-space calculation of 2D  $\delta$  bound-state energy in terms of cutoff, done directly instead of via S-matrix pole, as well as reinterpretation of  $\psi(\vec{0})$  in light of renormalization.
  - Momentum-space calculation of the 1D  $\delta'$  bound-state and scattering sectors, including observation that, although there is no anomalous energy-dependence in the phase shift, we get the same transmission magnitude as is found in the Griffiths boundary condition approach.
  - Characterization of position-space renormalization of 2D  $\delta$  as redefinition of  $\delta$  functional to  $\tilde{\delta}$ , which picks out rate of logarithmic divergence of a test function.
2. Calculations done by the author that are almost certainly not new, but were done without referencing any outside sources:
- Deriving the conserved charges  $D$  and  $K$  in classical mechanics from scale and conformal symmetry, respectively.
  - Applying Griffiths' 1D  $\delta'$  boundary conditions to the bound-state and scattering problems.
  - Finding the general set of self-adjoint boundary conditions on  $\mathbb{R} \setminus \{0\}$ , as well as verifying that the usual  $\delta$  and  $\delta'$  boundary conditions from Griffiths represent self-adjoint point interactions.
  - Verifying that the free-particle radial operator (with boundary conditions to ensure continuous differentiability) on the unpunctured plane is self-adjoint.
  - Momentum-space solution to 1D  $\delta$  potential.
3. Calculations paraphrased by the author, possibly with slight modifications, corrections, and/or reinterpretations, from outside sources:
- Derivation of  $SO(2, 1)$  invariance algebra for scale-symmetric potentials in quantum mechanics (Ref. [1]).
  - Position-space regularization of 2D  $\delta$  (Ref. [1]).

- Solving Schrödinger equation for 3D  $1/r^2$  potential and finding self-adjoint domains (Refs. [1], [39], and [33]).
- Presentation of mathematics behind self-adjoint extensions in Chapter 3 (Refs. [4] and [5]).
- Derivation of anomalous term in Ehrenfest theorem (Ref. [42]).

## Chapter 2

# Theory of Anomalies

In short, an anomaly is a symmetry breaking that occurs “upon quantization”; that is, when considering the same problem from a quantum mechanical point of view. The idea of quantizing theories may be fundamentally flawed [37]: why would you formulate a supposedly more robust theory in terms of a classical approximation? Nonetheless, quantizing classical Hamiltonians is still a useful and common technique because it guarantees reduction to classical mechanics in the classical limit. Therefore the process of quantization is itself an interesting object of study. The anomaly, by definition, is a symmetry breaking caused by quantization, so it is necessary for us to understand it.

There are different ways of quantizing a physical system. We explain two common methods, canonical quantization and Feynman’s path-integral formulation. We work in one space dimension to keep the formulae readable, as it is straightforward to generalize to higher dimensions.

### 1. Canonical quantization

The classical theory takes place on phase space (the  $x$ - $p$  plane), and the physical observables are functions on phase space, for example kinetic energy. The dynamics of a physical observable  $A$  is given by the equation

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \{A, H\} \tag{2.1}$$

which involves the observable’s explicit time-dependence as well as its *Poisson bracket* with the Hamiltonian,  $\{A, H\} \equiv \frac{\partial A}{\partial x} \frac{\partial H}{\partial p} - \frac{\partial H}{\partial x} \frac{\partial A}{\partial p}$ . It is straightforward to show that

$\{\cdot, \cdot\}$  is anti-symmetric, bilinear, and satisfies the Jacobi identity, and thus the space of all physical observables forms a Lie algebra structure with the Poisson bracket [50]. The quantum-mechanical theory, on the other hand, takes place in a Hilbert space of possible states, and observables are represented by self-adjoint operators on this Hilbert space. It turns out there is also an important anti-symmetric, bilinear function that satisfies the Jacobi identity on the space of Hilbert space operators known as the *commutator*  $[A, H]$ . Moreover, the commutator appears in the equation for the dynamics of observables, known as the Ehrenfest theorem:

$$\frac{d\langle A \rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [A, H] \rangle \quad (2.2)$$

Amid many seemingly irreconcilable differences between the classical and quantum approaches to mechanics, the dynamics of expectation values remains a fascinatingly straightforward connection between the two theories. Thus it is tempting to *define* their correspondence as follows:

$$\{A, B\} \mapsto \frac{1}{i\hbar} [A, B] \quad (2.3)$$

That is, we preserve the relevant Lie algebra structure underlying the physical observables. This mapping is known as *canonical quantization*. The jargon is that we “promote” classical functions on phase space to Hilbert space operators via this mapping.

## 2. Path-integral formulation

Attributed to Richard Feynman, the path-integral formulation is another elegant way of expressing quantum mechanics in terms of classical mechanics [17]. The relevant quantity is the transition amplitude  $\langle t'', x'' | t', x' \rangle$ , i.e. the probability amplitude that, for a given Hamiltonian, a particle observed at position  $x'$  at time  $t'$  will be observed at position  $x''$  at a later time  $t''$ . Of course, in quantum mechanics, the particle did not take any well-defined “path” to get from  $x'$  to  $x''$ ; that would violate the uncertainty principle. The assumption of the theory is that this probability amplitude can be

calculated in terms of the classical action associated with *every* possible path from  $x'$  to  $x''$  in  $t'' - t'$  seconds. Translated into an equation, this reads

$$\langle t'', x'' | t', x' \rangle = \int e^{\frac{i}{\hbar} S_\phi(t', t'')} \mathcal{D}\phi \quad (2.4)$$

where  $\phi = \phi(t)$  is a path that satisfies  $\phi(t') = x'$ ,  $\phi(t'') = x''$ ;  $S_\phi(t', t'')$  is the classical action associated with  $\phi$  from  $t'$  to  $t''$ ; and  $\mathcal{D}\phi$  is a “functional differential,” i.e., the equivalent of  $dx$  for a path integral, but now we’re integrating over an entire space of functions instead of the real line. Essentially, you consider every possible classical path the particle could take from  $x'$  to  $x''$ , calculate the classical action  $S_\phi$  associated with that path, and turn that into a phase shift  $e^{\frac{i}{\hbar} S_\phi}$ . You add up all of these unit-modulus phase factors—one for each path—and they will ultimately produce a single complex number as the transition amplitude, whose modulus squared gives the transition probability density.

More precisely, one can calculate the path integral by discretizing time, integrating over all space at each point in time, and taking the limit as the discretization gets finer:

$$\begin{aligned} & \int e^{\frac{i}{\hbar} S_\phi(t', t'')} \mathcal{D}\phi \\ &= \lim_{\Delta t \rightarrow 0} Q^{N/2} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp \left\{ \frac{i}{\hbar} \sum_{j=0}^{N-1} \left[ \frac{1}{2} m \left( \frac{x_{j+1} - x_j}{\Delta t} \right)^2 - V(x_j, t_j) \right] \Delta t \right\} dx_1 \dots dx_{N-1} \end{aligned}$$

where  $t_0 = t'$  and  $t_N = t''$ ,  $t_{j+1} - t_j = \Delta t = \frac{t_N - t_0}{N}$  and  $x_j = x(t_j)$  for a discrete path  $x(t)$ . The sum inside the exponent is the action for  $x(t)$  with linearized kinetic energy between  $t_j$  and  $t_{j+1}$ . The pre-factor  $Q^{N/2} = \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{N/2}$  essentially gives the measure on the function space, which tells us how much to “weigh” each function’s contribution of  $e^{\frac{i}{\hbar} S}$ , analogous to how we use the width of an interval  $\Delta x$  as the weight for a particular point’s contribution in a Riemann sum. It is chosen such

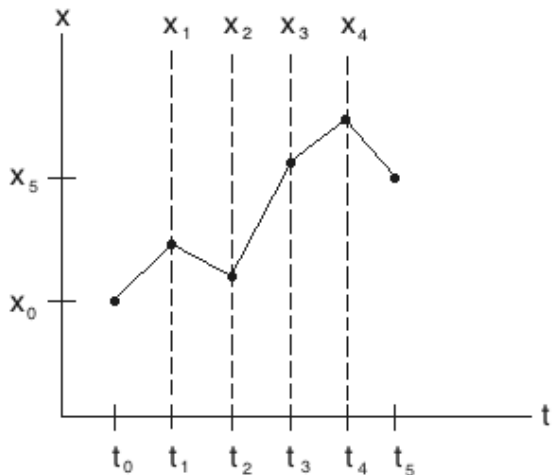


Figure 2.1: A discrete path  $x(t)$  for  $N = 5$ . The dotted vertical axes corresponding to the values of  $x_j$  for  $1 \leq j \leq N - 1$  are integrated over from  $-\infty$  to  $\infty$ .

that the path integral converges when taking the  $N \rightarrow \infty$  limit. (It is difficult to independently motivate the exact form of this pre-factor.) We present this expression in one dimension in order to not overwhelm the reader with even more indices, but the generalization to  $D$  dimensions is straightforward, even if  $D$  is non-integer, as is required in dimensional regularization.

Although there are some solvable examples, such as the free particle and the harmonic oscillator [22], in practice, to evaluate such a path integral is difficult, if not impossible, in most situations. This method of quantization is not so much important for its use as a calculational tool, but rather its use as a conceptual aid, for it gives a very direct correspondence between Lagrangian classical mechanics and quantum mechanical time evolution.

Moreover, there is an elegant argument for how this reduces to classical mechanics in the large-action limit (or, equivalently, the  $\hbar \rightarrow 0$  limit). Consider the neighborhood of any particular path with large action. Small relative changes in the action are still large relative to  $\hbar$  and thus will produce massive phase shifts  $e^{\frac{i}{\hbar}S}$ , winding around the unit circle so many times that even this tiny perturbation produces an effectively independent phase shift. A small neighborhood of perturbations, then, will have no



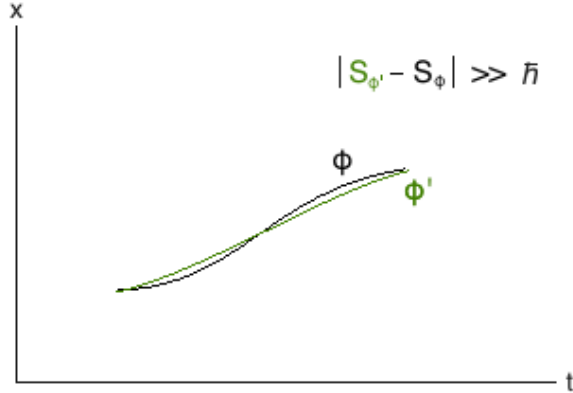


Figure 2.2: A small deviation  $\phi'$  from  $\phi$  will produce a change in action that is, in general, very large compared to  $\hbar$ , and so the resulting phases  $e^{\frac{i}{\hbar}S}$  for  $\phi$  and  $\phi'$  are essentially independent.

net effect on the path integral, as a sum of infinitely many independent “random variables” with mean 0 converges in probability to 0.

There is an exception, however, for a path that happens to have stationary action  $\delta S = 0$ . For a sufficiently small neighborhood centered around a path of stationary action, the action is approximately constant even relative to  $\hbar$ , and so the phases constructively interfere to produce some nonzero net contribution. Therefore this path and its neighborhood of perturbations contribute significantly more to the amplitude than does any other path’s neighborhood, hence this path is special in the classical limit. Incidentally, this argument also shows why the physical path in classical mechanics must have merely *stationary* action, not extremal action.

In each of these pictures, a quick and naive glance suggests that an anomaly is a mathematical impossibility. In canonical quantization, the defining mapping is between objects that express symmetries in each theory. In their respective theories, both the Poisson bracket and the commutator appear in the equation for a conserved quantity. A conserved quantity often originates in a symmetry, that is, the invariance of the classical action or quantum Hamiltonian under a particular transformation. The connection between symme-

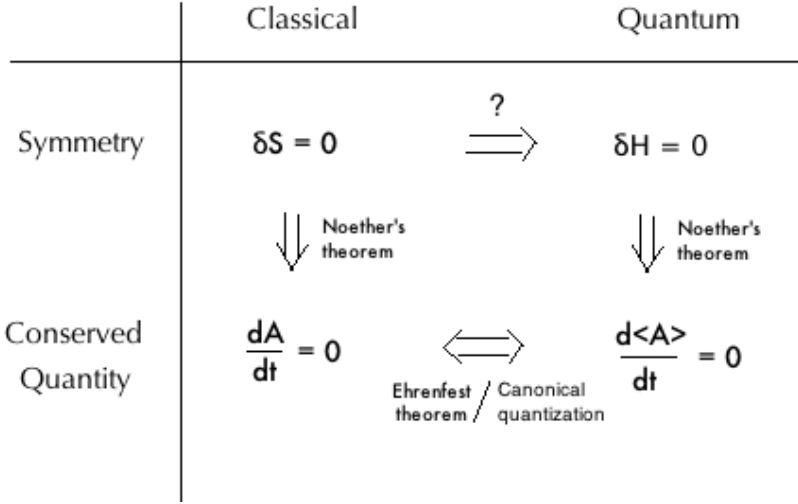


Figure 2.3: A diagram representing the naive argument against anomalies. A classical symmetry gives rise to a conserved quantity, whose corresponding quantum observable must also be conserved under canonical quantization and the Ehrenfest theorem. Then there is the same symmetry in the quantum picture, if the conservation of  $\langle A \rangle$  originates in its corresponding symmetry.

tries and conservation laws is given by Noether's theorem, which states that a continuous symmetry of a physical system implies that a particular quantity has no time-dependence, e.g. space-translation-invariant systems must conserve linear momentum. The converse of Noether's theorem does not hold, but of course the contrapositive does, and so the Poisson bracket or commutator can reveal time-dependence of a particular quantity, which would imply that the system does *not* contain a particular symmetry. Using the same example, if it could be shown that momentum is not conserved, then the system must not be invariant under space translations.

Moreover, in quantum mechanics,  $[U, H] = 0 \iff H = U^{-1}HU$ , so a transformation of the Hamiltonian via some unitary operator  $U$  (e.g. rotation or time evolution) is a symmetry if and only if it commutes with the Hamiltonian. The argument against the possibility of anomalies is that, since the Lie algebra structures in each theory contain so much information about the symmetries, a quantization procedure that explicitly ensures that these algebras are isomorphic ought to preserve symmetry. A diagrammatic representation of this logic is presented in Fig. 2.3.

In the path-integral approach, a similarly naive argument also suggests that classical symmetries must always carry over into the quantum picture. Classical symmetries are transformations that leave the action invariant, and so if transforming the system does not change the action  $S$ , then it certainly won't change  $e^{\frac{i}{\hbar}S}$  or  $\int e^{\frac{i}{\hbar}S_\phi} \mathcal{D}\phi$ .

But there are subtleties to these quantization methods that allow anomalous symmetry-breaking terms to sneak their way in. Esteve argues in Ref. [42] that this can happen in the canonical picture because of assumptions implicit in the derivation of the Ehrenfest theorem, which gives the time-dependence of expectation values in terms of the commutator:

$$\frac{d\langle A \rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [A, H] \rangle \quad (2.5)$$

(Note: to understand Esteve's argument requires knowledge of some definitions from Chapter 3; if the reader is unfamiliar with the basics of operator domains and self-adjointness, he or she should briefly consult Chapter 3 before reading.) The Ehrenfest theorem is often said to follow from  $H$  being a self-adjoint operator, because at some point in its derivation one must move  $H$  from a bra to a ket, but further assumptions are in fact required. Let's go through its derivation carefully, using the more precise notation  $(\psi, A\psi)$  instead of  $\langle \psi | A | \psi \rangle$ ; the latter sweeps issues of domains, adjoints, and self-adjointness under the rug by being vague about whether  $A$  acts "on the left" or "on the right." We also set  $\hbar = 1$  for the rest of this thesis. We start by explicitly evaluating the total time derivative of  $\langle A \rangle \equiv (\psi, A\psi)$  with the product rule:

$$\begin{aligned} \frac{d(\psi, A\psi)}{dt} &= \left( \frac{d\psi}{dt}, A\psi \right) + \left( \psi, \frac{\partial A}{\partial t} \psi \right) + \left( \psi, A \frac{d\psi}{dt} \right) = \left\langle \frac{\partial A}{\partial t} \right\rangle + (-iH\psi, A\psi) + (\psi, -iAH\psi) \\ &= \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i}(\psi, AH\psi) - \frac{1}{i}(H\psi, A\psi) =^* \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i} [(\psi, AH\psi) - (\psi, HA\psi)] \\ &= \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i} \langle [A, H] \rangle \end{aligned}$$

But the step  $=^*$  follows only if we can legally move  $H$  from  $\psi$  to  $A\psi$  in the inner product, which is okay if and only if  $A\psi$  is in the adjoint domain  $D(H^*)$ , or, more simply, iff  $A\psi \in D(H)$  since  $H$  is assumed to be self-adjoint, i.e.  $D(H^*) = D(H)$ . The inner product in

this context is an integral, and the Hamiltonian usually involves differentiation, so moving  $H$  from one function in the inner product to the other involves integration by parts. In practice, this term could be non-zero if applying integration by parts produces non-vanishing boundary terms, which would result from  $A\psi$  not satisfying the proper boundary conditions, i.e. not being in  $D(H)$ . We will see explicit examples of this process in later chapters.

Thus the Ehrenfest theorem holds only if the domain of the Hamiltonian is invariant under the operator of interest. If it is not, we can still manipulate the equation to look like the Ehrenfest theorem with a corrective, “anomalous” term added on:

$$\frac{d\langle\psi, A\psi\rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i} \langle [A, H] \rangle + \mathcal{A} \quad (2.6)$$

where  $\mathcal{A} = \frac{1}{i} [(\psi, HA\psi) - (H\psi, A\psi)]$  is what we call the anomalous term. An anomaly, then, occurs when this term adds time-dependence to a quantity that was conserved in the classical picture, thereby breaking the corresponding symmetry. In terms of the argument presented in Fig. 2.3, the bottom implication no longer holds, so  $\frac{d}{dt} \langle A \rangle \neq 0$ , implying that  $\delta H \neq 0$  by the contrapositive of the right-most instance of Noether’s theorem.

The path integral formulation can also produce anomalies, despite the naive argument that if  $\delta S = 0$ , then “of course”  $\delta \left( \int e^{iS_\phi} \mathcal{D}\phi \right) = 0$ . The key factor is the path-integral measure  $\mathcal{D}\phi$  in this expression for the propagator. The integrand  $e^{iS}$  may remain invariant under a classical symmetry transformation, but if that transformation induces a change in the function space measure, the propagator may change such that the classical symmetry is broken. This characterization of the anomaly, termed the “anomalous Jacobian,” is due to Fujikawa [31].

What is interesting to note from these two characterizations of the anomaly is that neither inherently requires any renormalization process. It should be possible, in theory, for a classical symmetry to break in quantum mechanics simply because the process of quantization isn’t clean enough to fully preserve the symmetry, without the aid of renormalization. If some authors refer to these characterizations of symmetry breaking as anomalous, while other authors define the anomaly as the failure of any regularization scheme to preserve symmetry, are they talking about the same thing? Is the anomaly the failure of a symmetry to

survive renormalization, or is it the failure of a symmetry to survive quantization?

## Chapter 3

# Self-Adjoint Extensions

The examples of the anomaly that we examine in this thesis all involve a singular potential, and the method of self-adjoint extensions is the most mathematically rigorous way of dealing with singularities in a potential. We present a somewhat informal introduction to the subject, primarily following Refs. [4] and [5], but also using Ref. [1]. We try to focus on the motivation for the results rather than the details behind them. Thus we have made liberal use of footnotes, to which we relegate the more arcane mathematical details that can be a distraction from the big picture.

In introductory quantum mechanics courses, the hermiticity of an operator is emphasized as the property that gives the quantum system a sensible physical interpretation, in particular real eigenvalues, orthogonal eigenstates, and unitary time evolution. However, the connection between hermiticity and these three properties follows only in the finite-dimensional case. The proof that a hermitian matrix  $A$  has real eigenvalues goes as follows: given an eigenvalue  $\lambda \in \mathbb{C}$  with corresponding eigenvector  $x \in \mathbb{C}^n$ ,

$$\begin{aligned}\lambda^\dagger x^\dagger x &= (\lambda x^\dagger x)^\dagger = (x^\dagger A x)^\dagger = x^\dagger A^\dagger x = x^\dagger A x = \lambda x^\dagger x \implies \lambda = \lambda^\dagger \\ &\implies \lambda \in \mathbb{R}\end{aligned}$$

since, by definition of eigenvector,  $x \neq \vec{0} \implies x^\dagger x \neq 0$ . The proofs for the existence of an orthonormal eigenbasis and for the unitarity of  $e^{-iAt}$  are similarly straightforward for finite-dimensional matrices. In infinite-dimensional linear algebra, however, there is a stronger condition required for these three coveted properties, namely that the operator

be *self-adjoint*, as opposed to merely hermitian. We will present the formal definition of self-adjointness after a brief introduction to infinite-dimensional linear algebra.

### 3.1 Domains and Adjoints

Linear operator theory in infinite dimensions departs from matrix theory in a number of important ways. In matrix theory, an  $n \times n$  matrix  $A$  is a linear map from  $\mathbb{C}^n \rightarrow \mathbb{C}^n$ , the vector space containing all possible “states” in a finite-dimensional quantum system, e.g. spin. The state space for a linear operator  $T$  is a Hilbert space  $\mathcal{H}$ , i.e. a complete<sup>1</sup> inner product space.<sup>2</sup> In quantum mechanics, this space is usually taken to be  $L^2(E)$ , the set of all functions  $f : E \rightarrow \mathbb{C}$  such that  $|f|^2$  is Lebesgue-integrable, with  $E \subseteq \mathbb{R}^n$ . Unlike in the finite-dimensional case, however,  $T$  is not a map defined on the entire state space, but rather  $T : D(T) \rightarrow \mathcal{H}$  where  $D(T) \subseteq \mathcal{H}$  is a dense<sup>3</sup> linear subspace of  $\mathcal{H}$ . This subspace is called the *domain* of  $T$ , and it is almost always a strict subset of  $\mathcal{H}$ . At first glance, that should seem strange: in matrix theory, it would be like saying  $A$  can only legitimately act on, say,  $\mathbb{Q}^n$ , even though you can obviously take linear combinations of any list of complex numbers. The reasons that specifying a subset of  $\mathcal{H}$  as a domain is necessary will become apparent soon.

Another important departure is that Hilbert space operators can have infinite spectra, whereas an  $n \times n$  matrix has at most  $n$  distinct eigenvalues. Clearly a finite set of eigenvalues has an upper bound, but an infinite spectrum can be *unbounded*.<sup>4</sup> Operators involving differentiation are usually unbounded, for example the derivative itself:  $\frac{d}{dx}e^{\lambda x} = \lambda e^{\lambda x}$  for any  $\lambda \in \mathbb{C}$ . The position space operator  $x$  is also unbounded.<sup>5</sup> Given that  $p = -i\frac{d}{dx}$ ,  $K = -\frac{d^2}{dx^2}$ , and  $V = V(x)$ , most operators we encounter in quantum mechanics are unbounded.

---

<sup>1</sup>If  $f_k \rightarrow f$ , i.e.  $\int |f_k - f| \rightarrow 0$ , and all  $f_k \in \mathcal{H}$ , then  $f \in \mathcal{H}$ .

<sup>2</sup>A vector space with an inner product  $(\cdot, \cdot) : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ . For  $L^2(E)$ , the inner product is  $(f, g) = \int_E \bar{f}g$ .

<sup>3</sup>That is, dense with respect to the norm induced by the inner product  $\|f\| = \sqrt{|(f, f)|}$ . One set  $A$  is said to be dense in another set  $B$  if for any point in  $B$ , there exists a sequence of points in  $A$  converging (in norm) to that point in  $B$ . For example,  $\mathbb{Q}$  is dense in  $\mathbb{R}$  with respect to the norm  $\|x\| = |x|$ .

<sup>4</sup>We say an operator  $T$  itself is “bounded” if there exists  $C > 0$  such that  $\|T\psi(x)\| \leq C\|\psi(x)\|$  for all  $\psi \in \mathcal{H}$ . Having an unbounded spectrum is clearly sufficient to break this condition.

<sup>5</sup>If  $f_k = 1$  on  $[k, k + 1]$  and 0 elsewhere, then  $\|Tf_k\| = \|xf_k\| = \int_k^{k+1} x dx = k + 1/2$  gets arbitrarily big, while  $\|f_k\| = 1$ .

As promised, we now present some reasons why an operator is usually not defined on all of  $\mathcal{H}$ :

1. The Hellinger-Toeplitz Theorem states that if  $T$  is a hermitian, linear operator with  $D(T) = \mathcal{H}$ , then  $T$  is bounded. A self-adjoint operator is hermitian in particular, and, as said earlier, we will rarely be dealing with bounded operators in quantum mechanics. So it is in fact a mathematical necessity that a physical operator have a strict subset of  $\mathcal{H}$  as its domain.
2. The codomain<sup>6</sup> of an operator  $T$  is by definition  $\mathcal{H}$ , so any state that  $T$  sends outside of  $\mathcal{H}$  cannot be in its domain. For example, returning to the position operator  $x$ , consider its action on  $\psi(x) = 1/x$ , an upstanding citizen of  $L^2(\mathbb{R})$ . Since  $x\psi(x) = 1 \notin L^2(\mathbb{R})$ ,  $\psi$  cannot be in  $D(x)$ .
3. The definition of the operator only makes sense on certain classes of functions. Perhaps  $x$  has a sensible definition on absolutely any function, but  $\frac{d}{dx}$  does not, and  $L^2(\mathbb{R})$  includes many (in fact, it is almost entirely composed of) pathological functions, for example Dirichlet's function.<sup>7</sup> Fortunately,  $C_0^\infty(\mathbb{R})$ , the set of all infinitely differentiable functions on  $\mathbb{R}$  with compact support<sup>8</sup> is dense in  $L^2(\mathbb{R})$ , so any element in  $L^2$  can be approximated by a well-behaved function. Thus we can find a domain for an operator involving derivatives of arbitrarily high order.
4. We want to impose *physical* boundary conditions on the problem. For example, in the 1D particle-in-a-box problem we consider the operator  $H = K = -\frac{d^2}{dx^2}$  on  $L^2([0, L])$ . For the domain of  $H$ , one typically requires that its members satisfy  $\psi(0) = \psi(L) = 0$  because this leads to quantized energy, an experimental observation. The process of applying boundary conditions in a physical problem is, formally, no more and no less than choosing a domain for the operator of interest.

---

<sup>6</sup>Also known as the target set, this is the set of possible outcomes of  $T(\psi)$ . It is not equal to, but does contain, the range of the function.

<sup>7</sup>A function usually defined on  $[0, 1]$  that sends every rational to 1 and every irrational to 0. It is continuous nowhere but *does* have a well-defined Lebesgue integral.

