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TOPICS IN PARTICLE PHYSICS, QUANTUM FIELD THEORY, AND COSMOLOGY

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Jaryd F. Ulbricht

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The Dissertation of Jaryd F. Ulbricht
is approved:

Professor Stefano Profumo, Chair

Professor Wolfgang Altmannshofer

Professor Michael Dine

Peter Biehl
Vice Provost and Dean of Graduate Studies

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Abstract

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Our understanding of particles physics derives, in large part, from our ability to do perturbative calculations by expanding around small coupling. This Feynman diagrammatic approach has been incredibly successful in providing physicists a means to approximate physical observables. However, there are many scenarios where a perturbative approach either does not exist or fails completely. In this thesis I will construct several nonperturbative (or singularly perturbative) methods that have applications in particle physics, quantum field theory, and cosmology. We will also investigate a broad range of topics, including grand unified theories, the hierarchy problem, dark matter phenomenology, the mathematical foundations of quantum mechanics, and a host of mathematical methods useful in physics.

To my wife Megan and our son Arlo, who give me purpose and so much joy.

Acknowledgments

I would like to thank my adisor, Professor Stefano Profumo, for helping me to navigate my doctoral career, and guiding my research with a gentle hand. I would also like to thank Professor Michael Dine for explaining to me a great number of subtle issues in theoretical physics, and for advising me on several projects.

I also owe a great deal of gratitude to Hiren Patel, who understood my research interests and shared with me many ideas that led to the content of this thesis. As well, Logan Morrison collaborated with me on a number of occasions, and I am very thankful to him, especially for his expertise in computational physics.

Introduction

Beyond Perturbation Theory

This is a collection of results derived by myself and in collaboration with others. These results focus primarily on topics in quantum field theory, but also touch on some other subjects such as cosmology and particle physics phenomenology. They share in the development and application of new mathematical methods and alternative approaches to problems in physics. The diversity of the spectrum of physical phenomena is, in large part, a consequence of nonlinear dynamics. Except for an extremely small number of special cases, we have no complete solutions of nonlinear systems. The existence of nontrivial relativistic quantum field theories is not even established, at least at the level of rigour of a mathematical proof. We then find ourselves investigating the natural world with a mathematical framework that we don't fully understand, whose dynamics we don't know how to solve. Let us begin with a historical perspective on how we have come to find ourselves in this situation.

In the early 20^{th} century our understanding of the physical world rested on the foundations of classical mechanics, whose mathematical structure is symplectic geometry. In this theory a system of N particles in 3 dimensions is described by the $6N$ generalized momenta p_i and coordinates q^i, with a closed nondegenerate differential 2-form (symplectic form). The motion of particles was described by their trajectories

through phase space, whose time evolution is governed by the Hamiltonian. This understanding of the universe led to a great number of incredibly successful theories, perhaps culminating in the kinetic theory of gases and the explanation of Brownian motion. I make this assertion because, before the papers by Einstein[1] and Smoluchowski[2], there was disagreement amongst physicists over whether the atom, whose existence is now regarded as obvious, was a mathematical construct or physical reality. The world, it seemed, was perfectly fluid and continuous. Atoms, with their ungainly discreteness, were an insult to our smooth existence in an unblemished cosmos. Of course, like freezing water in a granite spire, this discreteness would soon shatter the foundations of 20^{th} century physics.

As the physics community was overtaken by the theory of the quantum, shortly after the groundbreaking and Nobel prize winning research by Einstein on the photoelectric effect[3], the mathematical structure of physical theories shifted from symplectic geometry to the algebra of operators on Hilbert spaces. This shift resulted in a richer structure in physical theories, but it came with a cost: it was unintuitive and monstorously complicated. Nevertheless, the young theory of quantum mechanics lifted the clouds that obscured several outstanding problems in physics (to use the phrasing of Lord Kelvin[4]), such as the ultraviolet catastrophe in black body radiation.

Early successes of quantum mechanics, such as the energy levels of the hydrogen atom[5] and the quantum harmonic oscillator[6], consisted of exactly solvable problems[1]. Such problems, although incredibly useful in many regards, are not accu-

[1]The Bohr-Rutherford model of the hydrogen atom was built on the *old quantum mechanics* that existed during the period of 1905 and 1925, and was itself inconsistent. It was replaced with the more mature quantum mechanical theory of Pauli[7] and Schrödinger[8] in 1926

rate representations of the natural world. These relatively simple models could not reproduce the fine detail and heterogeneity of observation. To be sure, this is not a feature unique to quantum mechanics. Laplace and Lagrange were the first to consider the motions of celestial bodies as *perturbed* from their exactly solvable Keplerian orbits[9]. Perturbation theory, which it came to be called, was soon applied to quantum mechanics by Schrödinger[10] (time-independent) and Dirac[11] (time-dependent). More realistic models could then be investigated, such as the Stark effect and Zeeman effect on the spectrum of the hydrogen atom[7, 10], by considering small departures from the exactly solvable systems.

Despite these successes, quantum mechanics had a problem: it appeared inconsistent with special relativity[2]. Attempts to unite the two principals resulted in the proliferation of infinities at higher orders of perturbation theory. The Klein-Gordon equation[12–15] and the Dirac equation[16] were developed as fully relativistic wave equations, but it was not known how to calculate anything beyond the trivial free particle case. The leading order approximation from Dirac's theory of the anomalous magnetic dipole moment of the electron gave $g \sim 2$, in the limit that the electromagnetic coupling constant $\alpha_{\text{EM}} \to 0$. This was reasonably close to the experimental value (about 1 in 1000), and gave the correct splitting of the hydrogen atom spectrum, so Dirac's theory of the electron became the accepted theory at the time. However, this is essentially a classical result, since it ignores intermediate particle states. In the words of Sydney Coleman: "Even when relativistic effects are small, the kinematic effects of rela-

[2]It is still an open question of whether a general quantum theory is compatible with special relativity. There are affirmative results in 2 and 3 dimensions, and some negative results in dimensions greater than 4.

tivity are precisely the same order of magnitude as the effects of pair states and we have no business dealing with a system of only two bodies or one body in a potential."[17] In order to include the many particle states that should exist one formulates the theory in terms of fields, rather than individual particles. Since these fields are quantum in nature, this goes by quantum field theory (QFT).

The full theory of quantum electrodynamics is nonlinear in the fields, because of the coupling between the electron and photon. This makes the theory nonlinear and highly nontrivial. By assuming that the nonlinearities are small, that is that the theory is in some sense "nearly free", one might hope to make progress using perturbation theory. The first attempts at calculating radiative corrections were disastrous, everything beyond the leading order approximation was infinite. It took until the mid 1940s, in the works of Richard Feynman[18–20], Julian Schwinger[21], and Shin'ichirō Tomonaga[22–25], to resolve the infinities in a process that came to be known as *renormalization*. In renormalization the bare parameters of the theory are unphysical, and formally infinite. One then allows the divergent components of the bare parameters to exactly cancel with the divergences at each order in perturbation theory, so that the final result is finite. Feynman constructed an algorithmic procedure for doing this process by drawing little diagrams that represented each term in a perturbative expansion of observables in the theory, with a corresponding set of rules that are easily inferred from the diagram.

After Feynman, Schwinger, and Tomonaga put quantum field theory on firm footing (at least in the sense of being able to actually do perturbative computations), there have been a number of major advancements in the field of theoretical particle physics. Chen Ning Yang and Robert Mills extended the abelian gauge symmetry of

electromagnetism to non-abelian gauge groups in 1954[26], but non-abelian gauge bosons must be massless in order to maintain gauge invariance. This issue was resolved in the early 1960s by Yoichiro Nambu[27], Jefferey Goldstone[28, 29], Abdus Salam[29], and Steven Weinberg[29] with the inclusion of the spontaneous symmetry breaking mechanism of François Englert and Robert Brout[30], Peter Higgs[31], and Gerald Guralnik, Carl Hagen, and Tom Kiggle[32]. This set the stage for the development of our current theory of the universe on the smallest scales: the Standard Model of Particle Physics (SM).

The SM is a QFT, with gauge symmetry $\mathrm{SU}(3) \times \mathrm{SU}(2) \times \mathrm{U}(1)$, corresponding to the strong nuclear charge, weak nuclear charge, and hypercharge respectively. With the exception of the strong nuclear force (quantum chromodynamics, or QCD) the coupling parameters in the SM are relatively small, enabling a perturbative expansion of observables. In 1973 David Gross and Frank Wilczek[33], and independently David Politzer[34], showed that QCD was asymptotically free: the strong force becomes weaker at shorter distance scales. This also allows one to do perturbative calculations, provided the energy is sufficiently high.

There have been far more developments in the past 80 years that I have not mentioned. We will stop here though, because the point is beginning to become clear: most of the mathematical machinery we have at our disposal to understand particle physics is of the same ilk as of that used by Laplace and Lagrange. We write observables as an expansion around some small coupling (say λ):

$$\langle \mathcal{O} \rangle = c_0 + c_1 \lambda + c_2 \lambda^2 + \dots .$$

The leading order coefficient, c_0, is the free problem, which is exactly solvable. The higher order coefficients are calculated using Feynman rules, doing loop integrals, and renormalizing. We have reduced an unsolvable problem into an infinite number of solvable ones. Feynman diagrams and perturbation theory are the work horses of particle physics. This is a massively useful tool that has allowed physicists to make predictions at incredible precision.

However, there are physical phenomena which cannot be described using this brand of perturbation theory. These include the electroweak sphaleron[35, 36], the QCD instanton[37], soliton states[38], vacuum tunneling[39–41], and first order phase transitions[42, 43]. In these examples the leading order approximation corresponds to a nontrivial solution of a nonlinear boundary value problem, which typically has no known analytic solution (an exception being the QCD instanton). These effects can be approximated in a perturbative fashion, meaning we make an expansion around some small parameter[3], but this expansion involves a leading exponential term $\exp(-c/\lambda)$, and we reserve the phrasing *perturbative* to mean a Taylor series in positive powers of λ. Owing to their greater complexity, these phenomena are much less studied than perturbative effects, and there exist far fewer tools for their analysis in comparison.

Additionally, perturbative approximations of some observables may be valid in some region of parameter space, but fail in other regions. In most QFTs this is in fact true for all small coupling expansions. Using an argument originally by Freeman Dyson[44], the series expansion in powers of λ diverges for all $\lambda > 0$. At some order in perturbation theory, roughly $1/\lambda$, the coefficients begin to grow without bound[4]. This

[3] A better term for this kind of expansion would be *singularly perturbative*

[4] In fact we are quite lucky that the series is divergent. For two series representations of a meromorphic

is particularly apparent in QCD, where the strong coupling is divergent in the infrared (IR), which is believed to be the cause of color confinement (though no formal proof of such a claim exists). Again, we find ourselves with a dearth of options to analyze physical phenomena in cases where the perturbative method fails.

The major theme of this thesis is the development of mathematical methods useful in physics. This includes the investigation of nonperturbative methods, as well as some analysis and applications to phenomenology. In Chapter 1 we investigate a scenario where a perturbative analysis fails. It has been suggested that scattering cross sections at very high energies for producing large numbers of Higgs particles may exhibit factorial growth, and that curing this growth might be relevant to other questions in the Standard Model. We point out, first, that the question is inherently nonperturbative; low orders in the formal perturbative expansion do not give a good approximation to the scattering amplitude for sufficiently large N for any fixed, small value of the coupling. Focusing on $\lambda\phi^4$ theory, we argue that there *may* be a systematic approximation scheme for processes where N particles near threshold scatter to produce N particles, and discuss the leading contributions to the scattering amplitude and cross sections in this limit. Scattering amplitudes do not grow as rapidly as in perturbation theory. Additionally, partial and total cross sections do not show factorial growth. In the case of cross sections for $2 \to N$ particles, there is no systematic large N approximation available. That said, we provide evidence that nonperturbatively, there is no factorial growth in partial or

function, one convergent and one divergent, the divergent series will typically converge on the correct answer much more quickly than the convergent series, provided the divergent series is asymptotic. If the universe had been unkind observables in QFT would have convergent series expansions and we would have to calculate tens if not hundreds of terms to achieve even a modest level of precision. I encourage the reader to try this with their favorite transcendental function.

total cross sections. These results we found in collaboration with Michael Dine and Hiren Patel[45].

In Chapter 2 we develop a uniform WKB method to study the density of hypothetical dark matter particles as a function of the age of the universe. A solution to the Boltzmann equation governing the thermal relic abundance of cold dark matter is constructed by matched asymptotic approximations. The approximation of the relic density is an asymptotic series valid when the abundance does not deviate significantly from its equilibrium value until small temperatures. Resonance and threshold effects are taken into account at leading order and found to be negligible unless the annihilation cross section is negligible at threshold. Comparisons are made to previously attempted constructions and to the freeze out approximation commonly employed in the literature. Extensions to higher order matching is outlined, and implications for solving related systems are discussed. We compare our results to a numerical determination of the relic abundance using a benchmark model and find a fantastic agreement. The method developed also serves as a solution to a wide class of problems containing an infinite order turning point. This research was published in collaboration with Logan Morrison and Hiren Patel[46].

In Chapter 3 we turn our attention to effective field theories and analysis. New matter fields charged under the strong nuclear force would have dramatic phenomenological implications. Here, we systematically explore how these new states, which we postulate belong to some representation of SU(3) of QCD, could interact with SM fields: We analyze all lowest-dimensional "portal" operators for any SU(3) representation and, motivated by grand unification, we extend our results to SU(N), for $N > 3$. This

research was published in collaboration with Tesla Jeltema and Stefano Profumo[47].

In Chapter 4 we present a formula for calculating the regulated functional determinant of a second order elliptic operator that possesses radial symmetry. The formalism follows closely to what has been derived previously for second order elliptic operators acting on a single scalar field. The generalization from scalar operators to matrix operators is accomplished by identifying a privileged matrix solution of the differential equation known as the principal matrix solution. We obtain UV finite results by renormalizing the determinant ratio using zeta function regularization, and we also include a general procedure for the removal of zero modes. Explicit formula for dimensions $d = 2$, 3, and 4 are given. The generalization to higher dimensions is straightforward. This work is incredibly important and relevant for the study of nonperturbative effects in quantum field theory, as functional determinants are the one-loop contributions to correlation functions expanded around non-trivial saddle points of the classical action. These results also incorporate the matrix structure necessary to directly investigate nonperturbative effects in theories involving fermions. Finally, we note that the procedure developed is more general than a small coupling expansion, as we only require *some* large prefactor in the classical action (it need not be the inverse of some small coupling $1/\lambda$).

Chapter 1

Behavior of Cross Sections for Large Numbers of Particles

1.1 Introduction

The perturbation expansion of Greens functions in quantum field theories is typically asymptotic, with the coefficient of the n'th order terms exhibiting factorial growth in n[48]. This can be attributed to the factorial growth in the number of Feynman diagrams with n.For some time it has been noted that there is similar growth in the amplitudes for processes in scalar field theories with large numbers of final state particles N, e.g. in $2 \to N$ processes, already at the level of the leading order Feynman diagrams[49–52]. This happens because, near threshold, the amplitudes are only very weak functions of momenta, and there are $N!$ ways of rearranging the various final state particles in the lowest order diagrams. At extremely high energies estimates are more challenging, but there would seem likely to be factorially large numbers of contributions

to amplitudes with the same sign. Various attempts have been made to compute or estimate the behavior of amplitudes and cross sections in the limit of large N. These analyses are in some instances perturbative, and in some instances attempt to include non-perturbative effects. More recently it has been argued that the growth of amplitudes implies a physical cutoff at energies much less than the Planck mass $M_{\rm pl}$, thereby reducing the severity of the hierarchy problem[53, 54].

In this paper, we take a critical look at the question of the growth of scattering amplitudes and cross sections at very large N in $\lambda\phi^4$ theory. We start with the simple observation that the problem is *inherently non-perturbative* for $N \gg 1/\lambda$: at each order in λ, one obtains additional powers of N; the expansion parameter is λN. We will focus on two classes of processes: $2 \to N$ scattering and $N \to N$ particle scattering. We will work near threshold (with $|\vec{p}| = \epsilon m$, where m is the particle mass and ϵ is a small number which *does not* scale with N). In the first case, the scattering amplitude in lowest order of perturbation theory grows as $N!$. Bose symmetry gives a $1/N!$ factor, and the phase space integral gives neither $N!$ enhancement or suppression. So one has a cross section which grows as $N!$. In the case of $N \to N$ scattering there are, at large N, of order $(2N)!$ independent contributions to the scattering amplitude at low orders, suggesting $(2N)!$ growth of the scattering rate. But even near threshold the amplitudes have complicated dependence on the momenta. If we focus on the most singular momentum region, the perturbative rates do not exhibit factorial growth, and we give a crude argument that this singular region dominates the cross section.

In either case the perturbative analysis is not reliable when $N \gtrsim \lambda^{-1}$, and we would like some insight (and ideally a systematic approximation scheme) into these

processes. In the case of $N \to N$ scattering we describe a non-perturbative computation which we suspect to be the leading approximation in a systematic expansion in $1/\sqrt{N}$. This yields a cross section which *decreases* factorially with N as N becomes very large. In the case of $2 \to N$, we adopt a different approach. There does not appear to be a simple reorganization of the problem which would permit a systematic approximation in $1/N$. We describe an admittedly crude computation which suggests, again, that amplitudes grow more slowly than in perturbation theory and cross sections don't exhibit factorial growth.

As a strategy to explore the non-perturbative behavior we consider the problem from the perspective of the path integral. To cast the scattering problem in this language we employ the LSZ formalism. To render the LSZ result in a fashion which is convenient for a path integral analysis we can proceed in two ways. One approach is to reorganize the Feynman diagram expansion into a finite (power of N) number of classes of diagrams, each of which can be expressed as an integral of a Green's function weighted by external wave functions. Each of these Green's functions, in turn, can be simply expressed as a path integral. In some cases, taking the large N limit allows one to evaluate these by semiclassical methods. This statement relies critically on the use of normalizable wave packets, and the fact that there is a small space-time region where all of the wave packets coincide. From the path integral perspective, it is only in this small region of space-time, involving only a small subspace of the field space, where the large value of N is important. The amplitudes do indeed appear to be dominated by a particular classical configuration; more precisely a particular region of integration. This allows a simple determination of the scaling with N, and a possible systematic expansion in $1/N$

for the case of $N \to N$ scattering. For $2 \to N$, we adopt a different approach. The analysis is not systematic but strongly suggestive. As in the $N \to N$ case, this leads to an expectation that the growth of the amplitude is slower than in perturbation theory, and that the cross sections do not exhibit factorial growth with N.

In the rest of this note we investigate these questions. Other critiques and responses have appeared elsewhere[55–57]; the issues we raise are somewhat different. We will set aside the question of whether the theory has a sensible limit as its ultraviolet cutoff is taken to ∞, but will explain the analysis which leads to the results stated above. We first review, in section 1.2, the leading perturbative result for the cross section in $2 \to N$ scattering. We illustrate features of $N \to N$ scattering in section 1.3. While there are a vast number of diagrams we isolate a subset of them by examining a singular kinematic limit, where in low orders of perturbation theory there is not factorial growth of the coefficient of the most singular behavior. We then argue that while the non-singular diagrams are far more numerous, they are suppressed by factors of $1/N$ relative to the singular diagrams.

In both cases, as we note in section 1.4, perturbation theory becomes unreliable when $N \gtrsim 1/\lambda$, so any would-be conflicts with unitarity should arguably be viewed with skepticism when derived from a perturbative framework. To obtain some insight into the non-perturbative problem, in section 1.5, we review the behavior of a simple one-dimensional integral (zero-dimensional field theory) which possesses some of the features expected of actual ϕ^4 theory. In section 1.6.1 we review some basic aspects of scattering of wave packets in non-relativistic quantum mechanics in order to set the stage for our discussion of some aspects of the LSZ formula in section 1.6.2. In

particular, we focus on the scattering amplitude for normalizable initial and final states as well as aspects of the path integral. In section 1.7.1 we explain why, in the case of $N \to N$, this reorganization of the path integral is particularly effective and why the approximation appears systematic. We also show that the amplitude is substantially reduced over the leading perturbative contribution. On the other hand, for $2 \to N$, the approach provides, at best, a crude estimate. A more useful strategy, developed in section 1.7.2, involves the study of an effective action for $2 \to N$ processes, where the N final state particles are near threshold. This problem can also be expressed in path integral language and one can obtain a recursion relation for $\Gamma_{2\to N}$ for different values of N. The recursion relation, for $N \ll 1/\lambda$, reproduces the perturbative result, but it leads to slower growth at larger N. This, in turn, translates into a cross section which does not exhibit factorial growth.

In our concluding section we remark on implications of this work for unitarity at large N, and also suggest possible further directions which might give greater control over this particular limit of quantum field theories.

1.2 Perturbative Analysis of $2 \to N$ Scattering in $\lambda\phi^4$ Theory

We begin this section by reviewing a conventional perturbative analysis [49–52] of the production of N non-relativistic scalars near threshold in a $\lambda\phi^4$ theory from an initial state of two very highly energetic particles. The case where $N = 2\times 3^k$ lends itself to a simple analysis. In that case there is a diagram where the two incident scattered

particles produce two particles, and then each splits into three, each of these splits into three, and so on, $k-1$ times. All of the internal lines are far off shell, and one can neglect the small kinetic energies of the final states. As a result, there are $N!$ nearly identical contributions to the amplitude.

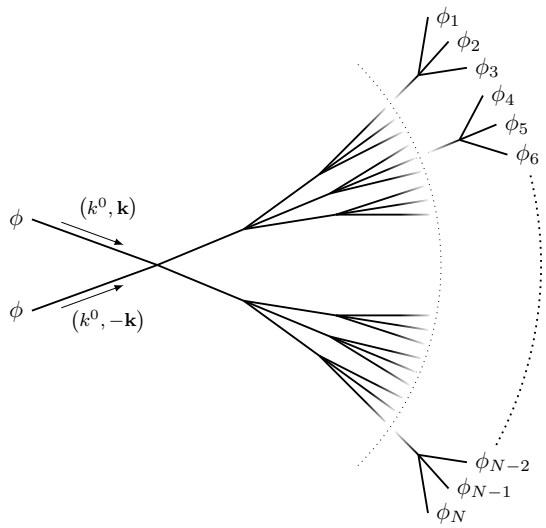


Figure 1.1: The initial state particles scatter to two very off shell particles, which then decay to three particles, and those particles decay to more particles, etc...

One might wonder whether there is suppression arising from the numerous propagators in the graph. The total number of vertices for this diagram is:

$$\begin{aligned} V =& 1 + 2\left(1 + 3 + 3^2 + \cdots + 3^{k-1}\right), \\ =& 1 + 2\left(\frac{3^k - 1}{2}\right), \\ =& \frac{N}{2}. \end{aligned} \tag{1.2.1}$$

The propagator suppression can be determined in a similar fashion. Take the initial momenta to be

$$k_1 \sim \left(\frac{Nm}{2}, 0, 0, \frac{Nm}{2} - \Delta\right), \quad (N \to \infty)$$
$$k_2 \sim \left(\frac{Nm}{2}, 0, 0, -\frac{Nm}{2} + \Delta\right), \quad (N \to \infty) \tag{1.2.2}$$

Where $\Delta \ll Nm$. The propagator suppression is (in units with the meson mass, m, set equal to one):

$$h(N) = \left[\frac{1}{\left(\frac{N}{2}\right)^2 - 1}\right]^2 \times \left[\frac{1}{\left(\frac{N}{2}\right)^2 3^{-2} - 1}\right]^6 \times \ldots \times \left[\frac{1}{\left(\frac{N}{2}\right)^2 3^{-2(k-1)} - 1}\right]^{2\times 3^{k-1}} \tag{1.2.3}$$

Taking the log and neglecting the factors of -1 in the propagator gives:

$$\ln(h(N)) \sim -3\ln(3)\frac{N}{2} + 2\ln\left(\frac{N}{2}\right) + \ln(3), \quad (N \to \infty) \tag{1.2.4}$$

There is no net $N!$ suppression from the large number of propagator factors. While we won't make claims as to the dominance of this set of diagrams, other classes of tree level graphs *do* have an $N!$ type kinematic suppression. For example, if most of the external lines connect in pairs to a single line, there is a substantial suppression. Considering only this class of diagrams, of which there are roughly $(3N/2)!$[1], and after dividing by a factor of $(N/2)!$ coming from the $N/2$ insertions of the interaction Lagrangian, we find:

$$\mathcal{M}_{2\to N} \sim 3^{-3N/2} N! \left(\frac{\lambda}{4}\right)^N \quad (N \to \infty) \tag{1.2.5}$$

[1]There are of order $N!$ ways to rearrange the external lines and $(N/2)!$ ways to relabel the vertices. In the $N \to \infty$ limit we write the product of $N! \times (N/2)! \Rightarrow (3N/2)!$ The sense in which we mean this is that both sides of the $\Rightarrow$ have factors of N^{cN} which are identical. In this paper we are primarily concerned with factors of N^{cN} and we will typically neglect factors such as a^N and N^b.

In the cross section there is a factor of $1/N!$ from Bose statistics. There is also a suppression from phase space when all of the particles are non-relativistic. If we assume that, in the center of mass frame, the total energy is

$$\sqrt{s} = N(1+\epsilon)m, \tag{1.2.6}$$

where we will think of ϵ as small compared to 1 but not $1/N$, we can consider final states where the momentum of each particle is of order ϵm. Then the phase space factor is of order

$$\prod_{i=0}^{N} \int^{\sqrt{\epsilon}m} \frac{\mathrm{d}^3 p_i}{2m} \sim \epsilon^{3/2N} m^{2N}. \quad (\epsilon \to 0, N \to \infty) \tag{1.2.7}$$

Multiplying by the squared amplitude (restoring the factors of m and multiplying by the Bose statistics factor) the cross section goes like

$$\sigma_{2\to N} \sim \left(\frac{\epsilon}{3}\right)^{3/2N} N! \left(\frac{\lambda}{4}\right)^{N/2}, \quad (\epsilon \to 0, N \to \infty)\,. \tag{1.2.8}$$

For ϵ a small, but fixed, number the suppression from the phase space integral does not compensate the factorial growth in the amplitude for $N > 1/(\epsilon\lambda^2)$. As we will elaborate in section 1.4, the perturbative analysis is generally invalid once $N \gtrsim \lambda^{-1}$. Our goal will be to get some idea of the behavior in this non-perturbative region. We will not be able to give a systematic analysis in λ and N, but we will argue shortly that the non-perturbative growth of the amplitude is no faster than $(N/2)!$ As a result cross sections do not show factorial growth and there are no conflicts with unitarity. In the next section we will study a different class of processes exhibiting factorial growth in

the number of Feynman diagrams, for which a systematic analysis *may* be possible.

1.3 $N \to N$ Scattering

Another interesting class of processes involves $N \to N$ scattering with all particles near threshold. Naïvely, given that there are of order $(N!)^2$ similar contributions to the amplitude, while the Bose statistics factor behaves as $1/N!$, potentially leading to a rapid growth in the cross section. It is necessary, however, to consider possible kinematic enhancement and suppression.

In particular, in leading order in perturbation theory, there are kinematical enhancements of certain classes of diagrams. A particularly singular region occurs when all (spatial) momenta are non-relativistic, and pairs of momenta are nearly equal: $\vec{p}_i = \vec{k}_i + \delta\vec{p}_i$. Then there are $N!$ contributions where all of the internal lines are within $\vec{p}_i \cdot \delta\vec{p}_i$ of the mass shell. To compute the amplitude we need to weight the Feynman diagrams with the initial and final wave functions and integrate. It is most convenient to work in momentum space.

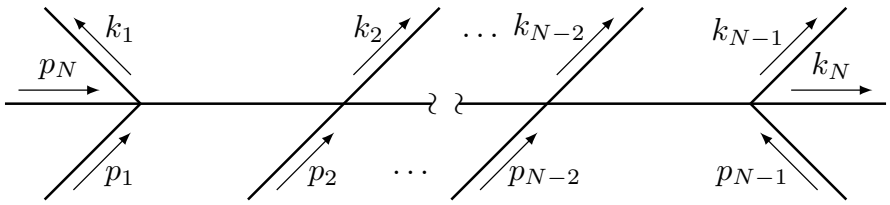


Figure 1.2: $N \to N$ scattering. At every vertex an initial state particle scatters to a final state particle with almost no momentum exchange. All of the propagators are then nearly on shell.

Consider the squared amplitude and integrate over final states for some fixed initial configuration. If the typical magnitude of the three-vector momentum is p, then

we restrict the final state momenta to all be of order p, and focus on the integration region:

$$\vec{k}_i = \vec{p}_i + \delta\vec{k}_i, \quad i = 1, \ldots, N; \quad \left|\delta\vec{k}_i\right| < \Delta k \ll p. \tag{1.3.1}$$

In this region of phase space we focus on the $(2N)!$ diagrams where (at all but two vertices, involving $\vec{k}_N$ and $\vec{p}_1$) the i^{th} final state particle emerges from the vertex from which the $(i+1)^{\text{th}}$ initial state particle enters. The resulting amplitude behaves as

$$\mathcal{M}_{N\to N} \sim \frac{(2N)!}{N!}\left(\frac{\lambda}{4}\right)^{N-1}\prod_{i=1}^{N-2}\frac{i}{2\sum_{j=1}^{i}\left(\vec{k}_1 - \vec{k}_{j+1}\right)\cdot\delta\vec{p}_j}, \quad (\delta\vec{p}_i \to 0, N\to\infty). \tag{1.3.2}$$

Note that because of the pairing, there is an $N!$ rather than $(2N)!$ factor. When we square the amplitude, integrate over the momenta $\delta\vec{p}_i$, divide by the Bose statistic factors for the initial and final states, and restrict $|\delta\vec{p}_i| \ll p$ we obtain

$$\sigma_{N\to N} \sim N!\frac{p^N(\Delta k)^N}{\mu^{2N}}, \quad (N\to\infty). \tag{1.3.3}$$

With a similar restriction on the momenta, but without the pairing, one has a suppression by at least two powers of $\Delta k/p$ for each unpaired momentum.

There are in fact, for fixed values of the initial and final momenta, vastly more diagrams which do not exhibit this pairing ($(2N)!$ rather than $N!$). However, these diagrams are further suppressed by powers of N coming from the large number of terms in some of the denominator factors. Roughly, the typical denominator is a sum of N^2 terms, with random signs, so we might expect the sum to be of order N for roughly half the order N propagators. The full propagator suppression might then be of order $1/N!$

from these diagrams, so that they are similar to those discussed previously, without the extra kinematic enhancement. Moreover, the diagrams have phases, so we might expect a factor of order $N!$ rather than $(2N)!$ contribution to the amplitudes from summing over all of the permutations in which not all momenta are paired.

We don't claim this analysis to be more than suggestive, but we do believe it is plausible that with these kinematic restrictions, even at the lowest non-trivial order in perturbation theory, the factorial growth of the amplitudes is bounded from above[2] by $(N/2)!$. This is despite the roughly $(3N/2)!$ Feynman diagrams that contribute to tree level processes. However, any estimate derived from perturbation theory is not reliable once $N \gtrsim \lambda^{-1}$.

We will argue in the following sections that, non-perturbatively and in the region with small paired momenta, there is actually a factorial *suppression* of the amplitude. We believe that this suppression can be rigorously established. For other regions of phase space, our arguments for suppression will be plausible but less rigorous. In any case, these considerations suggest that there is a region of phase space in which the cross section does not exhibit factorial growth, though it is enhanced by inverse powers of small momenta compared to naïve expectations.

[2]Here N is the total number of external particles. For a process that goes like $N \to N$ there are $2N$ external lines, so the bound should be stated as:

$$\mathcal{M}_{N\to N} = o\,(N!) \quad (N \to \infty).$$

1.4 Limitations of The Perturbative Analysis

Going Beyond

Perturbation theory is not reliable for either of the previously discussed processes for sufficiently large N. If $N \gg \lambda^{-1}$ then, for either $2 \to N$ or $N \to N$ scattering, one has an expansion in powers of λN. Once $N \gg 1/\lambda$ any partial sum of the perturbative series becomes a very poor approximation of the true amplitude.

A quick way to see that the expansion is a power series in λN is to consider coupling constant renormalization. At leading order we have seen that the scattering amplitude behaves as $\lambda^{N/2}$ or λ^N for $2 \to N$ or $N \to N$ processes respectively. The effect of one loop renormalization is to replace $\lambda \to \lambda(1 + A\lambda)$, so expanding in powers of λ we have a term of order $AN\lambda$. This counting is easily seen to be general by examining other classes of Feynman diagrams.

We have established that, order by order in perturbation theory, as one approaches the relativistic limit scattering amplitudes exhibit factorial growth for processes such as $2 \to N$ particles. However, it is not immediately clear how seriously to take these results. It is perhaps troubling to uncover a set of questions in quantum field theory which, even at weak coupling, we lack the tools to explore. We take some steps towards the non-perturbative study of large N amplitudes in the following sections.

1.5 A Model for Factorial Growth of Amplitudes

A Simple One Dimensional Integral

Certain features of the large order behavior of perturbation theory in quantum mechanics and quantum field theory can be modeled by an ordinary integral. One of our goals in this paper will be to reduce the scattering amplitudes for large N to similar integrals. In a theory with $\lambda\phi^4$ coupling, the one dimensional integral,

$$Z(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\phi \, e^{-\frac{1}{2}\phi^2 - \frac{\lambda}{4}\phi^4}, \tag{1.5.1}$$

counts (vacuum) Feynman diagrams. Indeed, we can expand in powers of λ using "Wick's Theorem" to write a Feynman diagram expansion. In this one dimensional problem, the "propagator" is just 1; there are no momentum integrals to do. So every diagram at order k gives simply $\frac{(-1)^k}{k!}\left(\frac{\lambda}{4}\right)^k$. Performing the expansion, order by order, gives:

$$Z(\lambda) = \sum_{k}^{\infty} z_k \left(\frac{\lambda}{4}\right)^k, \tag{1.5.2}$$

where

$$z_k = \frac{1}{\sqrt{\pi}} \frac{(-1)^k}{k!} 4^k \, \Gamma\left(2k + \frac{1}{2}\right). \tag{1.5.3}$$

So we see factorial growth of the number of diagrams, and that the perturbation expansion is an asymptotic expansion, reliable only for $k \lesssim 1/\lambda$. The original integral is, of course, finite for all $\lambda : \mathrm{Re}(\lambda) > 0$. The result can be written as a modified Bessel function (See Appendix A.1); it is easy to check numerically that the series gives good

agreement with the exact result if one only includes terms up to k somewhat smaller than $1/\lambda$.

For scattering in quantum field theory, we are interested in (connected) N-point functions. Correspondingly, we can start with the study of the simple one dimensional (Euclidean) integral:

$$\begin{aligned} Z(N,\lambda) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\phi\, \phi^N e^{-\frac{1}{2}\phi^2 - \frac{\lambda}{4}\phi^4}, \\ \sim& \frac{2^{N/2}}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} 4^k\, \Gamma\!\left(\frac{4k+N+1}{2}\right) \left(\frac{\lambda}{4}\right)^k, \quad (\lambda \to 0). \end{aligned} \tag{1.5.4}$$

Provided $N \lesssim 1/\lambda$, such that the asymptotic series reasonably approximates the function, we see that $Z(N,\lambda)$ exhibits factorial growth in N,

$$Z(N,\lambda) \sim \frac{1}{\sqrt{\pi}} 2^{\frac{N}{2}}\, \Gamma\!\left(\frac{N+1}{2}\right), \quad (\lambda \to 0). \tag{1.5.5}$$

The leading connected diagrams occur at order $k = (N-2)/2$. Correspondingly, we expect a contribution to Z:

$$\begin{aligned} Z(N,\lambda) \sim& -\frac{1}{\sqrt{\pi}} \frac{(-1)^{N/2}}{\left(\frac{N-2}{2}\right)!} 2^{\frac{3N-4}{2}}\, \Gamma\!\left(\frac{3N-3}{2}\right) \left(\frac{\lambda}{4}\right)^{(N-2)/2}, \quad (\lambda \to 0) \\ \sim& -(-1)^{N/2} \frac{54^{N/2}}{9\sqrt{2\pi}} N^{-3/2} e^{N\ln(N) - N} \left(\frac{\lambda}{4}\right)^{(N-2)/2}, \quad (\lambda \to 0, N \to \infty) \end{aligned} \tag{1.5.6}$$

So for this problem, perturbation theory is valid for $N < 1/\lambda$. We will explain shortly, and in an appendix, why this counting, which includes both connected and disconnected diagrams, gives the correct $N!$ dependence of the amplitudes in this limit.

For $\lambda N \gg 1/4$ the behavior is different, though the integral still exhibits factorial growth in N for fixed λ. The maximum of the integrand is located at

$$\phi_c^4 + \frac{1}{\lambda}\phi_c^2 - \frac{N}{\lambda} = 0 \tag{1.5.7}$$

For λN very large the location of the maximum is shifted substantially away from the origin, and the integrand is dominated by $\phi_c^4 \sim N/\lambda$.

$$Z(N,\lambda) \sim \frac{2^{(N+1)/2}}{N^{1/4}\lambda^{(N+1)/4}} \exp\left(\frac{N}{4}\ln\left(\frac{N}{4}\right) - \frac{N}{4} - \frac{1}{2}\sqrt{\frac{N}{\lambda}} + \frac{5}{16\lambda}\right), \quad (N \to \infty). \tag{1.5.8}$$

It is easy to check these statements numerically.

So we have learned that, for $N \gg 1/\lambda$, $Z(N,\lambda)$ exhibits factorial growth, but much slower than the factorial growth of perturbation theory. In subsequent sections, we will argue that the behavior of scattering amplitudes at large N is similar: they exhibit factorial growth, but *slower* than that of perturbation theory.

1.6 From an Ordinary Integral to the Path Integral

As a model for scattering amplitudes in field theory, the integral $Z(N,\lambda)$ is instructive, but has several limitations. The first is a relatively trivial one: the exponential should be a phase (the argument should be purely imaginary). This does not affect our large N estimate. Analytically continuing the integral (1.5.4) to the complex ϕ plane we find it is absolutely convergent in four wedges, which are rotated by the phase of the coupling (Figure 1.3).

So the integral defines a function of λ analytic in a wedge. The estimate above holds perfectly well if we simply rotate the variable ϕ by a constant phase angle of $\frac{\pi}{4}$ and simultaneously rotate the coupling by $-\frac{\pi}{2}$.

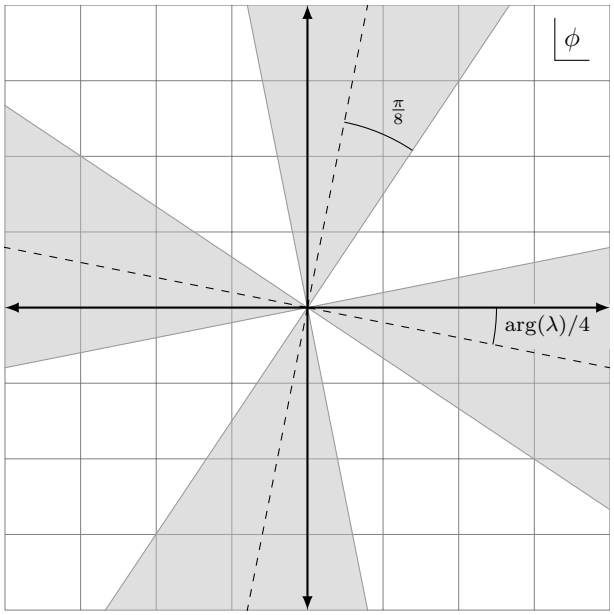


Figure 1.3: Regions of convergence of the integral in (1.5.4). Contour integrals beginning and ending in the gray shaded regions converge. The Euclidean version of the integral is related to the Minkowski version by $\arg(\phi) = \frac{\pi}{4}$, $\arg(\lambda) = -\frac{\pi}{2}$.

Another limitation is that the integral (1.5.4), in addition to generating connected diagrams, also generates vacuum and disconnected diagrams. However, the rough factorial growth of the generating function $Z(j)$ and $W(j) \coloneqq \ln(Z(j) \,/\, Z(0))$ is the same. This is readily proven by contradiction. Moving over to the full field theory, the generating functional $Z[J]$ is described by a convergent series in inverse powers N. As a result, so is $W[J]$. If terms in the expansion of W grow more rapidly with N than those of Z then, in fact, the growth of W must be faster than Z; similarly if terms in W grow more slowly.

This last issue will not be so severe in $3+1$ dimensions (as opposed to 0) when we work with wave packets, each of some average momentum. Due to momentum conservation, in processes with $2 \to N$ particles, the associated disconnected contributions to the Green's functions will largely vanish. So it is enough to divide out the vacuum

diagrams.

The path integral is certainly far more complicated than the ordinary integral, and the question is: to what degree is the behavior of this integral an indicator of what happens in field theory. Various approaches have been offered as solutions to this problem. We will argue that a particularly simple one is to use the LSZ formula, with normalizable wave packets. As a result, the effects of large N are important only in a small space-time region where the wave packets overlap. One might then expect that, limited to this region, the path integral *would* be much like the ordinary integral. Translating the results for the ordinary integral to the behavior of the field theory path integral is the subject of the next few subsections.