<sup>8</sup>The “support” of a function is the set on which it takes on a nonzero value, and a set is “compact” if it is closed and bounded.



5. We want the operator to be self-adjoint. Interestingly, this usually involves *extending* the domain rather than shrinking it. It is also possible for the domain to be too large for self-adjointness, but we usually start with a very small domain and so that is not an issue.

We are close to formally presenting the definition of self-adjointness. We must first define the *adjoint* of an operator and hermiticity more formally.

**Definition 3.1.1.** The **adjoint**  $T^*$  of a densely-defined linear operator  $T$  is itself a linear operator  $T^* : D(T^*) \rightarrow \mathcal{H}$ , where  $D(T^*) \subseteq \mathcal{H}$ . For a given  $\psi \in \mathcal{H}$ , we define  $T^*\psi$  as follows: if there exists  $\phi \in \mathcal{H}$  such that  $(\psi, T\sigma) = (\phi, \sigma)$  for every  $\sigma \in D(T)$ , then  $T^*\psi \equiv \phi$ . The domain of  $T^*$ , then, is the set of all  $\psi$  such that there exists such a  $\phi$ .

The definition is familiar: if you want to move the action of the operator from the ket to the bra, you have to take the adjoint. This  $\phi$  that may or may not exist for a given  $\psi$  (corresponding to whether or not  $\psi \in D(T^*)$ ) is  $T^*\psi$ . The astute reader will ask whether the adjoint is well-defined, since there could conceivably be multiple  $\phi$  (for a given  $\psi$ ) that satisfy  $(\psi, T\sigma) = (\phi, \sigma)$  for all  $\sigma$ . It turns out that, if  $D(T)$  is dense in  $\mathcal{H}$ , then the adjoint is in fact well-defined,<sup>9</sup> hence our previous insistence on dense domains.

We present the definition of hermiticity formally, since it also involves domain-related details that are ignored in matrix theory.

**Definition 3.1.2.** A densely-defined linear operator  $T$  is said to be **hermitian** or **symmetric** if, for every  $\psi, \sigma \in D(T)$ ,  $(\psi, T\sigma) = (T\psi, \sigma)$ .

It follows immediately that for a hermitian operator  $T$ ,  $D(T) \subseteq D(T^*)$ .<sup>10</sup> To achieve hermiticity necessarily requires choosing a domain small enough such that the adjoint domain is larger. Note how the more things we add to  $D(T)$ , the smaller  $D(T^*)$  becomes, because the  $\phi$  that must exist (carrying over notation from the definition) for  $\psi$  to be in  $D(T^*)$

---

<sup>9</sup>We present a quick proof. Suppose there existed  $\phi$  and  $\phi'$  satisfying the definition of the adjoint. Then for all  $\sigma \in D(T)$ ,  $(\phi - \phi', \sigma) = (\phi, \sigma) - (\phi', \sigma) = (\psi, T\sigma) - (\psi, T\sigma) = 0$ , i.e.  $\phi - \phi'$  is orthogonal to every element of the domain of  $D(T)$ . Let  $h = \phi - \phi'$ . By density of  $D(T)$ , we can choose a sequence  $\{\sigma_k\} \in D(T)$  such that  $\sigma_k \rightarrow h$ . Then  $\|h\|^2 = |(h, h)| = |(h, h) - 0| = |(h, h) - (h, \sigma_k)| = |(h, h - \sigma_k)| \leq \|h\|^2 \|h - \sigma_k\|^2 \rightarrow 0$ . So  $\|h\|^2 = 0 \implies h = 0 \implies \phi = \phi'$ .

<sup>10</sup>If  $\psi \in D(T)$ , then for all  $\sigma \in D(T)$ ,  $(T\psi, \sigma) = (\psi, T\sigma)$ . So  $T\psi$  is the “ $\phi$ ” that exists for  $\psi$ ; therefore  $\psi \in D(T^*)$ .

needs to satisfy a strictly *stronger* “for all” statement about all the elements  $\sigma$  of  $D(T)$ , because, well, we’re adding more elements to it.

There is often a “Goldilocks” domain you can choose so that  $D(T^*)$  shrinks to exactly  $D(T)$ . This, finally, is the definition of a self-adjoint operator.

**Definition 3.1.3.** A densely-defined linear operator  $T$  is said to be **self-adjoint** if it is hermitian and  $D(T) = D(T^*)$ .

The primary motivation for this definition is the following theorem.

**Theorem 3.1.4.** *If  $T$  is a self-adjoint operator, then*

- *The spectrum of  $T$  is a subset of the real line*
- *$U(t) = e^{itT}$  is a unitary operator for every  $t \in \mathbb{R}$ , and  $U(t + s) = U(t)U(s)$  for every  $s, t \in \mathbb{R}$*

Essentially,  $T$  has real eigenvalues and unitary time evolution. It is also true that  $T$  has a set of orthogonal eigenstates, but it is a bit arcane to even state this fact formally, let alone prove it. In short, a self-adjoint operator  $T$  can undergo a similarity transformation with a unitary operator such that it turns into a “multiplication operator,” the infinite-dimensional equivalent of a diagonal matrix. See Ref. [4], Sec. VIII.3 for details. In practice, the spectrum ends up being a discrete set of negative-energy bound states that satisfy a  $\delta_{ij}$  orthogonality relation with one another, as well as a continuum of positive-energy scattering states that satisfy a  $\delta(x - y)$  orthogonality relation. Although the scattering states are not in  $L^2$ , they get added in via the “rigged” Hilbert space construction discussed in Ref. [25].

We often encounter singular Hamiltonian operators that, with sufficiently strict boundary conditions, turn out to be hermitian. However, the boundary conditions we naively enforce on seemingly reasonable physical grounds usually end up being *too strict* for the operator to be self-adjoint. Thus we must *extend* the operator’s domain such that it becomes self-adjoint. The beauty of the self-adjointness requirement is that it can give physical insight into a problem by telling us what our boundary conditions ought to be. The physical sensibility of a real spectrum, orthogonal eigenstates, and unitary time evolution tells us to demand self-adjointness, and demanding self-adjointness in turn tells us what boundary

conditions we should enforce. But how do we find such a “Goldilocks” domain, and might there be more than one?

### 3.2 Finding Self-Adjoint Extensions “By Hand”

A classic example of a hermitian, but not self-adjoint, operator is  $T = i \frac{d}{dx}$  on  $[0, 1]$  with an initial domain of  $D(T) = \{\psi \in AC[0, 1] \mid \psi(0) = \psi(1) = 0\}$ , where  $AC[0, 1]$  is the set of functions on  $[0, 1]$  with a continuous derivative, i.e. those functions that can be integrated by parts. To prove  $T$ 's hermiticity, we perform integration by parts on the inner product of an arbitrary  $f, g \in D(T)$

$$(f, Tg) = \int_0^1 \overline{f} i \frac{dg}{dx} dx = i [\overline{f}g]_0^1 - i \int_0^1 \frac{d\overline{f}}{dx} g dx = 0 + \int_0^1 i \frac{d\overline{f}}{dx} g dx = (Tf, g)$$

The boundary terms in the integration by parts vanish because of our very strict domain, which requires  $f(0) = f(1) = g(0) = g(1) = 0$ , so of course  $\overline{f(1)}g(1) - \overline{f(0)}g(0) = 0$ . The problem is that this is *overkill*. If we instead allow  $f$  to come from the less restrictive adjoint domain  $D(T^*)$ , then  $T$  is hermitian if and only if, for every  $f \in D(T^*)$ ,  $g \in D(T)$ , we have

$$0 = (f, Tg) - (Tf, g) = i [\overline{f(1)}g(1) - \overline{f(0)}g(0)]$$

$$\iff \overline{f(1)}g(1) - \overline{f(0)}g(0) = 0 \tag{3.1}$$

The challenge, then, is to weaken the boundary condition on all  $g$  so that the *same* boundary condition is required for all  $f$  for Eq. 3.1 to hold. (That is precisely what  $D(T) = D(T^*)$  means.) If such a self-adjoint extension  $S$  exists, let us take an  $f$  in that domain  $D(S)$  that is *not* in  $D(T)$ . Then in the particular case where we take  $g = f$ ,

$$0 = \overline{f(1)}f(1) - \overline{f(0)}f(0) = |f(1)|^2 - |f(0)|^2 \iff |f(1)| = |f(0)|$$

i.e., Eq. 3.1 implies that every  $f \in D(S)$  satisfies  $f(1) = \alpha f(0)$  for *some*<sup>11</sup>  $\alpha$  with  $|\alpha| = 1$ . From that argument alone, this  $\alpha$  could certainly depend on  $f$ . But given some other

---

<sup>11</sup>This  $\alpha$  is unique for a given  $f$  precisely because we required  $f \in D(S) \setminus D(T)$ , which forces  $f(0) \neq 0$  so that we can divide by it to get  $|f(1)/f(0)| = 1$ . Otherwise any  $\alpha$  would give  $0 = \alpha \cdot 0$ .

$g \in D(S)$ , let  $\beta$  satisfy  $g(1) = \beta g(0)$ ,  $|\beta| = 1$ ; then applying Eq 3.1 in this more general case gives

$$0 = \overline{f(1)}g(1) - \overline{f(0)}g(0) = \overline{\alpha f(0)}\beta g(0) - \overline{f(0)}g(0) \iff 0 = \bar{\alpha}\beta - 1$$

$$\iff \alpha = \beta$$

since the conjugate and the inverse are the same for unit-modulus complex numbers. Thus this  $\alpha$  is fixed for all elements of the self-adjoint extension domain  $D(S)$ .

The claim is that all possible self-adjoint extensions  $T_\alpha$  of  $T$  are parameterized by  $\alpha$  on the complex unit circle, so that  $D(T_\alpha) = \{\psi \in AC[0, 1] \mid \psi(1) = \alpha\psi(0)\}$ . We already argued the reverse implication: that any self-adjoint extension of  $T$  must have such a domain. The forward implication is more obvious: any two elements of  $D(T_\alpha)$  clearly satisfy Eq. 3.1 for any  $\alpha$ .

### 3.3 Deficiency Subspace Method

We brute-forced our way through the above example by working straight from the definition of self-adjointness. It required some insight as to how to make Eq. 3.1 give equivalent restrictions on  $f$  and  $g$ . There is, fortunately, an algorithmic method for finding *all* self-adjoint extensions of *any* hermitian operator. We present the relevant definitions and theorems for this method, omitting the proofs. As such, how and why the method works will remain fairly mysterious, but the focus of this thesis is not the method itself, rather its application to the issue of anomalies in quantum mechanics.

**Definition 3.3.1.** Let  $T$  be a densely-defined linear operator. Then the eigenspace of  $i$ ,  $N_+ = \text{Ker}(T - i)$ , is termed the *positive deficiency subspace* of  $T$ , while the eigenspace of  $-i$ ,  $N_- = \text{Ker}(T + i)$ , is termed the *negative deficiency subspace* of  $T$ . The dimensions of these spaces  $\langle n_+, n_- \rangle$  are termed the *positive/negative deficiency indices*.

We usually care about the deficiency subspaces of  $T^*$ , since a failure of  $T$ 's self-adjointness manifests itself by  $D(T^*)$  being too large; in particular,  $D(T^*)$  may contain eigenvectors

with imaginary eigenvalues. The deficiency indices tell us how many parameters we'll need to describe the set of all self-adjoint extensions, via the following theorem from Ref. [5] Sec. X.1.

**Theorem 3.3.2.** *Let  $T$  be a densely-defined, linear hermitian operator. Then*

1. *If the deficiency indices of  $T^*$  are  $\langle 0, 0 \rangle$ , then  $T$  is said to be essentially self-adjoint, in that there is a unique self-adjoint extension.*
2. *If the deficiency indices of  $T^*$  are  $\langle n, m \rangle$  with  $n \neq m$ , then  $T$  does not have any self-adjoint extensions.*
3. *If the deficiency indices of  $T^*$  are  $\langle n, n \rangle$ , then the set of self-adjoint extensions of  $T$  is in one-to-one correspondence with the set of unitary linear transformations  $U : N_+ \rightarrow N_-$ .*

In Case 1 of the theorem, the self-adjoint extension is usually trivial, for example extending the domain of  $i\frac{d}{dx}$  from  $C_0^\infty(\mathbb{R})$  to  $C_0^1(\mathbb{R})$ . In this case, extending the operator amounts to simply closing it.<sup>12</sup> We won't worry about Case 2, since it doesn't come up in any of the potentials we address.

Case 3 is the most interesting case. The unitary group  $U(n)$  parameterizes all possible self-adjoint extensions of our operator  $T$ . The exact parameterization is as follows: for each  $U : N_+ \rightarrow N_-$  unitary, there is a self-adjoint operator  $T_U$  with domain

$$D(T_U) = \{\phi + \phi_+ + U\phi_+ \mid \phi \in D(T), \phi_+ \in N_+\} \quad (3.2)$$

And the operator, of course, acts on the domain by

$$T_U(\phi + \phi_+ + U\phi_+) = T\phi + i\phi_+ - iU\phi_+ \quad (3.3)$$

Let's apply this method to the previous example. The eigenvalue equations

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

---

<sup>12</sup>That is, taking the closure of the operator's graph in  $\mathcal{H} \times \mathcal{H}$ .

have solutions  $\phi_{\pm} = e^{\pm x}$ . Thus  $N_+ = \{\beta e^x \mid \beta \in \mathbb{C}\}$  and  $N_- = \{\beta e^{-x} \mid \beta \in \mathbb{C}\}$ . Since these spaces are one-dimensional, the unitary group is just the set of maps  $\beta \frac{\sqrt{2}}{\sqrt{e^2-1}} e^x \mapsto \gamma \beta \frac{\sqrt{2}e}{\sqrt{e^2-1}} e^{-x}$  with  $|\gamma| = 1$ . (We included normalization constants for  $e^x$  and  $e^{-x}$ , which are calculated via the usual quantum mechanical norm  $\sqrt{\int f^* f}$ , so that  $\gamma$  has unit modulus.) Therefore the domain of each  $T_\gamma$ , according to the theorem, is

$$D(T_\gamma) = \left\{ \phi + \beta \frac{\sqrt{2}}{\sqrt{e^2-1}} e^x + \gamma \beta \frac{\sqrt{2}e}{\sqrt{e^2-1}} e^{-x} \mid \phi \in D(T), \beta \in \mathbb{C} \right\} \quad (3.4)$$

Then for an arbitrary  $\psi \in D(T_\gamma)$ ,  $\psi(0) = \phi(0) + \beta \frac{\sqrt{2}}{\sqrt{e^2-1}} e^0 + \gamma \beta \frac{\sqrt{2}e}{\sqrt{e^2-1}} e^{-0} = 0 + \beta \frac{\sqrt{2}}{\sqrt{e^2-1}} + \gamma \beta \frac{\sqrt{2}e}{\sqrt{e^2-1}} = \beta \frac{\sqrt{2}}{\sqrt{e^2-1}} (1 + \gamma e)$ , and  $\psi(1) = \beta \frac{\sqrt{2}}{\sqrt{e^2-1}} (e + \gamma)$ , so

$$\left| \frac{\psi(1)}{\psi(0)} \right| = \left| \frac{e + \gamma}{1 + \gamma e} \right| = 1$$

(The fact that  $\left| \frac{e + \gamma}{1 + \gamma e} \right| = 1$  is not obvious from a quick glance, but it can be shown easily by splitting  $\gamma$  into its real and imaginary parts.) Thus we can identify  $\alpha = \frac{e + \gamma}{1 + \gamma e}$  from the “by-hand” solution, and we get the same result.

The most important step in this type of calculation is to physically interpret the different self-adjoint extensions. There is no “correct” extension to pick; each corresponds to a different physical scenario. In this case, the accepted interpretation is that  $|\psi(0)| = |\psi(1)|$  must hold because we want the space translation operator  $U(y) = e^{iyT_\alpha}$ , which acts on  $\psi(x)$  by  $U(y)\psi(x) = \psi(x - y)$ , to be unitary: if it sends some probability out of  $[0, 1]$  in one direction, probability must come out the other. Thus the two ends of the interval are in fact connected, with an arbitrary but constant phase shift  $\alpha$  given by the choice of self-adjoint extension.

### 3.3.1 Summary

In short, the method of self-adjoint extensions is a mathematical basis for choosing boundary conditions, motivated by the nice physical properties that self-adjoint operators have. The mechanics of the method work as follows:

1. Start with a preliminary domain  $D(T)$  that is very restrictive, requiring that any elements of the domain and derivatives of all orders vanish at boundary points of

$D(T)$ . Then the adjoint domain becomes essentially all of  $L^2$ , i.e. the set of all normalizable solutions regardless of boundary behavior. (This can be verified by examining boundary terms of  $(\phi, T\psi) - (T\phi, \psi)$ , which must vanish due to restrictions on  $\psi$  regardless of  $\phi$ .)

2. Find all  $L^2$  solutions to the equations  $T^*\psi = \pm i\psi$ . Since  $T$  is at least hermitian, the action of  $T^*$  is the same as that of  $T$ , so we are essentially solving  $T\psi = \pm i\psi$  but keeping any  $D(T^*) = L^2$  solution, not just those with proper boundary conditions for  $T$ . The number  $n_+$  of linearly independent solutions for  $+i$  and the number  $n_-$  of linearly independent solutions for  $-i$  are the deficiency indices  $\langle n_+, n_- \rangle$ .
3. If  $n_+ = n_-$ , which it usually will for the problems we consider, choose orthonormal bases for the solutions of  $T\psi = \pm i\psi$ , and then the matrix representations of unitary transformations relative to these bases will be unitary. Each  $n_+ \times n_+$ -dimensional unitary matrix  $U$  corresponds to some self-adjoint extension  $T_U$ .
4. The domain of  $T_U$  is formally  $D(T_U) = \{\phi + \phi_+ + U\phi_+ \mid \phi \in D(T), \phi_+ \in N_+\}$ . Since  $\phi \in D(T)$  must vanish at boundary points, we can find the boundary conditions for this domain by examining the behavior of  $\phi_+$  and  $U\phi_+$  at boundary points.
5. The set of possible self-adjoint extensions can usually be physically interpreted as the choice of some physical parameter, such as a bound state energy or phase shift.

## Chapter 4

# The Algebra of Scale Symmetry

The definition of a scale-symmetric potential is motivated by the consequences of having a scale-symmetric Hamiltonian. A re-scaling of the independent variable will come out of the kinetic energy operator squared, by the chain rule:  $-\frac{d^2}{d((1+\lambda)x)^2} = -\frac{1}{(1+\lambda)^2} \frac{d^2}{dx^2}$ . So if we want a scaling factor to pop out of the entire Hamiltonian  $-\frac{d^2}{dx^2} + V$ , we need the potential to behave in the same way under re-scaling.

**Definition 4.0.3.** A potential  $V(x)$  is said to be *scale symmetric* if for any  $\lambda \in (-1, \infty)$ ,  $V((1+\lambda)x) = \frac{1}{(1+\lambda)^2} V(x)$ .

We use  $1+\lambda$  as the scaling factor so that  $\lambda \approx 0$  represents a “small” scale change. Then if we scale a Hamiltonian with a scale symmetric potential, we have  $H_{(1+\lambda)x} = -\frac{d^2}{d((1+\lambda)x)^2} + V((1+\lambda)x) = -\frac{1}{(1+\lambda)^2} \frac{d^2}{dx^2} + \frac{1}{(1+\lambda)^2} V(x) = \frac{1}{(1+\lambda)^2} H_x$ .

This definition is consistent with the notion of scaling a state in  $L^2$ , which one would sensibly define as  $U_\lambda \psi(x) = \frac{1}{\sqrt{1+\lambda}} \psi((1+\lambda)x)$  so that  $U_\lambda$  is unitary. From this alone we can define how this scaling procedure should affect an operator:

$$U_\lambda H \psi(x) = U_\lambda H U_\lambda^{-1} U_\lambda \psi(x) = H' U_\lambda \psi(x) \tag{4.1}$$

Since  $H$  is a mapping from vectors to vectors (as opposed to covectors), it transforms as  $U_\lambda H U_\lambda^{-1}$ , hence the identification  $H' = U_\lambda H U_\lambda^{-1}$ . We can manipulate the far LHS to give

$$U_\lambda \left( \frac{d^2 \psi}{dx^2}(x) + V(x) \psi(x) \right) = \frac{1}{\sqrt{1+\lambda}} \left( \frac{d^2 \psi}{dx^2}((1+\lambda)x) + V((1+\lambda)x) \psi((1+\lambda)x) \right)$$



The parentheses after the second derivatives indicate evaluation. Note that  $U_\lambda$  acting on  $H\psi$  does *not* scale the  $x$  variable in the second derivative, since it only scales the variable at which we evaluate the function, once all differentiation is over with. The far RHS of Eq. 4.1 is clearly  $\frac{1}{\sqrt{1+\lambda}}H'\psi((1+\lambda)x)$ . Observe that differentiating  $\psi((1+\lambda)x)$  with respect to  $(1+\lambda)x$  gives the derivative of the original function with respect to  $x$ , so we can identify

$$H' = \frac{d^2}{d((1+\lambda)x)^2} + V((1+\lambda)x) = \frac{1}{(1+\lambda)^2}H$$

Thus a Hamiltonian with a scale-symmetric potential has a scale factor pop out to the  $-2$  power under a scaling transformation.

## 4.1 Continuum of Eigenstates

The most striking consequence of scale invariance is that the existence of any bound state implies the existence of a bound state of arbitrary (negative) energy:

$$H_x\psi(x) = E\psi(x) \implies H_x\psi((1+\lambda)x) = (1+\lambda)^2H_{(1+\lambda)x}\psi((1+\lambda)x) = (1+\lambda)^2E\psi((1+\lambda)x)$$

So then  $(1+\lambda)^2E$  is also an eigenvalue, which clearly can take on an arbitrary value of the same sign as  $E$  by a choice of  $\lambda$  [1]. So if we can find any negative energy that solves the Schrödinger equation, then there must in fact exist a continuum of bound states. That is a pathology that we do not accept, because it violates eigenstate orthogonality. The argument is that for very small changes in the eigenvalue, the corresponding eigenvector changes in a small way as well, such that their inner product must be approximately 1, and in particular not 0. A continuum is allowed in the scattering sector because solutions need not vanish at  $\infty$ , so for any small perturbation of the eigenvalue, the corresponding eigenfunction has infinite space to deviate significantly from the old eigenfunction. For example, even if  $k - k' \ll 1$ , we can still have  $\int_{-\infty}^{\infty} \sin(kx) \sin(k'x) dx = 0$  since eventually  $\sin(kx)$  and  $\sin(k'x)$  start to differ significantly. But in the bound-state sector, both eigenfunctions must eventually be close to 0 and therefore close to each other.

This consequence gives us another way of thinking about scale invariance, through the units of a coupling in  $V(x)$ . Take, for example,  $V(x) = g/x^2$ , which is clearly scale

symmetric. Setting  $\hbar = 2m = 1$  requires that  $E$  and  $V$  have units of  $[\text{length}]^{-2}$ . Then  $V(x) = g/x^2$  implies that the coupling  $g$  is unitless, so the coupling cannot set an energy scale. Any isolated bound-state energy would certainly vary with  $g$ , but  $g$  doesn't have the units necessary to non-arbitrarily define this energy.

There is a point of subtlety, however: the existence of arbitrary bound state energies requires that the state  $\psi((1 + \lambda)x)$  is *in the domain of the Hamiltonian*. It is common for an unbounded differential operator to have a continuous spectrum, and it is enforcing boundary conditions, i.e. choosing a subset of  $L^2$  as the domain, that picks out a discrete set of bound states. In some cases, there may be a unique  $\lambda$  that puts  $\psi((1 + \lambda)x)$  in the domain of the Hamiltonian.

## 4.2 Scale Invariance in Classical Mechanics

We have so far discussed scale symmetry in quantum mechanics. However, it is instructive to look at scale symmetry in classical mechanics as well, for the anomaly is a loss of symmetry upon quantizing a classical system. We will show that the  $1/r^2$  potential is scale symmetric in classical mechanics, in just one dimension for simplicity.

To demonstrate that this property is unique for the  $1/x^2$  potential out of all power potentials—which is more obvious in quantum mechanics than in classical mechanics—we will consider how the Lagrangian  $\mathcal{L}(x, \dot{x}, t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{x^n}$  for  $V = 1/x^n$  scales under the transformation  $x \mapsto (1 + \lambda)x$ . Time must be scaled by some factor as well, which we'll write as  $(1 + \lambda)^l$ .

$$\begin{aligned} \mathcal{L} \left[ (1 + \lambda)x, (1 + \lambda)^{1-l}\dot{x}, (1 + \lambda)^l t \right] &= \frac{1}{2}m \frac{(1 + \lambda)^2}{(1 + \lambda)^{2l}} \dot{x}^2 - \frac{1}{(1 + \lambda)^n} \frac{1}{x^n} \\ &= \frac{1}{(1 + \lambda)^n} \left( \frac{1}{2}m \frac{(1 + \lambda)^{2+n}}{(1 + \lambda)^{2l}} \dot{x}^2 - \frac{1}{x^n} \right) \end{aligned}$$

For the  $\frac{1}{(1 + \lambda)^n}$  factor to pop out of the original Lagrangian, we require  $(1 + \lambda)^{2+n} = (1 + \lambda)^{2l} \iff 2 + n = 2l$ . For this transformation to represent a *symmetry* of the theory, the action must remain invariant. So the scale factor that pops out of the Lagrangian must

cancel with the Jacobian of the action integral  $S = \int \mathcal{L}(x, \dot{x}, t) dt$ .

$$\int \mathcal{L} \left[ (1 + \lambda)x, (1 + \lambda)^{1-l}\dot{x}, (1 + \lambda)^m t \right] (1 + \lambda)^l dt = \int \frac{1}{(1 + \lambda)^n} \mathcal{L}(x, \dot{x}, t) (1 + \lambda)^l dt$$

which equals  $S$  if and only if  $l = n$ . Combining with the  $2 + n = 2l$  requirement yields  $n = l = 2$ .