1.6.1 Review of Non-Relativistic Scattering in Terms of Wave Packets

Our analysis of many particle scattering will rely on a wave packet approach. In particular, it assumes that we can think of the scattering amplitude in terms of normalizable initial and final wave packets labeled by a central momentum $\vec{p}_i$ and $\vec{p}_f$ respectively. It is helpful to review the problem of wave packet scattering in ordinary quantum mechanics. We first consider how to pass between the scattering amplitude in the plane wave basis to a basis of normalizable states[58]. Consider, in particular, the scattering amplitude of a particle in a potential, $V(\vec{x})$, with initial and final wave packets, $\psi_i(t, \vec{x})$ and $\psi_f(t, \vec{x})$. We write the Fourier transform of these wave packets as:

$$\begin{aligned}\psi_i(t,\vec{x}) &= \int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\tilde{\psi}_i(\vec{p})\,e^{-ip\cdot x},\\ \psi_f(t,\vec{x}) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\,\tilde{\psi}_f\Big(\vec{k}\Big)\,e^{-ik\cdot x}.\end{aligned} \tag{1.6.1}$$

where $k^0 \equiv E\Big(\vec{k}\Big)$ and $p^0 \equiv E(\vec{p})$ are the (on-shell) energy. We require the momentum space distribution of scattering states to be narrowly centered on the average momentum, a reasonable fulfillment of this requirement is to approximate the momentum distributions by very narrow Gaussians:

$$\begin{aligned}\tilde{\psi}_i(\vec{p}) =& \Big(2\pi\sigma^2\Big)^{-3/2} e^{-\frac{(\vec{p}-\vec{p}_i)^2}{2\sigma^2}} e^{i\vec{p}\cdot\vec{x_0^i}},\\ \tilde{\psi}_f\Big(\vec{k}\Big) =& \Big(2\pi\sigma^2\Big)^{-3/2} e^{-\frac{\left(\vec{k}-\vec{k}_f\right)^2}{2\sigma^2}} e^{i\vec{k}\cdot\vec{x_0^f}}.\end{aligned} \tag{1.6.2}$$

We have taken the spread in the momentum space wave packets to be identical for simplicity. At non-relativistic energies the coordinate space center of these wave packets propagate as

$$\begin{aligned}\langle\vec{x}\rangle_i &\sim \vec{x_0^i} + \frac{\vec{p}_i}{m}t, \quad (\sigma \to 0),\\ \langle\vec{x}\rangle_f &\sim \vec{x_0^f} + \frac{\vec{p}_f}{m}t, \quad (\sigma \to 0),\end{aligned} \tag{1.6.3}$$

and have a widths that increase with time. We will assume, again for simplicity, that this spreading can be neglected during the scattering process, so $\Delta x \approx \frac{1}{\sigma}$. To obtain an appreciable amplitude it is necessary that the trajectories of the two waves coincide during some time interval of order m/σ.

We'll confine our attention to the Born approximation for the scattering amplitude and work in the interaction picture. We first consider as a basis of scattering states

(non-normalizable) plane waves. We can write the S-matrix in terms of the interaction picture time-development operator, $U(t_1, t_2)$ as (taking the limit $T \to \infty$):

$$\langle \vec{p}_f | \, U(T/2, -T/2) \, | \vec{p}_i \rangle \coloneqq \langle \vec{p}_f | \, S \, | \vec{p}_i \rangle \tag{1.6.4}$$

where

$$\langle \vec{p}_f | \, S \, | \vec{p}_i \rangle = \langle \vec{p}_f | \vec{p}_i \rangle + (2\pi i) \delta \left(E_f - E_i \right) \langle \vec{p}_f | \, H' \, | \vec{p}_i \rangle \, . \tag{1.6.5}$$

The second term is the T matrix. In terms of the plane wave basis, the scattering amplitude for our wave packets, ψ_i, ψ_f is

$$\mathcal{A}_{i \to f} = \int \frac{\mathrm{d}^3 p_i}{(2\pi)^3} \frac{\mathrm{d}^3 p_f}{(2\pi)^3} \, \tilde{\psi}_f^*(\vec{p}_f) \, \langle \vec{p}_f | \, S \, | \vec{p}_i \rangle \, \tilde{\psi}_i(\vec{p}_i) \, . \tag{1.6.6}$$

Calculating the amplitude to first order in perturbation theory in terms of normalizable states in the interaction picture, we can understand the expression in Equation (1.6.6) in another way. In general, far away from the forward direction, the amplitude that an initial state $|\Psi_i\rangle$ time evolves into a state $|\Psi_f\rangle$ is:

$$\mathcal{A}_{i \to f} = \int_{-T/2}^{T/2} \langle \Psi_f | \, e^{iH_0 t} H' e^{-iH_0 t} \, | \Psi_i \rangle \, \mathrm{d}t \, . \tag{1.6.7}$$

We can rewrite this in terms of Schrödinger picture states:

$$\mathcal{A}_{i \to f} = \int \langle \Psi_f(t) | \, H' \, | \Psi_i(t) \rangle \, \mathrm{d}t \, . \tag{1.6.8}$$

So for our scattering problem,

$$\begin{aligned}\mathcal{A}_{i\to f} &= \int_{-T/2}^{T/2} \mathrm{d}t \int \frac{\mathrm{d}^3 p_f}{(2\pi)^3}\frac{\mathrm{d}^3 p_i}{(2\pi)^3}\, \tilde{\psi}_f^*(t,\vec{p}_f)\, \langle \vec{p}_f |\, H' \,| \vec{p}_i \rangle\, \tilde{\psi}_i(t,\vec{p}_i) \\ &= \int_{-T/2}^{T/2} \mathrm{d}t \int \frac{\mathrm{d}^3 p_f}{(2\pi)^3}\frac{\mathrm{d}^3 p_i}{(2\pi)^3}\, \tilde{\psi}_f^*(\vec{p}_f)\, e^{-i\left(E_i - E_f\right)t}\, \langle \vec{p}_f |\, H' \,| \vec{p}_i \rangle\, \tilde{\psi}_i(\vec{p}_i) \qquad (1.6.9) \\ &= 2\pi \int \frac{\mathrm{d}^3 p_f}{(2\pi)^3}\frac{\mathrm{d}^3 p_i}{(2\pi)^3}\, \tilde{\psi}_f^*(\vec{p}_f)\, \delta\left(E_f - E_i\right) \langle \vec{p_f} |\, H' \,| \vec{p_i} \rangle\, \tilde{\psi}_i(\vec{p}_i)\end{aligned}$$

The second line is equivalent to the coordinate space expression:

$$\mathcal{A}_{i\to f} = \int_{-T/2}^{T/2} \mathrm{d}t \int \mathrm{d}^3 x\, \psi_f^*(t,\vec{x})\, H'(\vec{x})\, \psi_i(t,\vec{x})\,. \qquad (1.6.10)$$

If H' is short range, then this last expression has support only when the wave functions overlap in a space-time region with size less than or order the range of the potential. Note that in order to obtain a cross section from this, one must take $|\mathcal{A}_{i\to f}|^2$, and integrate over $\left(\mathrm{d}^2 x_i\right)_\perp \equiv \mathrm{d}^2 b$ weighted by the flux (this assumes, for simplicity, identical wave packets up to translations). One also integrates over and $\mathrm{d}^3 x_f$, for fixed $\vec{b}$, $\vec{p}_i$, and $\vec{p}_f$. The result, again, is appreciable only for a range of $\vec{x}_f$ where the wave packet points back to the interaction point. In this range, one can replace $\mathrm{d}^3 x_f = r^2\, \mathrm{d}r\, \mathrm{d}\Omega$, allowing construction of the differential cross section. This will, in fact, give a contribution proportional to the "cross section" of the target, the fractional region over which the integrand is substantial. For a given $\vec{p}_f$, this fixes $\vec{x}_f$ to lie in a small region, $|\vec{x}_f| < \mu^{-1}$, the range of the potential.

This generalizes immediately to multichannel problems with, for instance, one particle initially impinging on a target (say a high Z atom), and many particles emerging. Again, one has an overlap of the Schrödinger wave function for the initial state, evolved with the free particle Hamiltonian to some time t, and the final state particles,

evolved back to time t. To obtain an appreciable result, there must be a time t where all of the wave functions coincide within a space-time region of order the range of the potential. Again, the (differential) cross section is obtained by integrating over $\mathrm{d}^2 x_i$ and dividing by the incoming flux.

If one formulates the amplitude in terms of the path integral, the integration $\int [\mathrm{d}x]$ is only significantly modified from the free particle result for the narrow range of variables $x(t)$ corresponding to the time interval where the wave packets overlap.

1.6.2 Scattering of Wave Packets using the LSZ Formula and the Path Integral

We want to consider processes with many particles in the initial and/or final state. Our goal is to determine the growth of the scattering amplitude for $N \gg 1/\lambda$.

The LSZ formula for scattering casts the problem of scattering in terms of Green's functions, so it is a natural setting in which to apply path integral methods. There is some discussion of wave packet scattering in this framework in textbooks, e.g. [59]. We will review this here, from a perspective close to the non-relativistic problem which we have described in the previous section, and which will be useful for the questions we are studying here.

Let's consider ϕ^4 theory. In the LSZ formula, for a scattering process with M particles in the initial state and N particles in the final state, we are instructed to evaluate the quantity:

$$\prod_{i=1}^{M+N} \left[\int \mathrm{d}^4 x_i \, f_i(x_i) \left(\partial_i^2 + m^2 \right) \right] \langle \phi(x_1) \dots \phi(x_{N+M}) \rangle \,, \tag{1.6.11}$$

where the functions f_i satisfy the free Klein-Gordan equation. We would like to treat this expression in the path integral, studying possible modifications associated with the large number of particles in the initial and final states, $M+N$. The inverse propagators in Equation (1.6.11) make this somewhat awkward, particularly when we attempt a large N, semiclassical treatment. One approach is to consider *classes* of diagrams where one contracts the external fields with fields in vertices, and evaluates the remaining Green's function. One then has to sum over the different classes.

An alternative is also useful. One traditional derivation of the LSZ formula starts with initial and final states at times $t = \pm T$, and evaluates:

$$\mathcal{M} = \prod_{i=1}^{M} \left[\int \mathrm{d}^3 x_i \, \psi_i(\vec{x}_i) \right] \prod_{j=1}^{N} \left[\int \mathrm{d}^3 y_j \, \xi_j(\vec{y}_j) \right]$$

$$\times \langle \phi(-T, \vec{x}_1) \dots \phi(-T, \vec{x}_M) \, \phi(T, \vec{y}_1) \dots \phi(T, \vec{y}_N) \rangle \,. \tag{1.6.12}$$

Here ψ_i, ξ_j are initial and final state wave functions at times $\pm T$. They are taken to be normalizable and non-overlapping. The correlation function can be studied perturbatively. A non-perturbative approach could involve construction of a one-particle irreducible effective action at $(N+M)^{\text{th}}$ order in ϕ. If this interaction, $\Gamma_{M \to N}$, is local the structure of the resulting path integral has many features in common with the toy integral. In particular, only the integration over a small local region of space-time is modified by large N.

1.7 Non-Perturbative Analysis

1.7.1 $N \to N$

We have argued that we can reduce the problem of computing the scattering rate for large numbers of particles to a problem of summing over a finite set of correlation functions which can be evaluated using the path integral. We might hope that large N might facilitate a non-perturbative evaluation, as in the case of the ordinary integrals we studied in previous sections. The use of wave packets of finite extent enhances the fields in a small region, mimicking some features of the ordinary integral at large N.

Consider, first, the case of $N \to N$ scattering. We saw that, in perturbation theory, there is a region of the phase space integral for which one class of diagrams is enhanced dynamically. There were of order $(N!)^2$ diagrams in this subset (coming from $N!$ rearrangements of the initial state particles and $N!$ rearrangements of the final state particles) and a factor of $1/N!$ due to the number of vertices, but the corresponding $(N!)^2$ enhancement in the squared amplitude was compensated by the Bose statistics factors associated with the initial and final states. The number of diagrams without any kinematic restriction grows as $(2N)!$, but arguably the dynamical dependence of the typical diagram on N compensates this growth. On the other hand, even for the class of diagrams where the growth is not factorial, we have not yet described a systematic approach to the computation of the amplitudes, and any claim for the general behavior is conjectural. Perturbatively, the kinematically enhanced region arises when pairs of initial and final momenta are nearly the same, $\vec{p}_i = \vec{k}_i + \delta\vec{p}_i$. So calling f_i the initial state wave functions, with momenta centered around $\vec{p}_i^{\,0}$ and width Δp, and similarly

denoting the final state wave functions and mean momenta by g_i, $\vec{k}_i$, we are interested in the set of correlation functions, of which one example (dropping terms of order 1) is:

$$\mathcal{A} = \prod_{i=1}^{N} \sum_{\text{perm } g_i} \int \mathrm{d}^4 x_i \left\langle \phi^2(x_1) \dots \phi^2(x_N) \right\rangle f_1(x_1)\, g_1^*(x_1) \dots f_N(x_N)\, g_N^*(x_N)\,. \quad (1.7.1)$$

This integral is much like our one dimensional toy example in two ways. First, writing this as a path integral and exponentiating the fields appearing in the Green's function:

$$\mathcal{A} = \int [\mathrm{d}\phi] e^{i\int \mathrm{d}^4 x \left\{ \frac{1}{2}(\partial_\mu \phi)^2 - \frac{m^2}{2}\phi^2 - \frac{\lambda}{4}\phi^4 \right\} + \sum_{i=1}^{N} \ln[\int \mathrm{d}^4 x f_i(x) g_i^*(x) \phi^2(x)]}. \quad (1.7.2)$$

The logarithmic term in the exponent is enhanced when all of the points nearly coincide. This enhancement is largest if pairs of the f_i's and g_i's are nearly the same, in which case the exponent is of order N. This is similar to the configurations of parallel momenta we discussed in perturbation theory. For random permutations, we might expect the exponent to be of order $\sqrt{N}$. If we assume that the path integral is dominated by a particular classical configuration, $\phi_{\mathrm{cl}}(x)$, we have:

$$\left(\partial^2 + m^2\right) \phi_{\mathrm{cl}}(x) = \lambda\, \phi_{\mathrm{cl}}^3(x) + 2 \sum_{i=1}^{N} \frac{f_i(x)\, g_i^*(x)\, \phi_{\mathrm{cl}}(x)}{\int \mathrm{d}^4 y\, f_i(y)\, g_i^*(y)\, \phi_{\mathrm{cl}}^2(y)} \quad (1.7.3)$$

For parallel or nearly parallel pairs of momenta and identical or nearly identical initial and final state wave packets, the second term on the right hand side is of order $N\phi_{\mathrm{cl}}^{-1}$. The right hand side of the equation can be made to vanish if $\phi_{\mathrm{cl}} \sim N^{1/4}$; the left hand side of the equation is then of order $N^{1/4}$, i.e. suppressed by $N^{-1/2}$ relative to the separate terms on the right hand side. In this case, the dominant term in the classical

action is of order $N\ln(N)/2$, giving an amplitude growing as $(N/2)!$, in contrast to the tree level growth of $N!$ found using perturbation theory. Alternatively, we can literally view the path integral as like our ordinary integral, thinking of $\phi(0)$ as a single variable. This yields the same $N!$ dependence as above.

For non-parallel momentum pairs, we might expect a suppression, as in the perturbative case. From this latter point of view, the contractions of the external fields where the pairs of fields have *different* momenta involve integrations over *different* variables. In this case, we might not expect the modification due to the large value of N to be captured by the model integral or the semiclassical solution. Indeed, we would not expect appreciable modifications from the perturbative result. If we attempt an analysis of the sort we did for parallel momenta in perturbation theory for non-parallel momenta, assuming that the terms in the exponent add with random phases, we would find a contribution for each contraction behaving as $(N/8)!$. The $N!$ contributions then would also add with random phases, yielding a contribution to the amplitude behaving as $(3N/8)!$. Squaring and dividing by the Bose statistics factors would yield a slightly larger contribution to the cross section, but still falling with N for large N.

We should ask: to what extent is this analysis systematic? For the subset of contributions where the momenta are paired, we can give a rough argument that corrections to the leading approximation are down by powers of N. We distinguish two types of corrections: corrections to the classical solution and "loop" corrections to the amplitude. Substituting back in the original equation and writing

$$\phi_{\rm cl} = \phi^0_{\rm cl} + \delta\phi_{\rm cl} + \delta\phi_{\rm quant}, \tag{1.7.4}$$

where $\delta\phi_{\rm cl} \sim N^{-1/4}$, i.e. the expansion of the classical solution about the leading result appears to be an expansion in powers of $N^{-1/2}$. Quantum (loop) corrections have a $\delta\phi_{\rm quant}$ propagator proportional to $N^{-1/2}$, and three point vertices of order $N^{1/4}$, so loop corrections appear to scale with $N^{-1/2}$ as well. So, while we will not investigate this further here, it appears that for these processes there is a systematic $1/N$ expansion. Establishing this requires demonstrating that classes of contributions with different contractions of the external fields are indeed suppressed.

1.7.2 $2 \to N$ Scattering

For $2 \to N$ processes we have not found a systematic $1/N$ expansion. If we proceed as we did for $N \to N$ scattering we encounter a functional integral whose integrand involves multiple integration variables (roughly $\phi\Big(nm, \vec{0}\Big)$ and $\phi\Big(rm, \vec{0}\Big)$), whose coupling is complicated. However, similar considerations suggest that the non-perturbative growth of the amplitude is far slower than the perturbative one. For instance, suppose we have computed an effective action for $2 \to N$ particles,

$$\mathcal{L}_I = \frac{\Gamma_{2\to N}}{N!}\phi^N. \tag{1.7.5}$$

We expect that if, in the center of mass frame, the typical spatial momenta is of order $|\vec{p}| \ll m$, then $\Gamma_{2\to N}$ is approximately independent of p. It is convenient to avoid the factors of inverse propagators, so with our N final state particles with wave functions $\psi_i(\vec{x})$ in the Schrödinger picture at some large time T, we need to study:

$$\mathcal{M}_{2\to N} = \frac{\Gamma_{2\to N}}{N!}\prod_i^N \left[\int \mathrm{d}^3x_i\,\psi_i(\vec{x}_i)\right]\int \mathrm{d}^4z\left\langle \phi^N(z)\,\phi(T,\vec{x}_1)\ldots\phi(T,\vec{x}_N)\right\rangle. \tag{1.7.6}$$

Note that the wave functions have support only when $\vec{x}_1,\ldots,\vec{x}_N$ are well separated at time $t=T$, and we have explicitly implemented the assumption of locality.

To determine the dependence of the scattering amplitude on N we will proceed in two steps. First, Then we will determine the N dependence of the Green's function appearing in the expression for $\mathcal{M}_{2\to N}$ in Equation (1.7.6).

Consider, first, the problem in perturbation theory. We can write an iterative relation between $\Gamma_{2\to N}$ and $\Gamma_{2\to N/3}$; these correspond to terms in the effective Lagrangian:

$$\mathcal{L}_{\text{eff}} = \Gamma_{2\to N}\frac{\tilde{\phi}^N\left(m,\vec{0}\right)}{N!} \qquad \mathcal{L}_{\text{eff}} = \Gamma_{2\to N/3}\frac{\tilde{\phi}^{N/3}\left(3m,\vec{0}\right)}{(N/3)!}. \tag{1.7.7}$$

where $\tilde{\phi}$ is the momentum space field and m is the scalar mass. For general N we can compute the N point Green's function, either starting with $\Gamma_{2\to N}$ or with $\Gamma_{2\to N/3}$, and expand the path integral to order $N/3$ in the interaction:

$$\frac{\Gamma_{2\to N}}{N!}\left\langle\tilde{\phi}^N\left(m,\vec{0}\right)\phi^N\left(m,\vec{0}\right)\right\rangle = \frac{\lambda^{N/3}}{(N/3)!}\frac{\Gamma_{2\to N/3}}{(N/3)!}\left\langle\tilde{\phi}^{N/3}\left(3m,\vec{0}\right)\tilde{\phi}^N\left(m,\vec{0}\right)\tilde{\phi}^N\left(m,\vec{0}\right)\tilde{\phi}^{N/3}\left(3m,\vec{0}\right)\right\rangle. \tag{1.7.8}$$

The correlation functions can be evaluated just as for our one dimensional integrals. For $N \ll 1/\lambda$ gives

$$\Gamma_{2\to N} = \frac{N!}{(N/3)!}\Gamma_{2\to N/3}. \tag{1.7.9}$$

This is solved by

$$\Gamma_{2\to N} = CN!, \tag{1.7.10}$$

where C is a constant, as expected from perturbation theory (the constant can be determined by matching to the perturbative result). If we consider the limit $N \gg 1/\lambda$, proceeding as in Equation (1.5.8) we obtain the recursion relation:

$$\begin{aligned} \frac{(N/2)!}{N!}\Gamma_{2\to N} =& (N/2)!(N/6)!\frac{1}{(N/3)!^2}\Gamma_{2\to N/3}, \\ \Rightarrow \Gamma_{2\to N} =& C(N/2)!\Gamma_{2\to N/3} \end{aligned} \tag{1.7.11}$$

This is solved by

$$\Gamma_{2\to N} = C\left(\frac{3N}{4}\right)!, \tag{1.7.12}$$

where, again, C is some arbitrary constant. With this result we can consider the scattering amplitude using the version of the LSZ formula of Equation (1.7.6). For the perturbative case we recover the result $\mathcal{M} \sim N!$. For the case when λN is large, we have instead:

$$\begin{aligned} \mathcal{M} \sim& \left(\frac{N}{2}\right)!\left(\frac{3N}{4}\right)!\frac{1}{N!}, \quad (N \to \infty), \\ \sim& \left(\frac{N}{4}\right)!, \quad (N \to \infty) \end{aligned} \tag{1.7.13}$$

The first factor of Equation (1.7.13) is that which we have just derived for $\Gamma_{2\to N}$; the second is from the correlation function of N fields near the same point, the third is from the definition of the effective action. This result gives a *cross section* which falls off as

$$\sigma_{2\to N} \sim \frac{1}{(N/2)!} \quad (N \to \infty) \tag{1.7.14}$$

This analysis is not systematic. In particular, in deriving our would-be non-perturbative recursion relation for $\Gamma_{2\to N}$, we performed an expansion of the exponent of the interaction term in powers of λ. Despite the previous concerns we make the following observations:

1. This analysis makes clear that the leading perturbative result is misleading and likely *vastly* overestimates the amplitude for large N.

2. Given that we have only considered, in effect, the summation of an infinite *subclass* of diagrams, it is likely that we still overestimate the result.

1.8 Conclusions

In quantum field theories perturbative expansions of observables around small coupling are almost always divergent asymptotic expansions; if λ is a typical coupling constant, the number of Feynman diagrams at order k is typically of order $(2k)!$, and the series approximates the actual theory only for $k \lesssim 1/\lambda$.

For scattering processes involving large numbers of particles there is also factorial growth of the number of diagrams, now with the *number of particles*, N, as well as the order of perturbation theory. This raises two prospects: First, that perturbation

theory is not a reliable tool for computing scattering amplitudes, for sufficiently large N; and second, that the amplitudes might themselves grow quickly with N, endangering unitarity. In this paper we have investigated both of these issues. We focused on two classes of processes: $N \to N$ particles scattering, with all particles near threshold, and $2 \to N$ scattering. We first reviewed the situation in the lowest non-trivial order in perturbation theory. In $N \to N$ scattering, there is $N!$ growth in the amplitude; Allowing for Bose statistics factors, this class of contributions to the cross section does not show factorial growth. Without this restriction there are vastly more diagrams, so there is the potential for such growth, even if the vast majority of the diagrams are not kinematically enhanced. We gave crude arguments that these other diagrams actually have factorial suppression. In the case of $2 \to N$ scattering the amplitude *does* grow as $N!$, so the amplitude-squared as $(2N)!$. There is a $1/N!$ from Bose statistics, so the lowest order contribution to the cross section *does* grow factorially.

In both cases we have noted that, for $N \gg 1/\lambda$, perturbation theory breaks down. It is not *a priori* clear that any standard non-perturbative tools are available for a systematic computation. To obtain some insight into the non-perturbative problem, we have studied scattering in $\lambda\phi^4$ theory in a path integral framework. To set up the problem we have considered scattering of normalizable wave packets and worked with the LSZ expression for the scattering amplitude. Because the wave packets are localized, there is a significant modification of the path integral from the free-field form only in a small space-time region where all of the wave packets overlap. We set up the path integral problem in two ways: one more suitable for the $N \to N$ process, the other more suitable for the $2 \to N$ process.

In the case of $N \to N$ scattering we argued that the dominant contribution is due to diagrams with pairs of momenta nearly equal. This corresponds to a class of contributions which can be treated semiclassically, with the amplitude growing factorially, but more slowly than in perturbation theory, and corrections which can be computed as a series in $1/\sqrt{N}$. As a result, the cross sections for large N are suppressed, and there are no issues with unitarity. We gave some arguments that the approximation is systematic, though we will not claim they are rigorous.

For $2 \to N$ scattering we reorganized the computation in terms of an effective action for $2 \to N$. Here our tool was a recursion relation for $\Gamma_{2\to N}$. Taking the limit $N \ll \lambda^{-1}$ reproduced the results from perturbation theory. For $N \gg \lambda^{-1}$, this relation yielded much slower growth, so that the scattering cross section does not show factorial growth. As we explained, the calculation is not systematic, but it likely *overestimates* the cross section.

We note that the authors of [53, 54] have also formulated the problem in terms of classical field evolution[60]. Such a system can be described in the language of coherent states, with large values for the field eigenvalue, corresponding to large occupation numbers. This problem is slightly different than the one we have considered here, where we had many widely separated particles; the coherent state problem would correspond to large numbers of particles in, say, two identical incoming and two identical outgoing states. But in this case, the problem is equivalent to classical evolution. The classical cross section is limited by energy conservation; one can't have the equivalent of factorial growth.

What is perhaps interesting in these problems is that there is a regime of

quantum field theory for which, even at weak coupling, our standard tools of analysis fail to yield reliable results. We view our work as providing a strategy to explore this domain. It would be desirable to make the $N \to N$ analysis more solid, and to make further inroads in the $2 \to N$ problem, perhaps proving rigorous bounds if not providing a systematic approximation procedure.

Chapter 2

Asymptotic Analysis of the Boltzmann Equation for Dark Matter Relic Abundance

2.1 Introduction

Successful cosmological theories must explain various observations, such as the structure of the cosmic microwave background, baryonic acoustic oscillations, structure formation, among others. These observations always require a cold, nearly (electromagnetically) neutral, non-baryonic matter component, which we call dark matter (DM) [61, 62]. Observations with Planck [63] show that 85% of all matter in the Universe consists of DM. While we know the basic properties of DM (it interacts gravitationally and at most weakly with the known Standard Model (SM) particles), the precise nature of DM is unknown. Some of the most popular theories of DM involve extending the SM by adding new particles. DM candidates often arise naturally in models trying to

address other outstanding issues such as the hierarchy problem, the strong CP problem, and neutrino masses (e.g., neutralinos in super-symmetry [64], axions [65] and sterile neutrinos [66], respectively.)

For any theory of particle DM to be viable, the theory must produce DM with the observed relic abundance of $\Omega_{\rm DM}h^2 \equiv \rho_{\rm DM}h^2/\rho_{\rm crit} \approx 0.12$ [63], where the relative uncertainty of today's value of Hubble's parameter H_0 is absorbed into the dimensionless Hubble parameter h

$$H_0 \equiv h \times 100 \text{ km s}^{-1} \text{ Mpc}^{-1}. \tag{2.1.1}$$

Therefore, it is necessary to be able to compute the abundance of DM for a given theory accurately. The standard method for determining the abundances of DM for a given theory is by solving the Boltzmann equation, which in the standard Friedman-Roberston-Walker cosmology is [67]:

$$\frac{\partial f_\chi}{\partial t} - H\frac{|\mathbf{p}|^2}{E}\frac{\partial f_\chi}{\partial E} = \mathcal{C}[f_\chi], \tag{2.1.2}$$

where $f_\chi(\mathbf{p}, t)$ is the DM phase-space distribution, $\mathbf{p}$ the DM momentum, E the DM energy $E = \sqrt{\mathbf{p}^2 + m_\chi^2}$, H the Hubble scale and $\mathcal{C}[f]$ the collision term which depends on the details of the DM model. In all but a select few cases it is sufficient to take the first moment of this equation[1], which, in the cases where the DM interacts with the SM via $\chi\bar{\chi} \leftrightarrow$ SM, takes the form of:

$$\frac{\mathrm{d}n_\chi}{\mathrm{d}t} + 3Hn_\chi = -\langle\sigma_{\chi\bar{\chi}\to\rm SM}v_{\rm Møl}\rangle\left(n_\chi^2 - n_{\chi,\rm eq}^2\right), \tag{2.1.3}$$

[1] See Ref. [68] for an example where more than just the first moment of the Boltzmann equation must be considered.

where n_χ is the DM number density

$$n_\chi = g \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3} f_\chi, \tag{2.1.4}$$

$n_{\chi,\mathrm{eq}}$ is the DM equilibrium number density obtained by setting $f_\chi = f_{\chi,\mathrm{eq}}$ given by a Bose-Einstein or Fermi-Dirac distribution: $1/[\exp(E/T) \pm 1]$ depending on the statistics of the DM particle, and $\langle \sigma_{\chi\bar{\chi}\to\mathrm{SM}} v_{\mathrm{M\o l}} \rangle$ (which we will shorten to $\langle \sigma v_{\mathrm{M\o l}} \rangle$) is the thermally-averaged cross section:

$$\langle \sigma v_{\mathrm{M\o l}} \rangle = \frac{\int \sigma v_{\mathrm{M\o l}} f_{\chi,\mathrm{eq}}(E_1) f_{\chi,\mathrm{eq}}(E_2)\, \mathrm{d}^3\mathbf{p}_1\, \mathrm{d}^3\mathbf{p}_2}{\int f_{\chi,\mathrm{eq}}(E_1) f_{\chi,\mathrm{eq}}(E_2)\, \mathrm{d}^3\mathbf{p}_1\, \mathrm{d}^3\mathbf{p}_2}, \tag{2.1.5}$$

with σ being the zero-temperature cross section for $\chi\bar{\chi} \to \mathrm{SM}$. This form of the Boltzmann equation is often modified to absorb the effects of the expanding Universe by scaling the solutions with the entropy density of the SM, s, through $Y \equiv n_\chi/s$. We then have the following differential equation:

$$\frac{\mathrm{d}\, Y(x)}{\mathrm{d}x} = -\lambda\, f(x) \left[Y^2(x) - Y_{\mathrm{eq}}^2(x) \right], \tag{2.1.6}$$

The dependent variable Y is the comoving number density of a particle species (it is common to refer to Y as the *abundance* for brevity), i.e. the number of particles per cosmic comoving volume element. The independent variable $x \equiv m_\chi/T$ is the ratio of the particle mass to the temperature of the thermal bath. The equilibrium abundance, Y_{eq}, is the comoving number density of a particle species when in thermal (chemical) equilibrium with the thermal bath. The prefactor λf contains the cross section of the particle species and is given by

$$\lambda\, f(x) \equiv \sqrt{\frac{\pi}{45}} \frac{m M_{\mathrm{pl}}}{x^2} \sqrt{g_{*,\mathrm{eff}}(x)}\, \langle \sigma v_{\mathrm{M\o l}} \rangle, \tag{2.1.7}$$

where $\langle \sigma v_{\text{Møl}} \rangle$ implicitly depends on x and $g_{*,\text{eff}}(x)$ is a function characterising the effective number of degrees of freedom contributing to the energy density and entropy density of the universe:

$$\sqrt{g_{*,\text{eff}}(x)} \equiv \frac{h_{\text{eff}}(x)}{\sqrt{g_{\text{eff}}(x)}} \left(1 + \frac{1}{3} \frac{\mathrm{d} \ln(h_{\text{eff}}(x))}{\mathrm{d} \ln(x)}\right). \tag{2.1.8}$$

The effective number of degrees of freedom contributing to the total energy density and entropy density are $g_{\text{eff}}(x)$ and $h_{\text{eff}}(x)$ respectively. The limiting behavior $Y_\infty \equiv \lim_{x \to \infty} Y(x)$ of the solution is the quantity of interest, and determines the thermal relic density.

The starting point for our analysis is Equation (2.1.6), but it cannot be solved exactly, and therefore one resorts to obtaining approximations. The most common method of approximation is direct numerical integration. The use of general-purpose integrators tend to fail due to the largeness of λ, and even sophisticated algorithms like Radau5 [69], LSODA [70] struggle because the differential equation is exceptionally stiff which requires high precision arithmetic. Dedicated software packages to obtain dark matter relic abundances from particle physics models such as `micrOMEGAS` [71], and DarkSUSY [72], etc. fare better due to additional heuristics supplied to their integrators. However, prepackaged software designed to solve (2.1.6) are compatible with only a small subset of beyond-standard-model (BSM) scenarios, which limits the end user from performing an analysis of more exotic models such as those with Lorentz violation or large $\mathcal{N}$ Yang-Mills [73].

An alternative approach to obtaining the limiting behavior of (2.1.6) is to look for analytic approximations. Several approximations exist in the literature such

as [67, 74], and can provide results accurate to 1-5%, confirmed by comparing against results of numerical integration. However, by nature of their construction it is not possible to systematically improve upon these approximations simply because there is no way to assign a parametric dependence on the error.

The mathematical technique allowing for the construction of approximations while bounding the error is *asymptotic analysis* (for an in depth review of perturbation theory and asymptotics see [75]). The error is managed by a controlling parameter such that, as the controlling parameter is taken arbitrarily close to some limit point, the error vanishes relative to the approximation. It is in this sense that we can consider the error to be 'small'. A natural choice for the problem at hand is to choose λ in (2.1.6) as the controlling parameter, and to attempt to construct an asymptotic approximation in the limit $\lambda \to \infty$.

The authors of [76] attempted to construct an asymptotic approximation by using boundary-layer-analysis, yielding a technically more correct result with the requisite scaling behavior of the error. However, we found their matching procedure to be inconsistent. We were able to correct these errors to arrive at similar results. But in order to get a good approximation we had to perform a resummation of the largest terms of a divergent series, and for this reason we found it more intuitive to take a different approach, based on the Wentzel–Kramers–Brillouin (WKB) technique.

In this paper, we present our asymptotic approximation to (2.1.6). Our final results are given by (2.5.1), (2.5.2), and (2.5.3). The paper is structured as follows: In Section 2.2 we derive the large and small x behavior of the solution as well as the large x asymptotic behavior of the thermal cross section and equilibrium abundance

for later reference. To (2.1.6) we associate a second order linear differential equation of Schrödinger type, making a WKB analysis possible. However, there exists an infinite order turning point (where the potential and all its derivatives vanish) at $x = \infty$. Such classes of differential equations are notoriously difficult to solve, so to circumvent this issue we employ a more robust *uniform* WKB ansatz in Section 2.3 that is better suited to the infinite order turning point problem, and construct asymptotic solutions in three subregions of $x \in (0, \infty)$: The thermal equilibrium region (I), freeze-out region (II), and post-freeze-out region (III). We preform an asymptotic match of region I and III in Section 2.4 at leading and next to leading order, removing all undetermined constants. After matching we take the limit $x \to \infty$, yielding an asymptotic approximation of the relic density. In Section 2.5 we collect our results and compare our approximation against a numerical determination of the relic density using a benchmark model. We find that our approximation, when compared to numerical results, gives sub-percent errors when the dark matter candidate freezes out at roughly $x = 25$. To our knowledge, we are the first to present an asymptotic approximation to Y_∞. We are also unaware of a previous application of this method to the infinite order turning point problem.

2.2 Asymptotic behaviors

We briefly discuss the asymptotic behavior of some of the quantities in (2.1.6) and the general large and small x behavior of the solution. The equilibrium abundance of a particle species is given by

$$Y_{\text{eq}}(x) = A \int_0^\infty \frac{s^2 \, \mathrm{d}s}{e^{\sqrt{s^2+x^2}} \mp 1}, \tag{2.2.1}$$

where the upper sign is for bosons and the lower for fermions, and A is given by

$$A \equiv \frac{45}{4\pi^4} \frac{g}{h_{\rm eff}(x)}, \tag{2.2.2}$$

where g is the number of internal degrees of freedom of the particle species and $h_{\rm eff}(x)$ is the number of relativistic degrees of freedom contributing to the entropy density. The large x behavior of the the equilibrium abundance is

$$Y_{\rm eq}(x) \sim \sqrt{\frac{\pi}{2}} A x^{3/2} e^{-x}, \quad (x \to \infty). \tag{2.2.3}$$

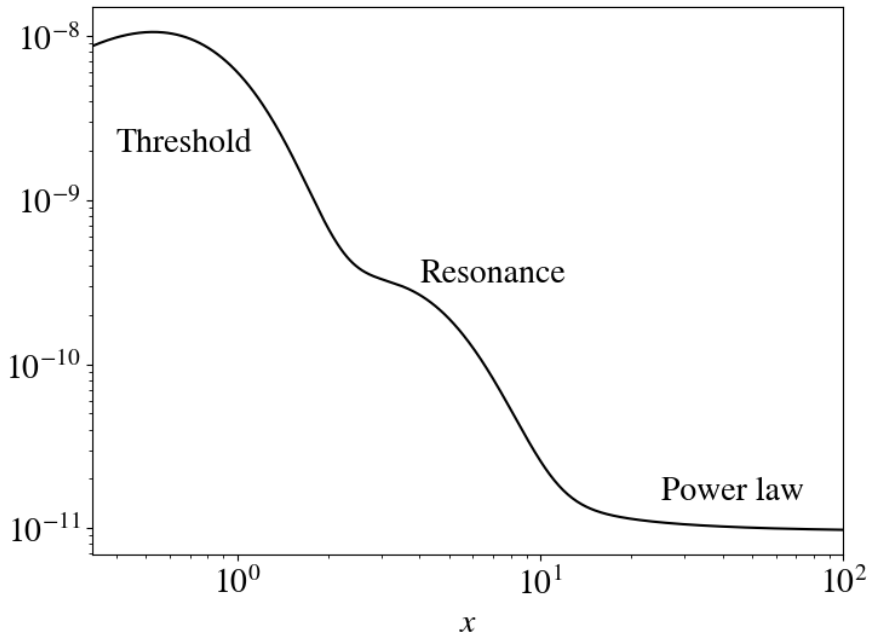


Figure 2.1: Typical behavior of the thermally averaged annihilation cross section $\langle \sigma v_{\rm M\o l} \rangle$ as a function of x, the vertical axis is GeV^{-2}. On the left threshold effects dominate. In the center threshold effects have decayed away and resonance contributions now dominate. On the right all threshold and resonance effects are negligible and the thermally averaged cross section assumes the form of a power law (in this case a constant).

For temperatures $T \lesssim 3m$, where m is the mass of particle species in question, the phase space distribution for all statistics is well approximated by the Maxwell-Boltzmann distribution. Making this substitution the $2 \to$ all thermally averaged anni-

hilation cross section reduces to a single integral [67],

$$\langle \sigma v_{\text{Møl}} \rangle \sim \int_0^\infty \mathrm{d}\epsilon \, \sigma v_{\text{lab}} \, \mathscr{K}(\epsilon, x) \,, \quad (x \to \infty), \tag{2.2.4a}$$

$$\mathscr{K}(\epsilon, x) = \frac{2x}{K_2^2(x)} \epsilon^{1/2} (1 + 2\epsilon) \, K_1\Big(2x\sqrt{1+\epsilon}\Big) \,, \tag{2.2.4b}$$

where

$$\epsilon \equiv \frac{s - 4m^2}{4m^2}. \tag{2.2.5}$$

We can further approximate the thermal kernel (2.2.4b) using the large argument expansion of the modified Bessel function.

$$\mathscr{K}(\epsilon, x) \sim \frac{2x^{3/2}}{\sqrt{\pi}} \frac{\epsilon^{1/2}(1+2\epsilon)}{(1+\epsilon)^{1/4}} e^{x\phi(\epsilon)}, \quad (x \to \infty), \tag{2.2.6a}$$

$$\phi(\epsilon) = -2\Big(\sqrt{1+\epsilon} - 1\Big), \tag{2.2.6b}$$

When x is very large we can estimate the integral using Laplace's method. We first located the maximum of the integrand in (2.2.4a), and denote this point ϵ_0. In the limit that $x \to \infty$ this maximum is just the maximum of $\phi(\epsilon)$. The approximation of the thermally averaged cross section then has a residual exponential character $\exp[x\,\phi(\epsilon_0)]$. If σv_{lab} is sufficiently smooth, i.e. any resonances are broad and all annihilation channels are of similar scale, then $\epsilon_0 = 0$ and $\phi(0) = 0$, so the thermally averaged cross section goes like some power of x. In this case a more thorough treatment, using Watson's lemma, yields:

$$\langle \sigma v_{\text{Møl}} \rangle \sim \sum_{k=0}^{\infty} \sigma_k x^{-k}, \quad (x \to \infty), \tag{2.2.7}$$

where the coefficients σ_k are easily found. There are two common scenarios in which the estimate (2.2.7) breaks down for intermediate values of x: when the annihilation

cross section contains a very narrow resonance or the dominant annihilation channel has support only when $s > 4m^2$. For a narrow resonance the annihilation cross section approaches a delta function in the limit that the width of the resonance goes to 0. If this narrow resonance is centered at $s = m_{\mathrm{R}}^2$ then $\epsilon_0 \sim (m_R^2 - 4m^2)/4m^2$ and

$$\phi(\epsilon_0) \sim -\frac{m_{\mathrm{R}} - 2m}{m}.$$

Alternatively, if there exists an annihilation channel that is kinematically unavailable when $s < s_{\mathrm{Th}} = 4m_{\mathrm{Th}}^2$, but that dominates the cross section when $s > s_{\mathrm{Th}}$, then $\epsilon_0 \sim (m_{\mathrm{Th}}^2 - m^2)/m^2$ and

$$\phi(\epsilon_0) \sim -\frac{2(m_{\mathrm{Th}} - m)}{m}.$$

Therefore, we can characterize the thermally averaged cross section for intermediate to large x by

$$\langle \sigma v_{\mathrm{M\o l}} \rangle \sim x^{\beta} e^{-\alpha x} \sum_{k=0}^{\infty} c_k x^{-k}, \quad (x \to \infty) \tag{2.2.8a}$$

$$\alpha = \begin{cases} 0 & \text{Power Law} \\ \frac{m_{\mathrm{R}} - 2m}{m} & \text{Resonance} \\ \frac{2(m_{\mathrm{Th}} - m)}{m} & \text{Threshold} \end{cases} \tag{2.2.8b}$$

The coefficients β and c_k generally depend on the choice of α. It is almost always the case that the leading order behavior of the thermally averaged cross section has no exponential decay (i.e. $\alpha = 0$) for very large x. We then expect that α will make rapid transitions as we move from intermediate x to large x, ultimately going to 0 once x becomes sufficiently large. We see that this assumption is correct in Fig. 2.1. For more complicated models, including those with coannihilation, determining the appropriate value for α analytically can be difficult. In Appendix B.1 we derive a

method of calculating α numerically for general models where the differential equation for the abundance can be reduced to (2.1.6).

Substituting the power law approximation (2.2.7) into (2.1.7) yields the standard behavior of $f(x)$ for large x,

$$f(x) \sim x^{-n-2}, \quad (x \to \infty), \tag{2.2.9}$$

where n is the order of the first non vanishing term in (2.2.7). The normalization of the thermally averaged cross section has been stripped away and included in the parameter λ.

For x not too large we approximate the solution to (2.1.6) by assuming a formal series expansion in powers of $1/\lambda$:

$$Y(x) \sim \sum_{k=0}^{\infty} Y_k(x)\, \lambda^{-k}, \quad (\lambda \to \infty). \tag{2.2.10}$$

This gives the approximate solution

$$Y(x) \sim Y_{\mathrm{eq}}(x) - \frac{Y'_{\mathrm{eq}}(x)}{2\lambda\, f(x)\, Y_{\mathrm{eq}}(x)}, \quad (\lambda \to \infty). \tag{2.2.11}$$

Because Y_{eq} decays exponentially fast this solution becomes invalid when $\lambda\, f(x)\, Y_{\mathrm{eq}}(x) = \mathcal{O}(1)$. When x is very large, such that $\lambda\, f(x)\, Y_{\mathrm{eq}}(x) \ll 1$ we can neglect the last term on the right hand side of (2.1.6), resulting in a second approximation

$$Y(x) \sim \left[\frac{1}{Y_\infty} - \lambda \int_x^\infty f(s)\, \mathrm{d}s\right]^{-1}, \quad (x \to \infty). \tag{2.2.12}$$

Assuming $Y_\infty > 0$, and because the integral

$$\lambda \int_x^\infty f(s)\, \mathrm{d}s$$

generally diverges as $x \to 0$, there necessarily exists some $0 < x_{\rm pole} < \infty$ such that

$$\frac{1}{Y_\infty} - \lambda \int_{x_{\rm pole}}^{\infty} f(s)\, \mathrm{d}s = 0$$

This approximation is therefore only valid when $x \gg x_{\rm pole} > 0$, and we cannot satisfy the boundary condition at $x = 0$.

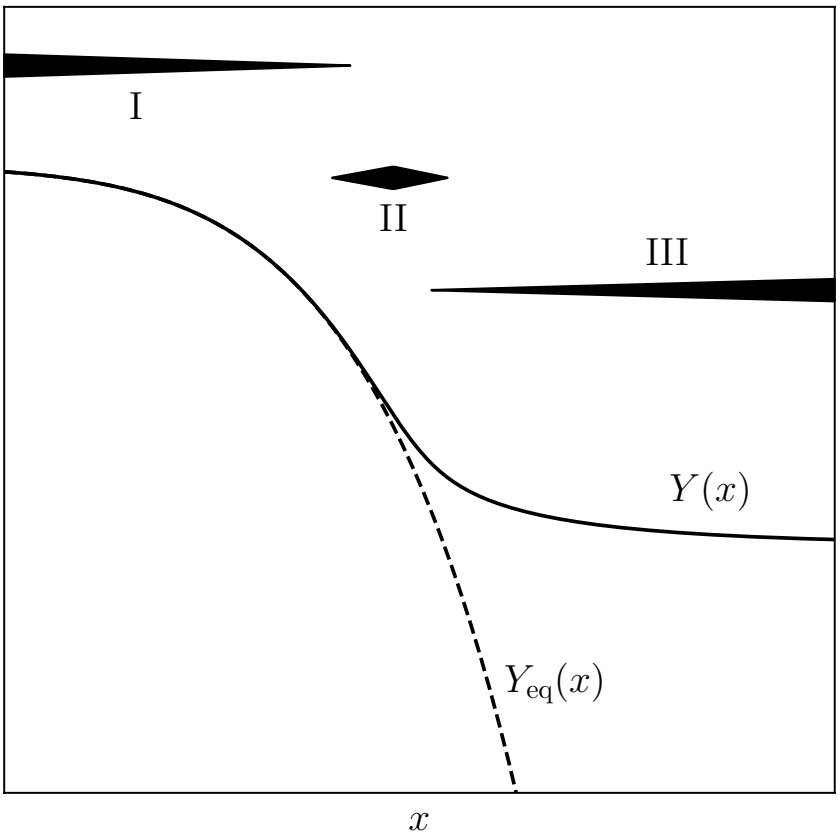


Figure 2.2: The abundance of a particle species as a function of $x \equiv m/T$. In region I the abundance closely tracks the equilibrium abundance. In region III the abundance asymptotes to a constant, denoted Y_∞. Region II represents the transition between region I and III. The wedges sketch the extent of each of the regions.

Generally the approximate solutions (2.2.11) and (2.2.12) have no overlap in their region of validity, so the arbitrary constant Y_∞ cannot yet be determined. One must either construct an intermediate solution whose region of validity overlaps with

both the large λ and the large x approximations, or modify one or both solutions such that they have some overlap. We take the latter approach, essentially resumming the largest components of (2.2.10) to all orders.

2.3 Construction of asymptotic solutions

We begin by transforming (2.1.6) from a first order non-linear differential (Riccati) equation into a second order linear differential equation of the Schrödinger type by changing the dependent variable to

$$Y(x) = \frac{1}{\lambda\, f(x)} \frac{\mathrm{d}}{\mathrm{d}x} \ln\Big(\sqrt{\lambda\, f(x)}\, u(x)\Big)\,, \tag{2.3.1}$$

so that

$$\begin{aligned} u'' - \Big[(\lambda f Y_{\mathrm{eq}})^2 + \frac{3}{4}\Big(\frac{f'}{f}\Big)^2 - \frac{1}{2}\frac{f''}{f}\Big] u = 0\,, \\ \frac{u'(0)}{u(0)} = \lambda\, f(0)\, Y_{\mathrm{eq}}(0) - \frac{f'(0)}{2f(0)} \end{aligned} \tag{2.3.2}$$

Using the canonical WKB ansatz,

$$u(x) \sim \exp\Big(\lambda \sum_{k=0}^{\infty} S_k(x)\, \lambda^{-k}\Big), \quad (\lambda \to \infty), \tag{2.3.3}$$

gives the solution for Y as a formal power series in $1/\lambda$.

$$Y(x) \sim \sum_{k=0}^{\infty} \frac{S_k'(x)}{f(x)} \lambda^{-k} + \frac{f'(x)}{2\lambda\, f^2(x)}, \quad (\lambda \to \infty). \tag{2.3.4}$$

We see that the $1/\lambda$ series solution of (2.1.6) is equivalent to the WKB solution of (2.3.2).

In what follows we construct asymptotic approximations for small x (Region I), large x (Region III), and intermediate x (Region II), shown schematically in Fig. 2.2. The region II approximation is superfluous, as we will see the domain of validity of the

region I and III solutions generally overlap (and hence the region I approximation can be asymptotically matched directly onto the region III approximation). However, the approximation in the overlap region motivates a definition of a freeze-out temperature that ensures a consistent asymptotic expansion in all three regions. In order to simplify our notation we define:

$$Q(x) \equiv f(x)\, Y_{\mathrm{eq}}(x)\,, \tag{2.3.5a}$$

$$P(x) \equiv \frac{3}{4}\left(\frac{f'(x)}{f(x)}\right)^2 - \frac{1}{2}\frac{f''(x)}{f(x)}, \tag{2.3.5b}$$

so that (2.3.2) becomes

$$u'' - \Big[\lambda^2\, Q^2(x) + P(x)\Big] u = 0. \tag{2.3.6}$$

Before proceeding we make some observations about the behavior of these two functions $Q(x)$ and $P(x)$. Consider, for example, the following large x behavior of f from (2.2.8a):

$$f(x) \sim x^{\beta} e^{-\alpha x}, \quad (x \to \infty). \tag{2.3.7}$$

The resulting behavior for $Q(x)$ and $P(x)$ is

$$Q(x) \sim \sqrt{\frac{\pi}{2}} A x^{\beta+3/2} e^{-(1+\alpha)x}, \quad (x \to \infty), \tag{2.3.8a}$$

$$P(x) \sim \frac{\alpha^2}{4} - \frac{\alpha\beta}{2x} + \frac{\beta(2+\beta)}{2x^2}, \quad (x \to \infty). \tag{2.3.8b}$$

and are shown in Fig. 2.3. Because of the exponential decay in (2.3.8a) $Q(x)$ and all its derivatives vanish as $x \to \infty$. Note that there are two linearly independent solutions to (2.3.6), and the WKB approximations of these two solutions are multivalued. Therefore, if we approximate the full solution as a specific combination of these two

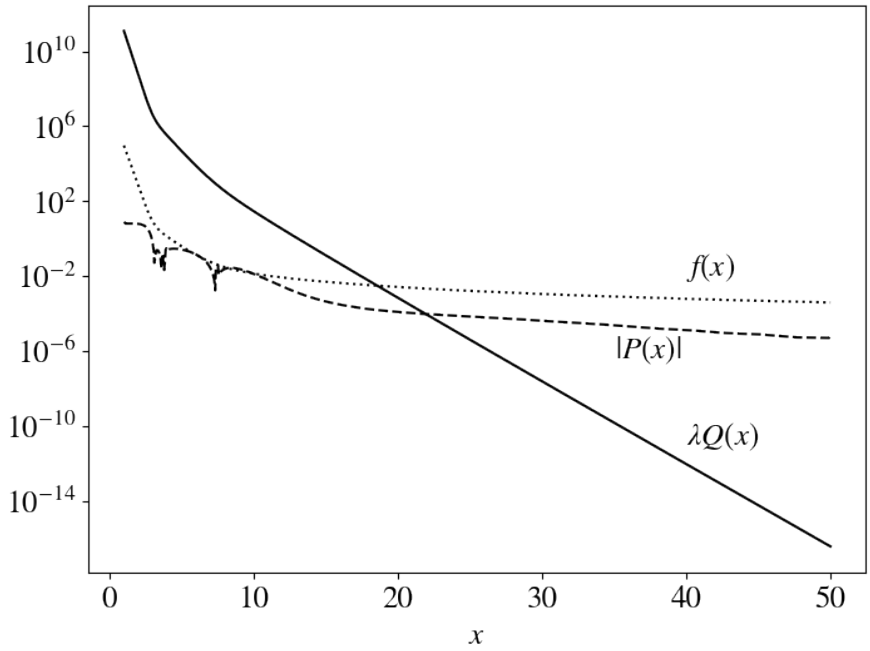


Figure 2.3: The functions $f(x)$, $P(x)$, and $\lambda Q(x)$ using a benchmark model (see Section 2.5).

linearly independent solutions near $x = \infty$, the same combination cannot be used for $xe^{2\pi i}$. This is known as the Stoke's phenomenon. Essentially, the problem is that the approximations are necessarily domain dependent. In this case, because $x = \infty$ is an essential singularity, in the neighborhood of the turning point there exists an infinite number of domains (bounded by Stoke's and Anti-Stokes lines), each requiring a different combination of linearly independent solutions. This is the infinite order turning point problem.

2.3.1 Thermal equilibrium region (Region I)

In the small x region, we construct a uniform WKB approximation to (2.3.2). The ansatz, originally constructed by Langer [77], is:

$$u^{\mathrm{I}}(x) = i\left(\frac{S}{S'}\right)^{1/2} K_\nu(\lambda S)\,, \tag{2.3.9}$$

where $K_\nu(z)$ is the modified Bessel function of the second kind, and $S(x)$ admits a series expansion in $1/\lambda$,

$$S(x) \sim \sum_{k=0}^{\infty} S_{2k}(x)\,\lambda^{-2k}, \quad (\lambda \to \infty). \tag{2.3.10}$$

The order parameter ν is left to be determined, it will be chosen to prolong the validity of the approximation. We remark that with the choice $\nu = \frac{1}{2}$ the ansatz (2.3.9) reduces to standard WKB. This construction is particularly well suited to the infinite order turning point problem, as can be seen by considering the exact solutions of

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} - \left[\lambda^2 e^{-2t} + \nu^2\right] y = 0, \tag{2.3.11}$$

which are linear combinations of modified Bessel functions $I_\nu(\lambda e^{-t})$, $K_\nu(\lambda e^{-t})$.

The prefactor of (2.3.9) is chosen so that (2.3.2) becomes a differential equation entirely in terms of $S(x)$, and the factor of i ensure the solution is real-valued for positive x. Substituting the ansatz (2.3.9) into (2.3.6) and then inserting (2.3.10) into the resulting equation allows one to solve for each term by equating powers of $1/\lambda$:

$$\begin{aligned} &-\frac{1}{2}\left(\frac{S'''}{S'}\right) + \frac{3}{4}\left(\frac{S''}{S'}\right)^2 + \left(\nu^2 - \frac{1}{4}\right)\left(\frac{S'}{S}\right)^2 + \lambda^2 (S')^2 - \lambda^2\, Q^2(x) - P(x) = 0. \\ &\lambda\, Q(0) - \frac{1}{2}\frac{f'(0)}{f(0)} = -\lambda\, S'(0)\,\frac{K_{\nu+1}(\lambda\, S(0))}{K_\nu(\lambda\, S(0))} + \frac{1}{2}\left[(1+2\nu)\frac{S'(0)}{S(0)} - \frac{S''(0)}{S'(0)}\right] \end{aligned} \tag{2.3.12}$$

Solving (2.3.12) at leading order gives

$$S_0(x) = -\int_0^x Q(s)\,\mathrm{d}s + S_0(0)\,. \tag{2.3.13}$$

The boundary condition dictates that the sign of $S_0'(x)$ must be negative, but the initial value is arbitrary. If the leading order solution changes sign at some finite value of x we will have to contend with the Stoke's phenomenon, so we require $S_0(x)$ be bounded from below. This is guaranteed with the choice $S_0(\infty) = 0$, yielding

$$S_0(x) = \int_x^\infty Q(s)\,\mathrm{d}s\,. \tag{2.3.14}$$

We now estimate $S_0(x)$ for large x . Begin by making a change of variables to $t \equiv s/x$.

$$S_0(x) = x\int_1^\infty Q(xt)\,\mathrm{d}t \tag{2.3.15}$$

If x is large $Q(xt)$ is exponentially suppressed everywhere along the range of integration. Then write

$$Q(x) \sim F(x)\,e^{-(1+\alpha)x}, \quad (x \to \infty), \tag{2.3.16}$$

where we assume that $F(x)$ contains no exponential terms. If resonance or threshold effects are negligible we will set $\alpha = 0$. Inserting (2.3.16) into (2.3.15) and expanding $F(xt)$ as a Taylor series around x then gives

$$S_0(x) \sim \frac{Q(x)}{F(x)}\sum_{n=0}^{\infty}\frac{1}{(1+\alpha)^{n+1}}\frac{\mathrm{d}^n F(x)}{\mathrm{d}x^n}, \ \ (x \to \infty). \tag{2.3.17}$$

The errors introduced are exponentially small as $x \to \infty$. Because $F(x)$ contains no exponential terms by assumption this series naturally organises itself as an expansion in powers of $1/x$.

Solving for the next to leading order term in (2.3.12) we find

$$S_2(x) = \frac{(4\nu^2-1)}{8}\left[\frac{1}{S_0(x)} - \frac{1}{S_0(0)}\right] \\ \underbrace{- \frac{1}{2}\int_0^x \frac{\mathrm{d}s}{Q(s)}\left\{P(s) + \frac{1}{2}\frac{Q''(s)}{Q(s)} - \frac{3}{4}\left[\frac{Q'(s)}{Q(s)}\right]^2\right\}}_{\text{Standard WKB}} + S_2(0)\,. \quad (2.3.18)$$

The integral can be approximated in a very similar way as for $S_0(x)$. We report only the leading order term:

$$S_2(x) \sim -\frac{1}{2(1+\alpha)}\frac{\phi(x)}{Q(x)}, \quad (x \to \infty), \quad (2.3.19)$$

where

$$\phi(x) \equiv P - \nu^2\left(\frac{S_0'}{S_0}\right)^2 - \sqrt{\frac{S_0'}{S_0}}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sqrt{\frac{S_0}{S_0'}}. \quad (2.3.20)$$

$S_2(x)$ is then exponentially increasing as $x \to \infty$. In order to extend the region of validity of our approximation we choose ν to cancel the leading order large x component of (2.3.20). The last term of (2.3.20) is at most of order $\mathcal{O}(1/x^3)$,

$$\sqrt{\frac{S_0'}{S_0}}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sqrt{\frac{S_0}{S_0'}} \sim -\frac{1}{2(1+\alpha)}\frac{\mathrm{d}^3}{\mathrm{d}x^3}\ln(F(x)), \quad (x \to \infty). \quad (2.3.21)$$

This fantastic cancellation of the lower order terms is due to the ansatz (2.3.9). On the other hand,

$$\frac{S_0'(x)}{S_0(x)} \sim -(1+\alpha) + \frac{F'(x)}{F(x)}, \quad (x \to \infty). \quad (2.3.22)$$

Therefore, if $P(x)$ is not asymptotic to a constant, we should choose $\nu = 0$. As stated previously $P(x)$ should only contain constant terms at large x if the cross section is decaying exponentially fast due to a low lying resonance or threshold. If this is the case then we should choose

$$\nu = \pm\frac{\alpha}{2(1+\alpha)}, \quad (2.3.23)$$

so that the constant term cancels. We can therefore guarantee that in the worst case scenario

$$S_2(x) \sim -\frac{1}{2}\frac{D}{x\,Q(x)}, \quad (x \to \infty). \tag{2.3.24}$$

for some constant D. This indicates an improvement over standard WKB, because $\lambda\, S_0(x) = 1$ occurs when $x = \mathcal{O}(\ln(\lambda))$. At this same point the correction $S_2(x)\,/\lambda = \mathcal{O}(1/\ln(\lambda))$ at most, and therefore our approximation extends into the region where $\lambda\, S_0(x) \ll 1$ (FIG. 2.4). We then define the upper bound of the thermal-equilibrium region by where the leading order term is equal in magnitude to the correction term,

$$\lambda^2\, Q^2(x_+) \coloneqq \frac{1}{x_+}. \tag{2.3.25}$$

The more common scenario is $\alpha = 0$ and $\beta = -2$, which yields a much larger upper bound

$$\lambda^2\, Q^2(x_+) \coloneqq \frac{1}{x_+^3}. \tag{2.3.26}$$

In any case $x_+ = \mathcal{O}(\ln(\lambda))$ due to the exponential decay of the equilibrium abundance, so that as $\lambda \to \infty$ the upper bound of the region of validity also goes to infinity as expected.

Finally, we have the approximation of the solution in the thermal equilibrium region:

$$u^{\mathrm{I}}(x) \sim \sqrt{\frac{\int_x^\infty \mathrm{d}s\, Q(s)}{Q(x)}}\, K_\nu\!\left(\lambda \int_x^\infty \mathrm{d}s\, Q(s)\right),$$

$$(\lambda \to \infty), \quad x \ll x_+$$

$$\nu = \begin{cases} 0 & \text{w/o res/thresh} \\ \frac{\alpha}{2(1+\alpha)} & \text{w/ res/thresh} \end{cases}. \tag{2.3.27}$$

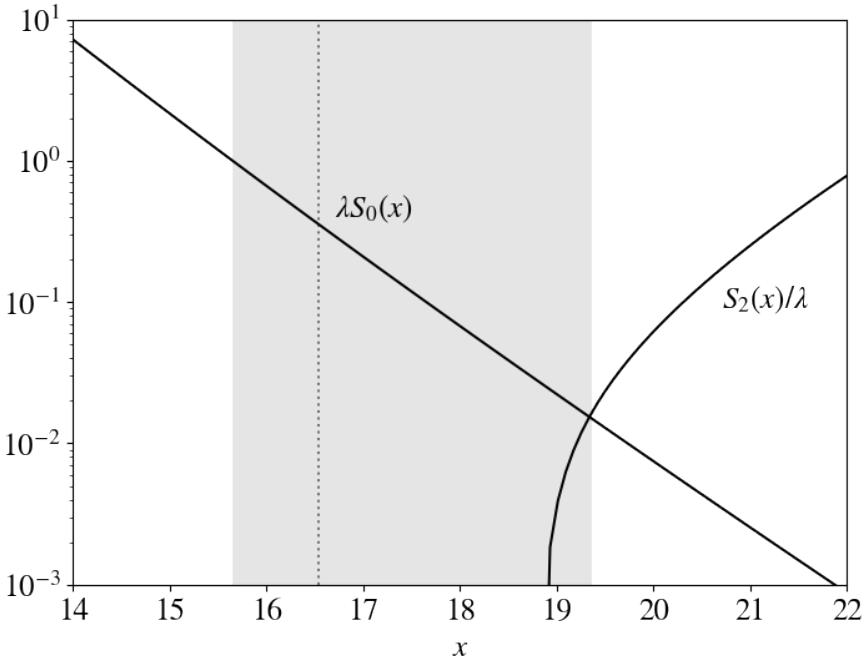


Figure 2.4: The leading order term $\lambda\, S_0(x)$ compared to the next to leading order term $S_2(x)\,/\lambda$. The shaded region corresponds to where $1 \geq \lambda S_0 \geq S_2/\lambda$. This shaded region also represents the extension of the region of validity over standard WKB. The vertical dotted line indicates the location of what will eventually be defined as the freeze-out temperature.

2.3.2 Post freeze-out region (Region III)

In the post-freeze out region, approximate (2.3.2) by taking the limit $x \to \infty$ while holding λ constant. Neglecting the first term at leading order in (2.3.2) (which is exponentially suppressed as $x \to \infty$), the differential equation becomes

$$u'' \sim P(x)\, u\,, \quad (x \to \infty) \tag{2.3.28}$$

Recalling the definition of $P(x)$ (2.3.5b), we see that (2.3.28) can be solved exactly, yielding

$$u^{\mathrm{III}}(x) \sim \frac{1}{\sqrt{f(x)}}\left[c_1 - c_2 \int_x^\infty f(s)\, \mathrm{d}s\right],\ (x \to \infty). \tag{2.3.29}$$

The arbitrary integration constants c_1 and c_2 cannot be determined because the boundary condition at $x = 0$ lies outside the region of validity of this approximation.

To obtain the higher order corrections to (2.3.29) we construct a series solution of the form

$$u^{\mathrm{III}}(x) \sim \sum_{k=0}^{\infty} u_k^{\mathrm{III}}(x)\, e^{-2(1+\alpha)kx}, \quad (x \to \infty). \tag{2.3.30}$$

The solution for $u_1^{\mathrm{III}}(x)$ can be obtained directly (and in closed form) using the method of variation of parameters. For the sake of clarity we retain only the largest component:

$$u_1^{\mathrm{III}}(x) \sim \frac{\lambda^2 F^2(x)}{4(1+\alpha)\sqrt{f(x)}}\left[c_1 - c_2 \int_x^{\infty} f(s)\,\mathrm{d}s\right], \quad (x \to \infty). \tag{2.3.31}$$

As was the case in the thermal equilibrium region, we require the higher order corrections to be negligible compared to the leading order result in order to claim a valid asymptotic approximation. This requirement then defines an estimate of the lower bound on the region of validity of the post-freeze-out approximation. We again obtain a transcendental definition of the lower bound estimate x_-:

$$\lambda\, Q(x_-) = 1. \tag{2.3.32}$$

Like the estimate of the upper bound of region I, x_- is $\mathcal{O}(\ln(\lambda))$.

Our final approximation of the solution in the post-freeze-out region is

$$u^{\mathrm{III}}(x) \sim \frac{1}{\sqrt{f(x)}}\left[c_1 - c_2 \int_x^{\infty} f(s)\,\mathrm{d}s\right], \quad (x \to \infty), \quad x \gg x_-. \tag{2.3.33}$$

Inserting (2.3.33) into (2.3.1) and taking the limit $x \to \infty$ yields the relic abundance

$$\begin{aligned} Y_\infty \equiv & \lim_{x\to\infty} Y(x)\,, \\ = & \frac{c_2}{\lambda c_1}. \end{aligned} \tag{2.3.34}$$

In section 2.4 we will approximate the coefficients c_1 and c_2.

2.3.3 Freeze-out region (Region II)

Comparing x_- to x_+ it is easy to see that there exists an overlap region where the thermal equilibrium and post-freeze-out approximations are both valid. Therefore, we can (and will) determine the constants c_1 and c_2 order by order by asymptotically matching the region I solution to the region III solution. However, it proves advantageous to construct an approximation in the overlap region in order to guide the asymptotic matching. We will define a *freeze-out* temperature $x_\mathrm{f} \in (x_-, x_+)$ with which we can organize the asymptotic limits. Because this x_f is order $\ln(\lambda)$ it is itself a large parameter if λ is large. We then construct a series solution in the overlap region by assuming

$$u^{\mathrm{II}}(t) \sim \sum_{k=0}^{\infty} \frac{u_k^{\mathrm{II}}(t)}{x_\mathrm{f}^k}, \quad (x_\mathrm{f} \to \infty), \tag{2.3.35}$$

where $t \equiv x - x_\mathrm{f}$. The relic abundance will not depend on the precise definition of x_f, but in order to obtain numerical values one must specify it explicitly. For now, we define the freeze-out temperature x_f to occur when

$$\lambda Q(x_\mathrm{f}) = \mathcal{O}(1), \quad (x_\mathrm{f} \to \infty), \tag{2.3.36}$$

so that the series representation (2.3.35) begins with an order 1 constant. Alternative definitions would require the leading order term to vanish in some cases (depending on

the asymptotic form of the thermally averaged cross section in the overlap region), and our choice avoids this inconvenience.

Next we expand the differential equation (2.3.6) around x_f using

$$Q(x_\mathrm{f}+t) \sim Q(x_\mathrm{f})\, e^{-(1+\alpha)t}, \quad (x_\mathrm{f}\to\infty), \tag{2.3.37a}$$

$$P(x_\mathrm{f}+t) \sim P(x_\mathrm{f}), \quad (x_\mathrm{f}\to\infty), \tag{2.3.37b}$$

for any finite t to yield

$$\frac{\mathrm{d}^2 u(t)}{\mathrm{d}t^2} \sim \left[\lambda^2 Q^2(x_\mathrm{f})\, e^{-2(1+\alpha)t} + P(x_\mathrm{f})\right] u(t)\,, \quad (x_\mathrm{f}\to\infty). \tag{2.3.38}$$

The solutions are linear combinations of modified Bessel functions. However, it is usually the case that we should not retain the $P(x_\mathrm{f})$ term. If the annihilation cross section does not vanish at threshold then $P(x_\mathrm{f})$ is at most of order $\mathcal{O}\left(x_\mathrm{f}^{-2}\right)$. We can enforce this distinction by allowing for two cases: $\alpha \ll 1/\sqrt{x_\mathrm{f}}$ and $\alpha \gtrsim 1/\sqrt{x_\mathrm{f}}$. The leading order solution is then

$$u_0^{\mathrm{II}}(t) = b_1\, K_\nu\left(\Lambda_\mathrm{f} e^{-(1+\alpha)t}\right) + b_2\, I_\nu\left(\Lambda_\mathrm{f} e^{-(1+\alpha)t}\right), \tag{2.3.39}$$

where $\Lambda_\mathrm{f} \equiv \lambda\, Q(x_\mathrm{f})\,/(1+\alpha)$ and

$$\nu = \begin{cases} 0 & \alpha \ll \frac{1}{\sqrt{x_\mathrm{f}}} \\ \frac{\sqrt{P(x_\mathrm{f})}}{1+\alpha} = \frac{\alpha}{2(1+\alpha)} & \alpha \gtrsim \frac{1}{\sqrt{x_\mathrm{f}}} \end{cases} \tag{2.3.40}$$

Note the exact agreement of the parameter ν as derived in section 2.3.1.

The leading order matching between region I and II is obvious:

$$b_1 = \frac{1}{\sqrt{1+\alpha}}, \tag{2.3.41a}$$

$$b_2 = 0. \tag{2.3.41b}$$

Because our choice of the freeze out temperature x_f lies near the lower bound of the overlap region we must also take $t \to \infty$. The solution in the overlap region is then approximately linear if $\alpha \ll 1/\sqrt{x_\mathrm{f}}$ or a sum of exponential terms $\exp(\alpha t/2)$ and $\exp(-\alpha t/2)$ if $\alpha \gtrsim 1\sqrt{x_\mathrm{f}}$. One could have chosen to define the freeze-out condition differently, and the behavior of the solution in the overlap region would be identical, but we could not have written it in such a simple way.

What we have learned is that, if we neglect α, the constant term and the term proportional to t must be considered the same order. Similarly, if α is not neglected, the exponential terms should also be considered the same order.

2.4 Asymptotic Matching

With asymptotic approximations in hand for the thermal-equilibrium region and post-freeze-out region we now asymptotically match the solutions in the region where both approximations are valid. We will utilize the following approximations of $S_0(x)$:

$$S_0(x_\mathrm{f}+t) \sim\ Q(x_\mathrm{f})\, e^{-(1+\alpha)t} \sum_{j=0}^{\infty} \sum_{k=0}^{j} \frac{[(1+\alpha)t]^k}{k!(1+\alpha)^{j+1}} \frac{1}{F(x_\mathrm{f})} \left.\frac{\mathrm{d}^j\, F(x)}{\mathrm{d}x^j}\right|_{x=x_\mathrm{f}}, \quad (x_\mathrm{f} \to \infty), \tag{2.4.1a}$$

$$S_0'(x_\mathrm{f}+t) \sim\ -Q(x_\mathrm{f})\, e^{-(1+\alpha)t} \sum_{j=0}^{\infty} \frac{t^j}{j!} \frac{1}{F(x_\mathrm{f})} \left.\frac{\mathrm{d}^j\, F(x)}{\mathrm{d}x^j}\right|_{x=x_\mathrm{f}}, \quad (x_\mathrm{f} \to \infty). \tag{2.4.1b}$$

These can be found by taking the Taylor expansion of $\mathrm{d}^j\, F(x)/\mathrm{d}x^j$ around $x_\mathrm{f}+t$ in (2.3.17). These representations are convenient because the sum over j yields a series in increasing powers of $1/x_\mathrm{f}$. We split the matching procedure into three categories:

leading order assuming $\alpha = 0$, next to leading order assuming $\alpha = 0$, and leading order for general α. Because our choice for the freeze-out condition is near the lower bound of the overlap region there will not be a true leading order matching condition for the $\alpha = 0$ case. What we label as leading order is in fact next to leading order, and what we have labeled as next to leading order is actually next to next to leading order.

2.4.1 Leading Order

Assuming that α is either large enough that resonance and threshold effects are negligible in the overlap region or that α is of order $1/x_\mathrm{f}$ or smaller we shift the dependent variable by $x \equiv x_\mathrm{f} + t$. In region I we retain only the leading order terms in (2.4.1a) and (2.4.1b).

$$u^\mathrm{I}(t) \sim C + t, \quad (x_\mathrm{f} \to \infty), \tag{2.4.2}$$

Where

$$C \equiv -\ln\!\left(\frac{\lambda\, Q(x_\mathrm{f})}{2}\right) - \gamma, \tag{2.4.3}$$

is an order 1 constant and γ is the Euler-Mascheroni constant. To obtain this approximation we have taken the limit $t \to \infty$ and used the small argument expansion of the modified Bessel function (with $\nu = 0$). In addition, there are terms that are exponentially suppressed at large t, but these can be neglected at leading order. Similarly, in region III we have

$$u^\mathrm{III}(t) \sim \frac{1}{\sqrt{f(x_\mathrm{f})}}\left[c_1 - c_2 \int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s + c_2\, f(x_\mathrm{f})\, t\right], \quad (x_\mathrm{f} \to \infty). \tag{2.4.4}$$

It may seem odd that the linear term in t is retained, because it is down by one power of x_f compared to the second constant term. However, as we learned in Section 2.3.3,

the constant term and the term proportional to t must be considered the same order. Large terms will cancel between the c_1 term and c_2 term, so that overall the constant term is of the same order as the term linear in t. It is then simple to determine the constants c_1 and c_2.

$$c_1 \sim \frac{1}{\sqrt{f(x_\mathrm{f})}}\left[\int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s + C\,f(x_\mathrm{f})\right],\ (x_\mathrm{f}\to\infty), \tag{2.4.5a}$$

$$c_2 \sim \frac{1}{\sqrt{f(x_\mathrm{f})}},\quad (x_\mathrm{f}\to\infty). \tag{2.4.5b}$$

Inserting these approximations into our expression for the relic abundance yields our leading order approximation:

$$Y_\infty \sim \frac{1}{\lambda\int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s + C\lambda\,f(x_\mathrm{f})},\quad (x_\mathrm{f}\to\infty). \tag{2.4.6}$$

So far we have derived the leading order asymptotic approximation of the relic abundance without specifying an exact value for x_f. In fact, these results do not depend strongly on the precise value of x_f. Allow $x_\mathrm{f}\to x_\mathrm{f}+\varepsilon$, where $\varepsilon \ll x_\mathrm{f}$. Under this shift

$$Q(x_\mathrm{f}) \to Q(x_\mathrm{f})\,e^{-\varepsilon}\left(1+\mathcal{O}\left(\frac{\varepsilon}{x_\mathrm{f}}\right)\right) \tag{2.4.7a}$$

$$C \to C+\varepsilon+\mathcal{O}\left(\frac{\varepsilon}{x_\mathrm{f}}\right) \tag{2.4.7b}$$

The ratio of the region III coefficients then transforms as

$$\begin{aligned}\frac{c_1}{c_2} &\to \int_{x_\mathrm{f}+\varepsilon}^{\infty} f(s)\,\mathrm{d}s + (C+\varepsilon)\,f(x_\mathrm{f}) \\ &= \int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s + C\,f(x_\mathrm{f})\,,\end{aligned} \tag{2.4.8}$$

which shows that the relic abundance is invariant under a small shift of the freeze-out temperature up to $\mathcal{O}(\varepsilon^2/x_\mathrm{f}^2)$.

2.4.2 Next to Leading Order

At next to leading order we retain terms up to $1/x_\mathrm{f}$ and t/x_f, but continue to drop terms like $1/x_\mathrm{f}^2$ and $\exp(-t)$. The approximations in each region become:

$$u^\mathrm{I}(t) \sim \alpha_1 + \beta_1 t, \quad (x_\mathrm{f} \to \infty). \tag{2.4.9}$$

$$u^\mathrm{III}(t) \sim \alpha_3 + \beta_3 t, \quad (x_\mathrm{f} \to \infty). \tag{2.4.10}$$

Where the coefficients are

$$\alpha_1 \equiv \left[1 + \frac{1}{2}\frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}\right] C - \frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}, \tag{2.4.11a}$$

$$\beta_1 \equiv 1 - \frac{1}{2}\frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}, \tag{2.4.11b}$$

$$\alpha_3 \equiv \frac{1}{\sqrt{f(x_\mathrm{f})}}\left[c_1 - c_2 \int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s\right], \tag{2.4.11c}$$

$$\beta_3 \equiv c_2\sqrt{f(x_\mathrm{f})} - \frac{1}{2}\frac{f'(x_\mathrm{f})}{f(x_\mathrm{f})}\alpha_3 \tag{2.4.11d}$$

Note the lack of a t^2 term in the region III solution, it has cancelled exactly. After a little algebra one can simultaneously solve for the coefficients c_1 and c_2.

$$c_1 \sim \frac{1}{\sqrt{f(x_\mathrm{f})}}\left\{\left[1 + \frac{C}{2}\frac{f'(x_\mathrm{f})}{f(x_\mathrm{f})} - \frac{1}{2}\frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}\right]\int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s + f(x_\mathrm{f})\left[C + \frac{1}{2}\frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}(C-2)\right]\right\}, \tag{2.4.12a}$$

$$c_2 \sim \frac{1}{\sqrt{f(x_\mathrm{f})}}\left[1 + \frac{C}{2}\frac{f'(x_\mathrm{f})}{f(x_\mathrm{f})} - \frac{1}{2}\frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}\right]. \tag{2.4.12b}$$

$$Y_\infty \sim \frac{1}{\lambda}\left\{\int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s + C\,f(x_\mathrm{f}) - \frac{C^2}{2}\,f'(x_\mathrm{f}) + (C-1)\,f(x_\mathrm{f})\,\frac{F'(x_\mathrm{f})}{F(x_\mathrm{f})}\right\}^{-1}, \quad (x_\mathrm{f} \to \infty). \tag{2.4.13}$$

We again check to ensure that the relic abundance does not depend strongly on the exact choice of freeze-out temperature. Shifting $x_{\rm f} \to x_{\rm f} + \varepsilon$, retaining the $\mathcal{O}(\epsilon^2/x_{\rm f}^2)$ term, and using

$$C \to C + \epsilon - \epsilon \frac{F'(x_{\rm f})}{F(x_{\rm f})} + \mathcal{O}\left(\frac{\varepsilon^2}{x_{\rm f}^2}\right), \tag{2.4.14}$$

we find that the $\mathcal{O}(\epsilon/x_{\rm f})$, $\mathcal{O}(\epsilon/x_{\rm f}^2)$, and $\mathcal{O}(\epsilon^2/x_{\rm f}^2)$ all cancel identically in the relic abundance. Therefore, we make the convenient choice for the freeze-out temperature of $C = 1$. This choice defines the numerical value of the freeze-out temperature by

$$\lambda\, Q(x_{\rm f}) = 2e^{-\gamma-1}. \tag{2.4.15}$$

The third term in (2.4.13) then vanishes identically, and the remaining three terms match exactly to

$$\int_{x_{\rm f}-1}^{\infty} f(s)\,\mathrm{d}s \sim \int_{x_{\rm f}}^{\infty} f(s)\,\mathrm{d}s + f(x_{\rm f}) - \frac{1}{2}\,f'(x_{\rm f})\,,$$

$$(x_{\rm f} \to \infty). \tag{2.4.16}$$

It is then a straightforward numerical exercise to determine the relic abundance up to order $1/x_{\rm f}^3$. One simply determines the freeze-out temperature using (2.4.15) and then integrates the thermally averaged cross section (with the appropriate cosmological factors) from $x_{\rm f} - 1$ to infinity.

This result is very similar to those in the literature, with some seemingly minor but important corrections. Writing

$$f(x) \sim x^{-n-2} \sum_{k=0}^{\infty} f_k x^{-k},\ f_0 = 1, \quad (x \to \infty), \tag{2.4.17}$$

the relic abundance can be written

$$Y_\infty \sim \frac{(n+1)x_{\rm f}^{n+1}}{\lambda\left[1+\frac{\Upsilon_1}{x_{\rm f}}+\frac{\Upsilon_2}{x_{\rm f}^2}\right]}, \quad (x_{\rm f}\to\infty), \tag{2.4.18}$$

with

$$\Upsilon_1 \equiv \frac{(n+1)(n+2)+f_1}{(n+2)} \tag{2.4.19a}$$

$$\Upsilon_2 \equiv \frac{(n+1)(n+2)(n+3)+2(n+3)f_1+2f_2}{2(n+3)} \tag{2.4.19b}$$

Dropping all but the first term in the denominator yields a result of the same form as in [74], but with a different choice for the freeze-out temperature. However, the $1/x_{\rm f}$ term is what guarantees that the result does not depend strongly on the choice of freeze-out temperature. The error then depends linearly on the choice of $x_{\rm f}$, which indicates that the approximation is, strictly speaking, invalid.

Keeping the $1/x_{\rm f}$ corrections in (2.4.18) reproduces the results of [76] after correcting for mistakes in their analysis (see Appendix B.2). This gives us confidence that boundary-layer-analysis can be used to construct approximate solutions to other Boltzmann equations.