So for the  $1/x^2$  potential, there exists a way of separately rescaling space and time such that the action is unchanged. We set equal to zero the generator of the transformation of the action integrand  $\mathcal{L} dt$  to find the corresponding Noether current.

$$0 = \left\{ \frac{d}{d\lambda} (1 + \lambda)^2 \mathcal{L} \left[ (1 + \lambda)x, \frac{1}{1 + \lambda} \dot{x}, (1 + \lambda)^2 t \right] \right\}_{\lambda=0} = 2\mathcal{L} + \frac{\partial \mathcal{L}}{\partial x} x - \frac{\partial \mathcal{L}}{\partial \dot{x}} \dot{x}$$

There is no explicit time-dependence in the Lagrangian; the time argument was included as a reminder that rescaling time affects  $\dot{x}$ . Assuming the equations of motion hold and writing  $p = \frac{\partial \mathcal{L}}{\partial \dot{x}}$ , we have

$$0 = 2\mathcal{L} + \dot{p}x - p\dot{x} = 2\mathcal{L} - 2p\dot{x} + \dot{p}x + p\dot{x} = -2\mathcal{H} + \frac{d}{dt}(px) = \frac{d}{dt}(-2tH + px)$$

since the Hamiltonian is conserved with a time-invariant potential. Thus we can identify a conserved quantity

$$D = \frac{1}{2}px - tH \tag{4.2}$$

It is then clear that  $\{D, H\} = H$ , which will become interesting when looking at the quantum version of this system.

There is another hidden symmetry of this potential, however. Consider the transformation

$$x \mapsto \frac{x}{1 + ct}, \quad t \mapsto \frac{t}{1 + ct}$$

Applying this to the action, we get

$$\begin{aligned}
S' &= \int \left[ \frac{1}{2}m \left( \frac{d\left(\frac{x}{1+ct}\right)}{d\left(\frac{t}{1+ct}\right)} \right)^2 - \frac{1}{\left(\frac{x}{1+ct}\right)^2} \right] d\left(\frac{t}{1+ct}\right) \\
&= \int \left[ \frac{1}{2}m (\dot{x}(1+ct) - cx)^2 - \frac{(1+ct)^2}{x^2} \right] \frac{1}{(1+ct)^2} dt \\
&= \int \left( \frac{1}{2}m\dot{x}^2 - \frac{1}{x^2} \right) dt + \int \frac{1}{2}m \left( -\frac{2c\dot{x}x}{1+ct} + \frac{c^2x^2}{(1+ct)^2} \right) dt \\
&= S + \frac{1}{2}m \left[ \frac{-cx^2}{1+ct} \right]_{t_1}^{t_2}
\end{aligned}$$

Since the Lagrangian varies by a total time derivative, we can still use Noether's theorem to find a conserved quantity. The generator of this term with respect to  $c$  is  $-\frac{1}{2}mx^2$ , and so equating the time derivative of this term to the variation of  $\mathcal{L}dt$ , we get

$$\begin{aligned}
\frac{d}{dt} \left( -\frac{1}{2}mx^2 \right) &= \left[ \frac{d}{dc} \frac{1}{(1+ct)^2} \mathcal{L} \left( \frac{x}{1+ct}, \dot{x}(1+ct) - cx \right) \right]_{c=0} \\
&= \left[ \frac{-2t\mathcal{L}}{(1+ct)^3} + \frac{1}{(1+ct)^2} \left( \frac{\partial \mathcal{L}}{\partial x} \left( \frac{-xt}{(1+ct)^2} \right) + \frac{\partial \mathcal{L}}{\partial \dot{x}} (\dot{x}t - x) \right) \right]_{c=0} \\
&= -2t\mathcal{L} - \dot{p}xt + p\dot{x}t - px = -2t(p\dot{x} - H) - \dot{p}xt + p\dot{x}t - px \\
&= -t(p\dot{x} + \dot{p}x) - px + 2tH = -t \frac{d}{dt}(px) - px + 2tH = \frac{d}{dt}(-pxt) + 2tH \\
&= \frac{d}{dt}(-pxt + t^2H) = \frac{d}{dt}(-2tD - t^2H) \\
\implies 0 &= \frac{d}{dt} \left( \frac{1}{2}mx^2 - 2tD - t^2H \right) = \frac{dK}{dt}
\end{aligned}$$

where we have defined  $K$  as the conserved quantity corresponding to conformal transformations. Although we used the  $1/x^2$  potential in this derivation, it would work for any scale-symmetric potential: we only needed the property that  $V(qx) = \frac{1}{q^2}V(x)$  for any  $q$  constant with respect to  $x$ , even if it includes time-dependence.

### 4.3 Scale Invariance in Quantum Mechanics

The conserved phase-space functions  $H$ ,  $D$ , and  $K$  from classical mechanics can be “promoted” to quantum mechanical operators via canonical quantization (modulo multiplication ordering), and assuming the Ehrenfest Theorem holds (see Chapter 2), the average values of

these observables are still conserved in quantum mechanics. But we can in fact derive these operators within the framework of quantum mechanics by assuming scale invariance. We present the same calculation as Gopalakrishnan in Ref. [1] but with some minor corrections. Recall that a scale transformation acts on a wave function by  $U_\lambda\psi(x) = \frac{1}{\sqrt{1+\lambda}}\psi((1+\lambda)x)$ . Assuming we can Taylor expand the operator, write

$$U_\lambda = 1 - iS\lambda + \mathcal{O}(\lambda^2) \quad (4.3)$$

for some operator  $S$ , which we can identify as the generator of scale transformations. Differentiating  $U_\lambda\psi(x)$  with respect to  $\lambda$  and evaluating at 0 allows us to find  $-iS$ :

$$\begin{aligned} -iS\psi(x) &= \left[ \frac{-1}{2(1+\lambda)^{3/2}}\psi((1+\lambda)x) + \frac{1}{\sqrt{1+\lambda}}\psi'((1+\lambda)x)x \right]_{\lambda=0} \\ &= -\frac{1}{2}\psi(x) + x\psi'(x) = \left( -\frac{1}{2} + ixp \right) \psi(x) \\ &\implies S = -\frac{i}{2} - xp \end{aligned}$$

Gopalakrishnan gets  $S = 1 + xp$ , which differs from our answer by a constant, but such a constant vanishes when taking commutators and/or time derivatives. We commute this operator with the Hamiltonian to see under what conditions the action of dilatation is a symmetry.

$$[S, H] = [xp, p^2 + V] = [x, p^2]p + x[p, V] = 2ip^2 - ixV'$$

We're stuck here unless we can use the scale invariance of  $V$  to further manipulate this expression for the commutator. Differentiating the relationship

$$V((1+\lambda)x) = \frac{1}{(1+\lambda)^2}V(x)$$

with respect to  $\lambda$  and examining the special case  $\lambda = 0$  shows that  $-2V = xV'$  for scale-invariant potentials. Then

$$[S, H] = 2i(p^2 + V) = 2iH$$

Using scale invariance does not get us to  $[S, H] = 0$ , but the commutator is proportional to the Hamiltonian, which in particular is constant in time and commutes with  $H$ . Then we can make a slight modification to  $S$  to create a conserved operator

$$D = \frac{1}{2}S - tH \tag{4.4}$$

by adding an explicit time-dependence that cancels out the  $-i\langle[S, H]\rangle$  term in the Ehrenfest theorem. Up to multiplication ordering and addition of constants, this operator is equivalent to the classical  $D = \frac{1}{2}px - tH$  we derived earlier.

As for the quantum mechanical  $K$ , Gopalakrishnan demonstrates a curious inconsistency. It is easy to show that the obvious promotion of  $K$  to a quantum mechanical operator is conserved (since the Ehrenfest Theorem explicitly ensures it), but it is *not* related to the generator of quantum mechanical conformal transformations

$$\psi(x) \mapsto (1 + cx)\psi\left(\frac{1}{1 + cx}\right)$$

Of course, to define a conformal transformation, which is inherently time-dependent, to a solution of the time-independent Schrödinger equation is difficult, and this must not be the correct way to do so.

## 4.4 SO(2,1) Algebra

These three operators  $H$ ,  $D$ , and  $K$  close under commutation in quantum mechanics—and therefore close under Poisson brackets in classical mechanics as well by the canonical correspondence. The commutation relations, from Ref. [44], are as follows

$$[D, H] = -iH$$

$$[K, H] = -2iD$$

$$[D, K] = iK$$

which, via some simple recombinations shown in Ref. [1], demonstrate that this Lie algebra is isomorphic to  $SO(2, 1)$ , the algebra of generators for the 2+1-dimensional Lorentz group. (This does not necessarily imply a connection to relativity, however; we are merely defining what  $SO(2, 1)$  means.)

Although finding a bound state is the simplest way to demonstrate the breaking of scale symmetry, another popular characterization of the anomaly is through the “breaking” of the  $SO(2, 1)$  algebra that generates the symmetry. One way to break the symmetry algebra is to find a non-vanishing time dependence in one of the expectation values [44]; we use this approach in examining the possibility of a “classical anomaly” in Chapter 6. Another way is to show that the commutator structure breaks down after renormalization or choosing a self-adjoint extension, as Gopalakrishnan does in [1].

## Chapter 5

# The $1/r^2$ Potential

The  $1/r^2$  potential is already an accepted example of the quantum mechanical anomaly in the literature [30]. Following the treatment in [1], we use the techniques outlined in Chapter 3 to derive a self-adjoint boundary condition for solutions to the Schrödinger equation for this potential on  $\mathbb{R}^3 \setminus \{0\}$ . The potential is still scale symmetric in any number of dimensions (unlike the  $\delta$  potential), but we work in three dimensions both because of some nice mathematical simplifications and because it is commonly encountered in physical applications.

### 5.1 Solving the Schrödinger Equation

The  $l = 0$  channel radial equation for the  $g/r^2$  potential, with the usual substitution of  $u = r\psi$ , becomes

$$-u'' + \frac{g}{r^2}u = -k^2u \tag{5.1}$$

where we write the eigenvalue as  $-k^2$  to look for bound, rather than scattering, states. For convenience later, let's parameterize the coupling as  $\zeta(\zeta + 1) = g$  and denote either modified Bessel function  $I_{\zeta+1/2}$ ,  $K_{\zeta+1/2}$  as  $Z_{\zeta+1/2}$ . We see by substitution into Eq. 5.1 that  $u(r) = \sqrt{r}Z_{\zeta+1/2}(kr)$  is an eigenstate:



$$\begin{aligned}
& -\frac{d^2}{dr^2} (\sqrt{r}Z_{\zeta+1/2}(kr)) + \left(\frac{g}{r^2} + k^2\right) \sqrt{r}Z_{\zeta+1/2}(kr) \\
&= -\left[-\frac{1}{4r^{3/2}}Z_{\zeta+1/2}(kr) + \frac{k}{\sqrt{r}}Z'_{\zeta+1/2}(kr) + k^2\sqrt{r}Z''_{\zeta+1/2}(kr)\right] + \left(\frac{g}{r^2} + k^2\right) \sqrt{r}Z_{\zeta+1/2}(kr) \\
&= -\sqrt{r}\left[k^2Z''_{\zeta+1/2}(kr) + \frac{k}{r}Z'_{\zeta+1/2}(kr) + \left(-k^2 - \frac{g+1/4}{r^2}\right)Z_{\zeta+1/2}(kr)\right] \\
&= -r^{-3/2}\left[r^2k^2Z''_{\zeta+1/2}(kr) + krZ'_{\zeta+1/2}(kr) - (k^2r^2 + (g+1/4))Z_{\zeta+1/2}(kr)\right] \\
&= -r^{-3/2}\left[r^2\frac{d^2}{dr^2}Z_{\zeta+1/2}(kr) + r\frac{d}{dr}Z_{\zeta+1/2}(kr) - (k^2r^2 + (g+1/4))Z_{\zeta+1/2}(kr)\right] \\
&= -r^{-3/2}(0) = 0
\end{aligned}$$

We have used the fact that the quantity in brackets is the modified Bessel equation, solved by  $Z_{\zeta+1/2}(kr)$  since  $\zeta + 1/2 = \pm\sqrt{g+1/4}$ .

The leading behavior of  $I_\alpha(z)$  is  $I_\alpha(z) \approx \frac{1}{\sqrt{2\pi z}}e^z$  for large  $z$  regardless of  $\alpha$  [12]. Thus  $I_{\zeta+1/2}$  blows up at  $\infty$  and so is not in  $L^2$ , no matter how it behaves at the origin. However, it is possible for  $\sqrt{r}K_{\zeta+1/2}(kr)$  to stay square-integrable at both 0 and  $\infty$ , depending on the value of  $\zeta$ . The leading-order behavior of this modified Bessel function is  $K_\alpha(z) \approx \frac{1}{2}\Gamma(\alpha)(\frac{1}{2}z)^{-\alpha}$ , so the radial probability density

$$|\psi|^2 r^2 = |u/r|^2 r^2 = |u|^2 = |\sqrt{r}K_{\zeta+1/2}(kr)|^2 \sim r(kr)^{-2(\zeta+1/2)} = k^{-2\zeta-1}r^{-2\zeta}$$

can be integrated at the origin if and only if  $\zeta < 1/2$ . For large arguments,  $K_\alpha(z) \approx \sqrt{\frac{\pi}{2z}}e^{-z}$ , and so if  $k > 0$ ,  $\sqrt{r}K_{\zeta+1/2}(kr)$  is always square-integrable at  $\infty$ .

It is easier to break this problem up into two cases: the “weak regime”  $|\zeta| < 1/2$  and the “strongly repulsive regime”  $\zeta \geq 1/2$ . (We set aside the third case  $\zeta < -1/2$  for now.) The strongly repulsive regime is fairly trivial. There are no square-integrable solutions to the Schrödinger equation, and so there is no bound state, as we would expect from the scale invariance of the potential. In the bound-state sector, the most basic requirement for a valid solution is that the state be in  $L^2$ , and any self-adjoint extension will still be contained in  $L^2$ ; thus no self-adjoint extension can force a bound state on the problem.

The weak regime is the more interesting case and illustrates some subtle issues related to domains. Once  $\zeta$  dips below  $1/2$ , our solution suddenly becomes square integrable *for every*  $k$ . This often happens in quantum mechanics, and boundary conditions narrow the solution set down to a discrete set of  $k$ . Applying boundary conditions within  $L^2$  is equivalent to specifying a domain, and we have to specify a domain such that  $H$  is self-adjoint.

We also want to study the attractive potential, that is, the  $g < 0$  case. Combined with the weak-regime restriction on  $\zeta$ , that requires  $-1/4 < g < 0$ .

## 5.2 Self-Adjoint Extensions

We can think of Eq. 5.1 as an eigenvalue equation for the operator  $T = -\frac{d^2}{dr^2} + \frac{g}{r^2}$ , so finding boundary conditions for the problem is equivalent to finding a domain  $D(T)$  for  $T$ . We start with the usual preliminary domain that requires  $0 = u(0) = u'(0) = \dots$ , ensuring that the adjoint domain  $D(T^*)$  contains any possible solution to  $Tu = \lambda u$ . Then we solve the deficiency-index equations, which effectively amounts to setting  $-k^2 = \pm i\mu^2$  in Eq. 5.1, where  $\mu > 0$  is an arbitrary parameter with dimensions of inverse length, which is necessary since  $T$  has units of inverse length squared.

A linearly independent pair of solutions for the  $\pm i$ -equation is  $\sqrt{r}I_{\zeta+1/2}(\sqrt{\pm i}\mu r)$  and  $\sqrt{r}K_{\zeta+1/2}(\sqrt{\pm i}\mu r)$ . But recall the asymptotic expansions  $I_{\zeta+1/2}(z) \approx \frac{1}{\sqrt{2\pi z}}e^z$  and  $K_{\zeta+1/2} \approx \sqrt{\frac{\pi}{2z}}e^{-z}$ , which are valid for any complex  $z$ . The principal values of both  $\sqrt{i}$  and  $\sqrt{-i}$  have positive real parts, so in each case we throw out  $\sqrt{r}I_{\zeta+1/2}(\sqrt{\pm i}\mu r)$  and keep  $K_{\zeta+1/2}(\sqrt{\pm i}\mu r)$ . The latter is well-behaved at 0 because we're still working in the case  $|\zeta| < 1/2$ . Thus we have deficiency indices of  $\langle 1, 1 \rangle$ .

Since  $\sqrt{r}K_{\zeta+1/2}(\sqrt{i}\mu r)$  and  $\sqrt{r}K_{\zeta+1/2}(\sqrt{-i}\mu r)$  each have the same norm, a unitary transformation from  $N_+$  to  $N_-$  using these functions as basis vectors can be represented by a unit-modulus complex number  $e^{i\theta}$ . By the main theorem from Chapter 3, then, the self-adjoint domain corresponding to  $e^{i\theta}$  contains all functions of the form

$$u(r) = \phi(r) + \beta \left[ \sqrt{r}K_{\zeta+1/2}(e^{i\pi/4}\mu r) + e^{i\theta} \sqrt{r}K_{\zeta+1/2}(e^{-i\pi/4}\mu r) \right] \quad (5.2)$$

where  $\phi$  is in the original domain (and therefore vanishes at the origin), and  $\beta$  is an arbitrary

complex coefficient. Then, following Ref. [1], we expand  $\Psi$  for small  $r$ , so  $\phi$  disappears and we once again use small-argument behaviors of the modified Bessel functions to derive our self-adjoint boundary condition

$$\begin{aligned} u(r) &\approx \beta \sqrt{r} \left( 2^{\zeta-1/2} \Gamma(\zeta + 1/2) e^{i\pi/4(-\zeta-1/2)} (\mu r)^{-\zeta-1/2} + e^{i\theta} 2^{\zeta-1/2} \Gamma(\zeta + 1/2) e^{-i\pi/4(-\zeta-1/2)} (\mu r)^{-\zeta-1/2} \right) \\ &= \beta \frac{\Gamma(\zeta + 1/2)}{\sqrt{2}} \frac{1}{\sqrt{\mu}} \left( \frac{\mu r}{2} \right)^{-\zeta} \left( e^{-i\pi(\zeta/4+1/8)} + e^{i\theta+i\pi(\zeta/4+1/8)} \right) \end{aligned}$$

It is tempting to try to match up this behavior with the small- $r$  behavior of a bound state  $\sqrt{r} K_{\zeta+1/2}(kr)$ . Then we would compare coefficients to identify the energy  $k_{bs}$  of the the bound state that gets added in by this particular self-adjoint extension corresponding to  $\theta$ , as is done in Section 6.3 with the 2D  $\delta$ . The problem is that all domains are vector spaces, which means they are closed under scalar multiplication (hence the arbitrary  $\beta$  in front of everything). So in fact, as we have written it here, *every* possible bound-state energy gets added in, giving the undesired continuum of negative-energy bound states. (This works for the 2D  $\delta$  because the small- $r$  behavior is logarithmic. Then rescaling  $r$  causes us to *add*, rather than multiply, a constant, so not every possible bound state is necessarily in a self-adjoint extension.) This treatment from Gopalakrishnan, therefore, is flawed.

It turns out that we want to look at a different characterization of the leading behavior of these functions. Refs. [33] and [39] get the result we desire in the  $-1/4 < g < 0$  regime via the approximation

$$K_{i\alpha}(z) \sim \sin \left( \alpha \log \left( \frac{1}{2} x \right) - \arg \Gamma(1 + i\alpha) \right) \quad (5.3)$$

Then, using a combination of the deficiency-indices technique and the simple “by-hand” approach to finding self-adjoint extensions, Ref. [33] finds that in this regime there is a unique bound state with energy given by

$$k_{bs} = \frac{2}{x_0} \quad (5.4)$$

in terms of a dimensioned self-adjoint-extension parameter  $x_0$  with dimensions inherited from  $\mu$ . We have not seen Gopalakrishnan’s treatment elsewhere in the literature, and it is

unclear exactly what goes wrong. But the focus of this thesis is not the  $1/r^2$  potential; it is primarily the point interactions  $\delta$  and  $\delta'$ . We present this result mostly because it is an interesting example in light of the discussion in Chapters 1, 2 and 4. The scale symmetry isn't broken by a regularization procedure or by a failure of the Ehrenfest theorem, but rather by being forced to choose a particular self-adjoint extension, which only contains one bound state. So the continuum promised by the scale invariance in Chapter 4 exists in  $L^2$ , but not in any one self-adjoint extension.

## Chapter 6

# The 2D $\delta$ Potential

The 2D  $\delta$  interaction  $V(x, y) = -g\delta(x, y)$  is another scale-invariant potential, as can be seen by the action of  $\delta(x, y)$  on a test function  $f(x, y)$  when everything is scaled by  $q = 1 + \lambda$ :

$$\begin{aligned}\iint_{[-\epsilon, \epsilon]^2} f(x, y)\delta(qx, qy)dx dy &= \iint_{[-q\epsilon, q\epsilon]^2} f(u/q, v/q)\delta(u, v)\frac{1}{q^2}dudv \\ &= \frac{1}{q^2} \iint_{[-q\epsilon, q\epsilon]^2} f(u/q, v/q)\delta(u, v)dudv = \frac{1}{q^2}f(0, 0) \\ &= \frac{1}{q^2} \iint_{[-\epsilon, \epsilon]^2} f(x, y)\delta(x, y)dx dy \\ &= \iint_{[-\epsilon, \epsilon]^2} f(x, y)\frac{1}{q^2}\delta(x, y)dx dy\end{aligned}$$

Then we can identify  $\delta(qx, qy) = \frac{1}{q^2}\delta(x, y)$ . From this scale invariance, we should expect to either see a continuum of states, an infinite-energy bound state, or no bound state at all.

But it is not straightforward to solve the Schrödinger equation with this potential, for the  $\delta$  function is defined by its behavior inside an integral, but solving a differential equation does not involve integration directly. There are a number of different ways of defining how the  $\delta$  function behaves in a differential operator.

### 6.1 Position-Space Regularization

Following Gopalakrishnan's treatment in Ref. [1], we model the 2D  $\delta$  potential as a limit of finite wells  $V_{g,a} = -g\theta(a - r)$ , where  $\theta(\cdot)$  is the Heaviside step function. (Unfortunately

the letter  $\theta$  will also be used as the angular variable.) We take  $ga^2$  constant in the limit so that  $\lim_{g \rightarrow \infty, a \rightarrow 0} \int V_{g,a} dA = 1$ , just like the actual  $\delta$  function.

In two-dimensional quantum mechanics with a circularly symmetric potential, we can rewrite the Schrödinger equation for  $\psi(r, \theta) = R(r)\Theta(\theta)$  with energy  $\pm k^2$  as two separate equations, one for the radial part  $R(r)$  and one for the angular part  $\Theta(\theta)$ .

$$r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} + [(\pm k^2 - V)r^2 - m^2] R = 0 \quad (6.1)$$

$$\frac{d^2 \Theta}{d\theta^2} + m^2 \Theta = 0 \quad (6.2)$$

An angular momentum quantum number  $m$  appears, which must be an integer for  $\Theta$  to be single-valued. We choose  $+k^2$  to solve the scattering problem, and  $-k^2$  to solve the bound-state problem. If  $V$  is a constant potential—and it will be piecewise constant in the finite well problem—Eq. 6.1 reduces to the Bessel equation of order  $m$  when  $\pm k^2 - V \geq 0$  and the modified Bessel equation of order  $m$  when  $\pm k^2 - V \leq 0$ . We use the Bessel and Neumann functions of order  $m$ , denoted  $J_m(qr)$  and  $Y_m(qr)$  respectively, as our linearly independent pair of solutions to the Bessel equation, and the modified Bessel functions  $K_m(qr)$  and  $I_m(qr)$  as our pair for the modified Bessel equation, where  $q^2 = |\pm k^2 - V|$ .

Here we can set  $m = 0$ , for in the bound-state problem, our primary concern is a ground state, and in the scattering problem, energy-dependence in the phase shift of the  $m = 0$  channel is sufficient to break scale symmetry. Then  $\Theta$  is a linear function, but any nonzero slope would result in a discontinuity at  $2\pi$ , so in fact  $\Theta$  is constant.

Let's start with the bound-state problem and accordingly use  $-k^2$  as our energy, which must be greater than the well depth  $-g$ . In the interior of the finite well, we solve Bessel's equation since  $-k^2 > -g \implies -k^2 - (-g) > 0$ , so  $J_0(qr)$  and  $Y_0(qr)$  are our solutions, though only  $J_0(qr)$  is regular near 0. Outside the well, we solve the modified Bessel equation, and the normalizable solution is  $K_0(kr)$ . We have two boundary conditions at  $a$ , the usual requirements of continuity and differentiability:

$$AJ_0(qa) = BK_0(ka) , \quad AqJ_0'(qa) = BkK_0'(ka) \quad (6.3)$$

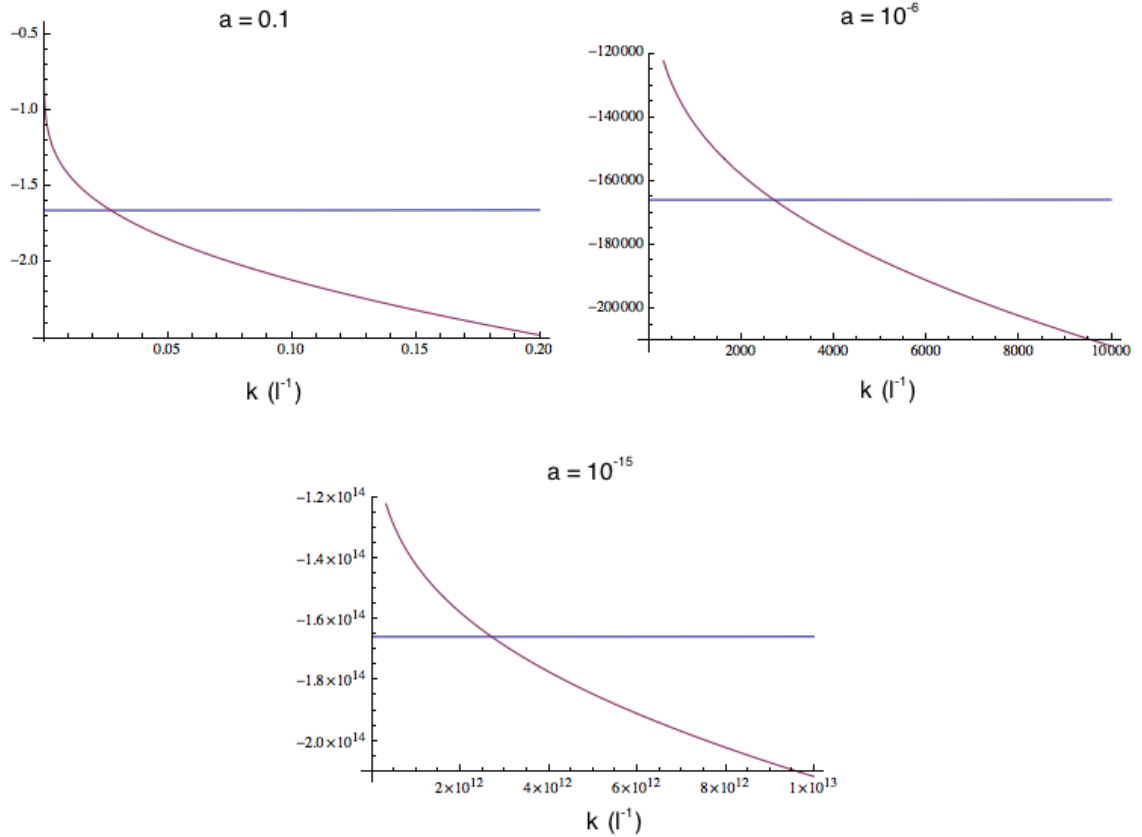


Figure 6.1: Plots of the LHS (blue) and RHS (red) of Eq. 6.4 as a function of  $k$  for different values of  $a$  and  $g = \frac{1}{\pi a^2}$ . As  $a \rightarrow 0$ , the bound-state energy  $k$ , the intersection point of the two curves, clearly blows up.

Dividing the second boundary condition by the first yields a transcendental equation for  $k$ :

$$q \frac{J'_0(qa)}{J_0(qa)} = k \frac{K'_0(ka)}{K_0(ka)} \quad (6.4)$$

Since we don't know how  $k$  behaves in the limit with  $ga^2$  constant, we can't make any small-argument approximations with the Bessel functions and so are forced to solve this numerically. Doing so in *Mathematica* demonstrates very clearly that the bound state energy blows up in the  $ga^2$  limit, so the 2D  $\delta$  potential does not have a finite-energy bound state.

But let's suppose there *were* a bound state, and give it a bound state energy  $k = k_{bs}$ . Then since  $k$  is constant, clearly  $ka$  becomes small in the  $a \rightarrow 0, g \rightarrow \infty$  limit. Let's also

force  $qa$  to be small by changing our mind about the limiting procedure and having  $ga^2 \rightarrow 0$ , so  $qa = a\sqrt{-k^2 + g} = \sqrt{-k^2a^2 + ga^2} \rightarrow 0$ . Then expanding out  $J_0$ ,  $J'_0$ ,  $K_0$ , and  $K'_0$  to first order, we have [12]

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

which simplifies to

$$\frac{2}{\log(ka)} = -q^2a^2 = -(-k^2 + g)a^2 \approx -ga^2$$

since  $-k^2$  is constant and  $g \rightarrow \infty$ . Solving for  $k$  yields

$$k_{bs} = \frac{1}{a}e^{-2/ga^2} \tag{6.5}$$

We can also find the scattering phase shift between incoming and scattered plane waves with positive energy  $k^2$ . Lapidus in Ref. [34] determines the scattering phase shift in the  $l = 0$  channel for the finite well to be

$$\tan(\phi) = \frac{kJ'_0(ka)J_0(qa) - qJ'_0(qa)J_0(ka)}{kN'_0(ka)J_0(qa) - qJ'_0(qa)N_0(ka)} \tag{6.6}$$

Still taking  $qa$  and  $ka$  to be small, we can plug in small-argument behavior for the Bessel functions, and we get

$$\tan(\phi) = \frac{-\pi}{2\log(k_{bs}/k)} \tag{6.7}$$

which is another hallmark of broken scale invariance: energy dependence in the phase shift. Without a dimensional parameter like  $k_{bs}$ , there would be no way for  $k$  to affect the dimensionless phase shift, as there must be a way for its dimensions to be cancelled out.

Recall that to find the bound state energy we had to change the regularization limit. We can now find exactly how quickly  $g$  must go to  $\infty$  relative to  $a$  for there to be a bound state by rearranging Eq. 6.5.

$$g \sim \frac{1}{a^2 \log\left(\frac{1}{k_{bs}a}\right)}$$



So  $g$  goes to  $\infty$  a little bit more slowly than in the original plan  $g \sim 1/a^2$ . The traditional interpretation (seen in Refs. [1], [2], and [8]) views the emergence of this bound-state energy as an anomaly, because it violates the properties of scale-invariant potentials presented in Chapter 4, in particular having one finite-energy bound state without also having a continuum of negative eigenvalues. The process of changing the limiting procedure is termed “renormalization,” an essential tool in the subject of quantum field theory, which is rife with unwanted infinities.

The renormalization process in normal quantum mechanics can be motivated similarly. Using the  $\delta$  function as our potential posits the patently absurd assumption that for every length in meters  $\epsilon > 0$  (including fractions of the Planck length), the probability density decays as a particle in free space, until something special happens *right at* the origin. Realistically, any situation that we might want to model as a  $\delta$  potential would actually be a very deep, very thin finite well with weird stuff happening at the cutoff scale that our existing physical theories cannot probe. Choosing a cutoff, a mostly mathematical consideration, is equivalent to choosing a bound-state energy, a physical observable. Ultimately, then, the process of renormalization can be thought of as turning mathematical limitations of a theory into measurable physical parameters. From this point of view, the seemingly questionable practice of changing our potential in the middle of the problem is a reasonable thing to do on physical grounds.

But how that factors into our interpretation of the scale-symmetry breaking as an *anomaly* is a separate question. To say that this emergence of a bound state is anomalous is to blame the transition from classical to quantum mechanics for the symmetry breaking. This brings us back to the question we raised in the introduction: is an anomaly, by definition, a symmetry broken by regularization, or is it a symmetry broken by quantization à la Esteve or Fujikawa?

Another interpretation is that we have changed the potential from the  $\delta$  potential to some other singular potential. As a functional, the  $\delta$  potential can be said to behave as follows in an integral with a sufficiently well-behaved test function  $f$ :

$$\int f(r)\delta(r)d^2\vec{r} = \begin{cases} c & \lim_{r \rightarrow 0} f(r) = c \\ \pm\infty & \lim_{r \rightarrow 0} f(r) = \pm\infty \end{cases} \quad (6.8)$$

We have taken  $f$  to be a circularly symmetric function  $f(r)$  to simplify the mathematics—which is fine because we only deal with circularly symmetric wave functions in this chapter. We can show that the regularization of the  $\delta$  potential  $V_{g,a} = g\theta(a-r)$  reproduces the behavior of the  $\delta$  function as a functional. (Note that we dropped the minus sign to simplify things. When we go back to quantum mechanics and want the attractive  $\delta$  potential, we can put it back in.) We put  $V_{g,a}$  next to  $f(r)$  in an integral and take the  $a \rightarrow 0$  limit outside the integral sign with  $g = \frac{1}{\pi a^2}$ :

$$\begin{aligned} \int f(r)\delta(r)d^2\vec{r} &= 2\pi \lim_{a \rightarrow 0} \int_0^\infty f(r) \frac{1}{\pi a^2} \theta(a-r) r dr = 2 \lim_{a \rightarrow 0} \frac{1}{a^2} \int_0^a f(r) r dr \\ &= 2 \lim_{a \rightarrow 0} \frac{\frac{1}{a} \int_0^a f(r) r dr}{a} \end{aligned}$$

By the fundamental theorem of calculus,  $\frac{1}{a} \int_0^a f(r) r dr \rightarrow f(0)(0) = 0$ . Thus we can use l'Hospital's rule (and the FTC again) to show that

$$2 \lim_{a \rightarrow 0} \frac{\frac{1}{a} \int_0^a f(r) r dr}{a} = 2 \lim_{a \rightarrow 0} \frac{\frac{-1}{a^2} \int_0^a f(r) r dr + \frac{1}{a} f(a) a}{1} = 2 \lim_{a \rightarrow 0} \frac{-1}{a^2} \int_0^a f(r) r dr + 2 \lim_{a \rightarrow 0} f(a)$$

The left-hand limit is the same limit that appeared a few equal signs ago but with a *minus* sign, so we can move it over to the other side of the equation and divide by 2. The result is

$$\int f(r)\delta(r)d^2\vec{r} = 2 \lim_{a \rightarrow 0} \frac{1}{a^2} \int_0^a f(r) r dr = \lim_{a \rightarrow 0} f(a)$$

Of course, this can be evaluated to  $f(0)$  if  $f$  is continuous, which we might as well assume since we needed that assumption along the way in using the FTC. It is not worth the space to prove it, but it should be fairly obvious that if  $f \rightarrow \pm\infty$ , then the  $\delta$  function returns  $\pm\infty$ .

By changing the limiting procedure for the  $\delta$  regularization from  $g = \frac{1}{\pi a^2}$  to  $g = \frac{2}{a^2 \log(1/ka)}$ , we've obviously changed the nature of the  $\delta$  functional. Let's call the new functional  $\tilde{\delta}$ . Then I claim

$$\int f(r)\tilde{\delta}(r)d^2\vec{r} = \begin{cases} 0 & \lim_{r \rightarrow 0} f(r) \in \mathbb{R} \\ 2\pi B & f \approx B \log(1/r) \text{ for small } r \\ \infty & f \rightarrow \pm\infty \text{ faster than } \log(1/r) \end{cases} \quad (6.9)$$

The proof goes similarly to the one for the original  $\delta$  functional. We'll show that  $\tilde{\delta}$  returns  $B$  if  $f$  goes as  $B \log(1/r)$ , since the other two cases are fairly obvious. We use the FTC and l'Hospital's rule in similar ways:

$$\begin{aligned} \int f(r)\tilde{\delta}(r)d^2\vec{r} &= 4\pi \lim_{a \rightarrow 0} \frac{1}{a^2 \log(1/ka)} \int_0^a f(r)rdr = 4\pi \lim_{a \rightarrow 0} \frac{\frac{1}{a} \int_0^a f(r)rdr}{a \log(1/ka)} \\ &= 4\pi \lim_{a \rightarrow 0} \frac{\frac{-1}{a^2} \int_0^a f(r)rdr + \frac{1}{a} f(a)a}{\log(1/ka) - 1} = 4\pi \lim_{a \rightarrow 0} \frac{\frac{-1}{a^2} \int_0^a f(r)rdr + \frac{1}{a} f(a)a}{\log(1/ka)} \\ &= 2\pi \lim_{a \rightarrow 0} \frac{f(a)}{\log(1/a)} \end{aligned}$$

The  $k = k_{bs}$  drops out because  $\log(1/ka) = \log(1/a) + \log(1/k)$ . We are being sloppy by putting dimensional quantities in logarithms, but this can always be fixed by sneaking in an arbitrarily dimensioned parameter with a value of 1.

This new potential is not scale invariant, since it requires a dimensional quantity  $k = k_{bs}$  to even make sense. This characterization of the renormalization process—that we are changing the potential itself to something explicitly not scale invariant—will become relevant when we look at the momentum-space approach to this problem, which uses the functional interpretation of the  $\delta$  potential more explicitly.

## 6.2 Momentum-Space Regularization

In this approach, we avoid having to “re-define” the  $\delta$  function as a limit of regularizing wells. We can use its original definition in terms of its action in an integral. The 2D  $\delta$  potential is both singular and scale symmetric, and both of those properties bring about complications in the momentum-space approach. Thus we'll take a brief tangent to illustrate the efficacy of this method with a merely singular potential, the 1D  $\delta$ .

### 6.2.1 1D $\delta$ Potential

Our potential is  $V(x) = -g\delta(x)$ . We start by taking the Fourier transform of the Schrödinger equation, with  $E = -k^2$  to look for a bound state. We denote the momentum-space wave function as  $\phi(p)$  and the position-space wave function as  $\psi(x)$ . Integrals in this subsection are assumed to go from  $-\infty$  to  $\infty$ .

$$p^2\phi(p) - g \int e^{-ipx} \delta(x)\psi(x)dx = -k^2\phi(p)$$

The  $\delta$  function makes the integral easy to evaluate, and a little bit of rearranging gives

$$\phi(p) = \frac{g\psi(0)}{p^2 + k^2}$$

Taking the inverse Fourier transform brings us back to  $\psi(x)$  in terms of a  $p$ -space integral.

$$\psi(x) = \frac{g\psi(0)}{2\pi} \int \frac{e^{ipx}}{p^2 + k^2} dp \quad (6.10)$$

Demanding consistency of  $\psi(0)$  gives us our energy-quantization condition:

$$\psi(0) = \frac{g\psi(0)}{2\pi} \int \frac{1}{p^2 + k^2} dp = \frac{g\psi(0)}{2\pi} \left(\frac{\pi}{k}\right) = \frac{g\psi(0)}{2k}$$

We can't have  $\psi(0) = 0$  since a free-space solution with negative energy decays outside the origin, so we must have  $k = g/2$ , or  $E = -g^2/4$ . To find the ground-state wave function, we can solve the integral in Eq. 6.10 via contour methods. We present the details because they illustrate how the discontinuity in the derivative of  $\psi(x)$  in the  $\delta$  potential arises in the momentum-space approach. We start with the case  $x > 0$  and draw a semi-circular contour in the upper half of the complex  $p$ -plane, depicted in Fig. 6.2.

The contour integral for any  $R$  is  $2\pi i \frac{e^{i(ik)x}}{2ik} = \frac{\pi}{k} e^{-kx}$  by the Cauchy Integral Formula since only the pole at  $ik$  is enclosed. Since  $x > 0$ , the hypotheses of Jordan's Lemma (see Ref. [11]) apply to this integral and thus the semi-circular part of the integral vanishes as  $R \rightarrow \infty$ , leaving

$$\psi(x) = \frac{g\psi(0)}{2\pi} \int_{-\infty}^{\infty} \frac{e^{ipx}}{p^2 + k^2} dp = \frac{g\psi(0)}{2\pi} \lim_{R \rightarrow \infty} \int_{-R}^R \frac{e^{ipx}}{p^2 + k^2} dp = \frac{g\psi(0)}{2\pi} \left(\frac{\pi}{k} e^{-kx}\right) = \psi(0) e^{-kx}$$

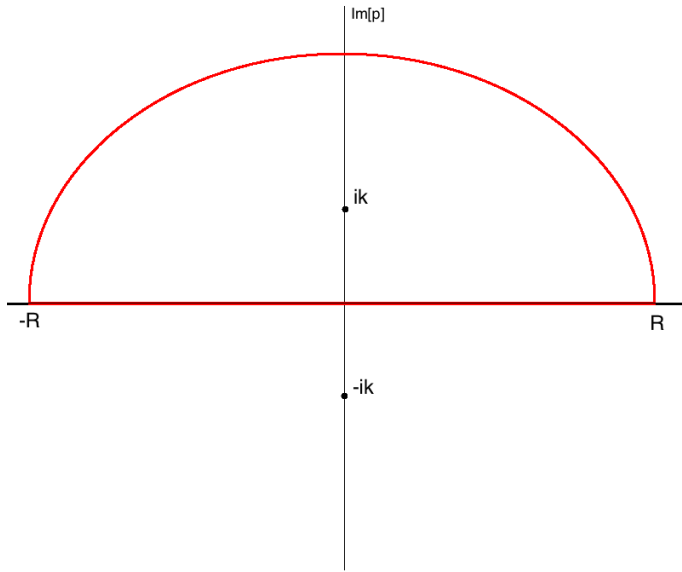


Figure 6.2: Contour for solving the integral expression for  $\psi(x)$ .

This method only worked for  $x > 0$ . To find  $\psi(x)$  for negative arguments, let  $x$  remain positive and plug  $-x$  into  $\psi$ . Then

$$\begin{aligned}\psi(-x) &= \frac{g\psi(0)}{2\pi} \int_{-\infty}^{\infty} \frac{e^{ip(-x)}}{p^2 + k^2} dp = \frac{g\psi(0)}{2\pi} \int_{\infty}^{-\infty} \frac{-e^{i(-p)x}}{(-p)^2 + k^2} d(-p) \\ &= \frac{g\psi(0)}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i(-p)x}}{(-p)^2 + k^2} d(-p) = \psi(x)\end{aligned}$$

So swapping  $x$  for  $-x$  effectively amounts to changing the dummy variable label from  $p$  to  $-p$ . Thus the function is even, and we can write it for all  $x$  as

$$\psi(x) = \psi(0)e^{-k|x|}$$

$\psi(0)$  is chosen to be  $k/2$  so that  $\psi$  is normalized.

This is a wonderful example, because it shows how the non-smooth behavior of the  $\delta$  potential's bound state can arise naturally from a sharp corner in a parameterized path integral. As  $x$  switches from positive to negative, we must draw a contour in the lower

half-plane instead of the upper half-plane to get the semi-circular integral to vanish. We are then enclosing a different pole, and so the derivative of  $\psi$  changes sharply. The result we get from this approach is exactly the same as we would get from a limit of finite wells or from directly integrating the Schrödinger equation to derive the discontinuity in the first derivative.

When we apply this same approach to scale-symmetric potentials, the result will not be as pretty, naturally: we're trying to find a bound state that shouldn't exist. But it is comforting to know that it is in fact the scale symmetry causing problems, not the singularity of the potential.

Before we move on to the 2D  $\delta$ , let us also solve the scattering problem in the 1D  $\delta$  using this method. We start with the Schrödinger equation but substitute  $-k^2$  for  $k^2$  to look for positive-energy eigenstates. The first few steps are almost identical with a minus sign in front of  $k^2$ , so we skip ahead to taking the inverse Fourier transform. (Compare with Eq. 6.10.) We also add in an “incoming wave”  $e^{ikx}$  to give a reference for the phase shift we eventually calculate.

$$\psi(x) = e^{ikx} + \frac{g\psi(0)}{2\pi} \int \frac{e^{ipx}}{p^2 - k^2} dp \quad (6.11)$$

As written, the integral should blow up due to the simple poles at  $k$  and  $-k$  along the contour of integration (the real line). We perform a very innocent “regularization” of sorts to correct for the problem, which amounts to nothing more than taking the *principal value* of the integral. Technically speaking, the integrand is not Lebesgue integrable since in particular the positive real part,  $\max\{\text{Re}[\frac{e^{ipx}}{p^2 - k^2}], 0\}$ , has an infinite integral. However, the negative real part also blows up in a way that perfectly “cancels” the positive part, and similarly for the imaginary parts, so we simply choose to allow this cancellation to happen. There are a number of ways to do this, such as drawing a contour in the complex  $p$ -plane that just skirts the poles, but it turns out the easiest method is to move the poles themselves [52].

We do have some choice, however, over how we move the poles. For  $x > 0$ , we must draw a contour in the upper-half plane to satisfy the hypotheses of Jordan's Lemma, and

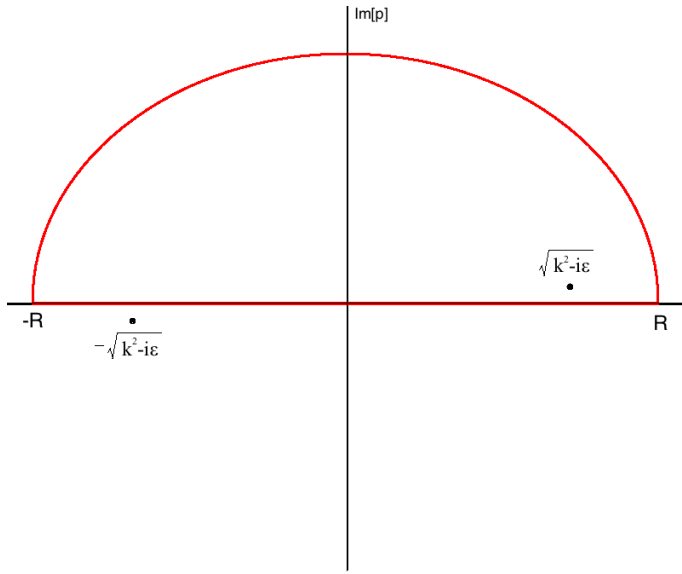


Figure 6.3: Contour for the scattering problem, with the poles very close to, but not on, the real axis.

so our choice amounts to whether we move one pole, the other pole, both, or neither inside the contour. On physical grounds, it turns out we want to move only the positive pole  $k$  inside the contour so that we get an out-going (scattered) wave. (One can also recognize this integral as the Green's function for the 1D Schrödinger equation, and we are choosing the retarded version [52].) To achieve this, we alter Eq. 6.11 by adding in  $-i\epsilon$  to the denominator for  $0 < \epsilon \ll 1$ .

$$\psi(x) = e^{ikx} + \frac{g\psi(0)}{2\pi} \int \frac{e^{ipx}}{p^2 - k^2 - i\epsilon} dp$$

Using Cauchy's integral formula, then, gives

$$\psi(x) = e^{ikx} + i \frac{g\psi(0)}{2\sqrt{k^2 + i\epsilon}} e^{i\sqrt{k^2 + i\epsilon}x} \rightarrow e^{ikx} + i \frac{g\psi(0)}{2k} e^{ikx} \text{ as } \epsilon \rightarrow 0$$

Recall, however, that the semi-circular part of the contour only vanishes for  $x > 0$ . As before, we can find  $\psi$  for negative  $x$  by the same simple argument that  $\psi$  is even. The minus sign on  $k^2$  and extra  $i\epsilon$  do not change the invariance of the integral under the change

of variables  $p \mapsto -p$ , which is equivalent to  $x \mapsto -x$  in this case. So for all  $x$ ,

$$\psi(x) = e^{ikx} + i \frac{g\psi(0)}{2k} e^{ik|x|} \quad (6.12)$$

We can find  $\psi(0)$  by demanding consistency of Eq. 6.12. Some simple algebra gives

$$\psi(0) = \frac{1}{1 - i \frac{g}{2k}}$$

allowing us to compute the phase shift. Unpacking Eq. 6.12 into a piecewise formula for  $\psi(x)$ , we see that the incoming wave from the left has an amplitude of 1, while the transmitted wave to the right has an amplitude of  $1 + i \frac{g\psi(0)}{2k} = \psi(0) = (1 - i \frac{g}{2k})^{-1}$ , giving a phase shift of

$$\tan(\theta) = \frac{g}{2k} = \frac{k_{bs}}{k} \quad (6.13)$$

where  $k_{bs}$  is related to the bound-state energy we found previously. This result is identical to the phase shift we would find by directly integrating the Schrödinger equation with a  $\delta$  potential for  $E = k^2$  and allowing the non-normalizable solutions  $e^{ikx}$ ,  $e^{-ikx}$ .

We present this calculation because it is a useful foil to the same approach for scale-invariant potentials. We see how the unusual wavefunction behavior brought about by the singularity of the potential elegantly arises from the complex analysis required in this approach. We have to make some seemingly questionable decisions, such as skirting the poles in the contour integration to get rid of an unwanted infinity, but in the end we recover the same answer as we'd get from a simpler approach. It will be useful to know which infinities are inherently a part of the momentum-space approach, and which infinities are a consequence of scale invariance.

### 6.2.2 2D $\delta$ Potential

Not surprisingly, we approach the bound-state problem in the same way as we did before but in two dimensions. Now position and momentum are vectors  $\vec{x}$  and  $\vec{p}$ . The zero vector is written as  $0$  instead of  $\vec{0}$  to keep the equations somewhat readable.



$$\begin{aligned}
-\nabla^2\psi(\vec{x}) - g\delta(\vec{x})\psi(\vec{x}) &= -k^2\psi(\vec{x}) \implies p^2\phi(\vec{p}) - g \int \psi(\vec{x})e^{-i\vec{p}\cdot\vec{x}}\delta(\vec{x})d\vec{x} = -k^2\phi(\vec{p}) \\
\implies p^2\phi(\vec{p}) - g\psi(0) &= -k^2\phi(\vec{p}) \\
\implies \phi(\vec{p}) &= \frac{g\psi(0)}{p^2 + k^2}
\end{aligned}$$

Taking the 2D inverse Fourier transform gives us our wave function  $\psi(\vec{x})$ . We go ahead and write the integral in 2D polar coordinates of the  $p_x$ - $p_y$  plane, with  $p = \sqrt{p_x^2 + p_y^2}$ .

$$\psi(\vec{x}) = \frac{g\psi(0)}{(2\pi)^2} \iint \frac{pe^{i\vec{p}\cdot\vec{x}}}{p^2 + k^2} dpd\theta \quad (6.14)$$

To find the bound-state wave function requires solving that tricky integral, but to merely quantize the energy requires only demanding consistency of  $\psi(0)$ . Doing so gives

$$\psi(0) = \frac{g\psi(0)}{(2\pi)^2} \iint \frac{p}{p^2 + k^2} dpd\theta = \frac{g\psi(0)}{4\pi} [\log |p^2 + k^2|]_0^\infty$$

If we divide out  $\psi(0)$ , then the log term evaluated at those limits must be finite. However, it is clearly not, unless  $k^2$  is infinite, i.e. we have a bound state at  $-\infty$ . To have a finite-energy bound state, then, requires imposing a ‘‘momentum-space cutoff’’  $\Lambda$ , by integrating to  $\Lambda$  instead of  $\infty$ . This is a renormalization: we decide that our theory cannot possibly capture the behavior of all possible momenta, and so we fix an arbitrary momentum at which the theory breaks down. A little algebra gives us the quantized energy  $k_{bs}$  in terms of the momentum cutoff:

$$k_{bs} = \frac{\Lambda}{\sqrt{e^{4\pi/g} - 1}} \quad (6.15)$$

Recall the position-space regularization approach to this problem. In that calculation, we effectively imposed a *position-space cutoff*  $a$  to keep the bound-state energy finite. Let’s see how  $a$  and  $\Lambda$  are related. First, we have to note that the lower-case  $g$ ’s we used in each problem are not the same. To keep them distinct, we’ll give the  $g$  we used in  $V_{g,a} = g\theta(a-r)$  the new  $g'$  and quickly get rid of it, noting that  $g = \int g\delta(x)dx = \lim \int V_{g',a}dx = \lim \pi g'a^2 =$

$\pi g' a^2$  since we take  $g' a^2$  constant in the limit. The bound-state energy we found previously was

$$k_{bs} = \frac{1}{a} e^{-2/g' a^2}$$

implying

$$\frac{\Lambda}{\sqrt{e^{4\pi/g} - 1}} = k_{bs} = \frac{1}{a} e^{-2/g' a^2} = \frac{1}{a} e^{-2\pi/g}$$

which is an equation purely in terms of the momentum cutoff, position cutoff, and dimensionless coupling for the  $\delta$  potential. Some straightforward algebra gives

$$a = \frac{1}{\Lambda} \sqrt{1 + e^{-4\pi/g}} \quad (6.16)$$

We would have expected this result, at least qualitatively: the position cutoff is inversely proportional to the momentum-space cutoff with a proportionality constant that depends on the coupling.