2.4.3 Including Resonance and Threshold Effects

We next assume that the thermally averaged cross section is exponentially decaying at leading order, with the coefficient in the exponent, α, being much larger than $1/x_{\rm f}$. In order to accommodate the additional Boltzmann suppression we write

$$f(x) \sim g(x)\, e^{-\alpha x}, \quad (x\to\infty). \tag{2.4.20}$$

Much like $F(x)$ we assume we have factored out all the exponential behavior so that $g(x)$ has a valid asymptotic approximation in powers of $1/x$ as $x \to \infty$. We will again shift the dependent variable to $x = x_\mathrm{f} + t$, and to further approximate the region III solution we split the integral into two parts,

$$\int_{x_\mathrm{f}+t}^{\infty} f(s)\,\mathrm{d}s \sim \int_{x_\mathrm{f}}^{\infty} f(s)\,\mathrm{d}s - \int_{x_\mathrm{f}}^{x_\mathrm{f}+t} f(s)\,\mathrm{d}s\,. \tag{2.4.21}$$

It is necessary to split the integral because in general the thermally averaged cross section will not be well approximated by this exponential behavior if x is sufficiently large for any finite set of parameters. We therefore leave the first integral to be evaluated numerically. The second integral can be evaluated to all orders assuming $g(x)$ is a slowing varying function over the range of integration.

$$\int_{x_\mathrm{f}}^{x_\mathrm{f}+t} f(s)\,\mathrm{d}s \sim \sum_{k=0}^{\infty} \frac{e^{-\alpha x_\mathrm{f}}}{\alpha^{k+1}}\,\gamma(k+1,\alpha t)\,g^{(n)}(x_\mathrm{f})\,, \tag{2.4.22}$$

where $g^{(n)}(x_\mathrm{f}) \equiv \mathrm{d}\,g(x)/\mathrm{d}x\,|_{x=x_\mathrm{f}}$ and $\gamma(x,z)$ is the lower incomplete gamma function,

$$\gamma(s,z) \coloneqq \int_0^z x^{s-1}e^{-x}\,\mathrm{d}x\,. \tag{2.4.23}$$

Each term in the series is suppressed by $1/(\alpha x_\mathrm{f})$ if α is large. If α is small the incomplete gamma function goes like $(\alpha t)^{k+1}$, which cancels all the factors of α in the denominator. In either case we can further approximate the region III solution by retaining only the first term in the series (2.4.22):

$$u^{\mathrm{III}}(x_\mathrm{f}+t) \sim \frac{1}{\sqrt{f(x_\mathrm{f})}}\left[\theta_\alpha^-(x_\mathrm{f})\,e^{\frac{\alpha t}{2}} - \theta_\alpha^+(x_\mathrm{f})\,e^{-\frac{\alpha t}{2}}\right] \tag{2.4.24}$$

where the constants are,

$$\theta_\alpha^-(x_\mathrm{f}) \equiv c_1 - c_2 \int_{x_\mathrm{f}}^\infty f(s)\,\mathrm{d}s + \frac{c_2}{\alpha}\, f(x_\mathrm{f})\,, \tag{2.4.25a}$$

$$\theta_\alpha^+(x_\mathrm{f}) \equiv \frac{c_2}{\alpha\sqrt{f(x_\mathrm{f})}}. \tag{2.4.25b}$$

Similarly, the region I approximation becomes

$$u^\mathrm{I}(t) \sim \frac{1}{\sqrt{1+\alpha}}\, K_\nu\!\left(\frac{\lambda\, Q(x_\mathrm{f})\, e^{-(1+\alpha)t}}{1+\alpha}\right), \quad (x_\mathrm{f} \to \infty), \tag{2.4.26}$$

where ν is defined by (2.3.23). We note that, for any value of α, the order of the Bessel function $\nu \in \left[0, \frac{1}{2}\right]$, we therefore let $t \to \infty$ and use the small argument expansion of the Bessel function for non integral orders.

$$u^\mathrm{I}(t) \sim B_\alpha\Big[\eta_\alpha^-(x_\mathrm{f})\, e^{\alpha t/2} - \eta_\alpha^+(x_\mathrm{f})\, e^{-\alpha t/2}\Big], \quad (x_\mathrm{f} \to \infty), \tag{2.4.27}$$

where the constants are

$$B_\alpha(x_\mathrm{f}) \equiv \frac{\pi}{2\sqrt{1+\alpha}\sin\!\left(\frac{\alpha\pi}{2(1+\alpha)}\right)} \tag{2.4.28a}$$

$$\eta_\alpha^+(x_\mathrm{f}) \equiv \frac{1}{\Gamma\!\left(\frac{2+3\alpha}{2+2\alpha}\right)}\left(\frac{\lambda\, Q(x_\mathrm{f})}{2(1+\alpha)}\right)^{\frac{\alpha}{2(1+\alpha)}} \tag{2.4.28b}$$

$$\eta_\alpha^-(x_\mathrm{f}) \equiv \frac{1}{\Gamma\!\left(\frac{2+\alpha}{2+2\alpha}\right)}\left(\frac{\lambda\, Q(x_\mathrm{f})}{2(1+\alpha)}\right)^{-\frac{\alpha}{2(1+\alpha)}} \tag{2.4.28c}$$

Both solutions exhibit the exact same exponential behavior. The coefficients c_1 and c_2 are easily found:

$$c_1 \sim c_2\left\{\int_{x_\mathrm{f}}^\infty f(s)\,\mathrm{d}s - \frac{f(x_\mathrm{f})}{\alpha}\left[1 - \frac{\eta^-(x_\mathrm{f})}{\eta^+(x_\mathrm{f})}\right]\right\}, \tag{2.4.29a}$$

$$c_2 \sim \frac{\alpha B_\alpha\, \eta_\alpha^+(x_\mathrm{f})}{\sqrt{f(x_\mathrm{f})}}, \quad (x_\mathrm{f} \to \infty). \tag{2.4.29b}$$

To simplify the notation and computational determination of the relic abundance we next define the parameter

$$\delta x := \frac{1}{\alpha} \ln\left(\frac{\eta_\alpha^-(x_\mathrm{f})}{\eta_\alpha^+(x_\mathrm{f})}\right). \tag{2.4.30}$$

This parameter has the following asymptotic behavior:

$$\delta x \sim 1 + \tfrac{1}{24}\Big(\psi^{(2)}(1) - 12\Big)\alpha^2, \quad (\alpha \to 0), \tag{2.4.31a}$$

$$\delta x \sim \frac{1 + \gamma - \ln(2) + \ln(\alpha)}{\alpha}, \quad (\alpha \to \infty), \tag{2.4.31b}$$

where $\psi^{(m)}(z)$ is the polygamma function of order m. Using this parameter we may write the relic abundance as

$$Y_\infty \sim \left[\lambda \int_{x_\mathrm{f}-\delta x}^{\infty} f(s)\,\mathrm{d}s\right]^{-1}, \quad (x_\mathrm{f} \to \infty). \tag{2.4.32}$$

The result (2.4.32) is valid for all values of α, and in the limit $\alpha \to 0$ reproduces the results of the previous section. It is correct up to $1/x_\mathrm{f}^2$ corrections for general α and up to $1/x_\mathrm{f}^3$ corrections when $\alpha \ll 1/x_\mathrm{f}$.

2.5 Results

We have determined an asymptotic approximation of the relic abundance in the limit that the number density of the particle species is very nearly its thermal equilibrium value until $T \ll m$, where m is the mass of the particle. We define the freeze-out condition as

$$\sqrt{\frac{\pi}{45}} \frac{m M_\mathrm{pl}\, g_{*,\mathrm{eff}}^{1/2}(x_\mathrm{f})}{x_\mathrm{f}^2} \langle \sigma v_{\mathrm{M\o l}} \rangle\, Y_\mathrm{eq}(x_\mathrm{f}) = 2e^{-1-\gamma}. \tag{2.5.1}$$

The asymptotic approximation of the relic abundance is

$$Y_\infty \sim \frac{\sqrt{45}}{\sqrt{\pi} m M_{\rm pl}} \left[\int_{x_{\rm f}-\delta x}^{\infty} \frac{g_{*,\rm eff}^{1/2}(s)}{s^2} \langle \sigma v_{\rm M\o l} \rangle \, {\rm d}s \right]^{-1}, \quad (x_{\rm f} \to \infty), \tag{2.5.2}$$

where the shift in the integration range δx is given by

$$\delta x = \frac{1}{\alpha} \ln \left(\frac{\Gamma\left(\frac{2+3\alpha}{2+2\alpha}\right)}{\Gamma\left(\frac{2+\alpha}{2+2\alpha}\right)} \right) + \frac{1+\gamma+\ln(1+\alpha)}{1+\alpha}. \tag{2.5.3}$$

In order to apply this approximation one must supply α as an input. If, as is usually the case, the thermally averaged cross section behaves like some power of $1/x$ near $x_{\rm f}$ then one should set $\alpha = 0$, i.e. $\delta x = 1$. On the other hand, if the leading order behavior near $x_{\rm f}$ of the annihilation cross section has an exponential character, i.e.

$$\langle \sigma v_{\rm M\o l} \rangle \sim x^\beta e^{-\alpha x},$$

then one should use the coefficient in the exponent, α, to determine δx from (2.5.3). We have provided the most common expressions for α in (2.2.8b), and in Appendix B.1 we derive a method to numerically calculate α for more complicated models:

$$\alpha \sim -\frac{1}{x_{\rm f}} \frac{{\rm d}^2}{{\rm d}\ln(x)^2} \ln(\langle \sigma v_{\rm M\o l} \rangle) \Big|_{x=x_{\rm f}}, \quad (x_{\rm f} \to \infty). \tag{2.5.4}$$

For models with only one stable relic one can often combine the Boltzmann equations for each particle species into a single equation that takes the form of (2.1.6), simply replacing the annihilation cross section σ with an effective annihilation cross section $\sigma_{\rm eff}$ (for example see [78]). Our analysis then also applies to such models, including those with coannihilation, by making the same replacement $\sigma \to \sigma_{\rm eff}$ in (2.5.4).

In order to estimate the fitness of our results we next compare our approximation to a numerical determination of the relic density using a benchmark model, which we now outline.

2.5.1 Benchmark Model

The benchmark model we will use is a simple extension of the SM in which we add a massive vector boson which kinetically mixes with the SM photon and a DM fermion. The Lagrangian is given by:

$$\mathcal{L} = \mathcal{L}_{\text{SM}} + \mathcal{L}_{\text{kin}} + \mathcal{L}_{\text{int}} \tag{2.5.5a}$$

$$\mathcal{L}_{\text{kin}} = -\tfrac{1}{4} V_{\mu\nu} V^{\mu\nu} + \tfrac{1}{2} M_V V_\mu V^\mu + \overline{\chi}\left(i\not{\partial} - m_\chi\right)\chi \tag{2.5.5b}$$

$$\mathcal{L}_{\text{int}} = \frac{\epsilon}{2} B_{\mu\nu} V^{\mu\nu} + g V_\mu \overline{\chi}\gamma^\mu \chi \tag{2.5.5c}$$

where V_μ is the new massive vector boson (with mass M_V), χ is the DM Dirac fermion (with mass m_χ) and B_μ is the hyper-charge gauge boson. We take the $\chi - V$ coupling g to be $\mathcal{O}(1)$ and the kinetic mixing parameter $\epsilon \ll 1$. The V-B mass matrix can be diagonalized by shifting $B_\mu \to B_\mu + \epsilon V_\mu$ and neglecting terms of $\mathcal{O}(\epsilon^2)$. After shifting the hyper-charge gauge boson, the vector mediator obtains interactions with the hyper-charge current:

$$\begin{aligned} \mathcal{L}_{\text{int}} &\supset \epsilon g' J_Y^\mu V_\mu \\ &= g'\epsilon V_\mu \left(\sum_i Q_i \overline{\psi}_i \gamma^\mu \psi + \sum_i \overline{\psi}_i^L \gamma^\mu T_3 \psi_i^L \right) \end{aligned} \tag{2.5.6}$$

where the first sum runs over all SM fermions ψ_i, the second over left-handed fermions ψ_i^L, and T_3 is essentially the third Pauli matrix $T_3 = \sigma_3/2$.

The thermally averaged $2 \to 2$ annihilation cross section for $\bar{\chi}\chi \to$ any for large x is given by

$$\langle \sigma v_{\text{Møl}} \rangle \sim \int_2^\infty \mathrm{d}z \, \mathscr{K}(x,z) \sum_{\mathbf{X}} \sigma_{\bar{\chi}\chi \to \mathbf{X}}(m_\chi z) \,, \tag{2.5.7}$$

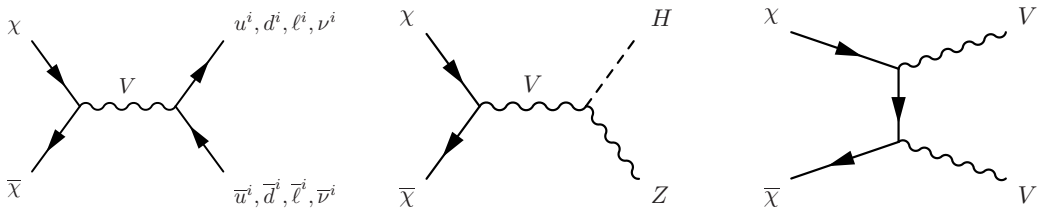


Figure 2.5: Feynman diagrams showing all possible $2 \to 2$ annihilation channels for DM in the benchmark model.

where the thermal kernel $\mathscr{K}(x, z)$ is

$$\mathscr{K}(x, z) \equiv \frac{x}{4\, K_2^2(x)} z^2 \Big(z^2 - 4\Big)\, K_1(xz)\,. \tag{2.5.8}$$

In the above expressions, z is the center-of-mass energy divided by the DM mass ($z \equiv \sqrt{s}/m_\chi$). In Fig. 2.5 we give all possible final states.

There are three interesting regions in parameters space for this model:

1. $m_\chi > M_V$: The DM is heavier than the vector mediator. There are neither thresholds nor any resonances. The dominant process is simply $\bar{\chi}\chi \to VV$. All other processes are negligible (assuming ϵ is small).

2. $M_V/2 < m_\chi < M_V$: The DM is lighter than the vector but heavier than half the vector mass. At large temperatures we will pass through a threshold in which, due to finite temperature, the final state $\bar{\chi}\chi \to VV$ opens up. For smaller temperatures, this final state becomes Boltzmann suppressed.

3. $m_\chi < M_V/2$: The DM is lighter than half the vector mass. At large temperatures, we will pass through both a resonance ($z = m_V/m_\chi$) and a threshold ($z = 2m_V/m_\chi$).

In Fig. 2.6 we show the magnitude of the relative error between a numerical

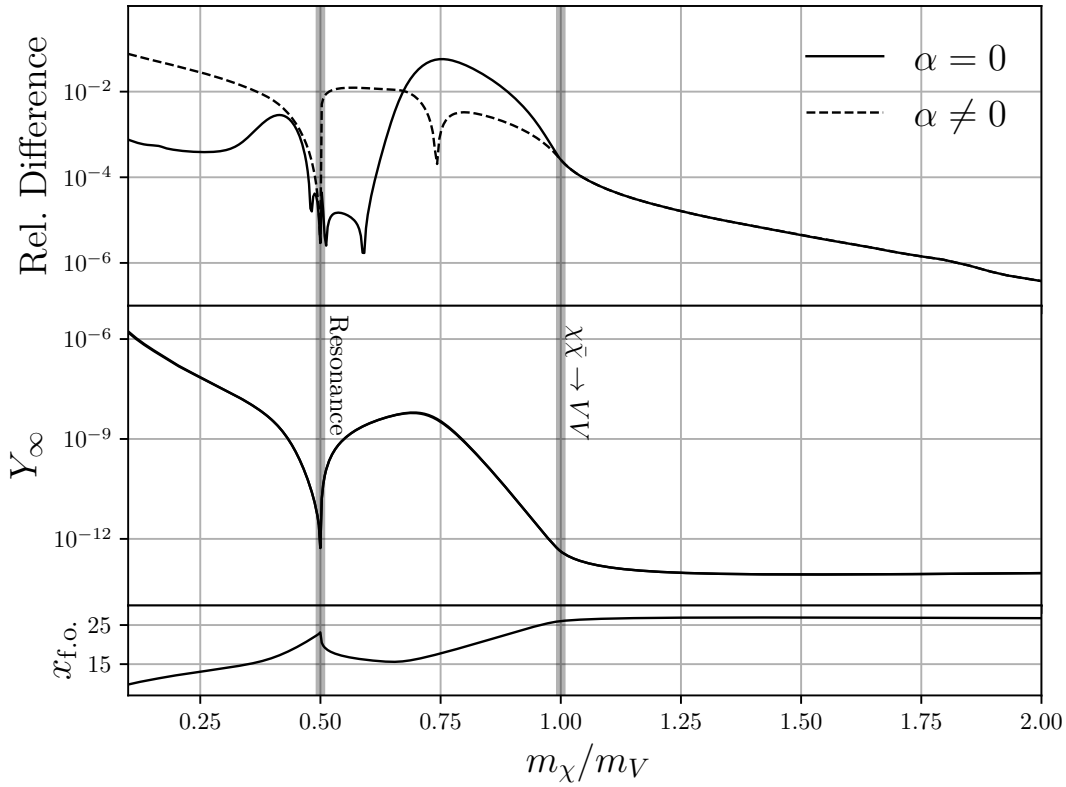


Figure 2.6: The asymptotic approximation of the thermal relic abundance compared to numerical results using a benchmark model. Top: The magnitude of the relative error between the asymptotic approximation and numerical results. Middle: The thermal relic abundance. Bottom: the freeze-out temperature. We set $M_V = 1\,\text{TeV}$, $g = 1$, $\epsilon = 10^{-3}$, and vary the mass of the DM particle from $m_\chi = 100\text{GeV} - 2\,\text{TeV}$. One can see the affect of the resonance and $\chi\bar{\chi} \to VV$ threshold from the rise in the power law ($\alpha = 0$) approximation near $m_\chi/M_V = 0.5$ and $m_\chi/M_V = 1$.

determination of the thermal relic density and the asymptotic approximations derived here using

$$\Omega_\chi h^2 = 2.744 \times 10^8 \frac{m_\chi}{\text{GeV}} Y_\infty. \tag{2.5.9}$$

The numerical results were obtained using the high-fidelity, order-switching, implicit RADAU integrator [79] taken from the author's website[2]. We recast the Boltzmann

[2]We use a slightly modified version of the C++ code from: https://unige.ch/~hairer/software.

equation into a logarithmic form in order to work with numbers of $\mathcal{O}(1-10)$:

$$\frac{\mathrm{d}W}{\mathrm{d}\ln(x)} = -\sqrt{\frac{\pi}{45}}\frac{mM_{\mathrm{pl}}}{x} g_{*,\mathrm{eff}}^{1/2} \langle \sigma v_{\mathrm{M\o l}} \rangle \left(e^{W} - e^{2W_{\mathrm{eq}}-W} \right), \tag{2.5.10}$$

with $W = \ln(Y)$ (and $W_{\mathrm{eq}} = \ln(Y_{\mathrm{eq}})$). The integration was performed over the interval $x = 1$ to $x = 5 \times 10^4$, beginning the integration with $W(x=1) = W_{\mathrm{eq}}(x=1)$ and maintaining a local error of $\mathcal{O}(10^{-10})$ (and a global error $\mathcal{O}(10^{-9})$). In order to reduce roundoff error we employ long double (80 bit floating point) precision arithmetic.

We vary the DM mass while keeping all other parameters fixed. Because resonance effects may be important for some values of the mass ratio we compare results using $\alpha = 0$ for all masses and the value of α obtained from (2.2.8b). With the exception of resonance and theshold effects, not accounted for in the $\alpha = 0$ approximation, as x_{f} becomes larger the relative error decreases, as is expected from the asymptotic nature of the approximation.

2.6 Conclusion

We have shown, using this benchmark model, that our results satisfy the requirements of an asymptotic approximation. The controlling parameter is x_{f}, and as x_{f} becomes large the relative error approaches 0. As well, our approximation yields outstanding results, giving sub percent relative errors for all parameters investigated. This is comparable or greatly exceeds the current measurement uncertainty of the Hubble parameter of roughly a percent or more [80–86]. The asymptotic approximation of the thermal relic density typically takes orders of magnitudes less time to compute than

`html`.

numerically integrating (2.1.6), making scans over models with large numbers of parameters more feasible. For the choices of parameters shown we typically have $\lambda \approx 10^{14}$, this results from weak scale cross sections but is already quite large. If one is interested in strongly interacting massive particles (SIMPs), or models with very large cross sections in general, (2.1.6) becomes exceptionally stiff, making numerical integration prohibitively difficult and quite unstable if not completely impossible. Reduction of order problems can also lead to overly optimistic error approximations, with no indication that anything is amiss. Our results do not suffer from such difficulties.

Having an analytic expression for the thermal relic density is useful in its own right, for instance in large $\mathcal{N}$ Yang-Mills models one may be interested in the analytic behavior of thermal relic density as one takes the number of colors $\mathcal{N}$ to infinity. This behavior can be found from (2.5.2) easily, but numerical methods must rely on extrapolation. All that is required to implement our results are standard cosmological parameters and the thermally averaged cross section as inputs, and a simple quadrature routine. The end user is not bound by the limitations of external software, thus making analysis of models that do not adhere to the typical requirements of prepackaged programs such as Lorentz invariance possible.

In addition, our method constitutes a global asymptotic approximation to the solution of a problem with an infinite order turning point. In fact, this procedure can be used to construct approximations to an entire class of problems of the form:

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} - \left[\lambda^2 F^2(x)\, e^{-2x} + P(x)\right] u = 0. \tag{2.6.1}$$

We have shown that the uniform WKB ansatz (2.3.9) allows one to extend the region

of validity of the small x approximation sufficiently close to the turning point at $x = \infty$ such that one can asymptotically match to the large x approximation. This has a large range of physics applications, including quantum mechanical scattering with a Yukawa type potential.

Our particular program could possibly generalize to a larger set of Boltzmann equations, but because our results rely on using a uniform WKB approximation we can only apply our procedure to systems that can be linearized. However, one could apply boundary-layer-analysis to obtain valid results for a multitude of Boltzmann equations.

Chapter 3

Lowest Dimensional Portals to SU(N) Exotics

3.1 Introduction

In the Standard Model of particle physics, matter fields are spin-1/2 Dirac fermions. Strong nuclear interactions are highly successfully modeled by an unbroken local gauge symmetry with gauge group SU(3). Matter fields that are strongly interacting belong to the fundamental (**3**) representation of SU(3), while their antimatter counterparts to the antifundamental ($\bar{\mathbf{3}}$) representation of SU(3). In terms of Dynkin labels, strongly interacting matter fields belong to the (1,0) representation, and antimatter, strongly interacting fields to the (0,1) representation of SU(3). The spin-1, massless force carriers, "gluons", belong to the adjoint (**8**) representation, the (1,1).

Grand unification schemes, where two or more of the Standard Model gauge groups arise from symmetry breaking, at some very high energy scale, of larger "unified"

gauge groups, have a similar structure. For instance, in Pati-Salam models based on $\mathrm{SU}(4)\times\mathrm{SU}(2)_\mathrm{L}\times\mathrm{SU}(2)_\mathrm{R}$ or $\mathrm{SU}(4)\times\mathrm{SU}(2)_\mathrm{L}\times\mathrm{SU}(2)_\mathrm{R}/\mathbb{Z}_2$ [87], matter fermions charged under strong interactions are accommodated in the fundamental representations $\mathbf{4}\cong(1,0,0)$ and $\bar{\mathbf{4}}\cong(0,0,1)$, with additional exotic states in the $\mathbf{6}\cong(0,1,0)$ representation; in Georgi-Glashow SU(5) grand unified theories [88] matter fermions are accommodated in the $\mathbf{5}\cong(1,0,0,0)$, $\mathbf{10}\cong(0,1,0,0)$, and their conjugate representations $\bar{\mathbf{5}}$ and $\bar{\mathbf{10}}$; in SU(6), Standard Model matter fermions are accommodated in the $\mathbf{6}\cong(1,0,0,0,0)$ and $\mathbf{15}\cong(0,1,0,0,0)$ and their conjugate representations $\bar{\mathbf{6}}$ and $\bar{\mathbf{15}}$, with possible additional beyond-the-Standard-Model matter fermions in the $\mathbf{20}\cong(0,0,1,0,0)$ (see e.g. [89] and [90]).

In constructing beyond-the-Standard-Model theories, new exotic states (by "exotic" state we indicate a physical state belonging to any representation of SU(N) different from the fundamental representation(s) and the adjoint representation) are assigned charges, or representations, under the Standard Model gauge groups (or under grand unified gauge groups as the case may be). If these exotic states belong to non-trivial gauge group representations it is of paramount importance for phenomenology to establish which interaction terms are allowed by gauge invariance to exist in the model's Lagrangian. Such interaction terms, of course, may not be renormalizable. If they are not, it is implicitly assumed that some high-scale physics is effectively integrated out, yielding the higher dimensional operators. In either case, the most important operators at low energies are those with the lowest mass dimension. In this study, we are precisely interested in which arrangement of matter fields and force mediators (in the adjoint representation) are needed to produce the *lowest mass dimension gauge-*

invariant operator between any given new exotic state and Standard Model fields. We refer to any operator containing both the field corresponding to the exotic state and Standard Model fields as a "portal", in that such operator would mediate interactions between the exotic states and the Standard Model, acting, as such, as a "portal" to new physics. Such terminology is common in particle physics, see e.g. [91–93].

In a non-perturbative regime, the question we address can be recast as the question of which arrangements of "quarks", "antiquarks" and "gluons" are needed to dress a given exotic state into a gauge-singlet, color-less combination: thus the question can be recast, borrowing the notion of "valence gluon" [94, 95], as what is the smallest SU(N) color-less bound state (see the recent study [96]).

From a group theoretic standpoint, we can reformulate the question as: given a gauge group SU(N) and a new exotic state, X, belonging to some irreducible representation (irrep) of SU(N), what is the most economical (in the sense of mass dimension of the corresponding operator) tensor product of fundamental and adjoint representations of SU(N) that contains the trivial representation? Since matter fermions have higher mass dimension than spin-1 force carriers in the adjoint representation, one seeks to minimize the number of matter fermions. Since it is necessarily the case that a tensor product containing the trivial representation has vanishing N-ality, it is then obvious that the solution includes a single tensor product with the one fundamental representation Q_i that takes the product $X \otimes Q_i$ to N-ality equal to zero, with as many copies k of the adjoint representation G_N as needed for the product $X \otimes Q_i \otimes G_N^{\otimes k}$ to eventually contain the trivial representation.

Technically, the intricacy of this problem lies in decomposing the *k-fold tensor*

product of adjoint representations into a direct sum of irreps of SU(N). While some general results are known, for example in the context of the Littlewood-Richardson rule (see e.g. [97]), we are not aware of any general result on the product of several copies of the adjoint representation. Here, we provide first, in the following section 3.2, a visually simple, algorithmic approach for building the gauge invariant operator, given the N-ality zero combination $X \otimes Q_i$, and provide examples and complete formulae for SU(N) with $N = 3,\ 4,\ 5$. We then discuss in sec. 3.3 the problem of what is the minimal k such that $\mathbb{1} \subset X \otimes G_N^{\otimes k_{\min}}$, or, equivalently, $X^* \subset G_N^{\otimes k_{\min}}$. The full problem of finding the minimal k such that $\mathbb{1} \subset X \otimes Q_i \otimes G_N^{\otimes k_{min}}$ is then solved in sec. 3.3.2. Because, especially for large N and large-dimensional representations for the exotic field X, the calculation is rather complicated, we describe in sec. 3.4 a python code, `tessellation`, which we make publicly available, to perform the needed calculations. We collect in two appendices the needed mathematical details, and a short user's manual for the `tessellation` code.

3.2 An algorithmic approach for building the gauge invariant operator

In this section, we present an algorithmic approach to finding the minimum number of copies, $k_{\min}$, of the adjoint representation, G_N, needed such that the product with a representation with vanishing N-ality contains the trivial representation; we believe this discussion will provide an intuitive understanding of the problem. We explicitly solve through $N = 4$, outline considerations for extending to $N > 4$, and

present formulae for $N = 3, 4, 5$ in Table 3.1. We also outline some considerations for arbitrary representations with non-zero N-ality before proceeding to a full solution in the following Sec. 3.3.

We begin by taking the tensor product of X with a single copy of the adjoint representation (see e.g. Ref. [98] for a general discussion of Young tableaux in the context of tensor products of group representations). We write the Dynkin label for X as $(p_1, p_2, \ldots, p_{N-1})$. The adjoint representation has Dynkin label $G_N \cong (1, 0, \ldots, 0, 1)$, and is composed of N boxes: two in the first row and one in each of the following $N - 2$ rows. The result of the tensor product is a direct sum of irreps, each with a unique tableau. Illustrated in Fig. 3.1 are several examples for the case of $N = 4$. The allowed configurations include placing one box on each row of X (including the bottom, or N^{th}, row which is assumed to initially have no boxes), or placing two boxes on the same row of X and one box on all but one of the remaining rows. The former possibility simply lengthens every row by one, effectively mapping X to itself ($(p_1, ..., p_{N-1}) \rightarrow (p_1, ..., p_{N-1})$), and thus adds a copy of the adjoint representation without getting closer to a representation containing the trivial representation. We will, therefore, only consider steps which add two boxes to one of the rows. Among these possibilities it is also never useful to add two boxes to the top row; in fact, the best step we can take is to add two boxes to the lowest row possible while maintaining rows which reduce in length from top to bottom. This allows us to complete at least one column and minimizes the steps needed to complete additional columns (see also the following sec. 3.3 for a formal proof of this statement).

In the best case scenario, the number of steps needed will simply be the number

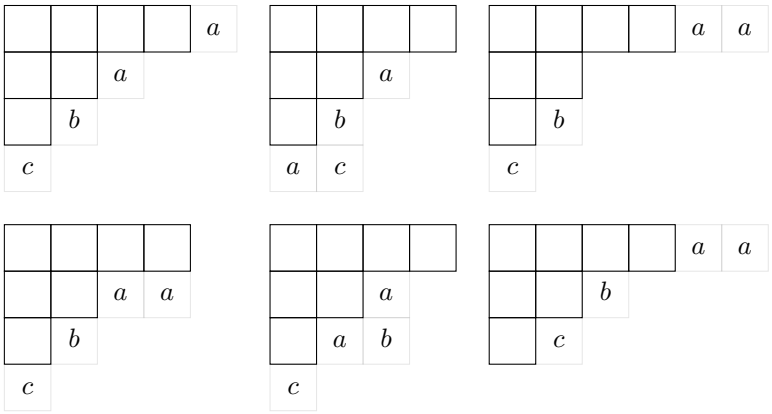


Figure 3.1: Representations resulting from the tensor product of the representation (2,1,1) of SU(4) with the adjoint representation of SU(4), (1,0,1), whose Young tableaux boxes are labeled by the letters a, b and c.

of boxes required to "fill in" the tableau for X. If the tableau for X has t boxes, where

$$t = \sum_{j=1}^{N-1} j p_j, \tag{3.2.1}$$

then the number of boxes in the resulting rectangle that just fits X will be the length of the first row of X times N:

$$\text{Area} = N \sum_{j=1}^{N-1} p_j. \tag{3.2.2}$$

Thus, the number of boxes needed to complete a rectangle is this area, less the number of boxes in X:

$$\begin{aligned} t^* &\coloneqq \text{Area} - t, \\ &= \sum_{j=1}^{N-1} (N-j) p_j. \end{aligned} \tag{3.2.3}$$

This t^* corresponds to the number of boxes in the *dual representation* to X. Because the tableau for the adjoint representation has N boxes, the *optimistic minimum number*

of steps is

$$\begin{aligned} k_{\text{opt}} &\coloneqq \frac{t^*}{N}, \\ &= \frac{1}{N}\sum_{j=1}^{N-1}(N-j)p_j. \end{aligned} \tag{3.2.4}$$

The true minimum number of steps required will always be equal to or exceed this optimistic minimum ($k_{\text{min}} \geq k_{\text{opt}}$).

We now state the algorithm as a theorem:

Theorem 3.2.1. *Consider an irrep, X, of* $\mathrm{SU}(N)$*, with Dynkin label $(p_1, p_2, \ldots, p_N)$. If*

$$\sum_{j=1}^{N} jp_j = 0 \mod N, \tag{3.2.5}$$

and $N \leq 4$, we can always take the tensor product of this X with k_{min} copies of the adjoint representation, where

$$k_{\text{min}} = \begin{cases} \dfrac{1}{N}\displaystyle\sum_{j=1}^{N-1}(N-j)p_j & p_1 \geq \displaystyle\sum_{j=2}^{N-1}(N-j)p_j, \\ \dfrac{2}{N}\displaystyle\sum_{j=1}^{N-1}(N-j)p_j - p_1 & p_1 < \displaystyle\sum_{j=2}^{N-1}(N-j)p_j, \end{cases} \tag{3.2.6}$$

to arrive at the trivial representation. The algorithm proceeds in three stages:

(1) Take p_{N-1} steps (i.e. tensor products with the adjoint representation), adding two boxes to the bottom row and one box to every row except the top, reducing $(p_1, p_2, \ldots, p_{N-1})$ to $(p_1 - p_{N-1}, p_2, \ldots, 0)$.

(2) While $p_1 > 0$, iteratively place two boxes on the next to lowest row followed by the lowest row until $p_{N-2} = p_{N-1} = 0$ after $2p_{N-2}$ steps; then follow a similar process of $3p_{N-3}$ steps to reduce to $p_{N-3} = p_{N-2} = p_{N-1} = 0$, etc. The total steps taken

from the starting representation is $p_{N-1} + 2p_{N-2} + 3p_{N-3} + \ldots$ *and the value of first Dynkin label is now* $p_1 - p_{N-1} - 2p_{N-2} - 3p_{N-3} - \ldots$.

(3) (conditional) If $p_1 = 0$*, add a box to row 1 increasing* p_1 *to one and reducing* p_2 *by one. Add the other* $N - 1$ *boxes on the lowest rows possible, reducing the value of the largest non-zero Dynkin label,* p_i*, by one.*

Proof. Starting from an initial representation with N-ality equal to zero, or which we have brought to N-ality of zero by taking the tensor product of X with the appropriate fundamental representation (see sec. 3.3.2), we ask what is the minimum number copies of the adjoint representation, $k_{\min}$, required to get to a direct sum of irreps that includes the trivial representation, effectively, and visually, constructing a rectangular tableau from X and $k_{\min}$ copies of G_N. Each stage of the algorithm is composed of multiple steps. At each step we will take the tensor product with an additional copy of the adjoint representation. The total number of steps needed to arrive at the trivial representation is then equal to $k_{\min}$.

We take advantage of the fact that the adjoint representation is self dual. It is convenient to choose, as the starting point, whichever of $(p_1, p_2, \ldots, p_{N-1})$ or $(p_{N-1}, p_{N-2}, \ldots, p_1)$ ensures $p_1 \geq p_{N-1}$. In step 1, we take the tensor product of X and G_N once, placing two boxes on the bottom row and one box on each row except the top row. The ordering with $p_1 \geq p_{N-1}$ ensures that this results in a valid tableau unless $p_1 = p_{N-1} = 0$. What happens in the case of $p_1 = 0$ is described later. This step has the effect of reducing both p_1 and p_{N-1} by one while leaving the other p_i unchanged, $(p_1, p_2, \ldots, p_{N-1}) \to (p_1 - 1, p_2, \ldots, p_{N-1} - 1)$ (see Fig. 3.2a). We can then repeat this

process p_{N-1} times until $p_{N-1} = 0$ (see Fig. 3.2b). This concludes the first stage of the algorithm.

With $p_{N-1} = 0$, the next step must add two boxes to row $N-1$ to ensure that it is longer than row N. Assuming our new p_1 (equal to $p_1 - p_{N-1}$) is greater than zero, we will also add one box each to the other rows except the top row. This step reduces p_1 by one, reduces p_{N-2} by one, and increases p_{N-1} to one (see Fig. 3.2c). In the following step we can again add two boxes to the bottom row, reducing p_{N-1} again to zero, reducing p_1 by one, and leaving the other p_i unchanged (see Fig. 3.2d). Thus it takes two steps to reduce p_{N-2} by one and have $p_{N-1} = 0$. This set of two steps may be repeated, while the first term p_1 is greater than zero, until $p_{N-2} = p_{N-1} = 0$ after $2p_{N-2}$ additional steps. At this point the lowest row on which we can place two boxes is $N-2$, which reduces the size of p_{N-3}. Reducing p_{N-3} by one and returning to $p_{N-2} = p_{N-1} = 0$ requires a set of three steps as we iteratively increase p_{N-2} and p_{N-1} to one and then bring them back to zero (i.e. we add two boxes first to row p_{N-2}, then to row p_{N-1}, and finally to p_N). Thus we conclude the second stage of the algorithm.

How this process concludes depends on whether the starting value of p_1 is equal to, greater than, or less than $\sum_{j=2}^{N-1}(N-j)p_j$. We consider each of these in turn. If $p_1 = \sum_{j=2}^{N-1}(N-j)p_j$ then we reduce p_1 to zero just as all of the other p_i go to zero. Here we form a complete rectangle (trivial representation) in the optimistic minimum number of steps, given the number of missing boxes in the starting state compared to a rectangle of height N and length $\sum_{j=1}^{N-1} p_j$.

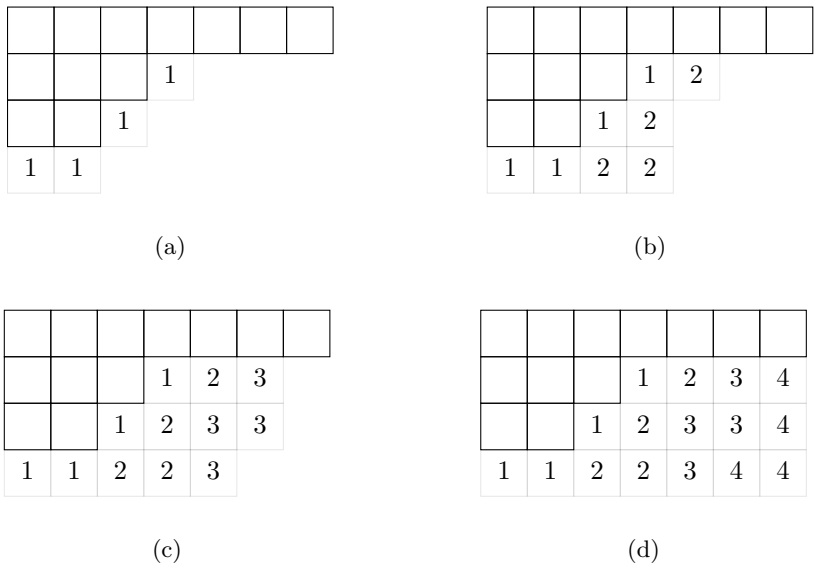


Figure 3.2: An example for $N = 4$ of a representation, here (4,1,2), which can be completed in the minimum possible number of steps.

$$k_{\min} = \sum_{j=2}^{N-1} (N-j)p_j, \quad \text{if} \quad p_1 = \sum_{j=2}^{N-1} (N-j)p_j. \tag{3.2.7}$$

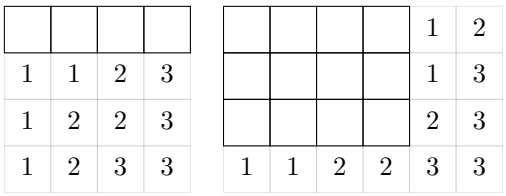


Figure 3.3: Examples for $N = 4$ of the symmetric representations, (4,0,0) and (0,0,4), which can be completed in the same number of steps.

If $p_1 > \sum_{j=2}^{N-1} (N-j)p_j$, we again complete the rectangle (i.e. get to a product of representations containing the trivial representation) in the optimistic minimum number of steps. This situation implies that we can bring all of the p_i with $i > 1$ to zero with some of the length of p_1 remaining. In this case, the remainder of p_1, which we shall call p_1', is necessarily a multiple of N given the starting condition of N-ality

zero. Writing $p_1' = jN$, presently we have a state of the form $(jN, 0, \ldots, 0)$. This representation can be reduced to the trivial representation in $(N-1)j$ steps (see e.g. the left panel of Fig. 3.3). The total number of steps from the initial representation in this case is

$$\begin{aligned} k_{\min} &= \sum_{j=2}^{N-1} (N-j)p_j + \frac{N-1}{N}\left(p_1 - \sum_{j=2}^{N-1}(N-j)p_j\right), \\ &= \frac{1}{N}\sum_{j=1}^{N-1}(N-j)p_j, \quad \text{if} \quad p_1 > \sum_{j=2}^{N-1}(N-j)p_j. \end{aligned} \tag{3.2.8}$$

If $p_1 < \sum_{j=2}^{N-1}(N-j)p_j$, then the p_1 term reaches zero before all of the other rows are zero. This situation requires that we expand beyond the bounds of our initial rectangle and take more than the optimistic minimum number of steps. Given the reordering we did in the beginning, we know that p_{N-1} is either zero or one at this point. In the step after the first term reaches zero, we add one box to the first row, increasing p_1 to one and reducing p_2 by one (see Fig. 3.4). The rest of this stage looks just like the previous ones we have taken; if $p_{N-1} = 1$, this term is reduced to zero and if it is not, the first non-zero term is reduced by one. The following step starts with $p_1 = 1$ and proceeds just like our previous steps reducing p_1 back to zero. Thus the effect of adding steps beyond the optimistic minimum (adding columns on to our rectangle) is to reduce p_2 by one and add two steps above the optimistic minimum for each extra column. We can then proceed as before, reducing each of the p_i in turn with the difference that when we get to reducing the p_2 term its value will be $p_2 - N_{\text{extra}}$, where N_{extra} is the number of extra columns. This concludes the third stage.

The total number of steps taken, assuming $p_2 - N_{\text{extra}}$ is greater than zero

until the final step, is then

$$k_{\min} = (N-2)(p_2 - N_{\text{extra}}) + \sum_{j=3}^{N-1}(N-j)p_j$$

$$= \frac{1}{N}\sum_{j=1}^{N-1}(N-j)p_j + N_{\text{extra}}, \tag{3.2.9}$$

$$\text{if} \quad p_1 < \sum_{j=2}^{N-1}(N-j)p_j.$$

Solving for the number of extra columns,

$$N_{\text{extra}} = \frac{1}{N}\sum_{j=2}^{N-1}(N-j)p_j - p_1, \tag{3.2.10}$$

and substituting (3.2.10) into (3.2.9) then gives

$$k_{\min} = \frac{N-2}{N}p_1 + \frac{2}{N}\sum_{j=2}^{N-1}(N-j)p_j$$

$$= \frac{2}{N}\sum_{j=1}^{N-1}(N-j)p_j - p_1 \tag{3.2.11}$$

$$\text{if } p_1 < \sum_{j=2}^{N-1}(N-j)p_j, \quad p_2 \geq \frac{1}{2}\left[\sum_{j=3}^{N-1}(N-j)p_j - p_1\right].$$

The total number of steps in this case is twice the optimistic minimum minus p_1, with p_1 being the number of steps we can take before adding extra columns. The condition on the size of p_2 comes from finding the value of p_2 such that it just reaches zero when the other p_j all reach zero. In this case, $k_{\min} = \sum_{j=3}^{N-1}(N-i)p_j$. At this point, we have fully solved for $N \leq 4$, since for $N = 4$, $p_3 = p_{N-1} \leq p_1$ by virtue of our starting representation and the condition on p_2 is always satisfied. □

For $N \geq 5$, there is the possibility that we arrive at a representation with zeros in the first two (or more) terms while the other p_j remain non-zero, e.g. $(0, 0, p_3', p_4')$. An easy method to see the number of steps remaining in this case is to consider the

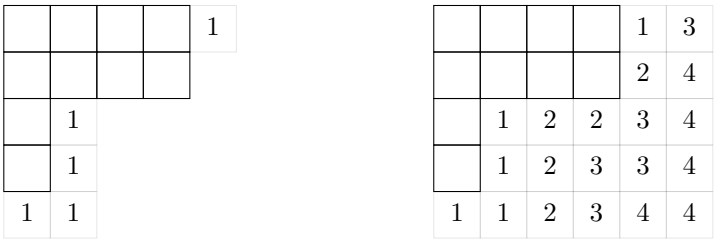


Figure 3.4: Example for $N = 5$ of a representation, here (0,3,0,1), for which completion requires expanding beyond the original length.

"symmetric" case, e.g. $(p'_4, p'_3, 0, 0)$, which will require the same number of steps to reduce (see Fig. 3.3 for one example). Here we know that p'_{N-1} is either 0 or 1 again by virtue of having started with $p_1 \geq p_{N-1}$. This means our "symmetric" representation automatically has $p_1 < \sum_{j=2}^{N-1}(N-j)p_j$ and the solution is given by Eqn. 3.2.11. The total number of steps taken is then the sum of the number of steps to get from an initial state $(p_1, p_2, \ldots, p_{N-1})$ to $(0, 0, p'_3, \ldots, p'_{N-1})$ plus the number of steps to reduce $(p'_{N-1}, \ldots, p'_3, 0, 0)$.

Explicit formulae for $k_{\min}$ for $N = 3, 4, 5$ are given in Table 3.1. For $N = 6$, there is the possibility of arriving at representations with three leading zeros $(0, 0, 0, p'_4, p'_5)$ or of the form $(0, 0, p'_3, 0, 0)$. The former can again be solved through symmetry. In the latter case, because N-ality is zero $p'_3 = iN/(N-3) = 2i$, for $N = 6$ and where i is a positive integer. To reduce from here $(N-3)i = 3i$ steps are needed. For $N > 6$, additional cases emerge, and we seek a fully general solution in the next section.

The following section also presents a general solution for non-zero N-ality. Here we discuss a few general considerations for this case. For a general representation X with N-ality equal to t, we can bring the initial representation to N-ality of zero in one step by adding a fundamental representation of $N - t$ boxes. Adding these

N	case (1)	case (2)	case (3)
3	$\frac{2p_1+p_2}{3}$	–	–
4	$\frac{3p_1+2p_2+p_3}{4}$	$\frac{2p_1+4p_2+2p_3}{4}$	–
5	$\frac{4p_1+3p_2+2p_3+p_4}{5}$	$\frac{3p_1+6p_2+4p_3+2p_4}{5}$	$\frac{2p_1+4p_2+6p_3+3p_4}{5}$

Table 3.1: Minimum number of steps, $k_{\min}$, for a state with N-ality of zero and $p_1 \geq p_{N-1}$. For a state with $p_{N-1} > p_1$, the number of steps is that of the symmetric state $(p_{N-1}, p_{N-2}, \ldots, p_1)$. The columns correspond to the three possible cases:
case (1) $\sum_{j=2}^{N-1}(N-j)p_j$;
case (2) $p_1 < \sum_{j=2}^{N-1}(N-j)p_j$ and $p_2 \geq \frac{1}{2}\sum_{j=3}^{N-1}(N-j)p_j - \frac{1}{2}p_1$;
case (3) $p_1 < \sum_{j=2}^{N-1}(N-j)p_j$ and $p_2 < \frac{1}{2}\sum_{j=3}^{N-1}(N-j)p_j - \frac{1}{2}p_1$

boxes to the lowest rows possible (while maintaining rows of decreasing length) will result in the representation which will then fill most efficiently (see Fig 3.5). If the term $p_t \neq 0$, boxes are added to the rows below row t and p_t is reduced by one. The resulting N-ality zero representation will be $(p_1, \ldots, p_t - 1, \ldots, p_{N-1})$. What happens if $p_t = 0$ depends on if the surrounding terms are also zero, but in general one of the zero terms increases to one while the non-zero terms above and below decrease by one. For example, if $p_t = 0$ and $p_{t+1}, p_{t-1} \neq 0$, then the resulting N-ality zero representation will be $(p_1, \ldots, p_{t-1} - 1, 0, p_{t+1} - 1, \ldots, p_{N-1})$.

3.3 Solution for General N

In the previous section we saw that the algorithmic procedure bifurcates at various stages depending on the particular irrep X that we start with. In general, as one proceeds through the algorithm there will be $N-1$ branch points between the initial

irrep and the trivial representation. As the gauge group parameter N becomes large the number of cases quickly becomes unmanageable, making a general solution elusive. In this section we take a different approach, motivated by the observation that

$$X^* \subset \mathrm{G}_N^{\otimes k} \implies \mathbb{1} \subset X \otimes \mathrm{G}_N^{\otimes k}, \tag{3.3.1}$$

where X^* is the dual representation to X. Therefore, we first decompose the tensor product of k copies of the adjoint representation into a direct sum of irreps of SU(N). Then, given any X with vanishing N-ality we will show that there exists a minimum $k = k_{\min}$ such that $X^* \subset \mathrm{G}_N^{\otimes k_{\min}}$. We then extend our analysis to cases when X does not have vanishing N-ality. This is accomplished by including an additional *matter field*, Q_i, in the tensor product, where the index i denotes the i^{th} fundamental representation. This index will be fixed by requiring $X \otimes Q_i$ have vanishing N-ality. The vector space $X \otimes Q_i$ further decomposes into a direct sum of irreps, with each subvector space generally resulting in a different value of $k_{\min}$. We conclude this section by developing an algorithmic procedure for determining the optimum irrep in $X \otimes Q_i$ that leads to the smallest value of $k_{\min}$ such that

$$\mathbb{1} \subset X \otimes Q_i \otimes \mathrm{G}_N^{\otimes k_{\min}}, \tag{3.3.2}$$

still holds.

3.3.1 Adjoint Product Decomposition

We need decompose the k-fold tensor product of the adjoint representation of SU(N) into a direct sum of irreps of SU(N). We will start with one irrep that is easily

found, and then build the remaining irreps from this one. The choice of starting point is made with the following Lemma:

Lemma 3.3.1. *The highest weight of the highest irrep,* $\bar{\Lambda}$*, of* $\mathrm{G}_N^{\otimes k}$ *is*

$$\bar{\Lambda} \coloneqq k\bar{\lambda} = (k, \underbrace{0, \ldots, 0}_{N-3}, k), \tag{3.3.3}$$

where $\bar{\lambda}$ *is the Dynkin label (highest weight) of* G_N*.*

Proof. Denote the weights of G_N by λ_i, with $\lambda_1 \equiv \bar{\lambda}$ and $i \in \{1, 2, \ldots, N^2 - 1\}$. Since $\bar{\lambda}$ is the highest weight of G_N,

$$\bar{\lambda} \succ \mu, \quad \forall \mu \in \{\lambda_2, \lambda_3, \ldots, \lambda_{N^2-1}\}. \tag{3.3.4}$$

where $\succeq$ constitutes a partial ordering of the weights. Every other weight of G_N can be constructed from $\bar{\lambda}$ by removing some number of positive roots:

$$\lambda_i = \bar{\lambda} - \theta_{ijk}\alpha^{jk}, \quad \theta_{ijk} \in \mathbb{R}^+, \ \alpha^{jk} \in \Delta^+, \tag{3.3.5}$$

where Δ^+ is the set of all positive roots of $\mathrm{SU}(N)$, and the θ_{ijk} cannot all vanish (except when $i = 1$). Every weight of $\mathrm{G}_N^{\otimes k}$ can be written

$$\Lambda_i = \xi_i^j \lambda_j, \quad \xi_i^j \in \mathbb{N}_0, \quad \sum_{j=1}^{N^2-1} \xi_i^j = k. \tag{3.3.6}$$

Substituting (3.3.5) into (3.3.6) then gives

$$\Lambda_i = k\bar{\lambda} - \sum_{j=2}^{N^2-1} \xi_i^j \theta_{jkl}\alpha^{kl}. \tag{3.3.7}$$

But then

$$k\bar{\lambda} - \Lambda_i = \sum_{j=2}^{N^2-1} \xi_i^j \theta_{jkl}\alpha^{kl}. \tag{3.3.8}$$

Defining $\bar{\Lambda} \equiv \Lambda_1 \coloneqq k\bar{\lambda}$ we then see that

$$\sum_{j=2}^{N^2-1} \xi_i^j \theta_{jkl} \in \mathbb{R}^+ \implies \bar{\Lambda} \succ \Lambda_i, \quad \forall i > 1. \tag{3.3.9}$$

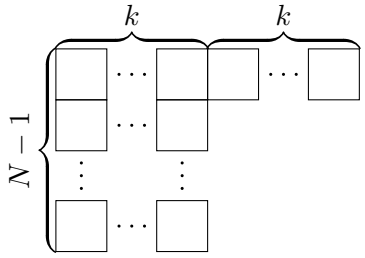
Therefore, $\bar{\Lambda}$ is the highest weight of $\mathrm{G}_N^{\otimes k}$. □

We cannot take the tensor product of any arbitrary X with some number of copies of the adjoint representation and expect to find the trivial representation. Intuitively, the tableau for X needs to have some integer multiple of N number of boxes in order for this to work (since the tableau for G_N has N boxes). This is the vanishing N-ality condition, which we state more formally in the following Theorem:

Theorem 3.3.2. *For a given irrep, X, of $\mathrm{SU}(N)$, with Dynkin label $(p_1, p_2, \ldots, p_{N-1})$ the following holds:*

$$\sum_{j=1}^{N-1} j p_j = 0 \mod N \implies \exists k \in \mathbb{N} \mid \mathbb{1} \subset X \otimes \mathrm{G}_N^{\otimes k}\,. \tag{3.3.10}$$

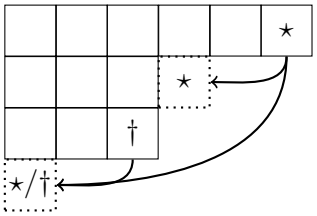
Proof. The weight $\bar{\Lambda}$ belongs to one and only one irrep in $\mathrm{G}_N^{\otimes k}$, which we denote $V_{\bar{\Lambda}}$. To $V_{\bar{\Lambda}}$ we associate the tableau

$V_{\bar{\Lambda}} \cong$ 

(3.3.11)

From Lemma 3.3.1 every other irrep has an associated tableau with fewer boxes in the first row. Therefore, to generate the other irreps in $\mathrm{G}_N^{\otimes k}$ we move boxes from the top rows of $V_{\bar{\Lambda}}$ to lower rows, and require that the resulting tableau remain valid (i.e. the number of boxes in each row are weakly decreasing). For example, with $k = 3$ and

$N = 4$ we can do the following moving only one box:



More generally, consider moving i_{jk} boxes from row j to row k with $j < k$. To this procedure we associate a totally antisymmetric $N \times N$ matrix:

$$M = \begin{pmatrix} 0 & i_{12} & i_{13} & \dots & i_{1N} \\ -i_{12} & 0 & i_{23} & \dots & i_{2N} \\ -i_{13} & -i_{23} & 0 & \dots & i_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -i_{1N} & -i_{2N} & -i_{3N} & \dots & 0 \end{pmatrix}. \tag{3.3.12}$$

The number of boxes *removed* from row j is

$$m_j \coloneqq \sum_{n=1}^{N} M_{jn}. \tag{3.3.13}$$

The Dynkin label of the resulting irrep is then given by taking $\bar{\Lambda}$ and for each row j subtracting the m_j boxes removed from that row and adding the m_{j+1} boxes removed from the row below it. We write this as a *correction* vector Δp, giving $\bar{\Lambda} - \Delta p$ as the Dynkin label of the resulting irrep.

$$\Delta p_{jk} \coloneqq m_j - m_k \tag{3.3.14a}$$

$$\Delta p_j \equiv \Delta p_{j\,j+1} = m_j - m_{j+1} \tag{3.3.14b}$$

$$\Delta p \equiv (\Delta p_1, \Delta p_2, \dots, \Delta p_{N-1}). \tag{3.3.14c}$$

It is not immediately obvious that every $\bar{\Lambda} - \Delta p$ corresponds to an irrep in the decomposition of $\mathrm{G}_N^{\otimes k}$. We reserve a proof of this for Appendix C.2, since it is a

little involved. Essentially, there is enough freedom in placing the boxes of the tableau that one can always construct the irreps such that they don't vanish from symmetry or antisymmetry. In other words, the multiplicity of every irrep with highest weight $\bar{\Lambda} - \Delta p$ in the direct sum decomposition of $\mathrm{G}_N^{\otimes k}$ is nonzero, which follows from Theorem C.2.3.

The m_j and Δp obey the following identities:

$$\sum_{j=1}^{N} m_j = 0, \tag{3.3.15a}$$

$$\sum_{j=n}^{N-1} \Delta p_j = m_n - m_N, \tag{3.3.15b}$$

$$\sum_{j=1}^{N-1} j \Delta p_j = -N m_N, \tag{3.3.15c}$$

$$\sum_{j=1}^{n} m_j \geq 0 \quad \forall n \leq N, \tag{3.3.15d}$$

The antisymmetry of M gives (3.3.15a) and (3.3.15d), (3.3.15b) follows from the definition of the Δp_j, and (3.3.15c) follows from (3.3.15a) and (3.3.15b). There are additional identities, but they will not be needed. Because $\mathrm{G}_N^{\otimes k}$ is self dual $X^* \subset \mathrm{G}_N^{\otimes k} \iff X \subset G_N^{\otimes k}$, which will save us from having to take the conjugate of X in (3.3.1). Equating the Dynkin label of X with $\bar{\Lambda} - \Delta p$ we see that

$$X \subset \mathrm{G}_N^{\otimes k} \implies p_j = \delta_j^1 k + \delta_j^{N-1} k - \Delta p_j, \tag{3.3.16}$$

for some Δp. Using (3.3.15c) we find that

$$\sum_{j=1}^{N-1} j p_j = N(k + m_N). \tag{3.3.17}$$

Because m_N and k are integral, the r.h.s. of (3.3.17) is an integer multiple of N. □

Corollary 3.3.2.1. *For a given irrep, X, of $\mathrm{SU}(N)$, with Dynkin label $(p_1, p_2, \ldots, p_{N-1})$, and*

$$\sum_{j=1}^{N-1} j p_j = 0 \mod N,$$

$\mathbb{1} \subset X \otimes \mathrm{G}_N^{\otimes k}$ if and only if

$$\forall n \in \mathbb{N} \mid 1 \leq n \leq N-1 \colon k \geq \frac{N-n}{N} \sum_{j=1}^{N-1} j p_j - \sum_{j=n+1}^{N-1} (j-n) p_j. \tag{3.3.18}$$

Proof. Construct the correction vector Δp as in Theorem (3.3.2). Sum over the p_j from $n \leq j \leq N-1$ and use (3.3.15b) to solve for the m_j:

$$\begin{aligned} m_n &= m_N + \sum_{j=n}^{N-1} \left(\delta_j^1 + \delta_j^{N-1}\right) k - \sum_{j=n}^{N-1} p_j, \quad n < N, \\ m_N &= \frac{1}{N} \sum_{j=1}^{N-1} j p_j - k. \end{aligned} \tag{3.3.19}$$

Substituting these values of m_j into (3.3.15d) then finishes the proof. □

We now have the final result for the case when X has vanishing N-ality:

Theorem 3.3.3. *Given an irrep, X, of $\mathrm{SU}(N)$, with Dynkin label $(p_1, p_2, \ldots, p_{N-1})$, and*

$$\sum_{j=1}^{N-1} j p_j = 0 \mod N,$$

define

$$k_n \coloneqq \frac{n}{N} \sum_{j=1}^{N-1} j p_j - \sum_{j=1}^{n} (n-j) p_{N-j}. \tag{3.3.20}$$

Then the quantity

$$k_{\min} \coloneqq \max\{k_1, k_2, \ldots, k_{N-1}\}, \tag{3.3.21}$$

obeys

$$\forall k \in \mathbb{N} \mid \mathbb{1} \subset X \otimes \mathrm{G}_N^{\otimes k},\ k_{\min} \leq k \tag{3.3.22}$$

Proof. Choose k such that $\mathbb{1} \subset X \otimes \mathrm{G}_N^{\otimes k}$. From Corollary 3.3.2.1

$$\forall n \in \mathbb{N} \mid 1 \leq n \leq N-1,\ k \geq k_n.$$

Next, assume $k < k_{\min}$. But then, because $k_{\min} = \max\{k_1, k_2, \ldots, k_{N-1}\}$, there exists a k_n such that $k < k_n$, a contradiction. □

3.3.2 Including Matter Fields

We next include an additional matter field in the tensor product

$$X \otimes Q_i \otimes \mathrm{G}_N^{\otimes k},$$

where X is some field in an arbitrary representation of SU(N), G_N is again a gauge field in the adjoint representation, and Q_i is a matter field in the

$$\dim(Q_i) = \frac{N!}{i!(N-i)!}, \quad 1 \leq i \leq N-1, \tag{3.3.23}$$

representation. The Dynkin label for Q_i is

$$\begin{aligned} Q_i &\cong (\underbrace{0, \ldots, 0}_{i-1}, 1, \underbrace{0, \ldots, 0}_{N-i-1}), \\ &\cong \left.\begin{array}{c}\square\\ \square\\ \vdots\\ \square\end{array}\right\}\sim. \end{aligned} \tag{3.3.24}$$

If the irrep X has highest weight p then the highest weight of the highest irrep in the tensor product $X \otimes Q_i$ is

$$(p_1, \ldots, p_{i-1}, p_i + 1, p_{i+1}, \ldots, p_{N-1}).$$

Only one irrep in the tensor product can have this weight in its weight space. The other irreps can again be built using a similar procedure to the previous section. Begin with the Dynkin label for the highest irrep above and move boxes to lower rows in all possible ways, keeping the vertical ordering of the boxes intact. The Dynkin label, $f = (f_1, f_2, \ldots, f_{N-1})$, for every irrep $V_f \subset X \otimes Q_i$ then takes the following form:

$$\begin{aligned} f_1 &= p_1 + \delta^i_1 - 2i_{12} + i_{23} \\ f_j &= p_j + \delta^i_j + i_{j-1\,j} - 2i_{j\,j+1} + i_{j+1\,j+2}, \\ f_{N-1} &= p_{N-1} + \delta^i_{N-1} - 2i_{N-1\,N} + i_{N-2\,N-1}, \end{aligned} \tag{3.3.25}$$

where the non-negative integers i_{jk} correspond to moving i_{jk} boxes from row j to row k. Again, we compact this procedure into an $N \times N$ matrix:

$$M \coloneqq \begin{pmatrix} 0 & i_{12} & 0 & 0 & \ldots & 0 \\ -i_{12} & 0 & i_{23} & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ & -i_{i-1\,i} & 0 & i_{i\,i+1} & 0 & \\ & 0 & -i_{i\,i+1} & 1 & i_{i+1\,i+2} & \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \ldots & \ldots & 0 & -i_{N-1\,N} & 1 \end{pmatrix}. \tag{3.3.26}$$

Then, as in the previous section, define

$$m_j \coloneqq \sum_{k=1}^{N} M_{jk}, \tag{3.3.27a}$$

$$\Delta p_j \coloneqq m_j - m_{j+1}. \tag{3.3.27b}$$

The Dynkin labels for the resulting irreps are then

$$f_j = p_j - \Delta p_j. \tag{3.3.28}$$

We now have the following lemma:

Lemma 3.3.4. *For a given irrep, X, of* $\mathrm{SU}(N)$*, with Dynkin label* $(p_1, p_2, \ldots, p_{N-1})$*,*

$$\exists k \in \mathbb{N} \mid \mathbb{1} \subset X \otimes Q_i \otimes \mathrm{G}_N^{\otimes k} \iff i = N - \left(\sum_{j=1}^{N-1} j p_j \mod N \right) \tag{3.3.29}$$

Proof. From Theorem (3.3.2):

$$\exists k \in \mathbb{N} \mid \mathbb{1} \subset V_f \otimes \mathrm{G}_N^{\otimes k} \iff \sum_{j=1}^{N-1} j f_j = 0 \mod N. \tag{3.3.30}$$

Using (3.3.25) we find

$$\sum_{j=1}^{N-1} j f_j = \sum_{j=1}^{N-1} j p_j + i + N(1 - i_{N-1\, N}). \tag{3.3.31}$$

The last quantity on the r.h.s. is already an integer multiple of N and can be dropped. Therefore, we require

$$\sum_{j=1}^{N-1} j p_j + i = 0 \mod N. \tag{3.3.32}$$

This, and the condition that $1 \leq i \leq N$, then gives the result. □

For every subvector space of $X \otimes Q_i$, with i determined from Lemma 3.3.4, we can apply Theorem 3.3.3 to find a $k_{\min}$. This gives a $k_{\min}$ for every unique set of f_j (for every irrep $V \subset X \otimes Q_i$). There will exist at least one set of f_j that gives the smallest $k_{\min}$, but to determine which set we must consider the restrictions on the irreps in $X \otimes Q_i$.

Lemma 3.3.5. *Consider an irrep, X, of* $\mathrm{SU}(N)$ *with Dynkin label* $(p_1, p_2, \ldots, p_{N-1})$*, and the i^{th} fundamental representation, Q_i, of* $\mathrm{SU}(N)$*. Then every irrep $V_f \subset X \otimes Q_i$ has a Dynkin label* $(f_1, f_2, \ldots, f_{N-1})$*, with $f_j = p_j - m_j + m_{j+1}$ subject to the following conditions:*

1)

$$\sum_{j=k}^{N-1} p_j - i_{N-1\,N} \leq \sum_{j=k}^{N-1} f_j \leq 1 - i_{N-1\,N} + \sum_{j=k}^{N-1} p_j, \tag{3.3.33}$$

where $i_{N-1\,N} \in \{0, 1\}$.

2)

$$0 \leq m_j \leq 1. \tag{3.3.34}$$

3)

$$\sum_{j=1}^{N} m_j = N - i. \tag{3.3.35}$$

4)

$$m_j - m_{j+1} \leq p_j. \tag{3.3.36}$$

Proof. Because Q_i corresponds to an antisymmetric combination of fundamental indicies[1] (for $i > 1$) we can place no more than a single box in each row. As well, we can move at most one box to the very bottom of the tableau (and remove the completed column). This implies $i_{N-1\,N} = 0$ or 1, which in turn implies $m_N = 0$ or 1. If no boxes are moved to the bottom of the tableau, i.e. $i_{N-1\,N} = 0$, then every row can have, at most, one more box than the same row in the original tableau for X. In addition, every row must have at least as many boxes than the same row in X. If $i_{N-1\,N} = 1$ then we eliminate the completed column, thus shortening each row by one box. In this case every row can contain *no more* boxes than the same row in X and *no fewer* than one less than the number of boxes in the same row in X. The length of row k in the tableau

[1] This irrep is generated by the Schur functor $\mathbb{S}^{(1,\ldots,1)}V = \wedge^{(1,\ldots,1)}V$, where $V = \mathbb{C}^N$, hence the antisymmetry.

of X is

$$\sum_{j=k}^{N-1} p_j,$$

while the length of row k in the tableau of V_f is

$$\sum_{j=k}^{N-1} f_j.$$

Thus, leaving $i_{N-1\,N}$ arbitrary yields the first condition. Then inserting (3.3.28) into (3.3.33) gives the second condition, summing over all of the m_j gives the third condition, and finally, requiring all of the $f_j \geq 0$ gives the last condition. □

We now have the final result:

Theorem 3.3.6. *Consider an arbitrary irrep, $X \neq \mathbb{1}$, of $\mathrm{SU}(N)$ with Dynkin label $(p_1, p_2, \ldots, p_{N-1})$, and the i^{th} fundamental representation, Q_i, of $\mathrm{SU}(N)$. Define the set*

$$L \coloneqq \{l \in \{1, 2, \ldots, N-1\} \mid p_l \neq 0\} \cup \{0, N\}. \tag{3.3.37}$$

Then the integers

$$\ell_1 \coloneqq \max\{l \in L \mid l \leq N - i\}, \tag{3.3.38}$$

$$\ell_2 \coloneqq \min\{l \in L \mid l > \ell_1\}, \tag{3.3.39}$$

define an irrep $V_f \subset X \otimes Q_i$, with Dynkin label $(f_1, f_2, \ldots, f_{N-1})$, where

$$f_j = p_j - \delta_j^{\ell_1} + \delta_j^{i-N+\ell_1-\ell_2} - \delta_j^{\ell_2}. \tag{3.3.40}$$

For this irrep V_f, defining

$$k_n(f) \coloneqq \frac{n}{N}\sum_{j=1}^{N-1} jp_j - \sum_{j=1}^{n}(n-j)p_{N-j} - \frac{(N-n)i}{N} - \sum_{j=0}^{N-n-1}(N-n-j)\Big(\delta_j^{\ell_1} - \delta_j^{i-N+\ell_1+\ell_2} + \delta_j^{\ell_2}\Big), \quad (3.3.41)$$

the minimum number of copies of the adjoint representation such that $\mathbb{1} \subset V_f \otimes \mathrm{G}_N^{\otimes k_{\min}(f)}$ is

$$k_{\min}(f) = \max\{k_n(f) \mid 1 \leq n \leq N-1\}. \quad (3.3.42)$$

Then, for any other $V_\lambda \subset X \otimes Q_i$, the following holds:

$$k_{\min}(f) \leq k_{\min}(\lambda). \quad (3.3.43)$$

Proof. For any irrep $V_\lambda \subset X \otimes Q_i$, indexed by its Dynkin label λ, we may use Theorem 3.3.3 to determine a $k_{\min}(\lambda)$. The first step is to calculate all of the k_n for each λ:

$$k_n(\lambda) = \frac{n}{N}\sum_{j=1}^{N-1} j\lambda_j - \sum_{j=1}^{n}(n-j)\lambda_{N-j},$$

where we have made the dependence on λ explicit. Using Lemma 3.3.4 and Lemma 3.3.5 we can construct every V_λ by writing $\lambda_j = p_j - m_j(\lambda) + m_{j+1}(\lambda)$, which then gives

$$k_n(\lambda) = \frac{n}{N}\sum_{j=1}^{N-1} jp_j - \sum_{j=1}^{n}(n-j)p_{N-j} + \sum_{j=N-n+1}^{N} m_j(\lambda) - \frac{(N-i)n}{N}. \quad (3.3.44)$$

For any fixed n the λ dependence factors in only through the term

$$E_n(\lambda) \equiv \sum_{j=N-n+1}^{N} m_j(\lambda). \quad (3.3.45)$$

Then choose any two arbitrary irreps, V_{λ_1} and V_{λ_2}, and suppose $k_{\min}(\lambda_2) \geq k_{\min}(\lambda_1)$.

If this is not the case then simply switch λ_1 and λ_2. It is obvious that

$$\exists n_1 \in \{1, 2, \ldots, N-1\} \mid k_{\min}(\lambda_1) = k_{n_1}(\lambda_1), \tag{3.3.46a}$$

$$\exists n_2 \in \{1, 2, \ldots, N-1\} \mid k_{\min}(\lambda_2) = k_{n_2}(\lambda_2). \tag{3.3.46b}$$

Generally, it will not be the case that $n_1 = n_2$. However, this then implies $k_{n_2}(\lambda_2) \geq k_{n_1}(\lambda_1)$. But, from Theorem 3.3.3 it must be that $k_{n_1}(\lambda_1) \geq k_n(\lambda_1)$ for any n, and in particular this holds for $n = n_2$. Therefore

$$k_{n_2}(\lambda_2) \geq k_{n_1}(\lambda_1) \implies E_{n_2}(\lambda_2) \geq E_{n_2}(\lambda_1). \tag{3.3.47}$$

Since this is true for arbitrary λ_1 and λ_2 it is true for all λ_1 and λ_2, and the implication becomes if and only if.

$$E_{n_2}(\lambda_2) \geq E_{n_2}(\lambda_1) \implies k_{\min}(\lambda_1) \leq k_{\min}(\lambda_2). \tag{3.3.48}$$

We therefore search for an irrep $V_f \subset X \otimes Q_i$ such that (3.3.48) holds for arbitrary n:

$$\forall n \in \{1, \ldots, N-1\} \colon \forall \lambda \in \mathbb{N}^{N-1} \mid V_\lambda \subset X \otimes Q_i,$$

$$E_n(f) \leq E_n(\lambda). \tag{3.3.49}$$

This implies $E_{n_f}(f) \leq E_{n_f}(\lambda)$, where n_f is such that $k_{\min}(f) = k_{n_f}(f)$, which in turn implies

$$k_{\min}(f) \leq k_{\min}(\lambda), \tag{3.3.50}$$

for arbitrary $V_\lambda \subset X \otimes Q_i$.

Take $n = 1$, then

$$E_1(\lambda) = m_N(\lambda). \tag{3.3.51}$$

If such a V_f exists in $X \otimes Q_i$, such that $m_N(f) = 0$, then $E_2(f) \leq E_2(\lambda)$ for any other V_λ for which $m_N(\lambda) \neq 0$. This is obvious because

$$E_2(f) = m_{N-1}(f)$$

$$E_2(\lambda) = m_{N-1}(\lambda) + m_N(\lambda).$$

A similar argument holds for any V_f such that $m_{N-1}(f) = m_N(f) = 0$. We can continue in this manner until finding a V_f such that

$$\begin{aligned} m_{N-i+1}(f) = m_{N-i+2}(f) = \ldots &= m_N(f) = 0, \\ m_1(f) = m_2(f) = \ldots &= m_{N-i}(f) = 1, \end{aligned} \tag{3.3.52}$$

where the second line is implied from (3.3.35) of Lemma 3.3.5. Such a V_f satisfies $E_n(f) \leq E_n(\lambda)$ for all n and all V_λ. However, we cannot guarantee that such a V_f exists. In particular, condition (3.3.36) of Lemma 3.3.5 gives the necessary condition:

$$m_{N-i}(f) - m_{N-i+1}(f) = 1 \implies p_{N-i} \geq 1, \tag{3.3.53}$$

which is clearly only a special case. We can make this more intuitive by introducing a vector for the m_j:

$$\bar{m} \coloneqq (\underbrace{1, \ldots, 1}_{N-i}, \underbrace{0, \ldots, 0}_{i}). \tag{3.3.54}$$

If $p_{N-i} = 0$ then we simply permute the entries of $\bar{m}$ until a vector is found that satisfies all of the conditions of Lemma 3.3.5. For instance, after one permutation we arrive at

$$(\underbrace{1, \ldots, 1, 1}_{N-i}, \underbrace{0, 0, \ldots, 0}_{i}) \to (\underbrace{1, \ldots, 1}_{N-i-1}, 0, 1, \underbrace{0, \ldots, 0}_{i-1}),$$

(the permuted entries have been highlighted in red for clarity) which requires $p_{N-i-1} > 0$ and $p_{N-i+1} > 0$. Start with the first condition: if $p_{N-i-1} = 0$ then we permute once

more and check p_{N-i-2}. If $p_{N-i-2} > 0$ we stop, if not we continue, until we find the first $l \leq N-i$ such that $p_l \neq 0$. This gives the definition of ℓ_1, and we arrive at

$$\bar{m} \to (\underbrace{1,\ldots,1}_{\ell_1},0,\underbrace{1,\ldots,1}_{N-i-\ell_1},\underbrace{0,\ldots,0}_{i-1}).$$

Next we check the second condition on p_{N-i+1}. If $p_{N-i+1} > 0$ we are finished, but if not we must continue permuting the entries of $\bar{m}$:

$$(\underbrace{1,\ldots,1}_{\ell_1},0,\underbrace{1,\ldots,1,1}_{N-i-\ell_1},\underbrace{0,0,\ldots,0}_{i-1})$$

$$\downarrow$$

$$(\underbrace{1,\ldots,1}_{\ell_1},0,\underbrace{1,\ldots,1}_{N-i-\ell_1-1},0,1,\underbrace{0,\ldots,0}_{i-2}).$$

This requires $p_{N-i} > 0$ and $p_{N-i+2} > 0$. But we already know that all of the $p_l = 0$ for $\ell_1 < l \leq N-i$, so we obviously must continue permuting until the second "0" is pushed up to the first "0":

$$\bar{m} \to (\underbrace{1,\ldots,1}_{\ell_1},0,0,\underbrace{1,\ldots,1}_{N-i-\ell_1},\underbrace{0,\ldots,0}_{i-2}).$$

We then continue to check if $p_\ell > 0$, where $\ell > N-i$. If so we are finished, if not we move another "0" through all of the $N-i-\ell_1$ "1"s, until a non zero p_ℓ is found. Clearly, this process terminates at the smallest value of ℓ, which is greater than $N-i$, and for which $p_\ell > 0$, which gives the definition of ℓ_2. Such ℓ_1 and ℓ_2 may not exist (for example, if $p_j = 0$ for $j > N-i$). This can be resolved by embedding the irrep X in a larger space:

$$\begin{aligned}\tilde{X} &\cong (\tilde{p}_0,\tilde{p}_1,\ldots,\tilde{p}_{N-1},\tilde{p}_N),\\ &\cong (1,\underbrace{p_1,\ldots,p_{N-1}}_{X},1).\end{aligned} \tag{3.3.55}$$

The set L can then be constructed as

$$L = \{l \mid \tilde{p}_l \neq 0\}, \tag{3.3.56}$$

and we similarly extend $f_j \to \tilde{f}_j$ and $m_j \to \tilde{m}_j$, where $f_j = \tilde{f}_j$ for $1 \leq j \leq N-1$ and $m_j = \tilde{m}_j$ for $1 \leq j \leq N$. Note that Lemma 3.3.5 does not apply to $\tilde{f}_0$, $\tilde{f}_N$, $\tilde{m}_0$, and $\tilde{m}_{N+1}$, but it does apply to all the other $\tilde{f}_j$ and $\tilde{m}_j$.

The process concludes when we arrive at the vector

$$m(f) = (\overbrace{\underbrace{1,\ldots,1}_{\ell_1},\underbrace{0,\ldots,0}_{\ell_2-N+i},\underbrace{1,\ldots,1}_{N-i-\ell_1}}^{\ell_2},\underbrace{0,\ldots,0}_{N-\ell_2}). \tag{3.3.57}$$

This configuration places as many "1"s near the front of the vector and as many "0"s at the end of the vector as possible. Because $\nexists \ell \in L \mid \ell > \ell_1 \wedge \ell < \ell_2$, between index $\ell_1 + 1$ and ℓ_2 there cannot exist a sequence of a "1" followed by a "0". The only other options are to move the "0"s from the end of the vector forward, move the "1"s at the front of the vector backward, or a combination of the two. We then have

$$E_n(f) = \begin{cases} 0 & n \leq N - \ell_2 \\ n - N + \ell_2 & N - \ell_2 < n \leq 2N - \ell_1 - \ell_2 - i \\ N - i - \ell_1 & 2N - \ell_1 - \ell_2 - i < n \leq N - \ell_1 \\ n - i & N - \ell_1 < n \end{cases}, \tag{3.3.58}$$

and by construction it is guaranteed that $E_n(f) \leq E_n(\lambda)$ for all n and any other irrep $V_\lambda \subset X \otimes Q_i$. This process, in fact, corresponds to moving as many of the i boxes coming from the tableau of Q_i to the bottom of the tableau of X as possible. Four examples have been given in Fig. 3.5.

From (3.3.57) we can directly read off the entries of the correction vector in the extended space:

$$\Delta\tilde{p}_j = \delta_j^{\ell_1} - \delta_j^{i-N+\ell_1+\ell_2} + \delta_j^{\ell_2} - \delta_j^N, \tag{3.3.59}$$

where j runs from 0 to N. The Dynkin labels (again in the extended space) are

$$\tilde{f}_j = \tilde{p}_j - \Delta\tilde{p}_j, \tag{3.3.60}$$

Note that if $\ell_1 = N - i$ the second and third term on the r.h.s. of (3.3.59) cancel. This is because ℓ_2 becomes irrelevant in this case since all of the i boxes can be placed below row ℓ_1, creating a complete column. If $\ell_2 = N$ it may not be possible to complete a column, and the last two terms on the r.h.s. of (3.3.59) cancel as expected.

Restricting j to values greater than 0 and less than N gives

$$f_j = \tilde{f}_j, \quad 1 \leq j \leq N-1, \tag{3.3.61}$$

which yields the first result (3.3.40). We can then substitute (3.3.40) directly into (3.3.20), yielding

$$\begin{aligned} k_n = \frac{n}{N}\sum_{j=1}^{N-1} j p_j - \sum_{j=1}^{n}(n-j)p_{N-j} \\ - \frac{n}{N}\sum_{j=1}^{N-1} j\Big(\delta_j^{\ell_1} - \delta_j^{i-N+\ell_1+\ell_2} + \delta_j^{\ell_2} - \delta_j^{N}\Big) \\ + \sum_{j=1}^{n}(n-j)\Big(\delta_{N-j}^{\ell_1} - \delta_{N-j}^{i-N+\ell_1+\ell_2} + \delta_{N-j}^{\ell_2} - \delta_{N-j}^{N}\Big). \end{aligned} \tag{3.3.62}$$

This can be simplified using

$$\begin{aligned} \sum_{j=1}^{N-1} j\Big(\delta_j^{\ell_1} - \delta_j^{i-N+\ell_1+\ell_2} + \delta_j^{\ell_2} - \delta_j^{N}\Big) \\ + N\delta_N^{\ell_1} - N\delta_N^{i-N+\ell_1+\ell_2} + N\delta_N^{\ell_2} - N \\ = \sum_{j=0}^{N} j\Big(\delta_j^{\ell_1} - \delta_j^{i-N+\ell_1+\ell_2} + \delta_j^{\ell_2} - \delta_j^{N}\Big) = -i, \end{aligned} \tag{3.3.63}$$

and

$$\sum_{j=1}^{n}(n-j)\Big(\delta_{N-j}^{\ell_1}-\delta_{N-j}^{i-N+\ell_1+\ell_2}+\delta_{N-j}^{\ell_2}-\delta_{N-j}^{N}\Big)$$

$$+n\delta_N^{\ell_1}-n\delta_N^{i-N+\ell_1+\ell_2}+n\delta_N^{\ell_2}-n$$

$$=-i$$

$$+\sum_{j=n+1}^{N}(n-j)\Big(\delta_{N-j}^{\ell_1}-\delta_{N-j}^{i-N+\ell_1+\ell_2}+\delta_{N-j}^{\ell_2}-\delta_{N-j}^{N}\Big) \quad (3.3.64)$$

After this simplification we have the result. □

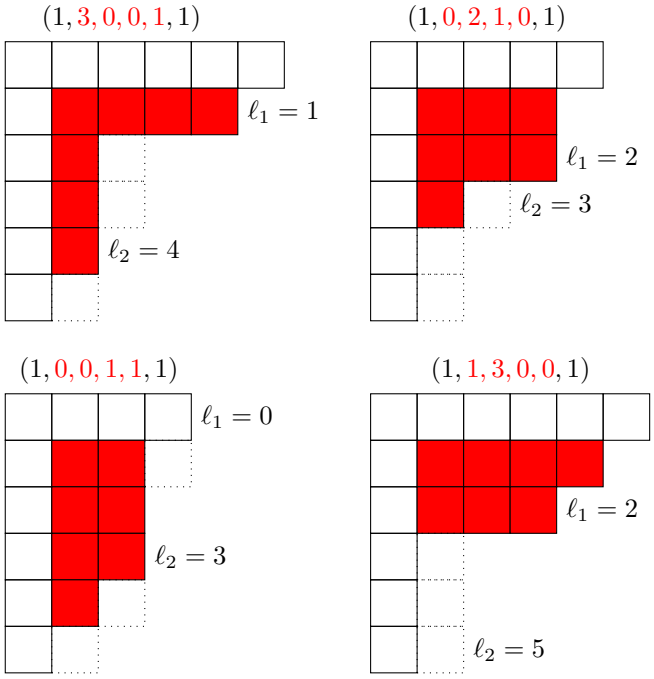


Figure 3.5: Four examples for determining the optimum irrep in $X \otimes Q_i$ with $N = 5$ and $i = 3$. Shown in red is the original irrep X, embedded inside the larger space $\tilde{X}$. The dotted boxes show the placement of boxes that guarantees the smallest possible $k_{\min}$. From left to right, the resulting minimum number of copies of the adjoint representation are $k_{\min} = 2, 2, 1,$ and 3.

Especially for large N, evaluating Eq. (3.3.42) becomes computationally in-

tensive and highly non-trivial. We therefore built and made publicly available the `tessellation` python code. We describe how to install and use the code in App. C.3.

3.4 The lowest dimensional portals

Consider an exotic species belonging to an irreducible representation X of SU(N). Assume that the quantum field associated with X has mass-dimension d_X, and that matter fields have mass-dimension d_q (for instance $d_q = 3/2$ for fermions, such as quarks or antiquarks) and that gauge-mediator fields in the adjoint representation have mass dimensions d_g (for instance, $d_g = 1$ for gluons). We are interested in gauge-invariant "portal" operators, with the structure

$$\mathcal{O}_j = \frac{c_j}{\Lambda^{n_j}} X \left(\prod_{i=1}^{N-1} Q_i^{n_{Q_i}} \right) g^{n_g}, \tag{3.4.1}$$

where Q_i represents the quantum field corresponding to one of the $N-1$ fundamental representations of SU(N), with Dynkin label

$$Q_i \cong (\underbrace{0,\ldots,0}_{i-1},1,\underbrace{0,\ldots,0}_{N-i-1}),$$

and where g is the quantum field corresponding to the gauge boson of SU(N), with Dynkin label (1,0,...,0,1). Note that we assume 4 space-time dimensions, so the mass dimensions of the operator in Eq. (3.4.1) must equal 4, and we assume that Λ has mass dimension 1, as customary. Also, we assume that the spin of X is such that $\mathcal{O}_j$ respects Poincaré invariance.

Here, we seek the lowest possible value of n_j such that the operator in Eq. (3.4.1) is gauge invariant, i.e. the lowest dimensional "portal" for X. Notice that the condi-

tion that the operator be gauge invariant is equivalent to the condition that the tensor product of the representations is such that

$$\mathbb{1} \subset X \otimes \bigotimes_{i=1}^{N-1} Q_i^{\otimes n_{Q_i}} \otimes G_N^{\otimes n_g}. \tag{3.4.2}$$

The results above address precisely this question: given the N-ality of X, say t, $n_i = 0$ $\forall i$ if $t = 0$, and $n_{Q_{N-t}} = 1$, $n_i = 0$ $\forall i \neq N - t$ for $t \neq 0$, while $n_g = k_{\min}$ with $k_{\min}$ given in Eq. (3.3.42). As a result, we find

$$\begin{gathered} 4 = -n_j + d_X + d_q + k_{\min} d_g \\ \Downarrow \\ n_j = d_X + d_q + k_{\min} d_g - 4. \end{gathered} \tag{3.4.3}$$

For instance, let's consider the QCD case in the Standard Model, with gauge group SU(3); let's assume $X \cong (p, q)$, thus $t = (p + 2q) \bmod 3$. We have the following cases:

(i) $t = 0$: this implies $n_{Q_i} = 0$ $(i = 1, 2)$,

$$k_{\min} = \begin{cases} \frac{p+2q}{3} & p \leq q \\ \frac{2p+q}{3} & p \geq q \end{cases},$$

and $n_j = d_X + k_{\min} d_g - 4$.

(ii) $t = 1$: this implies $n_{Q_1} = 0$, $n_{Q_2} = 1$,

$$k_{\min} = \begin{cases} \frac{p+2q-1}{3} & p - 1 \leq q \\ \frac{2p+q-2}{3} & p - 1 \geq q \end{cases},$$

and $n_j = d_X + d_q + k_{\min} d_g - 4$.

(iii) $t = 3$: this implies $n_{Q_1} = 1$, $n_{Q_2} = 0$,

$$k_{\min} = \begin{cases} \frac{p+2q-2}{3} & p \leq q - 1 \\ \frac{2p+q-1}{3} & p \geq q - 1 \end{cases},$$

and $n_j = d_X + d_q + k_{\min} d_g - 4$.

Similar cases for $N > 3$ and a different matter content can be readily computed utilizing the companion `tessellation` code.