To find the bound-state wave function, we simply solve the integral for general  $\vec{x}$  in Eq. 6.14—and we had better get something proportional to  $K_0(k_{bs})$  since that is the only normalizable solution to the free-space Schrödinger equation on  $\mathbb{R}^2 \setminus \{\vec{0}\}$  for negative energy. This time, we will use Cartesian coordinates, and we align our  $p_x - p_y$  coordinate system such that  $p_x$  points along  $\vec{x}$ , so that  $\vec{p} \cdot \vec{x} = p_x x$ .

$$\psi(\vec{x}) = \frac{g\psi(0)}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{ip_x x}}{p_x^2 + p_y^2 + k^2} dp_y dp_x$$

We first integrate in  $p_y$ , which is, by simple contour methods,

$$\begin{aligned} \frac{g\psi(0)}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{e^{ip_x x}}{2\sqrt{p_x^2 + k^2}} dp_x &= \frac{g\psi(0)}{2k(2\pi)^2} \int_{-\infty}^{\infty} \frac{e^{i\frac{p_x}{k} kx}}{\sqrt{\left(\frac{p_x}{k}\right)^2 + 1}} dp_x \\ &= \frac{g\psi(0)}{2(2\pi)^2} \int_{-\infty}^{\infty} \frac{e^{iu(kx)}}{\sqrt{u^2 + 1}} du = \frac{g\psi(0)}{(2\pi)^2} K_0(kx) \end{aligned}$$

where in the last line we used a standard integral representation of  $K_0$  [35]. We do in fact have something proportional to  $K_0$ , but the problem is that  $K_0$  blows up at the origin!

$$\psi(0) = \frac{g\psi(0)}{(2\pi)^2} K_0(0) = \infty \implies \psi(\vec{x}) = \frac{g\infty}{(2\pi)^2} K_0(kx) = \infty$$

Consistency of  $\psi(0)$  implies that  $\psi(\vec{x})$  is infinity everywhere, an obvious absurdity. We need  $\psi(0)$  to be finite and nonzero, but this is clearly not the case, as our bound state approaches  $\infty$  at the origin. The issue here is that, after renormalization,  $\psi(0)$  no longer means what it used to.

Recall the position-space regularization of the 2D  $\delta$ . We renormalized by changing the limiting behavior of the finite well: originally  $g \sim \frac{1}{a^2}$ , and then renormalization forced  $g \sim \frac{1}{a^2 \log(1/k_b s a)}$ . This “changing-limits” interpretation is equivalent to taking a very thin, very deep finite well via a position-space “cutoff”—although the well can’t be as deep as  $1/a^2$ , or else  $ka$  is not small enough for the Bessel function approximations. The momentum-space cutoff is, in turn, equivalent to the position-space cutoff via Eq. 6.16. Thus taking a momentum-space cutoff implicitly changes our  $\delta$  potential to the functional  $\tilde{\delta}$  discussed earlier, and  $\psi(0)$  is now interpreted to mean the *rate of logarithmic divergence* of  $\psi$  at 0 instead of the evaluation of  $\psi$  at 0. As  $x \rightarrow 0$ ,  $K_0(x) \sim \log(1/x)$ , so  $\psi(0)$  is finite. Therefore  $\psi(\vec{x})$  is in fact proportional to  $K_0(kx)$ , and normalization determines the proportionality constant.

### 6.3 Self-Adjoint Extensions Method

The 2D  $\delta$  potential is singular at the origin, so we shouldn’t expect it to behave regularly there in the way that we typically expect wave functions to behave. We can mathematically implement this consideration by treating the Hamiltonian as an operator on  $L^2$  functions from  $\mathbb{R}^2 \setminus \{(0,0)\}$  to  $\mathbb{C}$ . Since the  $\delta$  potential is 0 everywhere outside the origin, this approach amounts to treating the 2D  $\delta$  Hamiltonian as the free-particle Hamiltonian on the punctured plane.

The one issue with this approach is that, although  $-\nabla^2$  is self-adjoint on the plane, it is *not* on the punctured plane. So to be more precise, this approach treats the  $\delta$  Hamiltonian

as a *self-adjoint extension* of the free particle Hamiltonian on the punctured plane.

There are subtleties with regards to what it means to “puncture” the plane, because doing so breaks translational symmetry and forces us to use polar coordinates, which themselves have a troublesome singularity at the origin, independently of the puncture. In other words, it’s difficult to tell which abnormalities arise as a result of the puncture, which treats the point  $(0,0)$  as special, and which ones arise due to using a coordinate system which also treats  $(0,0)$  as special. Thus we begin by solving the free particle potential on the unpunctured plane.

### 6.3.1 Free Particle on the Unpunctured Plane

Due to the translational symmetry of the plane, we can write the time-independent Schrödinger equation in Cartesian coordinates.

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y) = k^2\psi(x,y) \quad (6.17)$$

One need not formally separate this equation to see that the separable solutions are

$$\psi(x,y) = e^{i\vec{k}\cdot\vec{r}} \quad (6.18)$$

for  $k^2 = |\vec{k}|^2$ . While a function such as  $K_0(k\sqrt{x^2+y^2})$  may satisfy the Schrödinger equation for negative energies almost everywhere, its poor behavior at 0 forces us to throw it out. Eq. 6.18 captures all possible solutions, and so the spectrum is  $(0, \infty)$ . We can see formally that  $-\nabla^2$  is (essentially) self-adjoint on  $\mathbb{R}^2$  because

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y) = i\psi(x,y) \quad (6.19)$$

has solutions

$$\psi_+(x,y) = e^{\pm\sqrt{-C_x}x}e^{\pm\sqrt{-C_y}y} \quad (6.20)$$

for some constants  $C_x, C_y$  such that  $C_x + C_y = i$  with any combination of pluses and minuses. Since  $C_x$  and  $C_y$  add up to  $i$ , they can’t both be real, and any complex number with an imaginary part must have a square root with a real part. Thus one of the factors

blows up in some direction, whether as  $x \rightarrow \infty$ ,  $x \rightarrow -\infty$ ,  $y \rightarrow \infty$ , etc. Therefore  $\psi_+$  cannot be in the rigged<sup>1</sup> Hilbert space corresponding to the plane. A similar argument for  $-i$  tells us that the deficiency indices are  $\langle 0, 0 \rangle$ , so  $-\nabla^2$  is essentially self-adjoint.

What if we did the same problem, but in polar coordinates? This approach is a bit tricky, because polar coordinates have a singularity at  $(0, 0)$ , even though the space we are working on does not. The singularity arises because  $r = 0$  implies  $(x, y) = (0, 0)$  regardless of  $\theta$ . Another way of thinking about it is that we treat the plane as  $[0, \infty) \times S^1$  instead of as  $\mathbb{R} \times \mathbb{R}$ , and the set  $[0, \infty)$  has 0 as a boundary point, while  $\mathbb{R}$  has no boundary.

Separating the equation in polar coordinates for  $m = 0$  causes us to find solutions of the form  $R(r)\Theta(\theta)$  instead of  $X(x)Y(y)$ . As was shown before,  $\Theta$  must be constant for  $m = 0$  while the radial part satisfies Bessel's equation

$$\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + k^2 R = 0 \quad (6.21)$$

But what boundary conditions do we impose on  $R$  at 0? We must continue to treat 0 as any other point, and we only demand that  $\psi$  be continuous and differentiable everywhere—so it wouldn't make sense to require anything extraneous like  $R(0) = 0$ . But to keep  $R(r)\Theta(\theta)$  differentiable in the plane, we must have  $R'(0) = 0$ , for we would otherwise have different left- and right-hand partial derivatives around the origin. A linearly independent pair of solutions to Eq. 6.21 is  $J_0(kr)$  and  $Y_0(kr)$ , but we throw out  $Y_0(kr)$  due to its divergent behavior at the origin. Although  $J_0(kr)$  is not in  $L^2$ , we allow it in the rigged Hilbert space as a positive-energy solution. Connecting this back to the eigenstates we found in Cartesian coordinates, we can see that  $J_0(kr)$  is just a “radially symmetrized” superposition of the plane waves  $e^{i\vec{k}\cdot\vec{r}}$ , via one of Bessel's integrals [12]:

$$J_0(kr) = \frac{1}{2\pi} \int_0^{2\pi} e^{ik \cos(\theta)r} \quad (6.22)$$

That is,  $J_0$  is an average of plane waves pointing in every direction.

---

<sup>1</sup>In positive-energy problems, we formalize the existence of the scattering sector through what is called a “rigged” Hilbert space, which is essentially the original Hilbert space with oscillatory solutions added in. Although functions like  $e^{ikx}$  are clearly not in  $L^2(\mathbb{R}^2)$ , they are well-behaved enough to be in the rigged Hilbert space and count as a part of the orthogonal energy eigenbasis. Functions like  $e^x$ , however, blow up faster than any polynomial and thus are thrown out. See Ref. [25].

Now we check for self-adjointness. We have shown that  $-\nabla^2$  is self-adjoint on  $\mathbb{R}^2$ , but is the  $m = 0$  radial operator  $\mathcal{R} = -(\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr})$  self-adjoint on  $D(\mathcal{R}) = \{R \in C_0^2([0, \infty)) \mid R'(0) = 0\}$  with integration measure  $rdr$ ?

To answer that question with the deficiency subspace method is difficult, because our initial domain isn't very restrictive. Normally, one chooses a very restrictive domain, requiring that any element of the domain and all of its derivatives be 0 at boundary points. Then the adjoint domain in turn becomes very large, and when finding the deficiency spaces of the adjoint we need not worry about what is or is not in  $D(\mathcal{R}^*)$ , because *everything* is [1]. In this case, however, we have to know which  $\psi$  satisfy  $\mathcal{R}^*\psi = \pm i\psi$  and are in  $D(\mathcal{R}^*)$ .

Therefore, for now, let us work straight from the definition of the adjoint and try to move  $\mathcal{R}$  from the ket to the bra in the expression  $(\phi, \mathcal{R}\psi)$  for  $\psi \in D(\mathcal{R})$ ,  $\phi \in D(\mathcal{R}^*)$  via repeated integration by parts.

$$\begin{aligned} (\phi, \mathcal{R}\psi) &= \int_0^\infty \bar{\phi} \left( -\psi'' - \frac{1}{r} \psi' \right) r dr = -[\bar{\phi} r \psi']_0^\infty + \int_0^\infty \overline{(\phi' r + \phi)} \psi' dr - [\bar{\phi} \psi]_0^\infty + \int_0^\infty \bar{\phi}' \psi dr \\ &= -[\bar{\phi} r \psi']_0^\infty - [\bar{\phi} \psi]_0^\infty + [\bar{\phi}' r \psi]_0^\infty - \int_0^\infty \overline{(\phi'' r + \phi')} \psi dr + [\bar{\phi} \psi]_0^\infty - \int_0^\infty \bar{\phi}' \psi dr + \int_0^\infty \bar{\phi}' \psi dr \\ &= [\bar{\phi}' r \psi - \bar{\phi} r \psi']_0^\infty - \int_0^\infty \overline{\left( \phi'' + \frac{1}{r} \phi' \right)} \psi r dr = [\bar{\phi}' r \psi - \bar{\phi} r \psi']_0^\infty + (\mathcal{R}\phi, \psi) \end{aligned}$$

So  $\mathcal{R}$  is hermitian if and only if the boundary term

$$(\phi, \mathcal{R}\psi) - (\mathcal{R}\phi, \psi) = [r(\bar{\phi}'\psi - \bar{\phi}\psi')]_0^\infty = [r(\bar{\phi}'\psi - \bar{\phi}\psi')]_{r=0}$$

vanishes for all  $\psi \in D(\mathcal{R})$ ,  $\phi \in D(\mathcal{R}^*)$ . Clearly the function vanishes at  $\infty$ , since  $L^2$  functions must go to 0 faster than  $r$ . (Although scattering solutions do not converge to 0 for large  $r$ , we can still work in  $L^2$  for the time being and think of scattering solutions such as plane waves and  $J_0(kr)$  as limiting cases of  $L^2$  wave packets.) Dividing out the measure factor  $r$ , the factor  $\bar{\phi}'\psi - \bar{\phi}\psi'$  vanishes on its own for all  $\phi, \psi \in D(\mathcal{R})$ . Moreover, this term vanishes in a way that is perfectly symmetric between the domain of the  $\mathcal{R}$  and the domain of the adjoint, since being in  $D(\mathcal{R})$  requires that  $\phi'(0) = \psi'(0) = 0$  while  $\phi(0)$  and  $\psi(0)$  can be anything. In other words, requiring  $\psi'(0) = 0$  forces precisely the same boundary

condition on  $\phi'$ , so they must come from the same domain, i.e.  $D(\mathcal{R}) = D(\mathcal{R}^*)$ . Thus the operator is self-adjoint, as expected.

### 6.3.2 Free Particle on the Punctured Plane

Now we finally solve the problem with a puncture, following the Gopalakrishnan's treatment in Ref. [1] with slight corrections. Of course, we can't separate in Cartesian coordinates because of the breaking of translational symmetry. So we return to the  $m = 0$  channel radial equation and this time start with a restrictive enough domain  $D(\mathcal{R}) = \{R \in L^2((0, \infty)) \mid 0 = R(0) = R'(0) = R''(0) = \dots\}$  to use the deficiency indices method. The equations  $\mathcal{R}^*\phi = \pm i\phi$  have normalizable solutions

$$\phi_{\pm}(r) = K_0\left(\sqrt{\pm ir}\right) \quad (6.23)$$

giving deficiency indices  $\langle 1, 1 \rangle$ . Since  $\phi_+$  and  $\phi_-$  have the same norm, we need not normalize, and we allow the following small- $r$  behavior in our domain:

$$R(r) \approx K_0\left(\sqrt{ir}\right) + \alpha K_0\left(\sqrt{-ir}\right) \quad (6.24)$$

for  $\alpha \in \mathbb{C}$  with  $|\alpha| = 1$ , which we can write as  $\alpha = e^{i\theta}$ . Expanding out the modified Bessel functions for small  $r$  via  $K_0(z) \approx -\log(z/2)$  for any small complex  $z$ , we get

$$\begin{aligned} R(r) &\approx -\log\left(\sqrt{ir}/2\right) - e^{i\theta} \log\left(\sqrt{-ir}/2\right) = -\left(e^{i\theta} + 1\right) \log(r/2) + i\frac{\pi}{4}\left(e^{i\theta} - 1\right) \\ &= \frac{1}{e^{i\theta} + 1} \left[-\log(r/2) - \frac{\pi}{4} \tan\frac{\theta}{2}\right] \propto -\log(r/2) - \frac{\pi}{4} \tan\frac{\theta}{2} \\ &= -\log(Cr/2) \approx K_0(Cr) \end{aligned}$$

where we have absorbed all of the constants into one parameter  $\log(C)$ , which we can do because  $\tan\frac{\theta}{2}$  spans all of the real numbers. There is a special extension corresponding to  $\theta = \pi$  that preserves the scale invariance, since in the first line above the log terms cancel and so we do not in fact add logarithmic divergence to the domain. Every other choice of  $\theta$  allows logarithmic divergence at the origin at some particular rate, which introduces a particular bound state  $K_0(k_{bs}r)$  where  $k_{bs} = C$ . Independently, we know that this bound

state must be unique since  $K_0(k_{bs}r) \geq 0$ , so  $K_0(k_{bs}r)$  and  $K_0(k'_{bs}r)$  cannot be orthogonal [1]. This boundary condition, when applied to the scattering sector, produces a phase shift (see Ref. [1]) of

$$\tan(\phi) = \frac{-\pi}{2 \log(k_{bs}/k)} \quad (6.25)$$

which is exactly the same anomalous phase shift we got in the position-space regularization.

A note about dimensions: although  $C$  appears to be dimensionless—and clearly needs dimensions of inverse length to cancel the dimensions of  $r$ —there is an arbitrary dimensioned term (whose value we set to 1) next to  $\pm i$  in the deficiency-index equations, which then reappears next to  $\sqrt{\pm i}$  in the solutions. In the purely mathematical treatment, we could ignore issues of dimension, but now that our operators are themselves dimensioned,  $\pm i$  must take on dimensions as well to compensate. Although this introduces yet another arbitrary constant, it can be subsumed into the also arbitrary self-adjoint extension parameter.

## 6.4 Dimensional Regularization

Speaking of dimensions, there is another avenue for renormalization that specifically targets the dependence of the dimensionless nature of the coupling on the dimension (in a different sense of the word) of the underlying space. This technique is known as *dimensional regularization*, a clever pun that exploits the homonym of unit dimension and space dimension in physics. It is popular in quantum field theory, for certain desired properties of the problem, for example unitarity, will hold independently of the number of dimensions, but would break via some other regularization scheme [32]. The idea is that, since the coupling is dimensionless only when  $D = 2$ , we solve the  $D$ -dimensional  $\delta$  potential for arbitrary—even non-integer— $D$  and take the limit as  $D \rightarrow 2$ .

Since  $D$ -dimensional integrals are easily generalizable, the best technique for this problem is the momentum-space approach, using  $D$ -dimensional Fourier transforms. The crucial generalization is the  $D$ -dimensional solid angle, which allows one to integrate functions with  $D$ -dimensional spherical symmetry. The details are in Ref. [14], and the result is



$$\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)} \quad (6.26)$$

With the identities  $\Gamma(1/2) = \sqrt{\pi}$ ,  $\Gamma(1) = 1$ , and  $\Gamma(3/2) = \sqrt{\pi}/2$ , it is trivial to verify that Eq. 6.26 holds for the well-understood cases  $D = 1$ ,  $D = 2$  and  $D = 3$ . Intuitively, we're just replacing the factorial that appears in the general equation for surface area in integer  $D$  dimensions with a Gamma function. Then the  $D$ -dimensional integral of a radially symmetric function  $f(r)$  is

$$\int_{\mathbb{R}^D} f(r) d^D \vec{r} = \Omega_D \int_0^\infty f(r) r^{D-1} dr \quad (6.27)$$

We return to the momentum-space derivation of the  $\delta$  potential's bound-state energy. Assuming the  $D$ -dimensional Fourier transform turns the  $D$ -dimensional Laplacian  $-\nabla_D^2$  into  $p^2$  and that the  $D$ -dimensional integral of  $\psi(\vec{r})\delta_D(r)$  returns  $\psi(0)$ , we follow the same steps as before to get

$$\phi(p) = \frac{g\psi(0)}{p^2 + k^2} \quad (6.28)$$

Then, to check consistency of  $\psi(0)$ , we take the inverse  $D$ -dimensional Fourier transform, plug in 0, and divide by  $\psi(0)$ .

$$1 = \frac{g}{(2\pi)^D} \int_{\mathbb{R}^D} \frac{1}{p^2 + k^2} d^D \vec{p} = \frac{g}{(2\pi)^D} \Omega_D \int_0^\infty \frac{p^{D-1}}{p^2 + k^2} dp \quad (6.29)$$

The integral on the far RHS of Eq. 6.19 is a special case of the Beta function identity [14]

$$\int_0^\infty \frac{x^{2\alpha-1}}{(x^2 + 1)^{\alpha+\beta}} dx = \frac{1}{2} B(\alpha, \beta) \quad (6.30)$$

and so, with a simple substitution  $u = p/k$  can be evaluated to give

$$\begin{aligned} 1 &= \frac{g\Omega_D}{(2\pi)^D} k^{D-2} \int_0^\infty \frac{u^{2(D/2)-1}}{(u^2 + 1)^{(D/2)+(1-D/2)}} du = \frac{gk^{D-2}}{2^D \pi^{D/2} \Gamma(D/2)} B(D/2, 1 - D/2) \\ &= \frac{gk^{D-2}}{2^D \pi^{D/2} \Gamma(D/2)} \frac{\Gamma(D/2)\Gamma(1 - D/2)}{\Gamma(1)} = g2^{-D} \pi^{-D/2} k^{D-2} \Gamma(1 - D/2) \end{aligned}$$

where we have used a characterization of the Beta function in terms of Gamma functions [12]. Then solving for a bound-state energy  $k$  gives

$$k = \left[ g 2^{-D} \pi^{-D/2} \Gamma(1 - D/2) \right]^{\frac{1}{2-D}} \quad (6.31)$$

If  $D$  approaches 2 from the right, then  $\Gamma(1 - D/2) \rightarrow -\infty$  and  $(2 - D)^{-1} \rightarrow -\infty$ , so  $|k| \rightarrow \infty$ . If we take the limit from the left, then  $\Gamma(1 - D/2) \rightarrow \infty$  and  $(2 - D)^{-1} \rightarrow \infty$ , in which case  $k \rightarrow \infty$ .

In either case, dimensional regularization by itself doesn't break the scale symmetry, which is to be expected: this process of working in arbitrary dimensions and limiting towards 2 does not in any way introduce a dimensional parameter that could define energy since  $k$  blows up. Furthermore, the units of  $g$  disappear in the  $D \rightarrow 2$  limit.

To produce a bound state then, requires renormalization. Previously, we renormalized by changing the limiting procedure for the finite well in position space or by taking a momentum cutoff in momentum space, and this time we make the renormalization process mathematically explicit by using a "running coupling." Since the potential's coupling is not a directly meaningful physical quantity, taking a variable coupling is not inherently problematic as long as it produces physically sensible results. We take  $g = g(\epsilon)$  for a renormalization parameter  $\epsilon = D - 2$ . Setting

$$g(\epsilon) = \left( \frac{1}{k_{bs}} \right)^\epsilon 2^{\epsilon+2} \pi^{\epsilon/2+1} \frac{1}{\Gamma(\epsilon/2)} \quad (6.32)$$

for some arbitrary parameter with dimensions of inverse length  $k_{bs}$ , when we take the  $\epsilon \rightarrow 0$  limit we now recover  $k \rightarrow k_{bs}$ . This may not seem like the most physically sensible renormalization process, compared to, say, the finite-well cutoff. From a modeling standpoint, it makes sense to accept that what we initially pretended to be a  $\delta$  function is actually just some really deep, really thin finite well; it may not be as mathematically trivial to deal with as a  $\delta$  function, but it is more in line with physical reality. With dimensional regularization, however, the corresponding physical reality posited by the renormalization scheme is one in which our world is *actually*  $2 + \epsilon$ -dimensional for some really small  $\epsilon > 0$ . Clearly, this technique, which is applicable in quantum field theory as well, is not motivated by physical

reality. Rather it is useful because of its aforementioned ability to preserve symmetries that a simple cutoff regulator does not, in particular the Ward identities in quantum field theories [48].

## 6.5 Path-Integral Approach

We can use the Feynman approach, as outlined in Chapter 2, to solve the bound-state and scattering problems for this potential, with the help of perturbative methods, as outlined in Ref. [21]. Doing so allows us to connect the symmetry breaking with Fujikawa’s “anomalous Jacobian” characterization of the anomaly. Anticipating the need for dimensional regularization, we will proceed in arbitrary  $D$  dimensions.

The path integral formulation of quantum mechanics gives a different way of finding the propagator  $\langle x'', t'' | x', t' \rangle$ , which in turn can indirectly tell us about the energy spectrum of  $H$ . Since this potential is time-independent, we can forget about  $t'$  and  $t''$ , and instead write the propagator as  $K(x'', x' | T) = \langle x'' | e^{-iTH} | x' \rangle$  for  $T = t'' - t'$ . The retarded, or “causal,” Green’s function for the Schrödinger equation is essentially the propagator but only going forwards in time, i.e.  $G(x'', x' | T) = \Theta(T)K(x'', x' | T)$ . The energy Green’s function is related to the time Green’s function via the energy-time Fourier transform

$$\begin{aligned} \tilde{G}(x'', x' | E) &= -i \int_{-\infty}^{\infty} e^{iTE} G(x'', x' | T) dT = -i \int_{-\infty}^{\infty} e^{iTE} \Theta(T) K(x'', x' | T) dT \\ &= -i \int_{-\infty}^{\infty} e^{iTE} \Theta(T) \langle x'' | e^{-iTH} | x' \rangle dT = -i \left\langle x'' \left| \int_0^{\infty} e^{-i(H-E-i0^+)T} dT \right| x' \right\rangle \\ &= \left\langle x'' \left| \frac{1}{E - H + i0^+} \right| x' \right\rangle \end{aligned}$$

with a small imaginary number  $i0^+$  added to both make  $\int_0^{\infty} e^{-i(H-E-i0^+)T} dT$  finite and to move the poles of  $(E - H + i0^+)^{-1}$  off the real axis. Inserting a complete set of eigenstates  $\mathbb{I} = \sum_n |n\rangle\langle n| + \int_{\alpha} |\alpha\rangle\langle\alpha| d\alpha$  shows how the energy Green’s function gives us the spectrum of  $H$ :

$$\tilde{G}(x'', x' | E) = \sum_n \frac{\psi_n^*(x') \psi_n(x'')}{E - E_n + i0^+} + \int_{\alpha} \frac{\psi_{\alpha}^*(x') \psi_{\alpha}(x'')}{E - E_{\alpha} + i0^+} d\alpha \quad (6.33)$$

Holding  $x'$  and  $x''$  fixed, we see that  $\tilde{G}(x'', x'|E)$ , as a function of  $E$ , is continuous except for poles at  $E_n$  and a branch cut along  $E_\alpha$ . We only needed the assumption of  $H$ 's self-adjointness to use the completeness relation in deriving Eq. 6.33. Therefore, if we have any self-adjoint Hamiltonian and use the path integral approach to calculate the corresponding propagator  $K(x'', x'|T)$ , we can find its spectrum by identifying poles and branch cuts of  $G(x'', x'|E)$ .

To compute the propagator for this problem is a long calculation. Since we are working with a radially symmetric potential, we want to separate the path integral into  $D$ -dimensional hyperspherical coordinates, which requires, in the discretization limit, an infinite number of Jacobians. Collecting the factors/integrations that depend only on angular variables and those that depend only on  $r$  allows us to identify a ‘‘radial propagator,’’ which is already a massive expression

$$K_{l+\nu}(r'', r'; T) = \int \exp \left[ i \int_0^T \left( \frac{1}{2} \dot{r}^2 - V(r) \right) dt \right] \mu_{l+\nu}[r^2] \mathcal{D}r \quad (6.34)$$

where  $\nu$  depends on the dimension  $D$  while  $l$  gives the angular-momentum channel. The factor

$$\mu_{l+\nu}^N[r^2] = \prod_{j=0}^{N-1} \sqrt{2\pi z_j} e^{-z_j} I_{l+\nu}(z_j) \quad (6.35)$$

is a function-space measure for the radial path integral (in the discretized version with  $N$  lattice points), where  $z_j = \frac{-ir_j r_{j+1}}{\Delta t}$ . Moreover, to solve the problem for the  $\delta$  potential requires writing it as a perturbative expansion and summing the perturbations to every order. Needless to say, the calculation is extensive, so we will just skip ahead to the end. We eventually find a Green's function in closed form since the perturbations form a geometric series:

$$G_D(\vec{r}'', \vec{r}'; E) = G_D^{(0)}(\vec{r}'', \vec{r}'; E) - \frac{G_D^{(0)}(\vec{r}'', \vec{0}; E) G_D^{(0)}(\vec{0}, \vec{r}'; E)}{G_D^{(0)}(\vec{0}, \vec{0}; E) - \frac{1}{g}} \quad (6.36)$$

where  $G_D^{(0)}(\vec{r}'', \vec{r}'; E)$  represents the Green's function for the zeroth-order perturbation, i.e. the free-particle Green's function in  $D$  dimensions, which is known to be (in terms of  $k = \sqrt{E}$ ,  $r = |\vec{r}'' - \vec{r}'|$ )

$$G_D^{(0)}(r; k) = -\frac{i}{4} \left( \frac{k}{2\pi r} \right)^{D/2-1} H_{\frac{D}{2}-1}^{(1)}(kr) \quad (6.37)$$

where  $H^{(1)}$  is the Hankel function of the first kind. From Eq. 6.36, poles are identified as bound states for the  $D$ -dimensional problem, and dimensional regularization eventually gives a bound-state energy for  $D = 2$ .

We gave a scant outline of this calculation to show how the path-integral approach, combined with a regularization scheme can solve the bound-state problem, and because it shows that *the Jacobian did not alone break the symmetry*—if it had anything to do with the symmetry breaking at all! It was entirely the dimensional regularization process that broke scale symmetry by forcing a bound state on the problem.

## 6.6 The Classical Problem

If anomalies are about the breaking of symmetries in the transition from the classical to the quantum picture, then it is worth investigating the classical picture on its own. As we showed in Chapter 4, a scale-symmetric potential such as the 2D  $\delta$  should have  $D = \frac{1}{2}px - tH$  conserved. Let's see if a classical regularization of the 2D  $\delta$  keeps  $D$  constant in time. We use the finite-well regularization  $V_{g,a}(r) = -g\theta(a - r)$  and consider for simplicity the case where a particle is on a trajectory to cross through the center of the well. This is essentially a one-dimensional problem, since in classical mechanics a particle moving in a straight line embedded in the plane is the same as just moving along a line. (The two-dimensional nature of the  $\delta$  potential comes in when we take the limit of the finite well with  $ga^2$  constant, as is appropriate for the 2D case.) Assuming  $a < 1$ , we can take the particle's trajectory  $x(t)$  to have initial position  $x(0) = -1$  and initial velocity  $p_0/m$ . It is straightforward to produce a piecewise expression for the particle's trajectory  $x(t)$ , as it is a free particle everywhere except for a kinetic-energy jump at  $-a$  and a dip at  $a$ , i.e. a change in momentum from  $p_0$  to  $\sqrt{p_0^2 + 2mg}$  and back to  $p_0$ . Letting  $t^{(1)} = \frac{m(1-a)}{p_0}$  and  $t^{(2)} = t^{(1)} + \frac{2ma}{\sqrt{p_0^2 + 2mg}}$  be the times at which the particle passes through the first and second edges of the well, respectively, we have

$$x(t) = \begin{cases} -1 + \frac{p_0}{m}t & t < t^{(1)} \\ -a + \frac{1}{m}\sqrt{p_0^2 + 2mg}(t - t^{(1)}) & t^{(1)} \leq t \leq t^{(2)} \\ a + \frac{p_0}{m}(t - t^{(2)}) & t > t^{(2)} \end{cases} \quad (6.38)$$

We are interested in how  $D$  varies with time. Since a constant potential is scale invariant,  $D$  should be piecewise conserved. Therefore we expect there to be discontinuities in  $D$  at  $t^{(1)}$  and  $t^{(2)}$ , but otherwise it should be constant. Using the fact that  $x$ ,  $t$  and  $H$  are continuous through the jumps at  $t^{(1)}$  and  $t^{(2)}$ , we can show that the discontinuity at  $-a$  is

$$\Delta D(-a) = \frac{1}{2}\sqrt{p_0^2 + 2mg}(-a) - t^{(1)}H - \left(\frac{1}{2}p_0(-a) - t^{(1)}H\right) = \frac{a}{2}\left(p_0 - \sqrt{p_0^2 + 2mg}\right)$$

and, similarly for  $a$ ,

$$\Delta D(a) = \frac{1}{2}p_0(a) - t^{(2)}H - \left(\frac{1}{2}\sqrt{p_0^2 + 2mg}(a) - t^{(2)}H\right) = \frac{a}{2}\left(p_0 - \sqrt{p_0^2 + 2mg}\right)$$

So if we squint and view this finite well as a very small but strong disturbance, as the particle passes through we get a total change in  $D$  of

$$\Delta D = a\left(p_0 - \sqrt{p_0^2 + 2mg}\right) \quad (6.39)$$

If we have a vanishingly thin but infinitely deep well with  $\pi ga^2 = 1$ , i.e. a  $\delta$ -like disturbance in two dimensions, then as  $a \rightarrow 0$ ,  $g \rightarrow \infty$ ,

$$\Delta D \rightarrow -\sqrt{\frac{2m}{\pi}} \quad (6.40)$$

which breaks the scale symmetry, since  $D$  is supposed to be conserved. We have found a failure of scale symmetry in a regularization of a scale-symmetric singular potential within the classical picture, and, ironically, we did so without any sort of limit fudging! Even more ironic, if we fudge the limits in the same way as we did for the quantum finite-well regularization by taking  $ga^2 \rightarrow 0$ , we actually *recover* the scale symmetry because then  $\Delta D \rightarrow 0$ .

These results are very perplexing. Since it obviously was not quantization that broke the scale symmetry, and it wasn't some sort of limit-fudging either, it must have been the

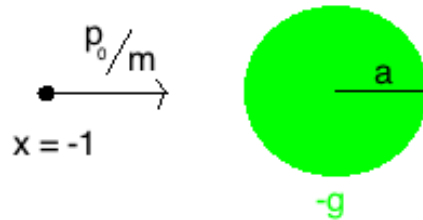


Figure 6.4: A classical particle in the plane with initial position  $x = -1$ ,  $y = 0$  and initial velocity  $\frac{p_0}{m}\hat{i}$  is on course to go through a finite potential well.

regularization process itself—even though this regularization process respects the scale symmetry! (Recall from earlier in Chapter 6 when we showed that the finite-well regularization of the 2D  $\delta$  is scale symmetric as a functional.) It is tough to know what to make of such a “classical anomaly,” except that the derivation of  $D$  as a conserved quantity must break down for singular scale-symmetric potentials and/or regularizations of such potentials.

## 6.7 Interpretation as Anomaly

We studied the 2D  $\delta$  potential more extensively than any other in this thesis, and there is a lot of “data” to work with. Its many pathologies include

1. It is not a “real” function, in the sense that it is equal to 0 almost everywhere but still has an integral of 1. Since the only difference between the  $\delta$  function and 0 is their integrals, to give meaning to  $\delta$  in the Schrödinger equation is difficult.
2. It is a singular potential.
3. Its coupling constant has no units, i.e. it is scale symmetric.

We used a variety of techniques to get around these pathologies in order to solve this potential, that is, to find its spectrum and basic scattering observables. These techniques included position-space regularization, momentum-space regularization, self-adjoint extensions, dimensional regularization, and renormalization of the path-integral formulation.

The common theme with all of these approaches is that, at some point, a renormalization of sorts is required, in which we force the problem to have a bound state and accept whatever consequences that entails: whether we have to fundamentally re-define the potential, impose an arbitrary cutoff on an improper integral, or take a “running-coupling” limit. Of course, such practices are commonplace in quantum field theory, as jarring as it may be to a mathematician, so these are not sufficient reasons to doubt the validity of these calculations. But it does raise the question: what if we take the unrenormalized versions at face value? Is there anything truly “pathological” about a potential having no bound state? Free space has none, after all. Why do we *choose* to use these techniques?

One exception, however, is the method using self-adjoint extensions. No fudging of any kind is required in this approach; we simply calculate using rigorous mathematics the self-adjoint extensions of  $-\frac{d^2}{dx^2}$  on the punctured plane. We started with a very restrictive domain, requiring derivatives of all order to vanish at the origin, which definitely has no bound states because it is strictly smaller than the usual domain for the plane. Then we found that all self-adjoint extensions introduce some bound state, with the bound-state energy a function of the self-adjoint-extension parameter. A tempting interpretation is that the scale symmetry of the  $\delta$  potential holds only if we naively choose a domain whose restrictions are overkill for hermiticity but too stringent for self-adjointness. Then requiring self-adjointness—a purely quantum-mechanical concept absent in classical mechanics—introduces a dimensional parameter to give the problem a bound state and break the scale symmetry. Viewed this way, this potential should be an uncontroversial example of the quantum anomaly.

But this interpretation fails, because *there is no reason to think this extended free-particle Hamiltonian is the  $\delta$  potential*. It is tempting to identify them, because they are both point interactions, and all interesting things happen at the origin. But at no point in the calculation do we ever use the definition of the  $\delta$  function, i.e. the fact that  $\int f(x)\delta(x)dx = f(0)$ .



Every other approach uses this at some point, whether in Fourier-transform integrals or through a finite-well regularization that behaves like the  $\delta$  function in the limit. There is nothing inherently scale-symmetric about point interactions in the plane: the  $\delta$  function is a special case. What this calculation actually produces is the set of all possible self-adjoint—and therefore physical—point interactions in the plane. There is the special extension  $\theta = \pi$ , which corresponds to no bound state, while every other self-adjoint domain has a unique bound state. It does *not* say which, if any, of these self-adjoint versions of the free-particle Hamiltonian ought to correspond to the  $\delta$  potential.

## Chapter 7

# The 1D $\delta'$ Potential

The 1D  $\delta'$  potential is another example of a scale-symmetric potential. A  $\delta$  potential in  $n$  dimensions transforms under re-scaling as  $\delta^n(qx) = q^{-n}\delta^n(x)$  to compensate for the  $n$ -dimensional Jacobian, so

$$\delta'(qx) = \frac{d\delta(x)}{dx}(qx) = \frac{d\delta(qx)}{d(qx)}(x) = \frac{1}{q} \frac{d\delta(x)}{d(qx)}(x) = \frac{1}{q^2} \frac{d\delta}{dx}(x) = \frac{1}{q^2} \delta'(x)$$

where we have abused notation slightly: parentheses just in front of  $\delta$  indicate evaluation before differentiation (so that the chain rule comes in), while parentheses right after a derivative indicate evaluation after differentiation. The key observation, in words, that makes this proof work is that evaluating the derivative of  $\delta$  at the scaled variable  $qx$  is the same as composing multiplication by  $q$  with  $\delta$ , differentiating with respect to  $qx$ , and then evaluating at  $x$ . An alternative way to see that this potential is scale invariant is that  $\int \delta(x)dx = 1$  implies  $\delta(x)$  has dimensions of inverse length, so then  $\frac{d\delta}{dx}$  has dimensions of inverse length squared, requiring that a coupling constant in front have no dimensions.

There is no consensus on how to treat the 1D  $\delta'$  potential in the Schrödinger equation. It is generally agreed that, in the most general setting, one defines the  $\delta'$  function to pick out the *negative* first derivative of a test function in an integral, due to an argument involving integration by parts:

$$\int_{-\infty}^{\infty} f(x)\delta'(x)dx = [f(x)\delta(x)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f'(x)\delta(x)dx = -f'(0)$$

But how to use this in a differential equation is still mysterious. Just as in the 2D  $\delta$

problem, there are a number of approaches for defining its effect in a differential equation.

However, unlike the 2D  $\delta$  potential, the different approaches end up giving mostly different results. In retrospect, it is quite spectacular that the several different means of treating the 2D  $\delta$  potential all ended up agreeing in some way: the position-space cutoff, momentum-space cutoff, and self-adjoint-extension parameter could be found in terms of one another such that they all produced the same bound state. We will not see the same consistency with the 1D  $\delta'$  potential.

## 7.1 Position-Space Regularization

If one believes that the most natural regularization of the  $\delta$  function in position space is the limit of finite wells, then one would agree the most natural treatment of  $\delta'$  is the double- $\delta$  regularization, as these regularizing potentials for  $\delta'$  are the derivatives of the corresponding finite wells for  $\delta$ , as demonstrated in Eq. 7.1.

$$\frac{d}{dx} [g (\theta(x - a) - \theta(x + a))] = g (\delta(x - a) - \delta(x + a)) \quad (7.1)$$

So we define  $V_{g,a} = g (\delta(x - a) - \delta(x + a))$ . Each  $\delta$  function enforces a boundary condition on the derivative of  $\psi$  at  $a$  and  $-a$ , which we can derive by directly integrating the Schrödinger equation from  $\pm a - \epsilon$  to  $\pm a + \epsilon$  for small  $\epsilon$ . The result is

$$\left[ \frac{\partial \psi}{\partial x} \right]_{\pm a^-}^{\pm a^+} = \pm g \psi(\pm a) \quad (7.2)$$

Enforcing continuity of  $\psi$  and this particular discontinuity of  $\psi'$  at  $a$  and  $-a$  gives four boundary conditions on energy eigenstates. Square integrability requires that the solutions be of the form

$$\psi(x) = \begin{cases} Ae^{\rho x} & \text{if } x < -a \\ Be^{\rho x} + Ce^{-\rho x} & \text{if } -a < x < a \\ De^{-\rho x} & \text{if } x > a \end{cases} \quad (7.3)$$

where  $\rho = \sqrt{-E}$ . Applying the boundary conditions leads to the following transcendental equation for the energy  $\rho$  (details in Appendix A):

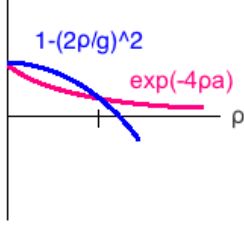


Figure 7.1: Plotting  $1 - \left(\frac{2\rho}{g}\right)^2$  and  $e^{-4\rho a}$  as functions of  $\rho$  for fixed  $a$  and  $g$  demonstrates graphically that there is a unique bound state.

$$1 - \left(\frac{2\rho}{g}\right)^2 = e^{-4\rho a} \quad (7.4)$$

We can visualize the energy solutions as intersection points of  $1 - \left(\frac{2\rho}{g}\right)^2$  and  $e^{-4\rho a}$ . Figure 7.1 includes a rough sketch of the solution. We see that there is a unique intersection for  $\rho > 0$ , but also a “stupid” solution at  $\rho = 0$ , which is explained in Appendix A. As  $g \rightarrow \infty$ , the blue curve, a parabola, gets wider and wider, pushing  $\rho$  to infinity. But simultaneously,  $a \rightarrow 0$  causes the pink curve to look more like a flat line, pushing  $\rho$  to 0.

To determine where  $\rho$  ends up in the limit, let’s assume it converges to something finite by fixing  $\rho = \rho_{bs}$  and look at small- $a$  behavior:

$$1 - \left(\frac{2\rho}{g}\right)^2 = e^{-4\rho a} = 1 - 4\rho a + O[a^2] \implies \rho = g^2 a + O[g^2 a^2]$$

As long as  $g^2 a$  is bounded and  $O[g^2 a^2] \rightarrow 0$  as  $a \rightarrow 0$ ,  $g \rightarrow \infty$ , we have a bound state for the  $\delta'$  potential. Both of these criteria are satisfied by taking the limit with  $g^2 a$  constant, since it implies  $O[g^2 a^2] = O[a] \rightarrow 0$ . Thus we have a bound-state energy  $\rho_{bs} = g^2 a$ . In the limit, the  $-a < x < a$  component of the wave function becomes irrelevant, so to find the corresponding bound state we find how  $A$  relates to  $D$ . It is shown in Appendix A that, in the limit where  $ga \rightarrow 0$ , we get  $A = D$ , and so the bound state is that of the 1D  $\delta$  function: a positive decaying exponential on each side, joining at a cusp at the origin. Normalization must dictate the value of  $A$  in terms of the decay constant/bound-state energy  $\rho$  the same way in each case. The difference between the two cases is that the 1D  $\delta'$  bound-state energy

is set by the renormalization parameter  $\rho_{bs}$ , while the 1D  $\delta$  bound-state energy is set by the dimensional coupling.

NB: It may be tempting it is to predict a  $\delta'$  bound state as having odd parity, i.e.  $A = -D$ , because the potential itself is odd, but there is in fact no reason to predict an odd bound-state wave function. The sign of the potential has bearing on the concavity of its eigenstates, not their sign. A smooth, odd potential would have no parity symmetry because on one side we would have decay and on the other we'd have oscillations.

Back on topic, the main takeaway from this calculation is that we have broken scale symmetry by introducing a bound state! However, the natural way to take the limit keeps  $ga$ , rather than  $g^2a$ , constant, for  $ga$  is the area of a finite well, which should not vanish in the limit, or else the integral of the  $\delta$  function is zero. This regularization is ultimately motivated by the finite-well regularization of the  $\delta$  function, so we should be consistent in how we take our limits. More directly, we can see that the  $ga$ -constant limit is correct by observing how this regularization acts on a test function in an integral:

$$\begin{aligned} \int_{-\epsilon}^{\epsilon} g (\delta(x-a) - \delta(x+a)) f(x) dx &= g (f(a) - f(-a)) = ga \left( \frac{f(a) - f(-a)}{a} \right) \\ &= ga \left( \frac{f(a) - f(0) + f(0) - f(-a)}{a} \right) = ga \left( \frac{f(a) - f(0)}{a} - \frac{f(-a) - f(0)}{a} \right) \\ &= ga \left( \frac{f(a) - f(0)}{a} + \frac{f(-a) - f(0)}{(-a)} \right) \rightarrow ga (f'(0) + f'(0)) = 2ga f'(0) \end{aligned}$$

Thus  $ga$  is constant, specifically  $ga = 1/2$ , which is not surprising since the width of the well is  $2a$ . Since we started by looking at the attractive  $\delta$  potential, which we wrote as  $-g\delta$  for  $g > 0$ , its derivative  $-g\delta'$  picks out the *positive* (negative-negative) derivative of a test function.

To get a bound state, then, we have to change our mind about the regularization scheme after the fact. We had a similar situation with the position-space regularization of the 2D  $\delta$  potential: the scale symmetry is quite directly broken by changing the regularization with the explicit purpose of producing a bound state.

The scattering problem goes similarly. The canonical approach to the problem has an incoming wave from the left, a reflected wave to the left, a transmitted wave to the right,

and any kind of constant-positive-energy oscillations in the middle:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x < -a \\ Ce^{ikx} + De^{-ikx} & \text{if } -a < x < a \\ Fe^{ikx} & \text{if } x > a \end{cases} \quad (7.5)$$

where  $k = \sqrt{E}$ . We apply the same boundary conditions as in the bound-state problem and find the phase shift by computing the complex argument  $\phi$  of  $F/A$ . Leaving the details to Appendix A, the result is

$$\tan(\phi) = \frac{g^2 a}{k} \frac{1}{\frac{ga}{2} + 1} \rightarrow \frac{\rho_{bs}}{k} \text{ in the } ga \rightarrow 0 \text{ limit}$$

which is another signature of an anomaly: an energy dependence in the phase shift. The more significant the bound-state energy is relative to the energy of the scattered particles, the greater the phase shift. Of course, if we take the sensible  $ga$ -constant limit,  $g^2 a \rightarrow \infty \implies \tan(\phi) \rightarrow \infty \implies \phi \rightarrow 0$ , which is independent of energy. So the anomalous behavior crucially depends on the renormalization process.

## 7.2 Momentum-Space Regularization

We can use the same momentum-space method as applied in the 2D  $\delta$  case by Holstein. For the bound-state problem, the Schrödinger equation starts as

$$-\frac{d^2}{dx^2}\psi(x) - g\delta'(x)\psi(x) = -k^2\psi(x) \quad (7.6)$$

and, upon taking the Fourier transform of both sides, can be rewritten as

$$p^2\phi(p) - g \int_{-\infty}^{\infty} \psi(x)e^{-ipx}\delta'(x)dx = -k^2\phi(p) \quad (7.7)$$

The  $\delta'$  function in the integral picks out the negative derivative of  $\psi(x)e^{-ipx}$  at 0, so our momentum-space equation is

$$(p^2 + k^2)\phi(p) = g(ip\psi(0) - \psi'(0)) \quad (7.8)$$

Rearranging and taking the inverse Fourier transform of both sides gives

$$\psi(x) = \frac{g}{2\pi} \left( i\psi(0) \int_{-\infty}^{\infty} \frac{pe^{ipx}}{p^2 + k^2} dp - \psi'(0) \int_{-\infty}^{\infty} \frac{e^{ipx}}{p^2 + k^2} dp \right) \quad (7.9)$$

It is useful to give these integrals names,  $I_1(x) = \int_{-\infty}^{\infty} \frac{pe^{ipx}}{p^2 + k^2} dp$  and  $I_2(x) = \int_{-\infty}^{\infty} \frac{e^{ipx}}{p^2 + k^2} dp$  so that Eq. 7.9 reads more easily as

$$\psi(x) = \frac{g}{2\pi} (i\psi(0)I_1(x) - \psi'(0)I_2(x)) \quad (7.10)$$

In the 1D and 2D  $\delta$  problems, we quantized energy by demanding consistency of  $\psi(0)$  in this equation, but here we must also do the same for  $\psi'(0)$ . It is tempting to differentiate under the integral sign to get an expression for  $\psi'$ , but we can actually just solve for  $I_1(x)$  and  $I_2(x)$  and take the derivative afterwards.  $I_2(x)$  is solved in Section 6.2.1, and  $I_1(x)$  is a similarly straightforward contour integral. We use the same contour for the  $x > 0$  case to find

$$I_1(x) = 2\pi i \frac{(ik)e^{-kx}}{2ik} = i\pi e^{-kx} \quad (7.11)$$

A simple argument shows that  $I_1(x)$  must be odd:

$$\begin{aligned} I_1(-x) &= \int_{-\infty}^{\infty} \frac{pe^{ip(-x)}}{p^2 + k^2} dp = \int_{-\infty}^{\infty} \frac{pe^{i(-p)x}}{p^2 + k^2} dp = \int_{\infty}^{-\infty} \frac{-(-p)e^{i(-p)x}}{(-p)^2 + k^2} (-d(-p)) \\ &= - \int_{-\infty}^{\infty} \frac{(-p)e^{i(-p)x}}{(-p)^2 + k^2} d(-p) = -I_1(x) \end{aligned}$$

which gives us the case  $x < 0$ . And for  $x = 0$ , the observation that the integrand is odd in  $p$  tells us that (the principal value of)  $I_1(x)$  is 0. Then we have

$$I_1(x) = \text{sign}(x)i\pi e^{-k|x|} \quad (7.12)$$

$$I_2(x) = \frac{\pi}{k} e^{-k|x|} \quad (7.13)$$

where  $\text{sign}(0) = 0$ . Note that  $I_2$  is sharp at the origin and  $I_1$  is discontinuous, but it still makes sense to interpret  $I_1(0)$  and  $I_2(0)$  as the averages of their left- and right-hand limits. Now we have an explicit expression

$$\psi(x) = -\frac{g}{2} \left( \psi(0)\text{sign}(x) + \psi'(0)\frac{1}{k} \right) e^{-k|x|} \quad (7.14)$$

for  $\psi$ . It must, however, be well-defined for  $\psi(0)$  and  $\psi'(0)$ . Plugging in  $x = 0$ , we have

$$\psi(0) = -\frac{g}{2k}\psi'(0) \quad (7.15)$$

Meanwhile, we can differentiate Eq. 7.14

$$\psi'(x) = \frac{g}{2} (k\psi(0) + \psi'(0)\text{sign}(x)) e^{-k|x|} \quad (7.16)$$

by observing that  $e^{-k|x|} = e^{-k\text{sign}(x)x}$ . Then plugging in  $x = 0$  yields our second consistency condition

$$\psi'(0) = k\frac{g}{2}\psi(0) \quad (7.17)$$

However, when we combine this with our first condition Eq. 7.15, the  $k$  drops out, so we don't get a quantization condition on  $k$ . We should have expected this failure all along, as  $k$  is a dimensional quantity (with dimensions of inverse length) while the coupling  $g$  is unitless in the  $\delta'$  case, unlike in the  $\delta$  case where  $k_{bs}$  inherits its units from the dimensional coupling. As usual when dealing with scale-symmetric potentials, renormalization is required to fix this problem, but unlike previous cases, *there doesn't seem to be an obvious way to renormalize*. There is no divergent integral we can cut off, no finite regularization whose limiting behavior we can fudge—just a pair of boundary conditions on our bound state that are impossible to satisfy regardless of  $k$ .

The scattering problem has a similarly boring outcome. The calculation starts out the same except for using  $+k^2$  as our eigenvalue in the Schrödinger equation.

$$-\frac{d^2}{dx^2}\psi(x) - g\delta'(x)\psi(x) = k^2\psi(x) \quad (7.18)$$

We perform the same manipulations as before and add in an incoming plane wave as a reference for calculating the phase shift.



$$\psi(x) = e^{ikx} + \frac{g}{2\pi} \left( i\psi(0) \int_{-\infty}^{\infty} \frac{pe^{ipx}}{p^2 - k^2 - i\epsilon} dp - \psi'(0) \int_{-\infty}^{\infty} \frac{e^{ipx}}{p^2 - k^2 - i\epsilon} dp \right) \quad (7.19)$$

We have also replaced  $k^2$  with  $k^2 + i\epsilon$  for small  $\epsilon > 0$  to move the poles off the real axis. Thus we are effectively taking the principal values of these integrals, which without these adjustments would be, strictly speaking, not integrable. But recall from Chapter 6 that this is necessary (and unproblematic) even for well-understood point interactions like the 1D  $\delta$ —this is not some trick for renormalizing the coupling. Anyway, the method for solving these integrals is essentially the same as that for solving  $I_1$  and  $I_2$  from the bound-state problem, as we still have exactly one pole  $\sqrt{k^2 + i\epsilon}$  in the upper-half plane. The result is

$$\psi(x) = e^{ikx} - \frac{g}{2} \left( \psi(0)\text{sign}(x) + i\psi'(0)\frac{1}{k} \right) e^{ik|x|} \quad (7.20)$$

We are close to finding the phase shift, but we must first find the values of  $\psi(0)$  and  $\psi'(0)$ . Following the same steps as in the bound-state problem, we find

$$\psi(0) = 1 - \frac{g}{2k} i\psi'(0) \quad (7.21)$$

$$\psi'(0) = ik \left( 1 - \frac{g}{2} \psi(0) \right) \quad (7.22)$$

which is an inhomogeneous  $2 \times 2$  system that can be easily inverted to find

$$\psi(0) = \frac{1 + g/2}{1 + g^2/4} \quad (7.23)$$

$$\psi'(0) = \frac{ik(1 - g/2)}{1 + g^2/4} \quad (7.24)$$

Then we have, as our final scattering solution,

$$\psi(x) = e^{ikx} - \frac{g}{2(1 + g^2/4)} [(1 + g/2)\text{sign}(x) - (1 - g/2)] e^{ik|x|} \quad (7.25)$$

The canonical form for a 1D scattering problem features an incoming wave, a reflected wave, and a transmitted wave. We can identify these components in Eq. 7.25 since for  $x < 0$ , the only right-going part is  $e^{ikx}$ , while for  $x > 0$ ,  $e^{ik|x|} = e^{ikx}$  and so the whole expression

represents a right-going wave. Thus the ratio of the transmitted coefficient to the incoming coefficient is

$$\frac{1 - g^2/4}{1 + g^2/4} \in \mathbb{R} \quad (7.26)$$

This is real regardless of  $g$ , so the corresponding phase shift is 0. Again, we should be unsurprised by this result, for there is no dimensional parameter to reference the energy dependence in a dimensionless phase shift. Some sort of renormalization must be necessary, yet again there was not much of an opportunity to renormalize the problem.