3.5 Summary and conclusions

In this study we have entertained the question of which is the lowest-possible mass dimension of SU(N) gauge invariant operators that contain an exotic new state in a given representation X of SU(N). We showed that to address this question one needs to find which is the smallest tensor product of the adjoint representation that contains the representation X. We fully solved this question, and built a numerical code that solves this problem for any N. We then solved the original question, pointing out that one needs to first take the tensor product of X with one of the fundamental representations of SU(N) to obtain a representation with vanishing N-ality, and then find the minimal number of copies of the adjoint representation that contains that product. We gave explicit formulae for any N, and explicit results for the mass dimension of the lowest-dimensional portal for the case of SU(3) of QCD. Our results are relevant for several areas of particle phenomenology which seek new physics beyond the Standard Model: the numerical tool `tessellation` is also per se relevant in the context of group theory.

Chapter 4

Functional Determinants in Quantum Field Theory

4.1 Introduction

In many physical applications one is tasked with calculating the determinant of an operator, which we denote as τ, that acts on some Hilbert space $\mathfrak{H}$. This situation arises in many branches of physics and mathematics, but in particular we encounter functional determinants in relativistic quantum field theories (for instant false vacuum decay rates[39–41], sphaleron transitions[35, 36, 99–101], and Casimir energies[102]). In these contexts functional determinants are the formal result of Gaussian integrals around a classical background in the path integral formulation.

We focus our attention on a subclass of elliptic operators, which take the most general form as

$$\tau f := \left[-g^{\mu\nu}\nabla^{\mathcal{V}}_{\mu}\nabla^{\mathcal{V}}_{\nu} + E\right] f, \tag{4.1.1}$$

where f is a section of a vector or spinor bundle $\mathcal{V}$ over a manifold $\mathcal{M}$, $\nabla_\mu^{\mathcal{V}}$ is the coordinate representation of the connection on $\mathcal{V}$, $g^{\mu\nu}$ is the metric on the manifold, and E is an endomorphism on $\mathcal{V}$. To be less precise, the first term is the Laplacian in d dimensions, including the possibility of a manifold with curvature. E is some finite dimensional matrix function on the manifold $\mathcal{M}$. We will take the dimension of $\mathcal{V}$ to be n.

The subclass of elliptic operators that we will consider are those operators where the vector or spinor bundle $\mathcal{V}$ is over flat Euclidean space, i.e. the manifold $\mathcal{M} = \mathbb{R}^d$ with Euclidean metric. Throughout this paper we will say that an $f \in \mathcal{V}$ is an element of some vector space V if every component of f is an element of V. For instance, we say that f is a vector in the space of square integrable functions over some interval $I \subseteq \mathbb{R}$ with Borel measure μ as $f \in L^2(I, \mathrm{d}\mu)$ if

$$\forall i \in \{1, \ldots, n\} \mid f_i \in L^2(I, \mathrm{d}\mu)\,, \tag{4.1.2}$$

where the f_i are the coefficient functions of f in some basis of $\mathcal{V}$.

Definition 1. We define the differential operator τ as

$$\tau f \coloneqq \left[-\nabla^2 + M^2 + V(x)\right] f, \qquad f \in \mathfrak{D}(\tau) \subseteq L^2\left(\mathbb{R}^d, \mathrm{d}^d x\right), \qquad x \in \mathbb{R}^d, \tag{4.1.3}$$

where M^2 is a constant $n \times n$ mass matrix (which we will assume is real and diagonal) and $V(x)$ is a $n \times n$ matrix function.

The maximal domain of definition of τ is

$$\mathfrak{D}(\tau) \coloneqq \Big\{ f \in L^2\left(\mathbb{R}^d, \mathrm{d}^d x\right) \mid f \in \mathrm{AC}\left(\mathbb{R}^d\right), \forall i \in \{1, \ldots, d\} \colon \frac{\partial f}{\partial x^i} \in \mathrm{AC}\left(\mathbb{R}^d\right), \\ \tau f \in L^2\left(\mathbb{R}^d, \mathrm{d}^d x\right) \Big\}, \tag{4.1.4}$$

where $\mathrm{AC}(\mathcal{M})$ is the set of absolutely continuous functions on the manifold $\mathcal{M}$.

We further assume that the matrix potential is spherically symmetric, i.e. $V(x) = V(r)$, where the Euclidean radius is $r = \sqrt{x^i x_i}$ (Einstein summation of repeated indices is assumed). The problem can then be reduced to an infinite number of 1-dimensional problems by separation of variables. In spherical coordinates the operator is given by

$$\tau u = \left[-\frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} - \frac{1}{r^2} \Delta_{S^{d-1}} + M^2 + V(r) \right] u, \tag{4.1.5}$$

where $\Delta_{S^{d-1}}$ is the Laplace-Beltrami operator on the $(d-1)$-sphere S^{d-1}. Requiring period boundary conditions on S^{d-1} then implies that every $u \in \mathfrak{D}(\tau)$ has a valid representation as

$$u(x) = \sum_{l=0}^{\infty} \sum_{\alpha} Y_l^{\alpha}(\Omega)\, u_l(r)\,, \tag{4.1.6}$$

where $\Omega \in S^{d-1}$ and the $Y_l^{\alpha}(\Omega)$ are the hyperspherical harmonic functions labeled by the multiindex α and the angular momentum quantum number l. The hyperspherical harmonics are the eigenfunctions of the Laplace-Beltrami operator, with eigenvalue

$$\Delta_{S^{d-1}}\, Y_l^{\alpha}(\Omega) = -l(l+d-2)\, Y_l^{\alpha}(\Omega)\,. \tag{4.1.7}$$

We then introduce a set of operators indexed by l from

$$\tau u = \sum_{l=0}^{\infty} \sum_{\alpha} Y_l^{\alpha}(\Omega)\, \tau_l\, u_l(r)\,. \tag{4.1.8}$$

We then consider the radial coefficient functions $u_l(r)$ to be elements of the Hilbert space

Definition 2.

$$\mathfrak{H} \equiv L^2\Big((0,\infty), r^{d-1}\,\mathrm{d}r\Big)\,, \qquad \langle f, g\rangle \coloneqq \int_0^{\infty} f^{\dagger}(r)\, g(r)\, r^{d-1}\,\mathrm{d}r\,. \tag{4.1.9}$$

Definition 3. The 1-dimensional radial operators over the interval $I = (0, \infty)$ are defined as

$$\mathfrak{D}(\tau_l) \coloneqq \Big\{ f \in \mathfrak{H} \mid f, r^{d-1} f' \in \mathrm{AC}(I)\,, \tau_l f \in \mathfrak{H} \Big\}, \tag{4.1.10}$$

$$\mathfrak{D}\Big(\tau_l^{\mathrm{free}}\Big) \coloneqq \Big\{ f \in \mathfrak{H} \mid f, r^{d-1} f' \in \mathrm{AC}(I)\,, \tau_l^{\mathrm{free}} f \in \mathfrak{H} \Big\}, \tag{4.1.11}$$

$$\tau_l f \coloneqq \Big[-\frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} + \frac{l(l+d-2)}{r^2} + M^2 + V(r) \Big] f, \quad f \in \mathfrak{D}(\tau_l)\,, \tag{4.1.12}$$

$$\tau_l^{\mathrm{free}} f \coloneqq \Big[-\frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} + \frac{l(l+d-2)}{r^2} + M^2 \Big] f, \qquad f \in \mathfrak{D}\Big(\tau_l^{\mathrm{free}}\Big)\,. \tag{4.1.13}$$

The ratio of functional determinants in d-dimensions can then be decomposed into a product of 1-dimensional functional determinants

$$\frac{\det(\tau)}{\det(\tau^{\mathrm{free}})} = \prod_{l=0}^{\infty} \left[\frac{\det(\tau_l)}{\det(\tau_l^{\mathrm{free}})} \right]^{\deg(d,l)}, \tag{4.1.14}$$

where the degeneracy factor,

$$\deg(d,l) \equiv \begin{cases} 1 & l = 0 \\ \dfrac{(2l+d-2)(l+d-3)!}{(d-2)!\,l!} & l > 0 \end{cases}, \tag{4.1.15}$$

gives the dimension of the subspace spanned by the hyperspherical harmonic functions $Y_l^{\alpha}(\Omega)$.

We have introduce the *free* operator τ_l^{free}, which is determined from τ_l by setting $V(r) = 0$. In order to avoid additional diverges we also make the following hypothesis on the matrix potential function:

Hypothesis H1. On the interval $I = (0, \infty)$

- $V(r) = V^{\dagger}(r)$,

- $V(r) \in L^1_{\text{loc}}\Big(I, r^{d-1}\,\mathrm{d}r\Big)$,
- $V(r) \in L^1_{\text{loc}}(I, \mathrm{d}r)$,

where † in this context is complex conjugate transpose and $L^1_{\text{loc}}(I, \mathrm{d}\mu)$ is the space of functions which are Lebesgue integrable on arbitrary compact subintervals of I.

In particular, (H1) supposes that $V(r)$ has the small r asymptotic behavior

$$V(r) \sim V_0 r^{-1+\epsilon_0}, \quad (r \to 0), \tag{4.1.16}$$

for some $\epsilon_0 > 0$ and arbitrary constant matrix V_0. In addition, it is also true that

$$V(r) \sim V_\infty r^{-d-\epsilon_\infty}, \quad (r \to \infty), \tag{4.1.17}$$

again, for some $\epsilon_\infty > 0$ and arbitrary constant matrix V_∞.

It is necessary to consider the free operator in physical problems because free energy functionals are always relative (ignoring gravity). However, it is also necessary from a mathematical perspective because self adjoint extensions of the operators defined by (4.1.12) usually have a spectrum with a continuous component. Hypothesis 1 ensures that the essential spectrum of the free operator is identical to that of τ_l, so that if we consider the ratio of functional determinants $\det(\tau_l)/\det\Big(\tau_l^{\text{free}}\Big)$ the essential spectrum cancels and we can consider only the discrete component of the spectrum.

In Section 4.2 we introduce the concept of Gel'fand-Yaglom formulas for functional determinants and motivate their use in physical and mathematical applications. In Section 4.3 we introduce the *principal solutions* of Reid, which are privileged matrix solutions of the same differential operators τ_l and τ_l^{free}. Using these principal matrix solutions we show in Section 4.4 that a self adjoint extension of τ exists, and its domain

is given by those $f \in \mathfrak{H}$ that obey *Friedrichs boundary condtions* (we explicitly give these boundary conditions in terms of the principal solutions). Once we have constructed a self adjoint extension we introduce the zeta function of τ, $\zeta(s|\tau)$, via a contour integral in Section 4.6. The zeta function provides a rigorous mathematical definition of the determinant of τ, however this contour integral representation needs to be analytically continued to the region near $s = 0$. In Section 4.7 we perform this analytic continuation to $s = 0$ in dimensions $d = 2, 3,$ and 4, yielding UV finite results. We have found zeta function regularization to be simpler and more efficient than other approaches, but many physicists are more familiar with dimensional regularization, so we also provide an explicit dictionary between the different regularization schemes. In Section 4.8 we consider the (common) case that zero modes exist, and give a general and very simple prescription for defining the functional determinant with zero modes removed. Finally in Section 4.9 we give some concluding remarks.

Additionally, we derive in Appendix D.1 the asymptotic behavior of the *Jost matrix function* in detail, which could be useful for an extension of our formula to dimensions greater that 4. In Appendix D.2 we provide some comments and recommendations on the use of our formula in numerical analysis.

A brute force method of determining the ratio of functional determinants $\det(\tau)/\det\left(\tau^{\text{free}}\right)$ is to numerically calculate the eigenvalues of $\tau f = \lambda f$ and $\tau^{\text{free}} f = \lambda f$, subject to some appropriate boundary conditions. Boundary value problems are notoriously difficult to solve numerically, and this method suffers from many issues including the computational difficulty of solving for a huge number of eigenvalues and loss of precision due to using finite precision floating point types when taking the product of

these eigenvalues. In Section 4.2 we show a more efficient method is to replace the boundary value problem with a much easier to solve initial value problem. Our results are summarized in the following theorem.

Theorem 4.1.1. *Define the $n \times n$ matrix function $T_l(r)$ as the solution to the matrix differential equation*

$$\frac{\mathrm{d}^2 T_l}{\mathrm{d}r^2} + \left[\frac{d-1}{r} + 2\left[U_{0,l}^{\text{free}}(r)\right]^{-1} \frac{\mathrm{d}}{\mathrm{d}r} U_{0,l}^{\text{free}}(r)\right] \frac{\mathrm{d}T_l}{\mathrm{d}r} - \left[U_{0,l}^{\text{free}}(r)\right]^{-1} V(r)\, U_{0,l}^{\text{free}}(r)\, T_l = 0, \tag{4.1.18}$$

subject to the initial conditions

$$T_l(0) = \mathbb{1}, \qquad \left.\frac{\mathrm{d}\, T_l(r)}{\mathrm{d}r}\right|_{r=0} = \mathbb{0},$$

where $\mathbb{1}$ is the $n \times n$ identity matrix, $\mathbb{0}$ is an $n \times n$ matrix of zeros, and $U_{0,l}^{\text{free}}(r)$ is the principal matrix solution of the free differential equation

$$\tau_l^{\text{free}} U_{0,l}^{\text{free}} = 0,$$

given by

$$\left[U_{0,l}^{\text{free}}(r)\right]_j^i = 2^\nu\, \Gamma(\nu+1)\, r^{\frac{2-d}{2}}\, m_i^{-\nu}\, I_\nu(m_i r)\, \delta_j^i,$$

where ν is

$$\nu \equiv \frac{2l+d-2}{2},$$

the masses m_i are the positive roots of the eigenvalues of the squared mass matrix M^2,

$$\left[M^2\right]_j^i = m_i^2 \delta_j^i,$$

and $I_\nu(z)$ is the modified Bessel function of the first kind.

Supposing that (H1) is satisified, the renormalized logarithm of the ratio of functional determinants of the operators τ and τ^{free}, defined by (4.1.3), is then given by

$$\ln\left(\frac{\det(\tau)}{\det(\tau^{\text{free}})}\right)\Big|_{d=2} = \operatorname{tr}[\ln(T_0(\infty))] + \sum_{l=1}^{\infty} 2\operatorname{tr}\left[\ln(T_l(\infty)) - \frac{1}{2l}\int_0^\infty V(r)\, r\, \mathrm{d}r\right] + \int_0^\infty \operatorname{tr}[V(r)]\left[\ln\left(\frac{\mu r}{2}\right) + \gamma\right] r\, \mathrm{d}r\,. \tag{4.1.19}$$

$$\ln\left(\frac{\det(\tau)}{\det(\tau^{\text{free}})}\right)\Big|_{d=3} = \sum_{l=0}^{\infty} (2l+1)\operatorname{tr}\left[\ln(T_l(\infty)) - \frac{1}{2l+1}\int_0^\infty V(r)\, r\, \mathrm{d}r\right]. \tag{4.1.20}$$

$$\ln\left(\frac{\det(\tau)}{\det(\tau^{\text{free}})}\right)\Big|_{d=4} = \sum_{l=0}^{\infty} (l+1)^2 \operatorname{tr}\left[\ln(T_l(\infty)) - \frac{1}{2(l+1)}\int_0^\infty V(r)\, r\, \mathrm{d}r + \frac{1}{8(l+1)^3}\int_0^\infty V(r)\left[V(r) + 2M^2\right] r^3\, \mathrm{d}r\right] - \frac{1}{8}\int_0^\infty \operatorname{tr}\left[V(r)\left[V(r) + 2M^2\right]\right]\left[\ln\left(\frac{\mu r}{2}\right) + \gamma + 1\right] r^3\, \mathrm{d}r\,. \tag{4.1.21}$$

In the above, tr *is a finite dimensional trace over matrices, μ is an arbitrary renormalization scale, γ is Euler's constant, the differential operator τ is defined by (4.1.3), and τ^{free} is obtained from τ by setting $V(r) = 0$.*

In Theorem 4.1.1 we have assumed that there are no zero modes. If zero modes exist in some partial wave component with angular momentum quantum number l then the term $\operatorname{tr}[\ln(T_l(\infty))]$ should be modified according to Section 4.8.

4.2 Gel'fand-Yaglom Formulas

Consider a flat d-dimensional Euclidean manifold $\mathcal{M}$, and the action

$$S[\Phi] = -\frac{1}{2}\int_{\mathcal{M}} \mathrm{d}^d x\, \Phi(x)\left[\Box_E - V(x)\right]\Phi(x)\,, \tag{4.2.1}$$

which describes a single scalar field Φ in the presence of a background potential $V(x)$. We could also consider the action associated with a fermionic field Ψ

$$S[\Psi, \bar{\Psi}] = i \int_{\mathcal{M}} \mathrm{d}^d x \, \bar{\Psi}(x) \left[\gamma^i \nabla_i + im \right] \Psi(x) \,, \tag{4.2.2}$$

in a background electromagnetic field A that enters via minimal coupling into the covariant derivative $\nabla_i = \partial_i + ieA_i$.

In the Euclidean path-integral formalism all of the information about the physical system is contained in the functional integral

$$\mathcal{Z}[V] = \int \mathscr{D}\Phi \, e^{-S[\Phi]}, \tag{4.2.3}$$

$$\mathcal{Z}[A] = \int \mathscr{D}\Psi \, \mathscr{D}\bar{\Psi} \, e^{-S[\Psi, \bar{\Psi}]}. \tag{4.2.4}$$

These functional integrals are not well defined however, even with the Euclidean signature in the exponent. There is an infinite normalization that we have neglected. This infinite normalization is formally removed by instead considering $\mathcal{Z}[V] \,/\, \mathcal{Z}[0]$ or $\mathcal{Z}[A] \,/\, \mathcal{Z}[0]$. If the manifold where Minkowski the situation is even worse, since the weight in the path integral becomes e^{iS}, and the integrand rapidly oscillates for large values of S. For this reason we choose to begin with the Euclidean signature, and analytically continue to Minkowski space in the end, if needed.

Because the action is quadratic in the fields we can, at least formally, perform the Gaussian integral over the fields:

$$\ln(\mathcal{Z}[V]) = -\frac{1}{2} \ln\Big(\det\Big[(-\Box_E + V)/\mu^2 \Big] \Big), \tag{4.2.5}$$

$$\ln(\mathcal{Z}[A]) = \frac{1}{2} \ln\Big(\det\Big[\Big(-\Box_E + ie\sigma^{jk} F_{jk} + m^2 \Big)/\mu^2 \Big] \Big), \tag{4.2.6}$$

where μ is an arbitrary parameter with dimensions of mass and

$$\sigma^{jk} = \frac{1}{4}\Big[\gamma^j, \gamma^k\Big],$$

$$F_{jk} = \partial_i A_j - \partial_j A_k.$$

We have not attempted to make this particularly rigorous, the Gaussian integration performed above is done by analogy to the finite dimensional case, discretizing the manifold $\mathcal{M}$ and integrating over a finite number of field points $\Phi(x_i)$. After performing an arbitrary number of integrations we then take the continuum limit to arrive at the result, neglecting any overall infinite normalization. A more rigorous definition will be provided in Section 4.6.

In interacting theories no analytic results exist (except for special cases such as Conformal Field Theories (CFT) in $d = 2$ dimensions). In this case we approximate the partition functional using Laplace's method. We reintroduce $\hbar$

$$\mathcal{Z}[\hbar, V] = \int \mathscr{D}\Phi \, e^{-\frac{1}{\hbar}S[\Phi]}, \tag{4.2.7}$$

$$\mathcal{Z}[\hbar, A] = \int \mathscr{D}\Psi \, \mathscr{D}\bar{\Psi} \, e^{-\frac{1}{\hbar}S[\Psi,\bar{\Psi}]}, \tag{4.2.8}$$

and approximate the functional integral in the limit $\hbar \to 0$. Expanding around the stationary points of the action, and then performing the Gaussian integration around the classical configuration yields

$$\ln(\mathcal{Z}[\hbar, V]) \sim -\frac{1}{\hbar}S[\Phi_{\text{cl}}] - \frac{1}{2}\ln\Big(\det\Big[\tau/\mu^2\Big]\Big), \qquad (\hbar \to 0), \tag{4.2.9}$$

$$\ln(\mathcal{Z}[\hbar, A]) \sim -\frac{1}{\hbar}S[\Psi_{\text{cl}}, \bar{\Psi}_{\text{cl}}] + \frac{1}{2}\ln\Big(\det\Big[\tau/\mu^2\Big]\Big), \qquad (\hbar \to 0), \tag{4.2.10}$$

where τ is the operator that results from a functional Taylor series of the action about

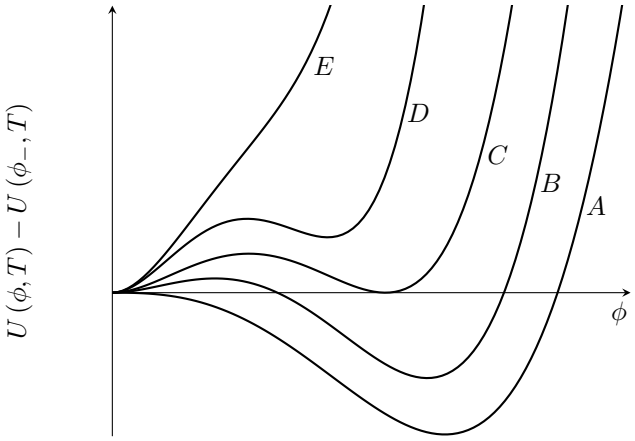


Figure 4.1: The effective potential $U(\phi, T)$ corresponding to a first order phase transition (adapted from [43, Linde 1983]). The horizontal axis has been shifted so the origin corresponds to $\phi = \phi_-$. (A) $0 < T < T_c$ (at the point T_c there appears the minimum at $\phi = \phi_-$); (B) $T_c < T < T_0$; (C) $T = T_0$; (D) $T_0 < T < T_{c1}$ (at the point T_{c1} the minimum at $\phi \neq \phi_-$ disappears; (E) $T_{c1} < T$.

its stationary points:

$$S[\Phi_{\rm cl} + \delta\Phi] \sim S[\Phi_{\rm cl}] + \frac{1}{2}\int_{\mathcal{M}} \mathrm{d}^d x\, \delta\Phi(x)\, \tau\, \delta\Phi(x)\,, \qquad (\delta\Phi \to 0), \tag{4.2.11}$$

$$S[\Psi_{\rm cl} + \delta\Psi, \bar{\Psi}_{\rm cl} + \delta\bar{\Psi}] \sim S[\Psi_{\rm cl}, \bar{\Psi}_{\rm cl}] + \frac{1}{2}\int_{\mathcal{M}} \mathrm{d}^d x\, \delta\bar{\Psi}(x)\, \tau\, \delta\Psi(x)\,, \qquad \Big(\delta\Psi, \delta\bar{\Psi} \to 0\Big). \tag{4.2.12}$$

To give a concrete example we consider the theory of a single scalar field ϕ at finite temperature. The action is given by, in the imaginary time formalism,

$$S_d[\beta, \phi] = \int_0^\beta \int_{\mathbb{R}^{d-1}} \mathrm{d}t\, \mathrm{d}^{d-1}x \left[\tfrac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 + \tfrac{1}{2}(\nabla\phi)^2 + U(\phi, \beta)\right]. \tag{4.2.13}$$

In the above $U(\phi, \beta)$ is the finite temperature effective potential. We assume that the behavior of the effective potential corresponds to a first order phase transition (shown schematically in Figure 4.1), so that at a temperature T_0 there exist two degenerate minima $U(\phi_-, \beta_0) = U(\phi_+, \beta_0)$.

As the temperature decreases below T_0 the vacuum at $\phi = \phi_-$ becomes metastable, and the system decays to the true vacuum at ϕ_+ (this process happens very slowly near T_0 however, so the phase transition actually occurs at a temperature slightly less than T_0 and there is a potential for the vacuum to supercool). The instability of the false vacuum corresponds to an imaginary component of the free energy

$$F = -\frac{1}{\beta} \ln(\mathcal{Z}[\beta]), \tag{4.2.14}$$

where $\beta = 1/T$ is the inverse temperature. If the first order phase transition temperature is much higher than the ground state energy of the system than thermal fluctuations dominate over quantum fluctuations, and the system decays via thermal nucleation of bubbles of true vacuum. The rate at which the phase transition occurs is proportional to the imaginary component of the free action[42]

$$\Gamma = \frac{\beta\omega_-}{\pi} \operatorname{Im}(F), \tag{4.2.15}$$

where ω_- is the frequency associated with the unstable mode. Further assuming that the characteristic size of the bubbles of true vacuum are much larger than β the partition functional can be estimated by a saddle point approximation. Technically, one should sum over all saddles in this approximation, but in practice one only needs to include the leading order saddles with minimum action, since higher order saddles will be exponentially suppressed. The trivial saddle ($\phi_{\text{cl}}(x) = \phi_-$) is removed by normalization, and the next to leading order saddle must be a function only of the radial distance from the center of the bubble (time dependent and rotationally inhomogeneous configurations are not disallowed, but will necessarily have larger actions). The action corresponding

to a critical-sized bubble or droplet is then dimensionally reduced to ($\bar{\phi}(t,\mathbf{x}) = \bar{\phi}(r)$)

$$\begin{aligned} S_d[\beta,\bar{\phi}] &= \beta \int_{\mathbb{R}^{d-1}} \mathrm{d}^{d-1}x \left[\frac{1}{2}\left(\nabla\bar{\phi}\right)^2 + U\left(\bar{\phi},\beta\right)\right] \\ &= \beta S_{d-1}[\beta,\bar{\phi}]. \end{aligned} \tag{4.2.16}$$

Expanding the free energy to leading order in exponentially small corrections then yields the relativistic rate for thermal nucleation per unit time per unit volume[42, 43]:

$$\Gamma \sim \frac{\omega_-}{\pi}\left(\frac{\beta S_{d-1}}{2\pi}\right)^{\frac{d-1}{2}} \left\{\frac{\det'\left(-\nabla^2 + U''\left(\bar{\phi},\beta\right)\right)}{\det(-\nabla^2 + U''(\phi_-,\beta))}\right\}^{-1/2} e^{-\beta S_{d-1}}, \quad (\beta S_{d-1} \to \infty). \tag{4.2.17}$$

The factors of S_{d-1} arise from integrating over the coordinates of the center of bubble, and the prime on the functional determinant signifies that zero modes have been removed. The determinant ratio is almost never evaluated because it would have to be done numerically. Instead, one often finds in the literature the approximation

$$\Gamma = T^d e^{-S_{d-1}/T} \qquad \text{or} \qquad \Gamma = T_c^d e^{-S_{d-1}/T},$$

but strictly speaking this is incorrect. First, the determinant prefactor can be orders of magnitude different than 1, so it is a numerically poor approximation. Second, the determinant ratio needs to be included in order for the approximation to be controlled, otherwise the relative difference between the full nonperturbative rate and the approximation does not tend to 0 in the limit that the critical-sized bubble tends to infinite radius.

The observable of interest is the temperature at which the first order phase transition actually occurs. This is done by comparing the thermal nucleation rate to the age of the universe. At the point that the nucleation rate exceeds the age of the universe

more than one critical-sized bubble will likely have appeared, and at this point the phase transition occurs, with the radius of the bubble of true vacuum quickly increasing at nearly the speed of light.

The previous calculation is also relevant to the question of baryogenesis. Electroweak sphalerons tend to annihilate any baryon excess inside the bubbles of true vacuum, so one attempts to calculate the rate of sphaleron transitions at temperatures large compared to M_W, but small compared to M_W/α_W (where M_W is the W-boson mass and α_W is the weak nuclear coupling constant). The calculation of the sphaleron rate is nearly identical to the thermal nucleation rate calculation, since both are topological quantum field theory effects. The sphaleron rate per unit space time volume is given as[35, 36, 99–101]

$$\Gamma \sim \frac{\omega_-}{2\pi}\mathcal{N}e^{-E_{\rm cl}/T}\kappa, \quad (E_{\rm cl}/T \to \infty), \tag{4.2.18}$$

where ω_- is again the absolute value of the eigenvalue of the unstable mode, the prefactor $\mathcal{N}$ includes the integration over collective coordinates of the sphaleron origin, $E_{\rm cl}$ is the classical sphaleron energy, and the factor κ is a ratio of functional determinants resulting from the Gaussian integration over thermal fluctuations about the sphaleron configuration

$$\kappa = \mathrm{Im}\left(\frac{\det(\Delta^0_{\rm FP})\,\det'\left(\Delta^S_{\rm GF}\right)}{\det(\Delta^S_{\rm FP})\,\det(\Delta^0_{\rm GF})}\right)^{-1/2}. \tag{4.2.19}$$

Here, Δ represents a quadratic fluctuation operator obtained by expanding the gauge-fixed (GF) action and the Faddeev-Popov (FP) action evaluated around the sphaleron (S) and the vacuum (0), respectively. The functional determinant $\det'\left(\Delta^S_{\rm GF}\right)$ contains

a negative eigenvalue due to the instability of the sphaleron, so

$$\left[\det{}'\left(\Delta^S_{\rm GF}\right)\right]^{-1/2} = \frac{i}{\omega_-}(\text{positive quantity})^{-1/2}, \tag{4.2.20}$$

so that κ is nonzero and the factors of ω_- cancel.

In analyzing the rates of both false vacuum decay and sphaleron transitions we observe the need to determine ratios of functional determinants. The most naive approach would be to assume that the spectra of these operators consists entirely of discrete eigenvalues (which is technically incorrect) and attempt to calculate each eigenvalue explicitly, then take the product of all these eigenvalues after regularization and normalization. This was the approach used in early calculations of the Standard Model electroweak sphaleron rate, using 35 CPU hours of vectorized computations on a Cray-2 supercomputer for a single parameter point[99]. Although modern computers have advanced significantly since the first sphaleron rates were calculated (a second generation iPad has nearly equivalent computational power to a Cray-2 supercomputer[103]), this is still an extremely computationally intensive task.

On could also put the theory on a lattice, and compute the partition functional directly. This has the added benefit of including more than just the one loop approximations. However, lattice computations are exceedingly difficult, and usually requires access to limited computational resources.

For some special cases alternatives to the brute force methods described previously exist. For theories of a single scalar field in one dimension Gel'fand and Yaglom discovered that the functional determinant of some operators can be expressed simply

by a single solution of an initial value problem[104]

$$\frac{\det\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+m^2+V(x)\right)}{\det\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+m^2\right)}=\lim_{x\to x_0}\frac{\phi(x)}{\phi^{\mathrm{free}}(x)}, \tag{4.2.21}$$

where $\phi(x)$ and $\phi^{\mathrm{free}}(x)$ are solutions of

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+m^2+V(x)\right]\phi=0, \qquad \phi(0)=0, \qquad \phi'(0)=1, \tag{4.2.22}$$

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+m^2\right]\phi^{\mathrm{free}}=0, \qquad \phi^{\mathrm{free}}(0)=0, \qquad \phi^{\mathrm{free}\prime}(0)=1, \tag{4.2.23}$$

and we have assumed the system is constrained to the interval $I=[0,x_0]$ (or $I=[0,\infty)$ if there is no boundary). In arriving at the above formula one must assume Dirichlet boundary conditions on the eigenfunctions of the respective operators

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+m^2+V(x)\right]\psi_n=\lambda_n\psi_n, \qquad \psi_n(0)=0, \qquad \psi_n(x_0)=0, \tag{4.2.24}$$

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+m^2\right]\psi_n^{\mathrm{free}}=\lambda_n\psi_n^{\mathrm{free}}, \qquad \psi_n^{\mathrm{free}}(0)=0, \qquad \psi_n^{\mathrm{free}}(x_0)=0. \tag{4.2.25}$$

In higher dimensions a similar formula holds, if we assume the potential function possesses a rotational symmetry. In this case we can use separation of variables to write

$$\frac{\det\left(-\nabla^2+m^2+V(r)\right)}{\det(-\nabla^2+m^2)}=\prod_{l=0}^{\infty}\left[\frac{\det(\mathcal{M}_l+m^2)}{\det(\mathcal{M}_l^{\mathrm{free}}+m^2)}\right]^{\deg(d,l)}, \tag{4.2.26}$$

where

$$\mathcal{M}_l\psi\coloneqq\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{d-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l(l+d-2)}{r^2}+V(r)\right]\psi, \tag{4.2.27}$$

$$\mathcal{M}_l^{\mathrm{free}}\psi^{\mathrm{free}}\coloneqq\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{d-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l(l+d-2)}{r^2}\right]\psi^{\mathrm{free}}, \tag{4.2.28}$$

and $\deg(d,l)$ is a degeneracy factor that counts the number of duplicate eigenvalues in the partial wave mode l. The partial wave determinants are now one dimensional, so we

may hope that we can apply the Gel'fand-Yaglom for each l, and then take the product of those results raised to the power of the appropriate degeneracy factor.

A problem immediately arises though, because the operators $\mathcal{M}_l$ and $\mathcal{M}_l^{\text{free}}$ are singular at the origin for $d > 1$. This is a regular singular point of the differential equation, so it is easily describe by the theory of Frobenius. However, we cannot apply the same boundary conditions that we could in the $d = 1$ case. For instance, choose $l = 0$ and approximate the solutions of

$$\left[\mathcal{M}_0 + m^2\right]\phi = 0, \tag{4.2.29}$$

$$\left[\mathcal{M}_0^{\text{free}} + m^2\right]\phi^{\text{free}} = 0, \tag{4.2.30}$$

as $r \to 0$. Assuming the potential function $V(r)$ is regular at $r = 0$ the linearly independent solutions have the following small r asymptotic behavior

$$\phi(r) \sim c_1, c_2 \ln(r), \quad (r \to 0), \tag{4.2.31}$$

for some constants c_1 and c_2. Therefore, no nontrivial solution exists with Dirichlet boundary conditions. The question then becomes: What boundary conditions should one impose for such a radial operator? The answer is more subtle than it initially appears, and it is worked out carefully in Section 4.3 and Section 4.4. It turns out that for this simple one field case the correct boundary conditions can be inferred from the results of scattering theory to be

$$\phi_l(r) \sim \phi_l^{\text{free}}(r) \sim r^l, \quad (r \to 0). \tag{4.2.32}$$

A second problem also arises in attempting to use the Gel'fand-Yaglom formula in dimensions $d > 1$: the product over l in (4.2.26) diverges. One then needs to regulate

and renormalize the product of determinants in some way. Dunne and Min[105] applied the heat kernel method with dimensional regularization and an angular momentum cutoff to renormalize the logarithm of the ratio of determinants for the case of $d = 4$ in the study of false vacuum decay at zero temperature. Zeta function regularization was used in the work of Dunne and Kirsten[106] to obtain explicit finite results in $d = 2$, $d = 3$, and $d = 4$, which would be suitable for finite temperature calculations using dimensional reduction.

Except for a small number of cases where exact results are known, there does not exist a general Gel'fand-Yaglom formula that incorporates the matrix structure necessary for multiple interacting scalar fields, gauge fields, or fermionic fields. Attempting to construct a formula directly from the path integral is prohibitively difficult, so we employ a mathematically rigorous method based on spectral theory.

The first step towards arriving at a general Gel'fand-Yaglom formula is to refine what we actually mean by a functional determinant. If the operator of interested was defined on a finite dimensional Hilbert space, then the determinant would simply be the product of a finite number of eigenvalues. The logarithm of the determinant would then be a sum,

$$\ln(\det(\tau)) = \sum_i \ln(\lambda_i).$$

We can generalize this to the infinite dimensional (separable) Hilbert space by considering the *resolvent set* of a densely defined closed operator A

Definition 4 (Resolvent Set)**.**

$$\rho(A) \coloneqq \left\{ z \in \mathbb{C} \mid (A - z)^{-1} \in \mathfrak{L}(\mathfrak{H}) \right\}, \tag{4.2.33}$$

where $\mathfrak{L}(\mathfrak{H})$ is the set of bounded linear operators on $\mathfrak{H}$. Essentially, $z \in \rho(A)$ if and only if $(A - z)\colon\ \mathfrak{D}(A) \to \mathfrak{H}$ is bijective and its inverse is bounded. We give this inverse a special name, the *resolvent* of A.

Definition 5 (Resolvent)**.**

$$\begin{aligned} R_A\colon\ \rho(A) &\to \mathfrak{L}(\mathfrak{H}) \\ z &\mapsto (A - z)^{-1}. \end{aligned} \tag{4.2.34}$$

The complement of the resolvent set is the *spectrum* of A.

Definition 6 (Spectrum)**.**

$$\sigma(A) \coloneqq \mathbb{C} \setminus \rho(A)\,. \tag{4.2.35}$$

This definition of the spectrum is the generalization we are looking for, since in the finite dimensional case we can alternatively write

$$\ln(\det(\tau)) = \sum_{\lambda \in \sigma(\tau)} \ln(\lambda).$$

There remain two difficulties with the above interpretation of the determinant of an operator. The first is that the spectrum generally consists of more than discrete eigenvalues. The second is that, even when the spectrum does consist of only discrete eigenvalues, the sum does not converge. A still more general interpretation, for the case where $\sigma(\tau) \subseteq \mathbb{R}$, would be

$$\ln(\det(\tau)) = \int_{\mathbb{R}} \ln(\lambda)\,\mathrm{d}\,\mu(\lambda)\,, \tag{4.2.36}$$

where $\mu(\lambda)$ is some finite Borel measure with support only on the spectrum of τ, i.e. $\mu(\mathbb{R} \setminus \sigma(\tau)) = 0$. The integral is still divergent in most cases, so we instead introduce the *zeta function* of a self-adjoint operator A

Definition 7 (Zeta Function)**.**

$$\zeta(s|A) = \int_{\mathbb{R}} \lambda^{-s} \, \mathrm{d}\, \mu_A(\lambda) \, . \tag{4.2.37}$$

Here, $\mu_A(\lambda)$ is the spectral measure of A. We then *define* the determinant of an operator in relation to its zeta function.

Definition 8 (Functional Determinant)**.** Suppose that A is a self adjoint operator with $\mathfrak{D}(A) \subseteq \mathfrak{H}$ and spectral measure μ_A. The logarithm of the determinant of A is related to the zeta function of A by

$$\ln(\det(A)) \coloneqq -\zeta'(0|A) \, . \tag{4.2.38}$$

This zeta function will turn out to be a meromorphic function on the complex plane, and its derivative at zero is finite.

The determinant of an operator τ is then constructed in two steps: we first need to find a self-adjoint extension of τ, and then we need to determine the spectrum of this self-adjoint extension. Therefore, we need to determine the domain of the adjoint of τ, which is equivalent to specifying the boundary conditions such that $\tau^* = \tau$. In Section 4.4 we remind the reader of a famous result of Friedrichs: for a symmetric operator bounded from below, a self-adjoint extension exists, and the domain of this extension is given by those $f \in \mathfrak{H}$ that satisfy Friedrichs boundary conditions. The Friedrichs boundary conditions are given explicitly in terms of the *principal solutions* of $\tau f = zf$. Once the self-adjoint extension is known we can construct the discrete component of the spectrum, also by utilizing the principal solutions. Therefore, we dedicate the next section to a thorough investigation of the principal solutions.

4.3 Principal Solutions

For sufficiently simple cases the relation between functional determinants of operators and particular solutions of those operators is well established. For radial operators (i.e. those operators in d-dimensions where symmetry arguments allow one to reduce the problem to 1-dimension) that act on scalar fields results are well known[106]. These results follow from a particular choice of boundary conditions, choosing the domain of the operator to be contained in the set of square integrable functions that are arbitrarily close to the "regular" solutions near the origin. The origin in such problems is a regular singular point of the differential equation, so there always exists at least one solution of Frobenius type, which behaves as some positive power of r as $r \to 0$. This choice is often motivated by a "physical" argument, i.e. that the physical fields should be bounded near the origin. Of course, in quantum mechanics the field values themselves are not observable, so such physical arguments lack a certain robustness. Even in the case of the nonrelativistic hydrogen atom, governed by the Schrödinger equation, there exist vectors in the Hilbert space that diverge logarithmically as $r \to 0$, that cannot be excluded by requiring square integrability. The true reason such states are excluded is because they do not belong to the domain of the Friedrichs extension of the hydrogen operator, which is the only self adjoint extension in this case. The spectrum of the operator depends crucially on the choice of boundary conditions, which is equivalent to specifying the domain of the operator. We will find that a self-adjoint extension exists, and the domain of the extended operator contains those square integrable functions that are arbitrarily close to the principal solutions of the differential

equation, which have been investigated thoroughly by Ried[107, 108].

We begin by collecting some results and definitions[108]. Consider the second order linear differential system, on an interval $I \subseteq \mathbb{R}$,

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[R(x)\,\frac{\mathrm{d}u}{\mathrm{d}x} + Q(x)\,u\right] - \left[Q^{\dagger}(x)\,\frac{\mathrm{d}u}{\mathrm{d}x} + P(x)\,u\right] = 0, \qquad x \in I, \tag{4.3.1}$$

where u is a n-dimensional vector function, and R, Q, and P are $n \times n$ matrix functions satisfying the following hypothesis

Hypothesis H2. On the interval I, the $n \times n$ matrix functions

- $R(x)$, $P(x)$ are hermitian,
- $R(x)$ is nonsingular,
- $R^{-1}(x)$, $R^{-1}(x)\,Q(x)$, and $P(x) - Q^{\dagger}(x)\,R^{-1}(x)\,Q(x)$ are locally (Lebesgue) integrable on I.

We introduce the *canonical variable* vector functions as

$$u(x)\,,\ v(x) \equiv R(x)\,\frac{\mathrm{d}\,u(x)}{\mathrm{d}x} + Q(x)\,u(x)\,. \tag{4.3.2}$$

This transforms the second order system into a first order system

$$L[y](x) \coloneqq \mathscr{J}\,\frac{\mathrm{d}y}{\mathrm{d}x} + \mathscr{A}(x)\,y = 0, \tag{4.3.3}$$

where

$$y(x) = \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}, \qquad \mathscr{J} \equiv \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \qquad \mathscr{A}(x) \equiv \begin{pmatrix} C(x) & -A^{\dagger}(x) \\ -A(x) & -B(x) \end{pmatrix}, \tag{4.3.4}$$

and

$$A(x) \equiv -R^{-1}(x)\,Q(x)\,, \quad B(x) \equiv R^{-1}(x)\,, \quad C(x) \equiv P(x) - Q^{\dagger}(x)\,R^{-1}(x)\,Q(x)\,. \tag{4.3.5}$$

We refer to (4.3.3) as a *Hamiltonian system*. It is easily shown that whenever R, P, and Q satisfy (H2), the following hypothesis is also satisfied.

Hypothesis H3. On the interval I the $n \times n$ matrix functions

- $B(x)$ and $C(x)$ are Hermitian, and
- $A(x)$, $B(x)$, and $C(x)$ are locally (Lebesgue) integrable on I.