That is, unless we change our mind about our decision to not differentiate under the integral sign. It is mathematically speaking correct to not do so in this case (which we know because it does not give the same answer), but some authors have done so [24], perhaps to find a regularization procedure, or perhaps because it was a mistake. Starting at Eq. 7.6 in the bound-state problem, we can check for the consistency of  $\psi'(0)$ , if we differentiate  $I_1$  and  $I_2$  under the integral sign, then our expression for  $\psi'(x)$  becomes

$$\psi'(x) = -\frac{g}{2\pi} \left( \psi(0) \int_{-\infty}^{\infty} \frac{p^2 e^{ipx}}{p^2 + k^2} dp + i\psi'(0) \int_{-\infty}^{\infty} \frac{p e^{ipx}}{p^2 + k^2} dp \right) \quad (7.27)$$

We know how to deal with the second integral, but the first is difficult to solve with contour methods. Fortunately, we only need its behavior at  $x = 0$  to check  $\psi'(0)$ . Plugging in  $x = 0$  reduces the expression to

$$\psi'(0) = \frac{g\psi(0)}{2\pi} \int_{-\infty}^{\infty} \frac{p^2}{p^2 + k^2} dp = \frac{g\psi(0)}{2\pi} [p - k \tan^{-1}(p/k)]_{-\infty}^{\infty}$$

by a simple trigonometric substitution. Of course, this integral blows up when you plug in the bounds, as expected since the integrand approaches 1. This gives us an opportunity to renormalize by taking a large-momentum cutoff  $\Lambda$ .

$$\psi'(0) = \psi(0) \frac{g}{\pi} (\Lambda - k \tan^{-1}(\Lambda/k)) \quad (7.28)$$

Combining with Eq. 7.15, we get a condition on  $k$  in terms of the dimensioned renormalization parameter  $\Lambda$ :

$$\tan^{-1}\left(\frac{\Lambda}{k}\right) = \frac{\Lambda}{k} + \frac{2\pi}{g^2} \quad (7.29)$$

Unfortunately, this has no solution for positive  $k$  and  $\Lambda$ , as is apparent from a quick sketch of the LHS and RHS as functions of  $\Lambda/k$ . It is unclear how exactly to interpret this calculation. If we allow  $k$  to be negative, then we get a unique bound-state energy of  $-k^2$  (which is still negative). If we allow  $\Lambda/k$  to intersect any branch of  $\tan^{-1}\left(\frac{\Lambda}{k}\right)$ , then we get infinite discrete energies all the way down to  $-\infty$ . None of these options is particularly appealing from a physical point of view, so we reject this form of renormalization, which began with questionable mathematics anyway.

### 7.3 Griffiths Method

A point interaction like  $\delta$  or  $\delta'$  is no more and no less than a boundary condition on the free-particle Hamiltonian at a particular point. In Ref. [6], David Griffiths shows a method of deriving the boundary condition for a point potential of the form  $\delta^n(x)$ , where the  $n$  indicates the  $n$ th derivative (not the  $n$ -dimensional  $\delta$  function). This method is only applicable in one dimension, hence we did not use it for the 2D  $\delta$ .

We present the derivation for  $n = 1$ , i.e. for the  $\delta'$  potential. It begins with the Schrödinger equation

$$-\frac{d^2}{dx^2}\psi(x) + g\delta'(x)\psi(x) = E\psi(x) \quad (7.30)$$

We integrate both sides from  $-\epsilon$  to  $\epsilon$  and find

$$-(\psi'(0^+) - \psi'(0^-)) - g\psi'(0) = 0 \quad (7.31)$$

so the first boundary condition we derive is that

$$\psi'(0^+) - \psi'(0^-) = -g\psi'(0) \quad (7.32)$$

where we interpret  $\psi'(0)$  to be the average of the left- and right-hand limits,  $\frac{1}{2}(\psi'(0^+) + \psi'(0^-))$ . There is in fact a way to squeeze a *second* boundary condition out of the Schrödinger

equation by integrating it twice. The first time, we integrate from some fixed  $-L < 0$  to an arbitrary  $x$ :

$$-(\psi'(x) - \psi'(-L)) + g \int_{-L}^x \delta'(x')\psi(x')dx' = E \int_{-L}^x \psi(x')dx' \quad (7.33)$$

The  $\delta'$  integral must be treated slightly differently than how we did at the beginning of the chapter. The boundary terms in the integration by parts no longer vanish, because we plan on integrating with respect to  $x$  later.

$$\int_{-L}^x \delta'(x')\psi(x')dx' = [\delta(x')\psi(x')]_{-L}^x - \int_{-L}^x \delta(x')\psi'(x')dx' = \delta(x)\psi(x) - \theta(x)\psi'(0)$$

The Heaviside step function appears because the integral returns  $\psi'(0)$  if and only if the interval  $[-L, x]$  includes 0. Then integrating Eq. 7.33 with respect to  $x$  from  $-\epsilon$  to  $\epsilon$  yields

$$-(\psi(0^+) - \psi(0^-)) + g(\psi(0) + 0) = 0 \quad (7.34)$$

since  $\theta(x)$  and  $\int_{-L}^x \psi(x')dx'$  have continuous antiderivatives. So our final boundary condition is

$$\psi(0^+) - \psi(0^-) = g\psi(0) \quad (7.35)$$

Intuitively, we can already see how these boundary conditions will not lead to a bound state. If either  $\psi$  or  $\psi'$  is continuous at origin, it must in fact be 0 at the origin. All of the solutions to  $-\frac{d^2}{dx^2}$  on  $\mathbb{R} \setminus \{0\}$  are spanned by  $e^{-k|x|}$  and  $\frac{x}{|x|}e^{-k|x|}$  where  $k = \sqrt{-E}$ , and neither of these two solutions satisfies either condition. However, some linear superposition could conceivably work, so we will go ahead and prove formally that there is no bound state. Any bound state would have to be of the form

$$\psi(x) = \begin{cases} Ae^{kx} & x < 0 \\ Be^{-kx} & x > 0 \end{cases} \quad (7.36)$$

Applying the two boundary conditions leads to the following equations:

$$-kB - kA = -g\frac{1}{2}(-kB + kA) \quad (7.37)$$

$$B - A = g\frac{1}{2}(B + A) \quad (7.38)$$

which, upon simplification and transforming into a matrix equation, becomes

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} k(g/2 - 1) & -k(g/2 + 1) \\ g/2 + 1 & g/2 - 1 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \quad (7.39)$$

The matrix has determinant  $k(g/2 - 1)^2 + k(g/2 + 1)^2 = k[(g/2 - 1)^2 + (g/2 + 1)^2] > 0$ . So the matrix is invertible, and thus the only solution to this system is  $A = B = 0$ , which is not a physical solution.

The scattering problem doesn't go any better for the anomaly fans. Now with  $E > 0$  and  $k = \sqrt{E}$ , any solution must be of the form

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ikx} & x > 0 \end{cases} \quad (7.40)$$

representing incoming, reflected, and transmitted waves. The  $\delta'$  boundary conditions manifest themselves as

$$ikC - ikA + ikB = -g\frac{1}{2}(ikA - ikB + ikC) \quad (7.41)$$

$$C - A - B = g\frac{1}{2}(A + B + C) \quad (7.42)$$

It is straightforward to solve these equations for  $C/A$ :

$$\frac{C}{A} = \frac{1 - g^2/4}{1 + g^2/4} \in \mathbb{R} \quad (7.43)$$

So the phase shift is a constant 0, which is of course independent of energy. Note that we got the same phase shift as in the momentum-space approach without renormalization. So we have found two distinct methods for solving the potential that give the same result: no bound state and a transmission coefficient of  $\frac{1-g^2/4}{1+g^2/4}$ . That's a first for the  $\delta'$ ! One definition of the anomaly is a breaking of symmetry through *any* possible renormalization scheme, and we have found two different approaches for deriving the same spectrum and scattering phase shift that don't even require renormalization. Thus we have evidence that perhaps the 1D  $\delta'$  is not, in fact, anomalous.

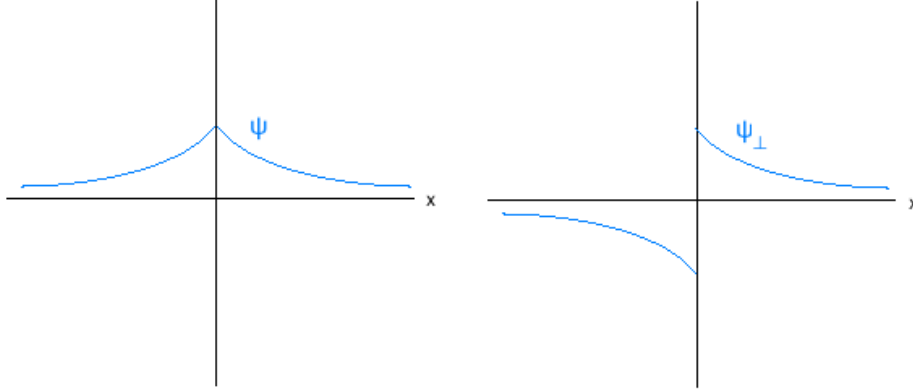


Figure 7.2: If  $\psi$  is an eigenstate of some linear operator separately on  $\mathbb{R}_{>0}$  and  $\mathbb{R}_{<0}$ , then  $-\psi$  is on  $\mathbb{R}_{<0}$  by linearity, so  $\psi_{\perp}$  is also an eigenstate. And clearly  $\psi \perp \psi_{\perp}$ .

## 7.4 Self-Adjoint Extensions

The real line has a crucial topological difference from the plane in that removing a single point breaks it into two connected components, while the plane remains connected [1]. For  $\mathbb{R}^2$ , since wave functions are required to be continuous, wave function behavior on one side of the origin must be related to wave function behavior on the other, despite the puncture. Conversely, for  $\mathbb{R}$ , the two connected pieces  $\mathbb{R}_{>0}$  and  $\mathbb{R}_{<0}$  can vary independently, allowing for the creation of an orthogonal eigenstate for any given eigenstate by reflecting half the wave function across the x-axis. Another way of thinking about this peculiarity of  $\mathbb{R} \setminus \{0\}$  is that a physical state can be identically 0 on half of the line while still being normalizable.

Let's examine the hermiticity of the free-particle Hamiltonian  $H = -\frac{d^2}{dx^2}$  on the punctured line for arbitrary boundary conditions at 0.

$$\begin{aligned}
 (\phi, H\psi) &= - \int_{-\infty}^{\infty} \bar{\phi} \psi'' dx = - \left( \int_{-\infty}^0 \bar{\phi} \psi'' dx + \int_0^{\infty} \bar{\phi} \psi'' dx \right) \\
 &= - [\bar{\phi} \psi']_{-\infty}^{0^-} - [\bar{\phi} \psi']_{0^+}^{\infty} + \int_{-\infty}^0 \bar{\phi}' \psi' dx + \int_0^{\infty} \bar{\phi}' \psi' dx \\
 &= [\bar{\phi}' \psi]_{-\infty}^{0^-} + [\bar{\phi}' \psi]_{0^+}^{\infty} - [\bar{\phi} \psi']_{-\infty}^{0^-} - [\bar{\phi} \psi']_{0^+}^{\infty} + (H\phi, \psi) \\
 &= [\bar{\phi} \psi' - \bar{\phi}' \psi]_{0^-}^{0^+} + (H\phi, \psi)
 \end{aligned}$$

To find a self-adjoint boundary condition, we need to choose a domain such that the boundary term  $[\overline{\phi}\psi' - \overline{\phi}'\psi]_{0^-}^{0^+}$  vanishes if and only if  $\phi$  and  $\psi$  are in that domain. As we will see, the space of such self-adjoint domains is parameterized by  $U(2)$  in this case instead of  $U(1)$ , so finding a fully general answer by hand is difficult—and wouldn't be particularly illuminating, for as we saw in the 2D  $\delta$  case, there is still no way to decide which self-adjoint extensions correspond to which point interactions. But we can verify that the 1D  $\delta$  and  $\delta'$  boundary conditions we derived earlier are in fact self-adjoint boundary conditions.

#### 7.4.1 Self-Adjointness of 1D $\delta$

It is non-controversial that the  $\delta$  potential  $V(x) = g\delta(x)$  enforces  $f(0^+) = f(0^-)$  and  $f'(0^+) - f'(0^-) = gf(0)$ . Let's call the domain of functions satisfying this boundary condition  $D(H)$ . The first half of the proof requires showing that the boundary term vanishes when we assume both  $\phi$  and  $\psi$  are in  $D(H)$ .

$$\begin{aligned} [\overline{\phi}\psi' - \overline{\phi}'\psi]_{0^-}^{0^+} &= \overline{\phi}(0)\psi'(0^+) - \overline{\phi}'(0^+)\psi(0) - \overline{\phi}(0)\psi'(0^-) + \overline{\phi}'(0^-)\psi(0) \\ &= \overline{\phi}(0) (\psi'(0^+) - \psi'(0^-)) - \psi(0) (\overline{\phi}'(0^+) - \overline{\phi}'(0^-)) \\ &= \overline{\phi}(0) (g\psi(0)) - \psi(0) (g\overline{\phi}(0)) = 0 \end{aligned}$$

We just showed that the free-particle Hamiltonian is hermitian on  $D(H)$ , but to show that it is self-adjoint requires proving that the adjoint domain  $D(H^*)$  is no larger than  $D(H)$ . So assuming  $\psi \in D(H)$ , we want to show that the boundary term vanishing forces  $\phi$  to also be in  $D(H)$ . Performing similar manipulations, using  $[\overline{\phi}\psi' - \overline{\phi}'\psi]_{0^-}^{0^+} = 0$  but *not* using  $\phi \in D(H)$ , we arrive at

$$\psi(0) (\overline{\phi}'(0^+) - \overline{\phi}'(0^-) - g\overline{\phi}(0^+)) = \psi'(0^-) (\overline{\phi}(0^+) - \overline{\phi}(0^-))$$

But since this must hold for arbitrary  $\psi \in D(H)$ , the only way for this equation to hold is for each side to be 0—otherwise we could choose a  $\psi \in D(H)$  with different behavior at the origin to break the equation that worked for a particular  $\phi \in D(H^*)$ . Then  $\overline{\phi}(0^+) = \overline{\phi}(0^-)$ ,

and  $\bar{\phi}'(0^+) - \bar{\phi}'(0^-) = g\bar{\phi}(0)$ , so  $\phi \in D(H)$ . So  $D(H) = D(H^*)$ , i.e.  $H$  is self-adjoint with the  $\delta$  boundary condition.

#### 7.4.2 Self-Adjointness of 1D $\delta'$

We also verify that the 1D  $\delta'$  domain we derived earlier (via the Griffiths method) is self-adjoint. To make the derivation a little more readable, we're going to relabel the eight different quantities in the boundary term with capital letters:

$$\bar{\phi}(0^+)\psi'(0^+) - \bar{\phi}'(0^+)\psi(0^+) - \bar{\phi}(0^-)\psi'(0^-) + \bar{\phi}'(0^-)\psi(0^-) = AG - CE - BH + DF$$

Then the  $\delta'$  boundary conditions manifest themselves as

$$\begin{aligned} A - B &= \frac{g}{2}(A + B) \\ C - D &= \frac{g}{2}(C + D) \\ E - F &= \frac{g}{2}(E + F) \\ G - H &= \frac{g}{2}(G + H) \end{aligned}$$

which we can apply to the boundary term

$$\begin{aligned} AG - CE - BH + DF &= AG - BG + BG - BH + DF - CF + CF - CE \\ &= G(A - B) + B(G - H) + F(D - C) + C(F - E) \\ &= \frac{g}{2} [G(A + B) - B(G + H) + F(C + D) - C(E + F)] \\ &= \frac{g}{2} (AG - CE - BH + DF) \end{aligned}$$

If  $g \neq 2$ , we must have  $AG - CE - BH + DF = 0$ , but in the case that  $g = 2$ , we can, instead of subtracting and adding  $BH$  and  $CF$ , subtract and add  $AH$  and  $DE$  to effectively tack on a minus sign to the RHS of the first line. Thus we have proved one direction of



self-adjointness. Without going through a similarly tedious proof, we can see the other direction must hold because, just as in the  $\delta$  case, we only “barely” got the boundary terms to equal 0, and it required using symmetric boundary conditions on  $\psi$  and  $\phi$ .

### 7.4.3 Deficiency Subspaces

Another consequence of the punctured line’s topology is that the imaginary eigenvalue equations of the free-particle Hamiltonian give deficiency indices of  $\langle 2, 2 \rangle$ . In particular, the positive- $i$  equation is

$$\frac{-d^2\psi}{dx^2} = i\psi \tag{7.44}$$

and has an orthogonal pair of  $L^2$  solutions

$$\begin{aligned} \psi_1^+(x) &= e^{q|x|} \\ \psi_2^+(x) &= \text{sign}(x)e^{q|x|} \end{aligned}$$

with  $q = \frac{-1+i}{\sqrt{2}}$ . (We choose this particular pair because it gives us a nice simplification later.) Similarly, the eigenvalue equation for  $-i$  has solutions

$$\begin{aligned} \psi_1^-(x) &= e^{\bar{q}|x|} \\ \psi_2^-(x) &= \text{sign}(x)e^{\bar{q}|x|} \end{aligned}$$

Choosing these as our bases for  $N_+$  and  $N_-$ , a unitary transformation  $\mathcal{U} : N_+ \rightarrow N_-$  represented by a unitary matrix

$$U = e^{i\omega} \begin{pmatrix} A & B \\ -\bar{B} & \bar{A} \end{pmatrix}, \text{ with } \omega \in [0, \pi), |A|^2 + |B|^2 = 1$$

sends an arbitrary state  $\alpha\psi_1^+ + \beta\psi_2^+$  of  $N_+$  to  $e^{i\omega} [(A\alpha + B\beta)\psi_1^- + (-\bar{B}\alpha + \bar{A}\beta)\psi_2^-]$  of  $N_-$ . The coefficients on  $\psi_1^-$  and  $\psi_2^-$  are just the results of the matrix multiplication  $U \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ , where  $\alpha$  and  $\beta$  are arbitrary complex coefficients parameterizing an element of  $N_+$ . Note that although  $\psi_{1,2}^\pm$  are not normalized, they all have the same norm  $\sqrt{2}$  and so  $U$  as written still

represents a unitary transformation. By examining how these functions and their derivatives behave on either side of the origin in terms of  $U$ , we can derive the fully general set of self-adjoint boundary conditions. However, to do so is very tedious, and not particularly enlightening since we already showed by hand that the point interactions we care about are in fact self-adjoint. We leave it to Appendix *B*.

## 7.5 Interpretation

The different approaches to the  $\delta'$  potential are not in as firm agreement as for the 2D  $\delta$ , but the Griffiths boundary condition and momentum-space approach give the exact same transmission coefficients. Perhaps renormalization is not, then, necessary to give a well-defined, physically sensible answer to the problem, even if it does not include a bound state. This potential may be an example of what we asked about in the introduction: a potential whose scale symmetry does *not* break under quantization/renormalization.

## Chapter 8

# Applications and Conclusion

There are two broad classes of applications this type of work can have: theoretical and experimental. The theoretical application of these quantum mechanical calculations usually lies in their function as approximations to or analogies for similar problems/concepts in quantum field theory. But there are experimental applications as well, for we are ultimately solving pathological quantum mechanical potentials, which in some cases can have a physical, experimental realization. Solving these potentials amounts to finding their spectra, which is of course experimentally relevant.

### 8.1 Theoretical Applications

Quantum mechanical anomalies are of interest to theorists because of the importance of the anomaly in quantum field theory. Quantum mechanics can serve as a simplifying approximation to quantum field theories, which are often rife with technical difficulties due to the need for perturbative methods even in problems that would be straightforward in quantum mechanics [21]. To find a bound state even of a simple quantum field theory is extremely difficult, and studying how renormalization allows a bound-state sector to emerge in quantum mechanics can give some insight into how it ought to work in quantum field theory. Camblong advocates for an approach involving path integrals, which, though cumbersome to work with computationally, can capture the non-perturbative nature of bound states in quantum field theory [20], [21].

We also lump pedagogical purposes into this category. Given how important renormalization and anomalies are in quantum field theory, it is crucial to help advanced undergrad-

uates build their intuition for these concepts. However, to do so in the context of quantum field theory is too difficult, and the same ideas are fairly translatable into quantum mechanics. Holstein strongly advocates studying quantum mechanical anomalies for this very reason.

## 8.2 Experimental Applications

The three potentials we studied were presented roughly in descending order of experimental relevance. The 3D isotropic  $1/r^2$  potential may be said to be unphysical, but it captures the radial behavior of an ideal electric dipole [30]. Incidentally, the breakdown of the  $1/r^2$ -like behavior at short distances for a real dipole is a physical manifestation of renormalization and therefore a good demonstration for why renormalization can be necessary. Another physical situation in which we get a pure  $1/r^2$  potential is a test charge interacting with an infinite, charged wire [30], which reduces to a 2D problem because of the cylindrical symmetry. Additionally, unknown interactions can be studied using power law perturbative methods, and so practically any potential of the form  $r^{-n}$ , at least for small  $|n|$ , is important to study—especially if it is pathological and/or involves symmetry-breaking.

The  $\delta$  potential, or any point interaction in general, has heavy application in solid-state physics [46]. It is useful as a first try at modeling a localized interaction as a part of larger physical system, e.g. it is common to put a  $\delta$  potential at each atom/molecule in a large lattice or ensemble [45]. In problems that reduce to two dimensions, the potential becomes pathological due to its scale invariance and no longer provides the option for a bound state without renormalization. The renormalization parameter  $k_{bs}$  then has to become an experimental measurement, for there is no *a priori* means to determine a bound-state energy, the way there can be for potentials with dimensioned couplings.

The  $\delta'$  potential is, admittedly, more of a theoretical curiosity than a useful model, but that is mostly because we don't understand it well enough to use it as a model—not because it is unphysical. For localized interactions, the default model is a  $\delta$  potential, even though this is just one out of infinitely many conceivable point interactions. (For example, the 1D point interaction is parameterized by the entire unitary group  $U(2)$ , even if we insist on

self-adjointness.) In quantum field theory, perturbative methods are often necessary to get some handle on a problem, and a natural-seeming way to expand a point interaction  $P(x)$  would be using  $\delta$  potentials and their derivatives:

$$P(x) = \sum_{n=1}^{\infty} c_n \delta^{(n)}(x) \quad (8.1)$$

where  $\delta^{(n)}$  indicates the  $n$ th derivative of the  $\delta$  potential. An example of a  $\delta'$ -like interaction is one that looks like a localized dipole: a strong attraction immediately followed by a strong barrier, or vice versa. But if we can't understand the  $\delta'$  potential in isolation, how could it possibly be useful as a term in a perturbative expansion? Papers with new ideas to solve and/or interpret the 1D  $\delta'$  potential are still being published regularly today, as is apparent from the bibliography of this thesis [8], [13], [24], [38]. It is an urgent problem to solve precisely because, at the moment, it has no obvious application.

### 8.3 Conclusion

We have calculated spectra and phase shifts of three different singular, scale-symmetric potentials using various methods of regularization, renormalization, and/or finding self-adjoint boundary conditions. The observations from these calculations can be summarized as follows:

- Producing a quantum anomaly inevitably requires some sort of mid-calculation fudging, or “renormalization” as it is technically called, to give a desired result based on physical reasoning.
- The theories of how a classical symmetry can naturally break upon quantization (see Chapter 2) do not seem to be borne out in practice: most of the time, the symmetry breaking happens due to renormalization. The anomaly is sometimes defined as a symmetry breaking upon quantization, and sometimes as a symmetry breaking upon renormalization. These are not the same effect, and we mostly observe the latter.
- Despite our initial doubts about the possibility of a non-anomalous scale-invariant potential, it seems as though the 1D  $\delta'$  potential could be said to preserve its scale

symmetry in quantum mechanics. The momentum-space approach gives a spectrum of  $E > 0$ , i.e. no bound state, with a real transmission coefficient, via a pretty smooth calculation with no unwanted infinities, as does the Griffiths approach. It is sometimes said that the anomaly is a symmetry breaking that occurs under *any* regularization procedure, so if we have found some that preserve the scale symmetry, by that definition we would have disproved the 1D  $\delta'$  anomaly.

- Self-adjoint extensions are a useful way of dealing with singular potentials, but in the case of point interactions, the scale symmetry is never really used in the definition of the interaction. Therefore it doesn't really make sense to say the scale symmetry “breaks,” since it never really existed to begin with.

## 8.4 Future Work

There are countless loose threads dangling from this thesis, and a future thesis student could do a lot with any of them. We mention the most urgent unresolved questions.

The problem closest to the frontier is understanding the 1D  $\delta'$  potential. There are still a number of ways of attacking the problem that we did not include, for example different ways of regularizing in position space. One could use a rectangular regularization with a dip followed by a bump

$$V_{g,a}(x) = \begin{cases} 0 & x < -a \\ -g & -a < x < 0 \\ g & 0 < x < a \\ 0 & x > a \end{cases} \quad (8.2)$$

and take the limit as  $a \rightarrow 0$ ,  $g \rightarrow \infty$  with  $g \sim 1/a^2$  so that the two disturbances become  $\delta$  functions with *infinite* coupling in the limit. Another possible way of regularizing in position space is to find families of smooth, exactly solvable potentials and see if there is a way of taking a limiting case that looks like a  $\delta'$  potential in the limit.

A big loose end that needs tying up is seeing if any of the existing examples of quantum mechanical anomalies—or new examples—can be expressed as Esteve's anomalous term in the Ehrenfest theorem and/or Fujikawa's anomalous Jacobian. We came too late to the

realization that the heart of the anomalies issue is whether they arise due to renormalization or due to quantization, and so we did not have time to address this question via any explicit calculations. As to the Fujikawa characterization of the anomaly, one could investigate whether scale transformations affect the function-space measure  $\mu_{l+\nu}[r^2]$  in a way that helps break the scale symmetry—although it is still clear from our calculation in Section 6.5 that the symmetry breaks mostly due to dimensional regularization. As to Esteve’s characterization, one could see whether in our examples the operator  $D$  leaves the domain of the Hamiltonian invariant, since that is the conserved quantity corresponding to scale symmetry.

# Appendix A

## 1D $\delta'$ Calculation Details

Here we present the details of calculations that were too lengthy for the body of the paper, in particular ones relevant to the 1D  $\delta'$ .