Given (H3), we can assert a further hypothesis for the matrix function $\mathscr{A}(x)$.

Hypothesis H4. On the interval I the $2n \times 2n$ matrix function $\mathscr{A}(x)$ is Hermitian and locally (Lebesgue) integrable.

It then follows from well know existence theorems that, given n-dimensional constant vectors u_0 and v_0, a unique solution exists such that $u(x_0) = u_0$ and $v(x_0) = v_0$ for arbitrary $x_0 \in I$. There are $2n$ linearly independent solutions of (4.3.1), and if we take any two solutions

$$y_1(x) = \begin{pmatrix} u_1(x) \\ v_1(x) \end{pmatrix}, \qquad y_2(x) = \begin{pmatrix} u_2(x) \\ v_2(x) \end{pmatrix}, \tag{4.3.6}$$

the sesquilinear form

$$\{y_1, y_2\}(x) \equiv y_2^{\dagger}(x)\,\mathscr{J}\,y_1(x) = v_2^{\dagger}(x)\,u_1(x) - u_2^{\dagger}(x)\,v_1(x)\,, \tag{4.3.7}$$

is independent of x in I. If the value of this constant is 0 we say that these solutions, y_1 and y_2, are *(mutually) conjoined*.

Corresponding to the vector Hamiltonian system (4.3.3) we can construct a matrix Hamiltonian system

$$L[Y](x) \coloneqq \mathscr{J}\frac{\mathrm{d}Y}{\mathrm{d}x} + \mathscr{A}(x)\,Y = 0, \tag{4.3.3$_\mathrm{M}$}$$

where Y is a $2n \times r$ matrix function on I. There is a matrix function analog of (4.3.7) for solutions of (4.3.3$_\mathrm{M}$). Given

$$Y_1(x) \equiv \begin{pmatrix} U_1(x) \\ V_1(x) \end{pmatrix}, \qquad\qquad Y_2(x) \equiv \begin{pmatrix} U_2(x) \\ V_2(x) \end{pmatrix}, \tag{4.3.8}$$

such that $Y_1(x)$ and $Y_2(x)$ are $2n \times r_1$ and $2n \times r_2$ matrix solutions of (4.3.3$_\mathrm{M}$) respectively, the matrix quantity

$$\{Y_1, Y_2\}(x) \equiv Y_2^\dagger(x)\,\mathscr{J}\,Y_1(x) = V_2^\dagger(x)\,U_1(x) - U_2^\dagger(x)\,V_1(x)\,, \tag{4.3.9}$$

is a $r_2 \times r_1$ constant valued matrix function on I. If Y is a $2n \times r$ matrix solution of (4.3.3$_\mathrm{M}$) whose columns are linearly independent solutions of (4.3.3), with $\{Y, Y\} = 0$, these solutions form a basis for a conjoined family of solutions of dimension r, consisting of the set of all solutions of (4.3.3) which are linear combinations of these column vectors. If Y is a $2n \times n$ matrix solution of (4.3.3$_\mathrm{M}$), whose columns form a n-dimensional conjoined family of solutions of (4.3.3), then we refer to $Y(x)$ as a *conjoined basis for* (4.3.3). The maximum dimension of a conjoined family of solutions of (4.3.3) is n, and any conjoined family of solutions of dimension $r < n$ is contained in a conjoined basis for (4.3.3$_\mathrm{M}$)[108, Lemma 3.1, pp. 260].

Definition 9 (Conjugate Points)**.** Two distinct points, x_1 and x_2, of the interval I are said to be *(mutually) conjugate* with respect to (4.3.3) if there exists a solution $y(x) = (u(x)\,; v(x))$ of this system with $u(x) \neq 0$ on the subinterval I_0 with endpoints

x_1 and x_2, while $u(x_1) = u(x_2) = 0$. If no two distinct points of a subinterval $I_0 \subseteq I$ are conjugate with respect to (4.3.3), then this equation is said to be *disconjugate* on I_0.

This notion of conjugacy and conjugate points provides an oscillation criterion for the solutions of (4.3.3), and is essential for the construction of the principal solutions. We also have equivalent statements summarized in the following theorem.

Theorem 4.3.1 (Reid[108, Theorem 6.3, pp. 284]). *If $[a, b] \subset I$, and $B(x) \geq 0$ for x a.e. on I, then the following conditions are equivalent:*

- *(4.3.3) is disconjugate on $[a, b]$;*
- *there is no point on $(a, b]$ conjugate to $x = a$;*
- *there is no point on $[a, b)$ conjugate to $x = b$;*
- *there exists a conjoined basis $Y(x) = (U(x)\,; V(x))$ of (4.3.3) with $U(x)$ nonsingular on the closed interval $[a, b]$.*

We can now state an existence theorem of constructive type for the *principal solutions* of Reid. We will assume that $I = (a_0, b_0)$, $-\infty \leq a_0 < b_0 \leq \infty$, is an open subset of the real line. We will also assume that (4.3.3) is identically normal, as this will always be the case for differential operators that we consider.

Theorem 4.3.2 (Reid[108, Theorem 11.3, pp. 331]). *Suppose that hypothesis (H4) holds for (4.3.3) on $I = (a_0, b_0)$, while on this interval the system is identically normal and $B(x) \geq 0$ for x a.e. on I, and that there is a subinterval $I_0 = (a_0, c_0)$ on which (4.3.3) is disconjugate. For s and a distinct values on I_0, let $Y_{sa}(x) = (U_{sa}(x)\,; V_{sa}(x))$ be the*

solution of (4.3.3$_{\mathrm{M}}$) *satisfying the boundary conditions*

$$U_{sa}(s) = \mathbb{1}, \qquad\qquad U_{sa}(a) = 0. \tag{4.3.10}$$

Then

$$Y_{sa_0}(x) = \begin{pmatrix} U_{sa_0}(x) \\ V_{sa_0}(x) \end{pmatrix} \coloneqq \lim_{a \to a_0} Y_{sa}(x)\,, \tag{4.3.11}$$

exists and is a principal solution of (4.3.3$_{\mathrm{M}}$) *at* a_0*, with* $U_{sa_0}(x)$ *nonsingular on* I_0*; in particular* $Y_{sa_0}(x)$ *is a conjoined basis for* (4.3.3) *on* I_0*, and*

$$Y_{ca_0}(x) = Y_{sa_0}(x)\, U_{ca_0}(x)\,, \tag{4.3.12}$$

for $(s, c, x) \in I_0 \times I_0 \times I_0$.

The principal solutions generalize some properties of the "small" and "large" solutions of the scalar differential equation that are well known from scattering theory. In particular, the principal solutions are, in a sense, unique. That is, if $Y_0(x)$ is a principal solution of (4.3.3$_{\mathrm{M}}$), the most general form for the principal solutions are[108, pp. 329]

$$Y(x) = Y_0(x)\, K, \tag{4.3.13}$$

where K is a nonsingular $n \times n$ matrix. Other important properties are summarized in the following theorem:

Theorem 4.3.3 (Reid[108, Theorem 11.4(c), pp. 334])**.** *Suppose the hypotheses of Theorem 4.3.2 are satisfied. If* $Y_0(x) = (U_0(x)\,; V_0(x))$ *is a principal solution of* (4.3.3$_{\mathrm{M}}$) *at* a_0*, then for a* $2n \times n$*-dimensional solution* $Y_2(x) = (U_2(x)\,; V_2(x))$ *of the system the* $n \times n$ *constant matrix* $\{Y_0, Y_2\}$ *is nonsingular if and only if* $U_2(x)$ *is nonsingular for* x *on some subinterval* (a_0, c_2) *and* $[U_2(x)]^{-1}\, U_0(x) \to 0$ *as* $x \to a_0$.

Contained in Theorem 4.3.3 is an important observation, that if $Y_0(x) = (U_0(x)\,;V_0(x))$ is a principal solution of (4.3.3$_\mathrm{M}$) at a_0, and $Y(x) = (U(x)\,;V(x))$ is any other $2n \times n$-dimensional solution of (4.3.3$_\mathrm{M}$) such that $\{Y_0, Y\}$ is nonsingular, then it is necessarily the case that

$$\lim_{x\to a_0} [U(x)]^{-1} U_0(x) = 0. \tag{4.3.14}$$

It is in this sense that $Y_0(x)$ is the "smallest" possible solution of (4.3.3$_\mathrm{M}$).

The radial operators of interest are obtained from (4.3.1) by choosing $I = (0,\infty)$ and

$$R(x) = r^{d-1}, \quad Q(x) = Q^\dagger(x) = 0, \quad P(x) = r^{d-1}\left[\frac{l(l+d-2)}{r^2} + M^2 - z + V(r)\right]. \tag{4.3.15}$$

Hypothesis (H2) is then satisfied provided M^2 and $V(r)$ are Hermitian and z is real. Hypothesis (H4) is then immediately implied.

Theorem 4.3.4. *For the second order differential system*

$$(\tau_l - z)u \coloneqq -r^{1-d}\frac{\partial}{\partial r} r^{d-1}\frac{\partial u}{\partial r} + \left[\frac{l(l+d-2)}{r^2} + M^2 - z + V(r)\right]u = 0, \tag{4.3.16}$$

there is a conjoined basis that is principal at $r = 0$.

Proof. Written in standard form (expanding the derivative terms) the differential equation becomes

$$(\tau_l - z)u = -\frac{\partial^2 u}{\partial r^2} - \frac{d-1}{r}\frac{\partial u}{\partial r} + \left[\frac{l(l+d-2)}{r^2} + M^2 - z + V(r)\right]u = 0. \tag{4.3.17}$$

Using Hypothesis (H1) and expanding around $r = 0$ it is then clear that a solution of Frobenius type exists, and the leading order term is

$$u(r) \sim r^{\frac{2-d}{2}} r^{\pm\frac{2l+d-2}{2}} \mathbf{e}_i, \quad (r \to 0), \tag{4.3.18}$$

where $\mathbf{e}_i$ is generally an arbitrary constant vector in $\mathbb{C}^n$, but for convenience we will always take it to be one of the standard unit vectors in $\mathbb{R}^n$. The solution with a negative sign in the exponent is not always well defined, one will typically need to include log terms as well. However, the existence of even one solution of Frobenius type is sufficient, since every other solution can be constructed by taking derivatives of the Frobenius solution with respect to the indicial exponent[75]. Therefore, for sufficiently small r, every solution can be approximated by a function of the form

$$u(r) \sim \ln(r)^{\beta} r^{\alpha} \mathbf{e}_i, \quad (r \to 0). \tag{4.3.19}$$

Then defining an interval $I_0 = [0, r_0)$, and taking r_0 sufficiently small, there can be at most one point in I_0 where $u(r) = 0$. This immediately implies that the differential equation $(\tau_l - z)u = 0$ is disconjugate near $r = 0$. Hence, for $z \in \mathbb{R}$ so that hypothesis (H4) holds, Theorem 4.3.2 applies, and a principal solution exists near $r = 0$. □

The solutions of $\left(\tau_l^{\text{free}} - z\right)u = 0$ are easily found. We construct two conjoined bases, first introducing

$$\nu \equiv \frac{2l + d - 2}{2}, \qquad\qquad k_i \equiv \sqrt{z - m_i^2}. \tag{4.3.20}$$

The free solutions are then

$$\left[U_{0,l}^{\text{free}}(r; z)\right]_j^i = 2^{\nu}\, \Gamma(\nu + 1)\, r^{\frac{2-d}{2}} k_i^{-\nu}\, J_{\nu}(k_i r)\, \delta_j^i, \tag{4.3.21}$$

$$\left[U_{\infty,l}^{\text{free}}(r; z)\right]_j^i = \frac{i\pi}{2^{\nu+1}\, \Gamma(\nu + 1)} r^{\frac{2-d}{2}} k_i^{\nu}\, H_{\nu}^{(1)}(k_i r)\, \delta_j^i, \tag{4.3.22}$$

where $J_\nu(z)$ is the Bessel function of the first kind and $H_\nu^{(1)}(z)$ is the Hankel function of the first kind. The choice of normalization is partly for convenience, but the factors

of k_i^{ν} and $k_i^{-\nu}$ will actually be essential when we analytically continue the zeta function for the operators.

Further defining

$$V_{0,l}^{\text{free}}(r;z) \equiv r^{d-1}\frac{\partial}{\partial r}U_{0,l}^{\text{free}}(r;z)\,, \qquad V_{\infty,l}^{\text{free}}(r;z) \equiv r^{d-1}\frac{\partial}{\partial r}U_{\infty,l}^{\text{free}}(r;z)\,, \tag{4.3.23}$$

and

$$Y_{0,l}^{\text{free}}(r;z) = \begin{pmatrix} U_{0,l}^{\text{free}}(r;z) \\ V_{0,l}^{\text{free}}(r;z) \end{pmatrix}, \qquad Y_{\infty,l}^{\text{free}}(r;z) = \begin{pmatrix} U_{\infty,l}^{\text{free}}(r;z) \\ V_{\infty,l}^{\text{free}}(r;z) \end{pmatrix}, \tag{4.3.24}$$

it is trivial to show that

$$\left\{Y_{\infty,l}^{\text{free}}, Y_{0,l}^{\text{free}}\right\} = \mathbb{1}, \qquad \left\{Y_{0,l}^{\text{free}}, Y_{0,l}^{\text{free}}\right\} = 0, \qquad \left\{Y_{\infty,l}^{\text{free}}, Y_{\infty,l}^{\text{free}}\right\} = 0. \tag{4.3.25}$$

Furthermore,

$$\lim_{r\to 0}\left[U_{\infty,l}^{\text{free}}(r;z)\right]^{-1} U_{0,l}^{\text{free}}(r;z) = 0. \tag{4.3.26}$$

We see that the matrix solution $U_{0,l}^{\text{free}}(r;z)$ is a principal solution at $r=0$, because the principal solution is unique (up to post multiplication by a nonsingular matrix). Note that the above properties are independent of the angular momentum eigenvalue l, the dimension d, and the spectral parameter z (provided $z \in \mathbb{R}$).

Next, we use the free solutions to construct the principal solutions of $(\tau_l - z)u = 0$. We define two conjoined bases by

$$U_{0,l}(r;z) \sim U_{0,l}^{\text{free}}(r;z)\,, \qquad (r\to 0), \tag{4.3.27}$$

$$U_{\infty,l}(r;z) \sim U_{\infty,l}^{\text{free}}(r;z)\,, \qquad (r\to 0). \tag{4.3.28}$$

The existence of these solutions follows immediately from Hypothesis (H1). The conjoined basis $U_{0,l}(r;z)$ is uniquely defined by (4.3.27), but $U_{\infty,l}(r;z)$ is not uniquely

defined by (4.3.28). We could add to $U_{\infty,l}(r;z)$ a factor of $U_{0,l}(r;z)\,\Omega$, with Ω an arbitrary $n \times n$ matrix, and (4.3.28) will be left unchanged, since $U^{\text{free}}_{\infty,l}(r;z)$ generally diverges as $r \to 0$.

Defining, in a similar fashion as for the free equation,

$$V_{0,l}(r;z) \equiv r^{d-1}\frac{\partial}{\partial r}\,U_{0,l}(r;z)\,, \qquad V_{\infty,l}(r;z) \equiv r^{d-1}\frac{\partial}{\partial r}\,U_{\infty,l}(r;z)\,, \tag{4.3.29}$$

and

$$Y_{0,l}(r;z) = \begin{pmatrix} U_{0,l}(r;z) \\ V_{0,l}(r;z) \end{pmatrix}, \qquad Y_{\infty,l}(r;z) = \begin{pmatrix} U_{\infty,l}(r;z) \\ V_{\infty,l}(r;z) \end{pmatrix}, \tag{4.3.30}$$

we can use the fact that (4.3.9) is independent of r to show that

$$\{Y_{\infty,l}, Y_{0,l}\} = \mathbb{1}, \qquad \{Y_{0,l}, Y_{0,l}\} = 0, \qquad \{Y_{\infty,l}, Y_{\infty,l}\} = 0, \tag{4.3.31}$$

by simply choosing r to be arbitrarily small and using (4.3.27), (4.3.28), and (4.3.25). Applying the same arguments as in the free case we can show that $U_{0,l}(r;z)$ is the principal solution of $(\tau_l - z)u = 0$ at $r = 0$.

So far we have only constructed the leading order approximation of the principal solutions of $(\tau_l - z)u = 0$ at $r = 0$ using the principal solutions of $\left(\tau_l^{\text{free}} - z\right)u = 0$ at $r = 0$. For clarity we state the differential equations obeyed by these solutions:

$$\left[-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r} + \frac{l(l+d-2)}{r^2} + M^2 + V(r)\right] U_{0,l}(r;z) = z\,U_{0,l}(r;z)\,, \tag{4.3.32}$$

$$\left[-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r} + \frac{l(l+d-2)}{r^2} + M^2\right] U^{\text{free}}_{0,l}(r;z) = z\,U^{\text{free}}_{0,l}(r;z) \tag{4.3.33}$$

In order to construct higher order approximations of $U_{0,l}(r;z)$ we represent the solutions as a Volterra integral equation

$$U_{0,l}(r;z) = U^{\text{free}}_{0,l}(r;z) + \int_0^r K_l(r,t;z)\,U_{0,l}(t;z)\,\mathrm{d}t\,, \tag{4.3.34}$$

where the kernel, $K(r,t;z)$, is a solution of the free matrix equation

$$\left[-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r}+\frac{l(l+d-2)}{r^2}+M^2\right]K(r,t;z)=z\,K(r,t;z)\,, \tag{4.3.35}$$

with boundary conditions

$$K(r,r;z)=0, \qquad \frac{\partial}{\partial r}K(r,t;z)\Big|_{t=r}=V(r)\,. \tag{4.3.36}$$

Because there exists some $r_0\in(0,\infty)$ for which (4.3.33) is disconjugate on $I_0=(0,r_0)$, the principal solution $U_{0,l}^{\text{free}}(r;z)$ is nonsingular on this interval (this holds for all l and z). Therefore, the kernel is a solution of (4.3.33) on the interval I_0 if and only if[108, Theorem 3.1, pp. 261]

$$K_l(r,t;z)=U_{0,l}^{\text{free}}(r;z)\left\{A(t;z)+\int_0^r\left[U_{0,l}^{\text{free}}(s;z)\right]^{-1}s^{1-d}\left[\left[U_{0,l}^{\text{free}}(s;z)\right]^{\dagger}\right]^{-1}\mathrm{d}s\,B(t;z)\right\}, \tag{4.3.37}$$

for some matrix functions $A(t;z)$ and $B(t;z)$. Using the first boundary condition in (4.3.36) we find

$$A(t;z)=-\int_0^t\left[U_{0,l}^{\text{free}}(s;z)\right]^{-1}s^{1-d}\left[\left[U_{0,l}^{\text{free}}(s;z)\right]^{\dagger}\right]^{-1}\mathrm{d}s\,B(t;z)\,. \tag{4.3.38}$$

Using the second boundary condition in (4.3.36) we find

$$B(t;z)=\left[U_{0,l}^{\text{free}}(t;z)\right]^{\dagger}V(t)\,t^{d-1}. \tag{4.3.39}$$

The general solution for the kernel is then

$$K(r,t;z)=U_{0,l}^{\text{free}}(r;z)\int_t^r\left[\left[U_{0,l}^{\text{free}}(s;z)\right]^{\dagger}U_{0,l}^{\text{free}}(s;z)\right]^{-1}s^{1-d}\,\mathrm{d}s\left[U_{0,l}^{\text{free}}(t;z)\right]^{\dagger}V(t)\,t^{d-1}. \tag{4.3.40}$$

We evaluate the integrals in (4.3.40) by making use of the first relation of (4.3.25), written as

$$r^{d-1}\left[\left(\frac{\partial}{\partial r}\left[U_{0,l}^{\text{free}}(r;z)\right]^{\dagger}\right)U_{\infty,l}^{\text{free}}(r;z)-\left[U_{0,l}^{\text{free}}(r;z)\right]^{\dagger}\left(\frac{\partial}{\partial r}\,U_{\infty,l}^{\text{free}}(r;z)\right)\right]=\mathbb{1}. \tag{4.3.41}$$

Insert (4.3.41) inside the integral in (4.3.40) and integrate by parts. Then using

$$\left(\frac{\partial}{\partial r}\left[U_{0,l}^{\text{free}}(r;z)\right]^{\dagger}\right)U_{0,l}^{\text{free}}(r;z)-\left[U_{0,l}^{\text{free}}(r;z)\right]^{\dagger}\left(\frac{\partial}{\partial r}\,U_{0,l}^{\text{free}}(r;z)\right)=0, \tag{4.3.42}$$

the remaining integrals cancel and we are left with only the boundary terms.

$$\begin{aligned}K(r,t;z)=&-U_{\infty,l}^{\text{free}}(r;z)\left[U_{0,l}^{\text{free}}(t;z)\right]^{\dagger}V(t)\,t^{d-1}\\&U_{0,l}^{\text{free}}(r;z)\left[U_{0,l}^{\text{free}}(t;z)\right]^{-1}U_{\infty,l}^{\text{free}}(t;z)\left[U_{0,l}^{\text{free}}(t;z)\right]^{\dagger}V(t)\,t^{d-1}\end{aligned} \tag{4.3.43}$$

This can be further simplified by noting that for all $z\in\mathbb{R}$ the principal solutions of the free equation near $r=0$ are real valued. This follows from

$$J_{\nu}(ikr)=e^{i\pi\nu/2}\,I_{\nu}(kr)\,.$$

The factor of $\exp(i\pi\nu/2)$ cancels exactly with a similar term coming from the prefactor $k_i^{-\nu}$ in (4.3.21). Furthermore the free solutions commute since they are diagonal. This leaves us with

$$K(r,t;z)=\left[U_{0,l}^{\text{free}}(r;z)\,U_{\infty,l}^{\text{free}}(t;z)-U_{\infty,l}^{\text{free}}(r;z)\,U_{0,l}^{\text{free}}(t;z)\right]V(t)\,t^{d-1}. \tag{4.3.44}$$

We can then write the Volterra integral equation for the interacting solutions as

$$\begin{aligned}U_{0,l}(r;z)=U_{0,l}^{\text{free}}(r;z)&\left[\mathbb{1}+\int_0^r U_{\infty,l}^{\text{free}}(t;z)\,V(t)\,U_{0,l}(t;z)\,t^{d-1}\,\mathrm{d}t\right]\\&-U_{\infty,l}^{\text{free}}(r;z)\int_0^r U_{0,l}^{\text{free}}(t;z)\,V(t)\,U_{0,l}(t;z)\,t^{d-1}\,\mathrm{d}t\,.\end{aligned} \tag{4.3.45}$$

We conclude this section with an important observation. First we remind the reader of the *kernel* of an operator (also *null space*):

Definition 10 (Kernel)**.**

$$\mathrm{Kern}(A - z) = \{f \in \mathfrak{D}(A) \mid (A - z)f = 0\}. \tag{4.3.46}$$

A $z \in \sigma(A)$ is an eigenvalue if and only if $\mathrm{Kern}(A - z) \neq \emptyset$. Additionally, every regular solution of (4.3.16) can be written as

$$f_l(r; z) = U_{0,l}(r; z)\,\zeta, \tag{4.3.47}$$

for some constant nonzero n-dimensional vector ζ. If we then assume that z is an eigenvalue, and that $f_l(r; z) \in \mathrm{Kern}(\tau_l - z)$, it then must be the case that

$$f_l(r; z) \sim U^{\mathrm{free}}_{\infty,l}(r; z)\,\xi, \quad (r \to \infty), \tag{4.3.48}$$

for some constant nonzero n-dimensional vector ξ (this follows from (H1)). If this were not the case then $f_l(r; z)$ would not be square integrable, since $U^{\mathrm{free}}_{0,l}(r; z)$ is not locally Lebesgue integrable on (r, ∞) for any z. However, $U^{\mathrm{free}}_{\infty,l}(r; z)$ does have locally Lebesgue integrable components on (r, ∞) if $z < m_i^2$ for some i. To see this we use the analytic continuation properties of the Hankel functions:

$$K_\nu(z) = \frac{\pi}{2} i^{\nu+1} H^{(1)}_\nu(iz)\,, \quad -\pi < \arg(z) \leq \frac{\pi}{2}. \tag{4.3.49}$$

We then have

$$\left[U^{\mathrm{free}}_{\infty,l}(r; z)\right]^i_i = \frac{1}{2^\nu\,\Gamma(\nu+1)} r^{\frac{2-d}{2}} \left(m_i^2 - z\right)^{\nu/2} K_\nu\left(\sqrt{m_i^2 - z}\,r\right), \quad \text{if} \quad z < m_i^2. \tag{4.3.50}$$

Then, taking the large r behavior of the principal solutions

$$U_{0,l}(r; z) \sim U^{\mathrm{free}}_{0,l}(r; z)\,F_l(z) + U^{\mathrm{free}}_{\infty,l}(r; z)\,F^\dagger_l(z)\,, \quad (r \to \infty), \tag{4.3.51}$$

for some arbitrary $n \times n$ matrices $F_l(z)$ and $F_l^\dagger(z)$ (again, this follows from (H1)), we immediately see that $F_l(z)\,\zeta = 0$. Since ζ is nonzero by assumption it must then be the case that the constant matrix $F_l(z)$ is not full rank, i.e. $\det(F_l(z)) = 0$. In the next section we show that

$$f \in \mathrm{Kern}(\tau - z) \implies f = U_{0,l}(r; z)\,\zeta, \tag{4.3.52}$$

for some nonzero ζ. This would immediately imply that $\det(F_l(z)) = 0$ holds only if z is an eigenvalue. Before we can utilize this result we must first construct a self-adjoint extension of τ.

4.4 Friedrichs Extension

From the spectral theorem[109, Theorem 3.6, pp. 109] the spectrum of a self-adjoint operator A is $\sigma(A) \subseteq \mathbb{R}$. The difficulty in constructing the spectrum of the operator typically lies in identifying a self-adjoint extension of the operator (if one exists at all). It is usually simple enough to construct a *symmetric* operator,

Definition 11 (Symmetric)**.**

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle\,, \quad \forall \phi, \psi \in \mathfrak{D}(A)\,, \tag{4.4.1}$$

where $\mathfrak{D}(A) \subseteq \mathfrak{H}$ is the *domain* of A, i.e. the set of vectors in $\mathfrak{H}$ on which A is defined to act. For finite dimensional Hilbert spaces the operator A is necessarily self-adjoint if it is symmetric, but for the infinite dimensional Hilbert space this no longer holds in general. If A is a differential operator acting on some L^2 space then a suitable choice of boundary conditions easily yields a symmetric operator, which is almost always shown

by an integration by parts procedure. The choice of boundary conditions is equivalent to choosing the domain of A.

Definition 12 (Adjoint)**.** If A is a densely defined linear operator the adjoint operator is defined as

$$\begin{aligned} \mathfrak{D}(A^*) &= \Big\{\psi \in \mathfrak{H} \mid \exists \tilde{\psi} \in \mathfrak{H} \colon\ \langle \psi, A\phi\rangle = \langle \tilde{\psi}, \phi\rangle, \forall \phi \in \mathfrak{D}(A)\Big\}, \\ A^*\psi &= \tilde{\psi}. \end{aligned} \tag{4.4.2}$$

In this sense the adjoint A^* is the *maximal symmetric extension* of A. If $A = A^*$ then we refer to A as *self-adjoint*. Except for a very small number of special cases constructing the adjoint is highly nontrivial. If A is symmetric then it is always the case that $\mathfrak{D}(A) \subseteq \mathfrak{D}(A^*)$, that is the adjoint A^* is an extension of A, which we write as $A \subseteq A^*$. Even if one has labored extensively to somehow construct the adjoint, it may be that no self-adjoint extension exists, or that there are an infinite number of self-adjoint extensions.

Because it is often very difficult, if not entirely impossible, to construct the adjoint of an operator several theorems have been developed in order to avoid having to construct the adjoint altogether. For example, if one is lucky it may happen that the closure of the operator, $\overline{A} \equiv A^{**}$, is self-adjoint, in which case we refer to A as *essentially self-adjoint*. If A is essentially self-adjoint than $\overline{A}$ is the unique self-adjoint extension of A, and it is usually (though maybe counterintuitively) much easier to construct the closure $\overline{A}$ than it is to construct the adjoint A^*.

In every case the problem comes down to choosing the domain of A. The naive choice of boundary conditions is almost always too restrictive, which yields a symmetric

operator whose domain is smaller than the domain of its adjoint. For any symmetric densely defined linear operator A which is bounded below, Friedrichs[110] constructed a self-adjoint extension A_F that preserves the lower bound of A. Fortunately, in physical problems it is almost always the case that the operator A is bounded from below. This is just the statement that there exists a stable ground state. If no stable ground state exists than any system could decay to a state with lower energy, which in turn could decay to another lower energy state *ad infinitum*. This should clearly be avoided for physical systems.

Definition 13 (Semi-bounded/bounded from below)**.** We say that a symmetric operator A is *semi-bounded*, respectively, *bounded from below*, if there exists a $\gamma \in \mathbb{R}$ such that

$$\langle \psi, A\psi \rangle \geq \gamma \|\psi\|^2, \quad \forall \psi \in \mathfrak{D}(A)\,. \tag{4.4.3}$$

We will write $A \geq \gamma$ for short. The special case of a densely defined operator which is semi-bounded (respectively bounded from below) by 0 is called *nonnegative* (respectively *positive*). In this case $\langle \psi, A\psi \rangle \geq 0$ (respectively $>$ for $\psi \neq 0$) for all $\psi \in \mathfrak{D}(A)$, and we can introduce a map

$$\begin{aligned} \langle \cdot, \cdot \rangle_A : \mathfrak{D}(A) \times \mathfrak{D}(A) &\to \mathbb{C} \\ (\phi, \psi) &\mapsto \langle \phi, (A+1)\psi \rangle\,, \quad A \geq 0, \end{aligned} \tag{4.4.4}$$

The map (4.4.4) is a scalar product, hence we might adopt the norm, $\|\psi\|_A \coloneqq [\langle \psi, \psi \rangle_A]^{1/2}$, defined on a suitable subvector space of $\mathfrak{H}$. Take $\mathfrak{H}_A \subseteq \mathfrak{H}$ to be the completion of $\mathfrak{D}(A)$ with respect to the scalar product (4.4.4). A Cauchy sequence (ψ_n) in $\mathfrak{D}(A)$ is then also

a Cauchy sequence in $\mathfrak{H}$, because

$$\|\psi\|_A^2 = \langle \psi, A\psi \rangle + \|\psi\|^2 \implies \|\psi\| \leq \|\psi\|_A, \quad \text{if} \quad A \geq 0. \tag{4.4.5}$$

We can then identify the limit in $\mathfrak{H}_A$ with the limit of (ψ_n) regarded as a sequence in $\mathfrak{H}$. This observation allows us to extend the domain of the quadratic form of A to all $\psi \in \mathfrak{H}_A$,

$$q_A(\psi) = \langle \psi, \psi \rangle_A - \|\psi\|^2, \quad \psi \in \mathfrak{Q}(A) = \mathfrak{H}_A. \tag{4.4.6}$$

The set $\mathfrak{Q}(A)$ is often called the *form domain* of A.

Clearly, if A is semi-bounded (respectively bounded) from below by γ, then the operator $A - \gamma$ is nonnegative (respectively positive). In the general case we can then define

$$\begin{aligned} \langle \cdot, \cdot \rangle_{A-\gamma} : \mathfrak{D}(A) \times \mathfrak{D}(A) &\to \mathbb{C} \\ (\phi, \psi) &\mapsto \langle \phi, (A + 1 - \gamma)\psi \rangle, \quad A \geq \gamma, \end{aligned} \tag{4.4.7}$$

and similarly take $\mathfrak{H}_{A-\gamma}$ as the completion of $\mathfrak{D}(A)$ with respect to $\langle \cdot, \cdot \rangle_{A-\gamma}$, and the quadratic form

$$q_A(\psi) = \langle \psi, \psi \rangle_{A-\gamma} - (1 - \gamma)\|\psi\|^2, \quad \psi \in \mathfrak{H}_{A-\gamma}. \tag{4.4.8}$$

The quadratic form $q_A(\psi)$, extended to the full form domain $\mathfrak{Q}(A)$, is often called an "energy" norm.

The Friedrichs extension is then given by the following theorem.

Theorem 4.4.1 (Friedrichs Extension[109], Theorem 2.13, pp. 80)**.** *Let A be a symmetric operator which is bounded from below by γ. Then there is a self-adjoint extension*

$$A_F\psi = A^*\psi, \qquad \mathfrak{D}(A_F) = \mathfrak{D}(A^*) \cap \mathfrak{H}_{A-\gamma}, \tag{4.4.9}$$

which is also bounded from below by γ. Moreover, A_F is the only self-adjoint extension with $\mathfrak{D}(A_F) \subseteq \mathfrak{H}_{A-\gamma}$.

In the following lemma take $\mathrm{AC}_{\mathrm{loc}}(I)$ to be the set of complex functions that are absolutely continuous on arbitrary compact subintervals of I, and $\mathrm{AC}_{\mathrm{c}}(I)$ to be those functions in $\mathrm{AC}_{\mathrm{loc}}(I)$ with compact support on I.

Lemma 4.4.2. *Consider the partial wave operators defined by (4.1.12) and (4.1.13). The operators defined by*

$$\mathfrak{D}(A) = \mathfrak{D}(\tau_l) \cap \mathrm{AC}_{\mathrm{c}}(0,\infty)\,, \qquad Af = \tau_l f, \qquad f \in \mathfrak{D}(A)\,, \tag{4.4.10}$$

$$\mathfrak{D}\Big(A^{\mathrm{free}}\Big) = \mathfrak{D}\Big(\tau_l^{\mathrm{free}}\Big) \cap \mathrm{AC}_{\mathrm{c}}(0,\infty)\,, \qquad A^{\mathrm{free}} f = \tau_l^{\mathrm{free}} f, \qquad f \in \mathfrak{D}\Big(A^{\mathrm{free}}\Big)\,, \tag{4.4.11}$$

are symmetric.

Proof. The proof follows easily using integration by parts. We show the proof only for τ_l since the proof for τ_l^{free} is identical.

$$\langle f, Ag\rangle = \int_0^\infty f^\dagger(r)\left[-\frac{1}{r^{d-1}}\frac{\mathrm{d}}{\mathrm{d}r}r^{d-1}\frac{\mathrm{d}}{\mathrm{d}r} + \frac{l(l+d-2)}{r^2} + M^2 + V(r)\right] g(r)\, r^{d-1}\,\mathrm{d}r\,,$$

$$f, g \in \mathfrak{D}(A)\,. \tag{4.4.12}$$

M^2 and $V(r)$ are Hermitian by assumption, so we have

$$\begin{aligned}\langle f, Ag\rangle = &-\int_0^\infty f^\dagger(r)\,\frac{\mathrm{d}}{\mathrm{d}r}r^{d-1}\frac{\mathrm{d}\,g(r)}{\mathrm{d}r}\,\mathrm{d}r \\ &+\int_0^\infty \left\{\left[\frac{l(l+d-2)}{r^2} + M^2 + V(r)\right] f(r)\right\}^\dagger g(r)\, r^{d-1}\,\mathrm{d}r\,.\end{aligned} \tag{4.4.13}$$

Then, since $r^{d-1}\, g'(r) \in \mathrm{AC}(0,\infty)$, we can integrate by parts:

$$-\int_0^\infty f^\dagger(r)\,\frac{\mathrm{d}}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}\, g(r)}{\mathrm{d}r}\,\mathrm{d}r = -\,f^\dagger(r)\, r^{d-1}\frac{\mathrm{d}\, g(r)}{\mathrm{d}r}\bigg|_0^\infty + \int_0^\infty \frac{\mathrm{d}\, f^\dagger(r)}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}\, g(r)}{\mathrm{d}r}\,\mathrm{d}r\,. \quad (4.4.14)$$

As well, $g \in \mathrm{AC}(0,\infty)$, so we can integrate by parts a second time.

$$-\int_0^\infty f^\dagger(r)\,\frac{\mathrm{d}}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}\, g(r)}{\mathrm{d}r}\,\mathrm{d}r = -\,f^\dagger(r)\, r^{d-1}\frac{\mathrm{d}\, g(r)}{\mathrm{d}r}\bigg|_0^\infty + \frac{\mathrm{d}\, f^\dagger(r)}{\mathrm{d}r} r^{d-1}\, g(r)\bigg|_0^\infty - \int_0^\infty \left[\frac{\mathrm{d}}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}\, f(r)}{\mathrm{d}r}\right]^\dagger g(r)\,\mathrm{d}r\,. \quad (4.4.15)$$

Then, because $f, g \in \mathfrak{D}(A)$ have compact support, the boundary terms vanish, leaving us with

$$-\int_0^\infty f^\dagger(r)\,\frac{\mathrm{d}}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}\, g(r)}{\mathrm{d}r}\,\mathrm{d}r = -\int_0^\infty \left[\frac{1}{r^{d-1}}\frac{\mathrm{d}}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}\, f(r)}{\mathrm{d}r}\right]^\dagger g(r)\, r^{d-1}\,\mathrm{d}r\,. \quad (4.4.16)$$

The result is then

$$\begin{aligned}\langle f, Ag\rangle &= \int_0^\infty \left\{\left[-\frac{1}{r^{d-1}}\frac{\mathrm{d}}{\mathrm{d}r} r^{d-1}\frac{\mathrm{d}}{\mathrm{d}r} + \frac{l(l+d-2)}{r^2} + M^2 + V(r)\right] f(r)\right\}^\dagger g(r)\, r^{d-1}\,\mathrm{d}r \\ &= \langle Af, g\rangle\,.\end{aligned} \quad (4.4.17)$$

□

From τ_l and τ_l^{free} Lemma 4.4.2 shows we can define the symmetric operators A and A^{free}. If it can be shown that these symmetric operators are bounded from below then we can invoke Theorem 4.4.1 to show that a self-adjoint extension exists. It might be tempting to use a variational principal to look for the minimum of $\langle \psi, A\psi\rangle$, but this generally fails. Suppose for a moment that there exists a $z_0 \in \mathbb{R}$, with $z_0 < 0$, such that

$\mathrm{Kern}(A - z_0) \neq \emptyset$. Then it would be the case that $\exists \psi_0 \in \mathrm{Kern}(A - z_0) : A\psi_0 = z_0\psi_0$, and $\langle \psi_0, A\psi_0 \rangle = z_0 \|\psi_0\|^2$. However, we could also consider any other $\psi \in \mathfrak{D}(A)$ with $\psi = c\psi_0$, for any $c \in \mathbb{C}$. Obviously this ψ would also be in $\mathrm{Kern}(A - z_0)$, so $\langle \psi, A\psi \rangle = z\|c\|^2\|\psi_0\|^2$. We could then take c to have norm greater than 1, and since z_0 is negative

$$\langle \psi, A\psi \rangle < \langle \psi_0, A\psi_0 \rangle \,, \tag{4.4.18}$$

for arbitrary c with $\|c\| > 1$. Therefore, $\langle \psi, A\psi \rangle$ cannot be bounded below if there are any negative eigenvalues, and any minimum of $\langle \psi, A\psi \rangle$ could only be local.

This situation can be avoided if we scale out the norm and instead consider $\langle \psi, A\psi \rangle / \|\psi\|^2$. It would then be the case that

$$\frac{\langle \psi_1, A\psi_1 \rangle}{\|\psi_1\|^2} = \frac{\langle \psi_2, A\psi_2 \rangle}{\|\psi_2\|^2} \quad \text{if} \quad \psi_1 = c\psi_2 \quad \text{for any} \quad c \in \mathbb{C}. \tag{4.4.19}$$

We could then consider minimizing $\langle \psi, A\psi \rangle$ on the subset of $\mathfrak{D}(A)$ for which $\|\psi\| = 1$.

Lemma 4.4.3. *Take A and A^{free} to be the symmetric operators as in Lemma 4.4.2. Then A^{free} is bounded below, and A is bounded from below if (H1) holds. More specifically,*

$$\exists z_0 \in \mathbb{R} \colon (\mathrm{Kern}(A - z_0) \neq \emptyset \wedge \forall z \in \mathbb{R} \colon z < z_0 \implies \mathrm{Kern}(A - z) = \emptyset) \implies A \geq z_0. \tag{4.4.20}$$

That is, if there exists a lowest real eigenvalue then A is bounded from below by this lowest eigenvalue.

Proof. For the free operator we have

$$\left\langle \psi, A^{\mathrm{free}}\psi \right\rangle = \int_0^\infty \psi^\dagger(r) \left[-\frac{1}{r^{d-1}} \frac{\mathrm{d}}{\mathrm{d}r} r^{d-1} \frac{\mathrm{d}}{\mathrm{d}r} + \frac{l(l+d-2)}{r^2} + M^2 \right] \psi(r)\, r^{d-1}\, \mathrm{d}r \,. \tag{4.4.21}$$

Using integration by parts this becomes

$$\left\langle \psi, A^{\text{free}}\psi \right\rangle = \int_0^\infty \frac{\mathrm{d}\,\psi^\dagger(r)}{\mathrm{d}r}\frac{\mathrm{d}\,\psi(r)}{\mathrm{d}r} r^{d-1}\,\mathrm{d}r + \int_0^\infty \psi^\dagger(r)\left[\frac{l(l+d-2)}{r^2} + M^2\right]\psi(r)\, r^{d-1}\,\mathrm{d}r\,. \quad (4.4.22)$$

Every term in the above is positive for all $l \geq 0$ and $d > 0$, so $A^{\text{free}} \geq 0$, at least.