Any bound state must solve the Schrödinger equation in each region and be normalizable, and hence is of the following form:

$$\psi(x) = \begin{cases} Ae^{\rho x} & \text{if } x < -a \\ Be^{\rho x} + Ce^{-\rho x} & \text{if } -a < x < a \\ De^{-\rho x} & \text{if } x > a \end{cases} \quad (\text{A.1})$$

But we must also enforce four boundary conditions. Two are for continuity of  $\psi$  at  $-a$  and  $a$ , and the other two are for particular step discontinuities in  $\psi'$  at  $-a$  and  $a$  given by the  $\delta$  potentials.

$$\left[ \frac{\partial \psi}{\partial x} \right]_{\pm a^-}^{\pm a^+} = \pm g \psi(\pm a) \quad (\text{A.2})$$

Applying these boundary conditions to Eq. A.1 yields

1.  $Ae^{-\rho a} = Be^{-\rho a} + Ce^{\rho a}$
2.  $B\rho e^{-\rho a} - C\rho e^{\rho a} - A\rho e^{-\rho a} = -gAe^{-\rho a}$
3.  $Be^{\rho a} + Ce^{-\rho a} = De^{-\rho a}$
4.  $-D\rho e^{-\rho a} - B\rho e^{\rho a} + C\rho e^{-\rho a} = gDe^{-\rho a}$

Since this system is linear in  $A, B, C$ , and  $D$ , we can use what is effectively Gaussian elimination to find which  $\rho$  give non-trivial solutions, i.e. to find the energy quantization



condition. If we are just interested in the energy, a shortcut is to set the determinant of the system equal to 0 and solve for  $\rho$ , because only singular matrices  $M$  have nontrivial solutions to  $M\vec{x} = \vec{0}$  and a physical wave function cannot have  $A = B = C = D = 0$ . We do this first to find the energy:

$$\begin{aligned}
0 &= \begin{vmatrix} e^{-\rho a} & -e^{-\rho a} & -e^{\rho a} & 0 \\ (g - \rho)e^{-\rho a} & \rho e^{-\rho a} & -\rho e^{\rho a} & 0 \\ 0 & e^{\rho a} & e^{-\rho a} & -e^{-\rho a} \\ 0 & -\rho e^{\rho a} & \rho e^{-\rho a} & -(\rho + g)e^{-\rho a} \end{vmatrix} = e^{-4\rho a} (-g^2 + e^{4\rho a} g^2 - 4e^{4\rho a} \rho^2) \\
&\iff g^2 = e^{4\rho a} (g^2 - 4\rho^2) \\
&\iff e^{-4\rho a} = 1 - \left(\frac{2\rho}{g}\right)^2
\end{aligned}$$

This recovers the energy quantization condition we used in Chapter 7, and, again, fixing  $\rho = \rho_{bs}$  to some finite, positive value forces  $g^2 a$  constant in the limit. Then  $\rho = g^2 a$  is that constant, which we can also consider to be renormalized, or dimensionally transmuted, coupling.

The  $\rho = 0$  solution, as follows immediately from (1) and (3), is special in that  $A = D = 0$ , so in the limit we have the non-physical 0 function as our bound-state wave function. In fact, we have the 0 function even before taking the limit, as  $B + C = 0$ , so all three regions are identically 0. (We still get non-trivial solutions to the matrix equation, because the determinant is zero for  $\rho = 0$ , and they are of the form  $B = -C$ .)

But we would also like to know the bound-state wave function for general  $\rho$ , which requires the full elimination process. We start by manipulating (1) and (2) to show that  $A = B + Ce^{2\rho a}$  and  $A = \rho \frac{B - Ce^{2\rho a}}{\rho - g}$ , which can be combined to find

$$B = Ce^{2\rho a} \left( \frac{2\rho}{g} - 1 \right)$$

Then we can combine with (3) to relate  $C$  to  $D$ :

$$D = C \left[ e^{4\rho a} \left( \frac{2\rho}{g} - 1 \right) + 1 \right]$$

Then, finally, we find the ratio  $A/D$  by using (1) and replacing  $B$  and  $C$  with expressions involving  $D$ :

$$\frac{A}{D} = \frac{e^{2\rho a} \left(\frac{2\rho}{g}\right)}{e^{4\rho a} \left(\frac{2\rho}{g} - 1\right) + 1} = \frac{2\rho e^{2\rho a}}{2\rho e^{4\rho a} + g(1 - e^{4\rho a})} = \frac{2\rho e^{2\rho a}}{2\rho e^{4\rho a} + g(-4\rho a + \mathcal{O}(a^2))} \rightarrow 1$$

And thus we get the symmetric bound state as promised in Chapter 7.

For the scattering problem, we solve the same boundary conditions but for a positive-energy, non-normalizable solution:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{if } x < -a \\ Ce^{ikx} + De^{-ikx} & \text{if } -a < x < a \\ Fe^{ikx} & \text{if } x > a \end{cases} \quad (\text{A.3})$$

We compute the phase shift at the origin by finding the complex argument of  $F/A$ . We apply the four boundary conditions, which manifest themselves as

1.  $Ae^{-ika} + Be^{ika} = Ce^{-ika} + De^{ika}$
2.  $Cike^{-ika} - Dike^{ika} - Aike^{-ika} + Bike^{ika} = -g(Ae^{-ika} + Be^{ika})$
3.  $Ce^{ika} + De^{-ika} = Fe^{ika}$
4.  $Fike^{ika} - Cike^{ika} + Dike^{-ika} = gFe^{ika}$

If we set  $A = 1$ , we have 4 equations and 4 unknowns, and we focus on solving for  $F$  in terms of  $a$ ,  $g$  and  $k$ . We can manipulate (4) to give

$$F(ike^{ika} - ge^{ika}) = Cike^{ika} - Dike^{-ika} \implies F = \frac{Cike^{ika} - Dike^{-ika}}{ike^{ika} - ge^{ika}} = \frac{1}{1 - \frac{g}{ik}} (C - De^{-2ika})$$

Then we need (3) to relate  $C$  and  $D$ :

$$Ce^{ika} = Fe^{ika} - De^{-ika} \implies C = F - De^{-2ika}$$

So now we have a new equation with just  $F$  and  $D$ :

$$\begin{aligned}
F &= \frac{1}{1 - \frac{g}{ik}} \left( F - De^{-2ika} - De^{-2ika} \right) \\
\implies F \left( 1 - \frac{1}{1 - \frac{g}{ik}} \right) &= \frac{1}{1 - \frac{g}{ik}} \left( -2De^{-2ika} \right) \\
\implies F &= \frac{\frac{1}{1 - \frac{g}{ik}} \left( -2De^{-2ika} \right)}{\left( 1 - \frac{1}{1 - \frac{g}{ik}} \right)} = \frac{-2De^{-2ika}}{\frac{-g}{ik}} = \frac{2ik}{g} De^{-ika}
\end{aligned}$$

Now we find  $D$  in terms of  $B$  (and  $F$ , unfortunately) using (2).

$$\begin{aligned}
Cike^{-ika} - Dike^{ika} - ike^{-ika} + Bike^{ika} &= -g \left( e^{-ika} + Be^{ika} \right) \\
\implies \left( F - De^{-2ika} \right) ike^{-ika} - Dike^{ika} - ike^{-ika} + Bike^{ika} &= -g \left( e^{-ika} + Be^{ika} \right) \\
\implies D \left( -ike^{-3ika} - ike^{ika} \right) &= ike^{-ika} - Bike^{ika} - g \left( e^{-ika} + Be^{ika} \right) - Fike^{-ika} \\
\implies D &= \frac{ike^{-ika} - Bike^{ika} - g \left( e^{-ika} + Be^{ika} \right) - Fike^{-ika}}{-ike^{-3ika} - ike^{ika}} \\
&= \frac{-e^{-2ika} + B + \frac{g}{ik} \left( e^{-2ika} + B \right) + Fe^{-2ika}}{1 + e^{-4ika}} \\
&= \frac{1}{1 + e^{-4ika}} \left( B \left( 1 + \frac{g}{ik} \right) + Fe^{-2ika} + e^{-2ika} \left( \frac{g}{ik} - 1 \right) \right)
\end{aligned}$$

Now we use (1) to find  $B$  in terms of  $D$  and  $F$ . We also use (3) in the third equals sign.

$$\begin{aligned}
B &= Ce^{-2ika} + D - e^{-2ika} = e^{-2ika} \left( C + De^{2ika} \right) - e^{-2ika} = e^{-2ika} \left( F - De^{-2ika} + De^{2ika} \right) - e^{-2ika} \\
&= D \left( 1 - e^{-4ika} \right) + Fe^{-2ika} - e^{-2ika}
\end{aligned}$$

If we plug this back into our previous expression for  $D$ , we get

$$\begin{aligned}
D &= \frac{1}{1 + e^{-4ika}} \left[ \left( D \left( 1 - e^{-4ika} \right) + F e^{-2ika} - e^{-2ika} \right) \left( 1 + \frac{g}{ik} \right) + F e^{-2ika} + e^{-2ika} \left( \frac{g}{ik} - 1 \right) \right] \\
&\implies D \left( \left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik} \right) = F e^{-2ika} + \frac{g}{ik} F e^{-2ika} - e^{-2ika} - \frac{g}{ik} e^{-2ika} \\
&+ F e^{-2ika} + \frac{g}{ik} e^{-2ika} - e^{-2ika} = F e^{-2ika} \left( 2 + \frac{g}{ik} \right) - 2e^{-2ika} \\
&\implies D = \frac{F e^{-2ika} \left( 2 + \frac{g}{ik} \right) - 2e^{-2ika}}{\left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik}}
\end{aligned}$$

Then plugging into our relationship between  $F$  and  $D$ ,

$$\begin{aligned}
F &= \frac{2ik}{g} e^{-ika} \frac{F e^{-2ika} \left( 2 + \frac{g}{ik} \right) - 2e^{-2ika}}{\left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik}} \\
&\implies F \left( 1 - \frac{2ik}{g} e^{-ika} \frac{e^{-2ika} \left( 2 + \frac{g}{ik} \right)}{\left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik}} \right) = \frac{2ik}{g} e^{-ika} \frac{-2e^{-2ika}}{\left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik}} \\
&\implies F \left( \left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik} - \frac{2ik}{g} e^{-ika} e^{-2ika} \left( 2 + \frac{g}{ik} \right) \right) = \frac{-4ike^{-3ika}}{g} \\
&\implies F = \frac{-4ike^{-3ika}}{g} \frac{1}{\left( 2 + \frac{g}{ik} \right) e^{-4ika} - \frac{g}{ik} - \frac{2ik}{g} e^{-ika} e^{-2ika} \left( 2 + \frac{g}{ik} \right)} \\
&= \frac{-4ik}{g \left( \left( 2 + \frac{g}{ik} \right) e^{-ika} - \frac{g}{ik} e^{3ika} - \frac{2ik}{g} \left( 2 + \frac{g}{ik} \right) \right)} = \frac{4k}{g \left( \left( 2i + \frac{g}{k} \right) e^{-ika} - \frac{g}{k} e^{3ika} + \frac{4k}{g} - 2i \right)} \\
&= \frac{4k}{\frac{g^2}{k} e^{-ika} + 2gie^{-ika} - \frac{g^2}{k} e^{3ika} + 4k - 2gi} = \frac{4k}{4k + \frac{g^2}{k} (e^{-ika} - e^{3ika}) + i2g (e^{-ika} - 1)} \\
&= \frac{1}{1 + \frac{g^2}{4k^2} (e^{-ika} - e^{3ika}) + i\frac{g}{2k} (e^{-ika} - 1)}
\end{aligned}$$

Now letting  $a$  be small,

$$F = \frac{1}{1 + \frac{g^2}{4k^2} (-4ika) + i\frac{g}{2k} (-ika)} = \frac{1}{1 + \frac{ga}{2} - \frac{g^2 ai}{k}}$$

This corresponds to a phase shift of

$$\tan(\phi) = \frac{\frac{g^2 a}{k}}{1 + \frac{ga}{2}} \rightarrow \frac{\rho_{bs}}{k} \text{ as } a \rightarrow 0, g \rightarrow \infty \text{ since } ga \rightarrow 0$$

## Appendix B

# Self-Adjoint Extensions On $\mathbb{R} \setminus \{0\}$

We stay completely general for now, even though it is unsightly, because we want to derive the family of all possible self-adjoint boundary conditions for the punctured line.

The next step is to find the left- and right-hand limiting behaviors of elements of the self-adjoint domain

$$D(T_{\mathcal{U}}) = \{\phi + \phi_+ + \mathcal{U}\phi_+ \mid \phi \in D(T), \phi_+ \in N_+\} =$$

$$= \{\phi + \alpha\psi_1^+ + \beta\psi_2^+ + e^{i\omega} [(A\alpha + B\beta)\psi_1^- + (-\bar{B}\alpha + \bar{A}\beta)\psi_2^-] \mid \phi \in D(T), \alpha, \beta \in \mathbb{C}\}$$

where  $T_{\mathcal{U}}$  is the self-adjoint extension of  $T = -\frac{d^2}{dx^2}$  corresponding to  $\mathcal{U}$ , represented by  $U$  relative to the bases  $\{\psi_1^+, \psi_2^+\}$  and  $\{\psi_1^-, \psi_2^-\}$  of  $N_+$  and  $N_-$  respectively. In the original domain, we require that wave functions vanish at 0, so the behavior of an arbitrary  $\psi \in D(T_{\mathcal{U}})$  is

$$\psi(0^+) = \alpha + \beta + e^{i\omega} [(A\alpha + B\beta) + (-\bar{B}\alpha + \bar{A}\beta)] = (1 + Ae^{i\omega} - \bar{B}e^{i\omega})\alpha + (1 + Be^{i\omega} + \bar{A}e^{i\omega})\beta$$

$$\psi(0^-) = \alpha - \beta + e^{i\omega} [(A\alpha + B\beta) - (-\bar{B}\alpha + \bar{A}\beta)] = (1 + Ae^{i\omega} + \bar{B}e^{i\omega})\alpha + (-1 + Be^{i\omega} - \bar{A}e^{i\omega})\beta$$

$$\psi'(0^+) = q\alpha + q\beta + e^{i\omega} [\bar{q}(A\alpha + B\beta) + \bar{q}(-\bar{B}\alpha + \bar{A}\beta)] = (q + \bar{q}Ae^{i\omega} - \bar{q}\bar{B}e^{i\omega})\alpha + (q + \bar{q}Be^{i\omega} + \bar{q}\bar{A}e^{i\omega})\beta$$

$$\psi'(0^-) = -q\alpha + q\beta + e^{i\omega} [-\bar{q}(A\alpha + B\beta) + \bar{q}(-\bar{B}\alpha + \bar{A}\beta)] = (-q - \bar{q}Ae^{i\omega} - \bar{q}\bar{B}e^{i\omega})\alpha + (q - \bar{q}Be^{i\omega} + \bar{q}\bar{A}e^{i\omega})\beta$$

A general set of boundary conditions relates the discontinuities of  $\psi$  and  $\psi'$  at 0 to the average values of  $\psi$  and  $\psi'$  at 0. For example, the boundary conditions for the  $-g\delta$  potential can be derived from the Schrödinger equation to be

$$\psi(0^+) - \psi(0^-) = 0$$

$$\psi'(0^+) - \psi'(0^-) = -\frac{g}{2}(\psi(0^+) + \psi(0^-))$$

We can solve for the most general self-adjoint boundary conditions given by the set of self-adjoint extensions by writing  $\Delta\psi(0) = X\psi(0) + Y\psi'(0)$ ,  $\Delta\psi'(0) = X'\psi(0) + Y'\psi'(0)$  and solving for  $X, Y, X'$ , and  $Y'$  in terms of  $A, B$ , and  $e^{i\omega}$ . To do so is a tedious but straightforward process of rearranging our expressions for  $\psi(0^\pm)$  and  $\psi'(0^\pm)$  and solving a 2x2 linear system. For starters, we can add/subtract those expressions to get

$$\begin{aligned}\psi(0^+) - \psi(0^-) &= -2(\bar{B}e^{i\omega})\alpha + 2(1 + \bar{A}e^{i\omega})\beta \\ \psi'(0^+) - \psi'(0^-) &= 2(q + \bar{q}Ae^{i\omega})\alpha + 2(\bar{q}Be^{i\omega})\beta \\ \frac{1}{2}(\psi(0^+) + \psi(0^-)) &= (1 + Ae^{i\omega})\alpha + (Be^{i\omega})\beta \\ \frac{1}{2}(\psi'(0^+) + \psi'(0^-)) &= -(\bar{q}\bar{B}e^{i\omega})\alpha + (q + \bar{q}\bar{A}e^{i\omega})\beta\end{aligned}$$

Demanding  $\Delta\psi(0) = X\psi(0) + Y\psi'(0)$  as a general boundary condition means it must hold for all  $\alpha, \beta \in \mathbb{C}$ .

$$\begin{aligned}\psi(0^+) - \psi(0^-) &= X\frac{1}{2}(\psi(0^+) + \psi(0^-)) + Y\frac{1}{2}(\psi'(0^+) + \psi'(0^-)) \\ \iff -2(\bar{B}e^{i\omega})\alpha + 2(1 + \bar{A}e^{i\omega})\beta &= X[(1 + Ae^{i\omega})\alpha + (Be^{i\omega})\beta] + Y[-(\bar{q}\bar{B}e^{i\omega})\alpha + (q + \bar{q}\bar{A}e^{i\omega})\beta] \\ \iff X(1 + Ae^{i\omega}) + Y(-\bar{q}\bar{B}e^{i\omega}) &= -2\bar{B}e^{i\omega} \\ \text{and } X(Be^{i\omega}) + Y(q + \bar{q}\bar{A}e^{i\omega}) &= 2(1 + \bar{A}e^{i\omega})\end{aligned}$$

A simple 2 x 2 matrix inversion allows us to find

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \frac{1}{q + 2\text{Re}(qA)e^{i\omega} + \bar{q}e^{2i\omega}} \begin{pmatrix} -2\bar{B}e^{i\omega}(q + \bar{q}\bar{A}e^{i\omega}) + 2\bar{q}\bar{B}e^{i\omega}(1 + \bar{A}e^{i\omega}) \\ 2 + 4e^{i\omega}\text{Re}(A) + 2e^{2i\omega} \end{pmatrix}$$

And similarly, demanding  $\Delta\psi'(0) = X'\psi(0) + Y'\psi'(0)$  yields

$$\begin{pmatrix} X' \\ Y' \end{pmatrix} = \frac{1}{q + 2\text{Re}(qA)e^{i\omega} + \bar{q}e^{2i\omega}} \begin{pmatrix} 2q + 4\text{Re}(A)e^{i\omega} + 2\bar{q}^2e^{2i\omega} \\ -2Be^{i\omega}(q + \bar{q}Ae^{i\omega}) + 2\bar{q}Be^{i\omega}(1 + Ae^{i\omega}) \end{pmatrix}$$

Although unpleasant to read, we have derived the fully general set of boundary conditions for this problem in terms of the unitary matrix corresponding to the self-adjoint extension. There is, however, no way to decide, without external motivation, which of these self-adjoint extensions corresponds to  $\delta'$ . All this accomplishes is to enumerate all of the possible legal boundary conditions, and it's for us to figure out which physically ought to correspond to which point interactions.

# Bibliography

- [1] S. Gopalakrishnan, “Self-Adjointness and the Renormalization of Singular Potentials,” unpublished senior thesis, Amherst College, 2006
- [2] B. Holstein, “Understanding an anomaly,” *AJP* 82, 591 (2014)
- [3] V. Araujo, F. A. B. Coutinho, J. Perez, “Operator domains and self-adjoint operators,” *AJP* 72, 203-213 (2004)
- [4] M. Reed, B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis*, Academic Press, San Diego, 1975
- [5] M. Reed, B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic Press, San Diego, 1975
- [6] D. Griffiths, “Boundary conditions at the derivative of a delta function,” *J. Phys. A: Math*, 26, 2265 (1993)
- [7] G. Bonneau, J. Faraut, G. Vallent, “Self-adjoint extensions of operators and the teaching of quantum mechanics,” *AJP* 69, 322 (2001)
- [8] R. Lange, “Point and surface interactions in quantum mechanics,” arXiv:1401.7627
- [9] R. Jackiw, “Delta-Function Potentials in Two- and Three-Dimensional Quantum Mechanics,” MIT-CTP-1937, 1991
- [10] H. Camblong, “Anomaly in conformal quantum mechanics: From molecular physics to black holes,” *Phys.Rev. D*68, 125013 (2003)



- [11] J. Brown, R. Churchill, *Complex Variables and Applications*, McGraw-Hill Science/Engineering/Math, New York, 1995
- [12] M. Abramowitz, I. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Dover Publications, New York, 1964
- [13] T. Cheon, T. Shigehara, “Realizing discontinuous wave function with renormalized short range potentials,” *Phys.Lett.* A243 (1998)
- [14] H. Camblong, “Dimensional Transmutation and Dimensional Regularization in Quantum Mechanics,” *Annals Phys.* 287 (2001)
- [15] A. V. Zolotaryuk, P.L. Christiansen, S. V. Iermakova, “Scattering properties of point dipole interactions,” *J. Phys. A: Math. Gen.* 39 (2006)
- [16] D. Griffiths, S. Walborn, “Dirac deltas and discontinuous functions,” *Am. J. Phys.* 67, 446 (1999)
- [17] R. P. Feynman, A. R. Hibbs, *Quantum mechanics and path integrals*, McGraw-Hill, New York, 1965
- [18] D. Griffiths, *Introduction to quantum mechanics*, Pearson Prentice Hall, Upper Saddle River, 2005
- [19] H. Camblong, C. Ordonez, “Anomaly in conformal quantum mechanics: From molecular physics to black holes,” *Phys.Rev.* D68 (2003)
- [20] H. Camblong, C. Ordonez, “Renormalized path integral for the two-dimensional delta function interaction,” *Phys.Rev.* A65 (2002)
- [21] H. Camblong, C. Ordonez, “Path Integral Treatment of Singular Problems and Bound States: Quantum Mechanics,” *Int.J.Mod.Phys.* A19 (2004)
- [22] C. Grosche, “An Introduction into the Feynman path integral,” Nov 1992. 92 pp. NTZ-29-92

- [23] H. Kleinert, *Path integrals in quantum mechanics, statistics, polymer physics, and financial markets*, World Scientific, Hackensack, 2006
- [24] M. H. Al-Hashimi, A. M. Shalaby, “The Solution of the Relativistic Schrödinger Equation for the  $\delta'$ -Function Potential in 1-dimension Using Cutoff Regularization,” arXiv:1503.00786
- [25] L. Ballentine, *Quantum mechanics : a modern development*, World Scientific, River Edge, 1998
- [26] F. A. B. Coutinho, Y. Nogami, J. Perez, “Generalized point interactions in one-dimensional quantum mechanics,” *J. Phys. A: Math. Gen.* 30 (1997)
- [27] B. Holstein, “Anomalies for pedestrians,” *Am. J. Phys.* 61, 142 (1993)
- [28] A. Khelashvilia, T. Nadareishvilia, “Singular Behavior of the Laplace Operator in Polar Spherical Coordinates and Some of Its Consequences for the Radial Wave Function at the Origin of Coordinates,” *Physics of Particles and Nuclei Letters.* vol.12. pp11-25 (2015)
- [29] R. Jackiw, “Introducing scale symmetry,” *Phys.Today* 25N1 (1972)
- [30] S. Coon, B. Holstein, “Anomalies in quantum mechanics: The  $1/r^2$  potential,” *Am.J.Phys.* 70 (2002)
- [31] R. Bertlmann, “Anomalies in quantum field theory,” Oxford University Press Inc., New York, 2000
- [32] G. Hooft, M. Veltman, “Regularization and renormalization of gauge fields,” *Nuclear Physics B*44 (1972)
- [33] A. Essin, D. Griffiths, “Quantum mechanics of the  $1/x^2$  potential,” *Am. J. Phys.* 74 (2006)
- [34] I. Lapidus, “Scattering by two-dimensional circular barrier, hard circle, and delta function ring potentials,” *Am. J. Phys.* 54, 459 (1986)

- [35] I. Gradshteyn, I. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, San Diego, 1994
- [36] G. Watson, *A Treatise on the Theory of Bessel Functions*, Cambridge University Press, Cambridge, 1996
- [37] D. Tong, “Lectures on Quantum Field Theory,” University of Cambridge
- [38] M. Maroun, “Generalized Spectrum of the Derivative of a Dirac Delta Function as a Schrodinger Potential,” Department of Mathematics, UC Riverside (2015)
- [39] D. Gitman, I. Tyutin, B. Voronov, “Self-adjoint Extensions in Quantum Mechanics,” Birkhäuser Basel, 2012
- [40] H. Camblong, et. al., “Renormalization of the inverse square potential,” *Phys.Rev.Lett.* 85 (2000)
- [41] E. Gozzi, D. Mauro, “Scale symmetry in classical and quantum mechanics,” *Phys.Lett.* A345 (2005)
- [42] J. Esteve, “Origin of the anomalies: The modified Heisenberg equation,” *Phys.Rev.* D66 (2002)
- [43] V. de Alfaro, S. Fubini, G. Furlan, “Conformal Invariance in Quantum Mechanics,” *Nuovo Cim.* A34 (1976)
- [44] G. Ananos, H. Camblong, C. Ordonez, “SO(2,1) conformal anomaly: Beyond contact interactions,” *Phys.Rev.* D68 (2003)
- [45] B. Dasannacharya, P. Goyal, “Investigation of hydrogenous materials using neutrons,” *Bull. Mater. Sci.* V6 N.2 (1984)
- [46] P. Christiansen, et. al., “On the existence of resonances in the transmission probability for interactions arising from derivatives of Diracs delta function,” *J. Phys. A: Math. Gen.* 36 (2003)

- [47] T. Gherghetta, “Phenomenological consequences of supersymmetry with anomaly induced masses,” Nucl.Phys. B559 (1999)
- [48] L. Rosen, J. Wright, “Dimensional regularization and renormalization of QED,” Communications in Mathematical Physics Volume 134, Issue 3 (1990)
- [49] A. Jaffe, “Introduction to Quantum Field Theory,” Harvard University, 2005
- [50] H. Goldstein, C. Poole, J. Safko, “Classical Mechanics,” 3rd Ed., Addison Wesley, San Francisco, 2002
- [51] F. Olver, D. Lozier, R. Boisvert, C. Clark, editors. *NIST Handbook of Mathematical Functions*, Cambridge University Press, New York, 2010
- [52] P. Morse, H. Feshbach, *Methods of Theoretical Physics, Part I*, McGraw-Hill, New York, 1953