The operator A looks identical, except for the potential matrix $V(r)$, hence we need only to check that

$$\langle \psi, V\psi \rangle = \int_0^\infty \psi^\dagger(r)\, V(r)\, \psi(r)\, r^{d-1}\,\mathrm{d}r$$

is bounded from below. We can consider only those $\psi \in \mathfrak{D}(A)$ such that $\|\psi\| = 1$, since

$$\langle \psi_1, A\psi_1 \rangle \geq \gamma \|\psi_1\|^2 \implies \langle \psi_2, A\psi_2 \rangle \geq \gamma \|\psi_2\|^2, \quad \text{if} \quad \psi_1 = c\psi_2 \quad (4.4.23)$$

for any fixed γ and nonzero $c \in \mathbb{C}$. Take as example the simple function $\psi_i \in \mathfrak{D}(A)$ with components

$$\psi_i^j(r) = \sqrt{\frac{d}{(b^d - a^d)}}\, \chi_{(a,b)}(r)\, \delta_i^j, \quad (4.4.24)$$

where χ_Ω is the characteristic function on a subset Ω, i.e.

$$\chi_\Omega(c) = \begin{cases} 1 & \text{if } c \in \Omega \\ 0 & \text{else} \end{cases}. \quad (4.4.25)$$

Then

$$\langle \psi_i, V\psi_i \rangle = \frac{d}{b^d - a^d}\int_a^b V_{ii}(r)\, r^{d-1}\,\mathrm{d}r\,. \quad (4.4.26)$$

This quantity is finite for an arbitrary interval (a, b), since from (H1)

$$\left| \int_a^b V(r)\, r^{d-1}\,\mathrm{d}r \right| \leq \int_a^b |V(r)| r^{d-1}\,\mathrm{d}r < \infty, \quad (4.4.27)$$

where the expression above holds component-wise. This continues to hold for arbitrary simple functions ψ with $\|\psi\| = 1$. Since the simple functions are dense in $\mathfrak{H}$ we have,

$$\forall \psi \in \mathfrak{D}(A) : \|\psi\| = 1 \implies |\langle \psi, V\psi \rangle| < \infty. \tag{4.4.28}$$

Next, we look for a minimum of the functional $\langle \psi, A\psi \rangle$ with the constraint $\|\psi\| = 1$. Enforce the constraint with a Lagrange multiplier by defining the action integral

$$S[\psi, z] \coloneqq \langle \psi, A\psi \rangle - z\Big(\|\psi\|^2 - 1\Big). \tag{4.4.29}$$

$S[\psi, z] = \langle \psi, A\psi \rangle$ if ψ has norm 1. Taking the variation with respect to ψ and z, and setting the variation to 0 yields

$$(A - z_0)\psi_0 = 0, \qquad \|\psi_0\|^2 = 1. \tag{4.4.30}$$

Thus, if a minimum exists then $\mathrm{Kern}(A - z_0)$ is nonempty and $S[\psi_0, z_0] = z_0$. $\langle \psi, A\psi \rangle$ is then bounded from below by the smallest eigenvalue. □

From Theorem 4.4.1, if a symmetric densely defined linear operator A is bounded below then a self-adjoint extension exists. However, as previously stated, constructing the adjoint A^* (not to mention the form domain $\mathfrak{H}_{A-\gamma}$) is highly nontrivial in most cases. The domain of linear differential operators are uniquely determined by specifying boundary conditions, but Theorem 4.4.1 makes no explicit reference to boundary conditions. The question is then: what are the boundary conditions associated to the Friedrichs extension of a linear differential operator?

For a special class of regular Sturm-Liouville operators Friedrichs answered this question[111], showing that the domain of the Friedrichs extension corresponds to

imposing Dirichlet boundary conditions at the endpoints. This result was extended to all regular Sturm-Liouville operators[112] (with minimal restrictions on the coefficients and weight function) and for classical and quasi-differential operators of even order[113, 114].

The connection between the principal solutions of Reid and the Friedrichs extension is first seen by considering the case where the endpoints are regular. In this case Theorem 4.3.2 gives precisely those solutions which vanish at the boundary, corresponding to Dirichlet boundary conditions. Consider the linear differential operator

$$\tau f \coloneqq \frac{1}{r(x)}\left[-\frac{\mathrm{d}}{\mathrm{d}x}\, p(x)\, \frac{\mathrm{d}f}{\mathrm{d}x} + q(x)\right], \quad f, pf' \in \mathrm{AC}(a,b)\,, \tag{4.4.31}$$

on an arbitrary open interval $I = (a,b) \subseteq \mathbb{R}$. The appropriate Hilbert space is

$$\mathfrak{H} = L^2((a,b), r\,\mathrm{d}x)\,, \qquad \langle f, g\rangle = \int_a^b f^\dagger(x)\, r(x)\, g(x)\,\mathrm{d}x\,. \tag{4.4.32}$$

We also require

Hypothesis H5. The following hold a.e. on I:

(i) $p^{-1} \in L^1_{\mathrm{loc}}(I, \mathrm{d}x)$, is positive;

(ii) $q \in L^1_{\mathrm{loc}}(I, \mathrm{d}x)$, is real-valued;

(iii) $r \in L^1_{\mathrm{loc}}(I, \mathrm{d}x)$, is positive.

Definition 14 (Regular)**.** If a is finite and if $p^{-1}, q, r \in L^1((a,c), \mathrm{d}x)$ for some $c \in I$, then the Sturm-Liouville equation (4.4.31) is called *regular at* a. Similarly for b. If it is regular at both a and b, it is called *regular*.

The maximal domain of definition for τ in $L^2(I, r\,\mathrm{d}x)$ is given by

$$\mathfrak{D}(\tau) = \Big\{ f \in L^2(I, r\,\mathrm{d}x) \mid f, pf' \in \mathrm{AC}(a,b)\,, \tau f \in L^2(I, r\,\mathrm{d}x) \Big\}. \tag{4.4.33}$$

If τ is regular and bounded from below then, from our previous discussion, the Friedrichs extension is given by

$$\begin{aligned} &\mathfrak{D}(A_F) = \{u \in \mathfrak{D}(\tau) \mid u(a) = u(b) = 0\}, \\ &A_F u = \tau u, \qquad\qquad u \in \mathfrak{D}(A_F)\,. \end{aligned} \tag{4.4.34}$$

Since τ is regular, the equation $(\tau - z)u = 0$ is disconjugate at both endpoints for $z \in \mathbb{R}$, hence a principal solution exists near both endpoints. The principal solutions are uniquely defined (up to an overall multiplicative constant) as

$$(\tau - z)u_a = 0, \qquad u_a(a) = 0, \qquad p(a)\,u_a'(a) = 1, \tag{4.4.35}$$

$$(\tau - z)u_b = 0, \qquad u_b(b) = 0, \qquad p(b)\,u_b'(b) = 1. \tag{4.4.36}$$

Further defining

$$y_a(x) = \begin{pmatrix} u_a(x) \\ v_a(x) \end{pmatrix}, \qquad v_a(x) = p(x)\,\frac{\mathrm{d}}{\mathrm{d}x}\,u_a(x)\,, \tag{4.4.37}$$

$$y_b(x) = \begin{pmatrix} u_b(x) \\ v_b(x) \end{pmatrix}, \qquad v_b(x) = p(x)\,\frac{\mathrm{d}}{\mathrm{d}x}\,u_b(x)\,, \tag{4.4.38}$$

as the associated solutions of the first order equation, we see that for any $y(x) = (u(x)\,; v(x))$ such that $v(x)$ is everywhere finite

$$\{y, y_a\}\,(a) = 0 \implies u(a) = 0, \tag{4.4.39}$$

$$\{y, y_b\}\,(b) = 0 \implies u(b) = 0. \tag{4.4.40}$$

The Friedrichs extension is therefore equivalently defined by

$$\mathfrak{D}(A_F) = \{u \in \mathfrak{D}(\tau) \mid y(x) = (u(x)\,; v(x)), v(x) = p(x)\,u'(x)\,,$$

$$\{y, y_a\}\,(a) = 0, \{y, y_b\}\,(b) = 0\}\,,$$

$$A_F u = \tau u, \qquad\qquad u \in \mathfrak{D}(A_F)\,. \tag{4.4.41}$$

In fact Rellich[115] and Niessen & Zettl[116] showed that (4.4.41) continues to hold even when τ is singular at one or both endpoints, provided τ is bounded below and $(\tau - z)u = 0$ is disconjugate near both endpoints for all $z \in \mathbb{R}$.

Generalizing to the case of n coupled second order differential equations we have similar results, due to an analysis by Marletta & Zettl[117].

Definition 15 (Quasi-derivatives)**.** Let $I = (a, b)$, $-\infty \le a < b \le \infty$ be an open subset of the real line and let $m = 2n$ be an even positive integer. Suppose $p_{ij} \in L^1_{\mathrm{loc}}(I, \mathrm{d}x)$ for $i, j = 0, 1, \ldots, n$, $(i, j) \neq (n, n)$ and $p_{nn}^{-1} \in L^1_{\mathrm{loc}}(I, \mathrm{d}x)$. Assume moreover that $p_{ij} = p_{ji}$. The quasi-derivatives $f^{[r]}$ are defined as

(i) $f^{[r]} \coloneqq \dfrac{\mathrm{d}^r f}{\mathrm{d}x^r}, \qquad r = 0, 1, \ldots, n-1;$

(ii) $f^{[n]} \coloneqq \displaystyle\sum_{j=0}^{n} p_{nj} \frac{\mathrm{d}^j f}{\mathrm{d}x^j};$

(iii) $f^{[n+r]} \coloneqq -\dfrac{\mathrm{d}}{\mathrm{d}x} f^{[n+r-1]} + \displaystyle\sum_{j=0}^{n} p_{n-r,j} \frac{\mathrm{d}^j f}{\mathrm{d}x^j}, \qquad r = 1, 2, \ldots, n.$

We consider very general quasi-differential operators of the form

$$A_{\max} f \coloneqq \frac{1}{r(x)} f^{[2n]}, \qquad f^{[r]} \in \mathrm{AC}_{\mathrm{loc}}(I), r = 0, 1, \ldots, n-1. \tag{4.4.42}$$

where $r(x) \in L^1_{\mathrm{loc}}(I, \mathrm{d}x)$ is a weight function and $\mathrm{AC}_{\mathrm{loc}}(I)$ denotes the set of all complex-valued functions which are absolutely continuous on arbitrary compact subintervals of

I. We further assume $r > 0$ a.e. on I. For sufficiently smooth coefficient functions p_{ij} this operator can also be written as

$$A_{\max} f = \frac{1}{r(x)} \sum_{i=0}^{n} (-1)^i \frac{\mathrm{d}^i}{\mathrm{d}x^i} \left\{ \sum_{j=0}^{n} p_{ij}(x) \frac{\mathrm{d}^j f}{\mathrm{d}x^j} \right\}. \tag{4.4.43}$$

The maximal domain of definition of the operator (4.4.42) is

$$\begin{aligned} \mathfrak{D}(A_{\max}) = \Big\{ & f \in L^2(I, r\,\mathrm{d}x) \mid \\ & \forall r \in \{0, 1, \ldots, 2n-1\} \colon f^{[r]} \in \mathrm{AC}_{\mathrm{loc}}(I), A_{\max} f \in L^2(I, r\,\mathrm{d}x) \Big\}. \end{aligned} \tag{4.4.44}$$

We want to obtain a symmetric operator and hence we choose

$$Af = A_{\max} f, \qquad \mathfrak{D}(A) = \mathfrak{D}(A_{\max}) \cap \mathrm{AC}_{\mathrm{c}}(I). \tag{4.4.45}$$

Next, we consider the expression

$$Af = \lambda f, \quad \lambda \in \mathbb{R}, \tag{4.4.46}$$

which is a differential equation of order $2n$. In order to consider the principal solutions of this expression we fix a value of $\lambda = \hat{\lambda}$ and consider the endpoint $x = b$.

Hypothesis H6. There exists a $\mu \in \mathbb{R}$, with $\mu > \hat{\lambda}$, and $d < b$ such that the differential equation $Af = \mu f$ is disconjugate on (d, b).

Remark. If the differential equation $Af = \mu f$ is disconjugate on some interval, then so is $Af = \lambda f$ on the same interval for any $\lambda < \mu$.

Theorem 4.4.4 (Marletta & Zettl[117], Theorem 12)**.** *Suppose that for the operator A defined by (4.4.45), (H6) holds and that $x = a$ is a regular point of the differential equation $Af = \mu f$. Then the domain of the Friedrichs extension A_F over $I = (a, b)$ is*

given by

$$\mathfrak{D}(A_F) = \left\{ y \in \mathfrak{D}(A_{\max}) \mid u(a) = 0, \forall k \in \{1, \dots, n\} \colon \left\{ y, y_b^{(k)} \right\}(b) = 0 \right\}, \tag{4.4.47}$$

where $y_b^{(k)}(x)$ *is the* k^{th} *principal solution of* $A_{\max} y = \mu y$.

Similar results hold if a is a singular point, provided the differential equation $\tau f = \lambda f$ is disconjugate at a. The general case is then clear: for a singular endpoint (say a) we replace Dirichlet boundary conditions with Friedrichs boundary conditions:

$$u(a) = 0 \to \left\{ y, y_a^{(k)} \right\}(a) = 0. \tag{4.4.48}$$

For our radial operators defined by (4.1.12) and (4.1.13) there is no boundary at $r = \infty$ at which to apply boundary conditions, so there are no conditions to enforce there except square integrability. We can now explicitly construct self adjoint operators from τ_l and τ_l^{free}.

Theorem 4.4.5. *Given the partial wave operators* τ_l *and* τ_l^{free} *on the interval* $I = (0, \infty)$*, defined by* (4.1.12)*,* (4.1.13)*, the Friedrichs self-adjoint extensions are given by*

$$\begin{aligned} \mathfrak{D}(A_F) &= \left\{ f \in \mathfrak{D}(\tau_l) \mid \forall k \in \{1, \dots, n\} \colon \left\{ y, y_{0,l}^{(k)} \right\}(0) = 0 \right\}, \\ A_F f &= \tau_l f, \quad f \in \mathfrak{D}(\tau_l), \end{aligned} \tag{4.4.49a}$$

$$\begin{aligned} \mathfrak{D}\left(A_F^{\text{free}}\right) &= \left\{ f \in \mathfrak{D}\left(\tau_l^{\text{free}}\right) \mid \forall k \in \{1, \dots, n\} \colon \left\{ y, y_{0,l}^{\text{free}(k)} \right\}(0) = 0 \right\} \\ A_F^{\text{free}} f &= \tau_l^{\text{free}} f, \quad f \in \mathfrak{D}\left(\tau_l^{\text{free}}\right), \end{aligned} \tag{4.4.49b}$$

where the vectors y *are constructed from*

$$y(r) = \begin{pmatrix} f(r) \\ r^{d-1} \frac{\mathrm{d} f(r)}{\mathrm{d} r} \end{pmatrix}, \tag{4.4.50}$$

and the principal solutions $y_{0,l}^{(k)}(r;z)$ *and* $y_{0,l}^{\mathrm{free}(k)}(r;z)$ *are given by*

$$y_{0,l}^{(k)}(r;z) = \begin{pmatrix} u_{0,l}^{(k)}(r;z) \\ v_{0,l}^{(k)}(r;z) \end{pmatrix}, \qquad y_{0,l}^{\mathrm{free}(k)}(r;z) = \begin{pmatrix} u_{0,l}^{\mathrm{free}(k)}(r;z) \\ v_{0,l}^{\mathrm{free}(k)}(r;z) \end{pmatrix} \tag{4.4.51a}$$

$$u_{0,l}^{(k)}(r;z) = U_{0,l}(r;z)\,\mathbf{e}_k, \qquad v_{0,l}^{(k)}(r;z) = r^{d-1}\frac{\mathrm{d}\,u_{0,l}^{(k)}(r;z)}{\mathrm{d}r}, \tag{4.4.51b}$$

$$u_{0,l}^{\mathrm{free}(k)}(r;z) = U_{0,l}^{\mathrm{free}}(r;z)\,\mathbf{e}_k, \qquad v_{0,l}^{\mathrm{free}(k)}(r;z) = r^{d-1}\frac{\mathrm{d}\,u_{0,l}^{\mathrm{free}(k)}(r;z)}{\mathrm{d}r}, \tag{4.4.51c}$$

and $\mathbf{e}_k$ *is the* k^{th} *unit vector of* $\mathbb{R}^n$.

Proof. Using Lemma 4.4.2 we can construct the symmetric operators A and A^{free}. Lemma 4.4.3 shows that these operators are bounded below, and hence from Theorem 4.4.1 a self-adjoint extension exists. In Section 4.3 we showed that the linear differential systems $(\tau_l - z)f = 0$ and $\left(\tau_l^{\mathrm{free}} - z\right)f = 0$ are disconjugate at $r = 0$ for arbitrary l and z. Hence, from Theorem 4.3.2 a principal solution exists at $r = 0$, and we constructed these principal solutions in Section 4.3. Finally, Theorem 4.4.4 applies since (H6) holds and a $2n$-order linear differential system is equivalent to some first order linear differential system. □

From now on we substitute τ_l and τ_l^{free} for the Friedrichs extensions A_F and A_F^{free} of Theorem 4.4.5. Since we explicitly know the domain of the self-adjoint operators we can derive (at least formally) the spectrum. The *discrete spectrum* of any self-adjoint operator A, $\sigma_{\mathrm{d}}(A)$, is the set of all eigenvalues which are isolated points of the spectrum and whose corresponding eigenspace is finite dimensional. The complement of the discrete spectrum is the *essential spectrum*, $\sigma_{\mathrm{ess}}(A) = \sigma(A) \setminus \sigma_{\mathrm{d}}(A)$, which consists of all accumulation points of the spectrum plus all isolated eigenvalues of infinite multiplicity.

Theorem 4.4.6. *Take τ_l and τ_l^{free} to be the Friedrichs realizations of the partial wave radial operators, and m^2 to be the smallest eigenvalue of the squared mass matrix*

$$m^2 = \min\Big\{m_i^2, \ldots, m_n^2\Big\}. \tag{4.4.52}$$

The essential spectrum of τ_l and τ_l^{free} are given by

$$\sigma_{\text{ess}}(\tau_l) = \sigma_{\text{ess}}\Big(\tau_l^{\text{free}}\Big) = [m^2, \infty). \tag{4.4.53}$$

The discrete spectrum of τ_l is given by those $\lambda \in \mathbb{R}$ such that $\forall i \in \{1, \ldots, n\}\colon \lambda < m_i^2$, and

$$\lim_{R\to\infty} \det\bigg(\Big[U_{0,l}^{\text{free}}(R;\lambda)\Big]^{-1} U_{0,l}(R;\lambda)\bigg) = 0. \tag{4.4.54}$$

The discrete spectrum of τ_l^{free} is empty.

Proof. The spectrum of the free operator is easy enough to construct, since we know the exact solutions of $\Big(\tau_l^{\text{free}} - z\Big) f = 0$ for all z. For $z \in \rho\Big(\tau^{\text{free}}\Big)$

$$\begin{aligned}\Big(\tau_l^{\text{free}} - z\Big)^{-1} g = {} & U_{\infty,l}^{\text{free}}(r;z) \int_0^r \Big[U_{0,l}^{\text{free}}(t;z)\Big]^\dagger g(t)\, t^{d-1}\, \mathrm{d}t \\ & + U_{0,l}^{\text{free}}(r;z) \int_r^\infty \Big[U_{0,l}^{\text{free}}(t;z)\Big]^{-1} U_{\infty,l}^{\text{free}}(t;z) \Big[U_{0,l}^{\text{free}}(t;z)\Big]^\dagger g(t)\, t^{d-1}\, \mathrm{d}t\,. \end{aligned} \tag{4.4.55}$$

If z is such that the free solutions have components that are purely oscillatory then the resolvent will be unbounded. Otherwise the resolvent is bounded, so

$$\sigma\Big(\tau_l^{\text{free}}\Big) = [m^2, \infty). \tag{4.4.56}$$

The $\text{Kern}\Big(\tau_l^{\text{free}} - z\Big) = \emptyset$ for all z, which shows that $\sigma_{\text{d}}\Big(\tau_l^{\text{free}}\Big) = \emptyset$ since the discrete spectrum is a subset of the eigenvalues. The spectrum of the free operator then consists only of the essential spectrum.

From Weyl's theorem (given in the next section as Theorem 4.6.1) and (H1) we have $\sigma_{\text{ess}}(\tau_l) = \sigma_{\text{ess}}\left(\tau_l^{\text{free}}\right)$. Since the essential spectrum of both operators is identical we need only consider those eigenvalues of $(\tau_l - \lambda)f = 0$ for which $\lambda < m^2$. But for $z < m^2$ every solution of $(\tau_l - z)f = 0$ is either an exponentially growing or decaying function. Writing the asymptotic behavior of the principal solutions for large r,

$$U_{0,l}(r;z) \sim U_{0,l}^{\text{free}}(r;z)\, F_l(z) + U_{\infty,l}^{\text{free}}(r;z)\, F_l^{\dagger}(z)\,, \quad (r \to \infty),$$

and since $U_{\infty,l}^{\text{free}}(r;z)$ has only exponentially decaying components for $z < m^2$, the limit

$$\lim_{R\to\infty} \left[U_{0,l}^{\text{free}}(R;z)\right]^{-1} U_{0,l}(R;z) = F_l(z)\,, \tag{4.4.57}$$

exists and defines the *Jost matrix function* $F_l(z)$. If $\lambda < m^2$ is an eigenvalue then there must exist some $\zeta \in \mathbb{R}^n$ such that

$$F_l(\lambda)\,\zeta = 0. \tag{4.4.58}$$

This immediately implies that $\det(F_l(\lambda)) = 0$ if $U_{0,l}(r;\lambda)\,\zeta \in \mathfrak{D}(\tau_l)$.

The multiplicity, α, of the eigenvalue λ is given by the limiting behavior of

$$\det(F_l(z)) \sim (z-\lambda)^{\alpha} c, \quad (z \to \lambda), \tag{4.4.59}$$

for some nonzero constant c. If there exists only one $\zeta \in \mathbb{R}^n$ such that $F_l(\lambda)\,\zeta = 0$, then in some basis one and only one column of $F_l(\lambda)$ vanishes, so $\det(F_l(z)) \sim (z-\lambda)c$ as $z \to \lambda$. If there exist two linearly independent vectors $\zeta_1, \zeta_2 \in \mathbb{R}^n$ such that $F_l(\lambda)\,\zeta_1 = F_l(\lambda)\,\zeta_2 = 0$, then it must be the case that, in some basis, two columns of $F_l(z)$ vanish. Each column must vanish linearly, so $\det(F_l(z)) \sim (z-\lambda)^2 c$ as $(z \to \lambda)$. Continuing in this manner we see that the multiplicity α is equal to the number of linearly independent

$\zeta_i \in \mathbb{R}^n$ such that $F_l(\lambda)\,\zeta_i = 0$. Since there can be no more than n linearly independent vectors in $\mathbb{R}^n$ the multiplicity is bounded by n. Therefore, since λ is an eigenvalue with finite multiplicity it is in the discrete spectrum of τ_l.

Finally, because the determinant is a continuous function of R we can pull the limit outside the determinant,

$$\begin{aligned}\det(F_l(z)) &= \det\left(\lim_{R\to\infty}\left[U_{0,l}^{\text{free}}(R;z)\right]^{-1} U_{0,l}(R;z)\right) \\ &= \lim_{R\to\infty}\det\left(\left[U_{0,l}^{\text{free}}(R;z)\right]^{-1} U_{0,l}(R;z)\right).\end{aligned} \tag{4.4.60}$$

Replacing z with an eigenvalue λ then proves the theorem. □

The results of Theorem 4.4.6 can then be used to show that the function

$$\frac{\mathrm{d}}{\mathrm{d}z}\ln(\det(F_l(z))) \sim \frac{\alpha}{z-\lambda}, \quad (z\to\lambda), \tag{4.4.61}$$

has simple poles in the complex z plane at the $\lambda \in \sigma_{\mathrm{d}}(\tau_l)$. In Section 4.6 we use this fact to construct the zeta functions of τ and τ^{free} via contour integration. The resulting sum over the angular momentum quantum number l is divergent for dimensions $d > 1$, so this sum needs to be regulated and renormalized. To preform this regularization and renormalization we need to know the asymptotic behavior of the Jost matrix function at large values of l and z, to which we dedicate the next section.

4.5 Jost Matrix Function

The condition for convergence of the zeta function comes from the large l behavior of the Jost matrix function (bear in mind that our definition of the Jost matrix function is slightly different from what is usually called the Jost function in scattering

theory). For z real and smaller than any of the masses in the squared mass matrix M^2 the free solutions are real and either grow or decay exponentially as $r \to \infty$. In this case

$$F_l(z) = \lim_{r\to\infty} \left[U_{0,l}^{\text{free}}(r;z)\right]^{-1} U_{0,l}(r;z)\,.$$

Using the Volterra integral equation for $U_{0,l}(r;z)$ (4.3.45) we can write this as

$$F_l(z) \equiv \mathbb{1} + \int_0^\infty U_{\infty,l}^{\text{free}}(t;z)\, V(t)\, U_{0,l}(t;z)\, t^{d-1}\, \mathrm{d}t\,. \tag{4.5.1}$$

The above expression is only valid for $\mathrm{Re}(z)$ smaller than the smallest mass in the squared mass matrix M^2. If z exceeds this value then there is an extra term (which we dropped when taking the large r limit). The large l behavior can be found in several ways. One method is to directly use radial WKB to approximate $U_{0,l}(r;z)$ in the limit $l \to \infty$, $k_i \to \infty$, holding k_i/l fixed. One needs to generalize radial WKB to the case where the principal solutions are matrix valued (this is often referred to as a *phase integral approximation*)[118]. The radial WKB procedure is not too difficult, but for values of the spectral parameter z such that $z > m_i^2$ there will be turning points and one needs to asymptotically match the solutions across the turning points. A more straightforward procedure is to simply observe that the physical optics approximation neglects the potential matrix entirely, so it must be the case that

$$U_{0,l}(r;z) \sim U_{0,l}^{\text{free}}(r;z) + \mathcal{O}\left(\frac{1}{l}\right), \quad (l \to \infty, k_i \to \infty). \tag{4.5.2}$$

This of course is simply the first iteration of the Volterra integral equation (4.3.45). Hence, further iterations of (4.3.45) must produce terms that are higher order in $1/l$.

In order to illustrate this we first proceed with the calculation by keeping only

the leading term. In this case the Jost matrix function is approximated by

$$F_l(z) \sim \mathbb{1} + \int_0^\infty U^{\text{free}}_{\infty,l}(t;z)\, V(t)\, U^{\text{free}}_{0,l}(t;z)\, t^{d-1}\, \mathrm{d}t\,, \quad (l \to \infty, k_i \to \infty). \tag{4.5.3}$$

Taking the logarithm and summing the diagonal elements then yields

$$\mathrm{tr}[\ln(F_l(z))] \sim \int_0^\infty \mathrm{tr}\Big[U^{\text{free}}_{\infty,l}(t;z)\, V(t)\, U^{\text{free}}_{0,l}(t;z)\Big] t^{d-1}\, \mathrm{d}t\,, \quad (l \to \infty, k_i \to \infty). \tag{4.5.4}$$

(4.5.4) can then be approximated further using the uniform asymptotic expansion of the modified Bessel functions:

$$I_\nu(\nu z) \sim \frac{e^{\nu\eta}}{(2\pi\nu)^{1/2}(1+z^2)^{1/4}} \sum_{k=0}^{\infty} W_k(p)\, \nu^{-k}, \qquad (\nu \to \infty), \tag{4.5.5a}$$

$$K_\nu(\nu z) \sim \left(\frac{\pi}{2\nu}\right)^{1/2} \frac{e^{-\nu\eta}}{(1+z^2)^{1/4}} \sum_{k=0}^{\infty} (-1)^k\, W_k(p)\, \nu^{-k}, \qquad (\nu \to \infty), \tag{4.5.5b}$$

where

$$\eta \equiv \left(1+z^2\right)^{1/2} + \ln(z) - \ln[1 + \left(1+z^2\right)^{1/2}], \qquad p \equiv \left(1+z^2\right)^{-1/2}, \tag{4.5.6}$$

and

$$W_{k+1}(p) = \frac{1}{2}p^2\left(1-p^2\right) W_k'(p) + \frac{1}{8}\int_0^p \left(1-5t^2\right) W_k(t)\, \mathrm{d}t\,, \qquad W_0(p) = 1. \tag{4.5.7}$$

Retaining only the leading order terms in (4.5.5) we then have

$$\Big[U^{\text{free}}_{0,l}(t;z)\, U^{\text{free}}_{\infty,l}(t;z)\Big]_{ij} \sim t^{2-d}\frac{1}{2\nu}\left(1 + \frac{k_i^2 t^2}{\nu^2}\right)^{-1/2} \delta_{ij}, \quad (\nu \to \infty, k_i \to \infty). \tag{4.5.8}$$

The leading order approximation of the trace of the logarithm of the Jost Matrix function is then

$$\mathrm{tr}[\ln(F_l(z))] \sim \frac{1}{2\nu}\sum_{i=1}^{N}\int_0^\infty V_{ii}(t)\left(1 + \frac{k_i^2 t^2}{\nu^2}\right)^{-1/2} t\, \mathrm{d}t\,, \quad (\nu \to \infty, k_i \to \infty). \tag{4.5.9}$$

Note that this holds in arbitrary dimensions d, and for arbitrarily many coupled equations N. Thus, the sum

$$\sum_{l=0}^{\infty} \deg(l,d)\,\mathrm{tr}[\ln(F_l(0))],$$

converges only for $d \leq 1$.

Going to higher order becomes tedious, but not technically difficult. The calculation of the higher order terms is carried out in Appendix D.1.

In dimensions $d \leq 4$ we will require no more than the following terms:

$$\begin{aligned} U_{0,l}(r;z) \sim U_{0,l}^{\mathrm{free}}(r;z) + U_{0,l}^{\mathrm{free}}(r;z) \int_0^r U_{\infty,l}^{\mathrm{free}}(r';z)\, V(r')\, U_{0,l}^{\mathrm{free}}(r';z)\, r'^{d-1}\,\mathrm{d}r' \\ - U_{\infty,l}^{\mathrm{free}}(r;z) \int_0^r U_{0,l}^{\mathrm{free}}(r';z)\, V(r')\, U_{0,l}^{\mathrm{free}}(r';z)\, r'^{d-1}\,\mathrm{d}r' \,. \end{aligned} \tag{4.5.10}$$

We then have

$$\begin{aligned} \mathrm{tr}(\ln(F_l(z))) \sim \int_0^{\infty} \mathrm{tr}\Big[U_{\infty,l}^{\mathrm{free}}(r;z)\, V(r)\, U_{0,l}^{\mathrm{free}}(r;z)\Big] r^{d-1}\,\mathrm{d}r \\ - \int_0^{\infty}\int_0^{r} \mathrm{tr}\Big[U_{\infty,l}^{\mathrm{free}}(r;z)\, V(r)\, U_{\infty,l}^{\mathrm{free}}(r;z)\, U_{0,l}^{\mathrm{free}}(r';z)\, V(r')\, U_{0,l}^{\mathrm{free}}(r';z)\Big] r'^{d-1}\,\mathrm{d}r'\, r^{d-1}\,\mathrm{d}r \end{aligned} \tag{4.5.11}$$

In arriving at the above expression we have canceled two terms when expanding the logarithm of a matrix

$$\ln(\mathbb{1} + \epsilon A) \sim \epsilon A - \tfrac{1}{2}\epsilon^2 A^2, \quad (\epsilon \to 0).$$

Using the uniform asymptotic expansion of the modified Bessel functions we determine

the first two non vanishing terms.

$$\begin{aligned}\mathrm{tr}(\ln(F_l(z))) \sim & \frac{1}{2\nu}\sum_{i=1}^{n}\int_0^\infty \frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}} \\ & + \frac{1}{16\nu^3}\sum_{i=1}^{n}\int_0^\infty \left[1-\frac{6}{1+\frac{k_i^2r^2}{\nu^2}}+\frac{5}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^2}\right]\frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{3/2}} \\ & - \frac{1}{4\nu^3}\sum_{i,j=1}^{n}\int_0^\infty \frac{V_{ij}(r)\,V_{ji}(r)\,r^3\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}+\left[1+\frac{k_j^2r^2}{\nu^2}\right]\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}},\end{aligned}$$

$$(\nu\to\infty, k_i\to\infty, k_i/\nu \text{ fixed}) \quad (4.5.12)$$

For most cases this expansion is sufficient to renormalize the determinant ratio. If one is interested in dimensions $d > 4$ additional terms should be retained. This is a tedious, but straightforward exercise.

4.6 Zeta Function Approach

For a symmetric operator A on a N-dimensional Hilbert space we define the zeta function as

$$\zeta(s|A) \coloneqq \sum_{i=1}^{N}\lambda_i^{-s}, \quad (4.6.1)$$

where $\{\lambda_i\}$ are the eigenvalues of the operator. The zeta function is related to the determinant via

$$\ln(\det(A)) = -\,\zeta'(0|A)\,, \quad (4.6.2)$$

where the prime denotes the derivative with respect to s. More generally, if A is a self-adjoint operator on a separable Hilbert space we may formally define the zeta function

as

$$\zeta(s|A) \coloneqq \mathrm{tr}\big(A^{-s}\big), \tag{4.6.3}$$

where $\mathrm{tr}(\cdot)$ in this context may include a functional trace over the Hilbert space. This definition holds for A an invertible elliptic operator of order greater than zero[119]. Provided A^{-s} is trace class, the functional trace can be written as

$$\mathrm{tr}(A^{-s}) = \sum_{i=1}^{\infty} \left\langle \phi_i, A^{-s}\phi_i \right\rangle, \tag{4.6.4}$$

where $\{\phi_i\}$ is some orthornormal basis on the Hilbert space and $\langle\cdot,\cdot\rangle$ is the inner product on the Hilbert space. This definition of the trace is finite for $\mathrm{Re}(s)$ sufficiently large, and is independent of the choice of basis. Hence if the spectrum of the operator A is purely discrete the basis can be chosen to be the normalized eigenfunctions of A, and we have

$$\zeta(s|A) = \sum_{i=0}^{\infty} \lambda_i^{-s}. \tag{4.6.5}$$

The determinat is then the product of the eigenvalues

$$\det(A) = \exp\big(-\zeta'(0|A)\big) = \prod_{i=1}^{\infty} \lambda_i,$$

as expected (note that some of the λ_i may be identical). The eigenvalues will have the same mass dimension as the operator A, so the determinant defined in this way will have some (formally infinite) normalization that depends on the physical units. We can remove this dependence on the units by considering the dimensionless operator A/μ^2, where μ is some arbitrary mass scale. From the formal definition of the zeta function we see that

$$\zeta\Big(s|A/\mu^2\Big) = \mu^{2s}\,\mathrm{tr}(A^{-s}) = \mu^{2s}\,\zeta(s|A)\,. \tag{4.6.6}$$

The dimensionless functional determinant then becomes

$$\ln\Big(\det\Big(A/\mu^2\Big)\Big) = -\ln\Big(\mu^2\Big)\,\zeta(0|A) - \zeta'(0|A)\,. \tag{4.6.7}$$

The factor of $\zeta(0|A)$ will diverge with the volume of the system, but this divergence will cancel when we compare this determinant with the determinant of the corresponding free operator. We therefore include the factor of μ^2 in the determinants, but work with the zeta function $\zeta(s|A)$ as in (4.6.7).

If the spectrum of A is not purely discrete (4.6.5) needs to be generalized to include the entire spectrum. To this end we can invoke the spectral theorem to write

$$A^{-s} = \int_{\mathbb{R}} \lambda^{-s}\,\mathrm{d}P_A(\lambda)\,, \tag{4.6.8}$$

where $P_A(\Omega)$ is the *unique* projection valued measure associated to the operator A. Taking the trace then gives

$$\zeta(s|A) = \sum_{i=1}^{\infty} \int_{\mathbb{R}} \lambda^{-s}\,\mathrm{d}\mu_{\phi_i}(\lambda)\,, \tag{4.6.9}$$

where, again, $\{\phi_i\}$ is any orthonormal basis, and the measure $\mu_{\phi_i}(\lambda)$ can be reconstructed from the resolvant operator, $R_A(z) = (A-z)^{-1}$, by the Stieltjes inversion formula:

$$\mu_{\phi_i}(\lambda) = \lim_{\delta\downarrow 0}\lim_{\epsilon\downarrow 0}\frac{1}{\pi}\int_{-\infty}^{\lambda+\delta} \mathrm{Im}(\langle\phi_i, R_A(t+i\epsilon)\,\phi_i\rangle)\,\mathrm{d}t\,. \tag{4.6.10}$$

Consider multiplication operators on $L^2(\mathbb{R},\mathrm{d}\mu)$, with $\mathrm{d}\mu$ a finite Borel measure. The set of all growth points,

$$\sigma(\mu) = \{\lambda\in\mathbb{R} \mid \mu((\lambda-\epsilon,\lambda+\epsilon)) > 0 \text{ for all } \epsilon > 0\}, \tag{4.6.11}$$

is the spectrum of μ. Thinking of A as multiplication by λ in $L^2(\mathbb{R},\mathrm{d}\mu)$, i.e.

$$A\,f(\lambda) = \lambda\,f(\lambda)\,, \qquad \mathfrak{D}(A) = \Big\{f\in L^2(\mathbb{R},\mathrm{d}\mu) \mid \lambda\,f(\lambda)\in L^2(\mathbb{R},\mathrm{d}\mu)\Big\}, \tag{4.6.12}$$

the spectrum of A is simply the spectrum of μ, that is[109, Theorem 3.7, pp. 110]:

$$\sigma(A) = \sigma(\mu)\,. \tag{4.6.13}$$

The zeta function then takes the most general possible form for self-adjoint operators as

$$\zeta(s|A) = \int_{\mathbb{R}} \lambda^{-s}\,\mathrm{d}\mu(\lambda)\,. \tag{4.6.14}$$

The spectrum of A is equivalently given as

$$\begin{aligned}\sigma(A) &= \{\lambda \in \mathbb{R} \mid \mu((\lambda-\epsilon,\lambda+\epsilon)) > 0 \text{ for all } \epsilon > 0\} \\ &= \{\lambda \in \mathbb{R} \mid P_A((\lambda-\epsilon,\lambda+\epsilon)) \neq 0 \text{ for all } \epsilon > 0\}.\end{aligned} \tag{4.6.15}$$

The task is then to construct the measure $\mu(\Omega)$. In fact, we will not need to construct the entire measure, but only the part of the measure that has support on the discrete spectrum. First we define

$$\sigma_{\mathrm{d}}(A) = \{\lambda \in \sigma_{\mathrm{p}}(A) \mid \mathrm{rank}(P_A((\lambda-\epsilon,\lambda+\epsilon))) < \infty \text{ for some } \epsilon > 0\}, \tag{4.6.16}$$

and

$$\sigma_{\mathrm{ess}}(A) = \{\lambda \in \mathbb{R} \mid \mathrm{rank}(P_A((\lambda-\epsilon,\lambda+\epsilon))) = \infty \text{ for all } \epsilon > 0\}. \tag{4.6.17}$$

We then have a theorem due to Weyl:

Theorem 4.6.1 (Teschl[109], Theorem 6.19, pp. 171)**.** *Denote by $\mathfrak{C}(\mathfrak{H})$ the closure of the set of all finite rank operators in $\mathfrak{L}(\mathfrak{H})$ (referred to as the set of compact operators). Then suppose that A and B are self-adjoint operators. If*

$$R_A(z) - R_B(z) \in \mathfrak{C}(\mathfrak{H})\,, \tag{4.6.18}$$

for one $z \in \rho(A) \cap \rho(B)$*, then*

$$\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)\,. \tag{4.6.19}$$

Comparing the interacting and free operators,

$$\tau_l = \tau_l^{\text{free}} + V(r)\,. \tag{4.6.20}$$

From Theorem 4.6.1 and Hypothesis (H1), we then have

$$\sigma_{\text{ess}}(\tau_l) = \sigma_{\text{ess}}\left(\tau_l^{\text{free}}\right). \tag{4.6.21}$$

The difference between the zeta functions $\zeta(s|\tau_l)$ and $\zeta\left(s|\tau_l^{\text{free}}\right)$ can therefore depend only on the discrete spectrum of the operators. This immediately implies that

$$\zeta(s|\tau_l) - \zeta\left(s|\tau_l^{\text{free}}\right) = \sum_{\lambda_i \in \sigma_{\text{d}}(\tau_l)} \alpha_i \lambda_i^{-s}, \tag{4.6.22}$$

where α_i is the multiplicity of the i^{th} eigenvalue. Using the Cauchy integral formula we can write

$$\alpha_i \lambda_i^{-s} = \frac{1}{2\pi i} \oint_{C_i} \frac{\alpha_i z^{-s}}{z - \lambda_i}\,\mathrm{d}z\,, \tag{4.6.23}$$

where the contour C_i encloses the eigenvalue λ_i. From the previous section we recognize the asymptotic behavior of the Jost matrix function near an eigenvalue

$$\frac{\mathrm{d}}{\mathrm{d}z} \ln(\det(F_l(z))) \sim \frac{\alpha_i}{z - \lambda_i}, \quad (z \to \lambda_i),$$

so we can equivalently write the contour integral as

$$\alpha_i \lambda_i^{-s} = \frac{1}{2\pi i} \oint_{C_i} z^{-s} \frac{\mathrm{d}}{\mathrm{d}z} \ln(\det(F_l(z)))\,\mathrm{d}z\,, \tag{4.6.24}$$

where it is to be understood that the contour C_i encloses only the eigenvalue λ_i. Summing over all eigenvalues then yields

$$\zeta(s|\tau_l) - \zeta\left(s|\tau_l^{\text{free}}\right) = \frac{1}{2\pi i} \oint_{C} z^{-s} \frac{\mathrm{d}}{\mathrm{d}z} \ln(\det(F_l(z)))\,\mathrm{d}z\,, \tag{4.6.25}$$

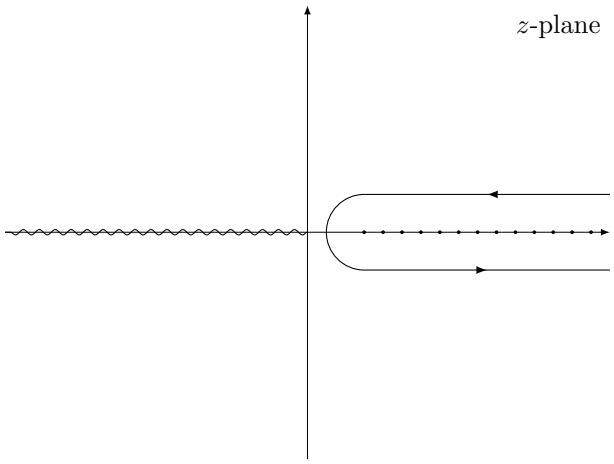


Figure 4.2: The contour C. Locations of eigenvalues are indicated by small circles on the positive z axis.

where the contour C encloses all eigenvalues on the positive real axis, and is shown in Figure 4.2 (we assume for now that there are no zero or negative eigenvalues).

In order to determine the full functional determinant ratio

$$\ln\left[\frac{\det(\tau/\mu^2)}{\det(\tau^{\text{free}}/\mu^2)}\right] = \sum_{l=0}^{\infty} \deg(d,l) \ln\left[\frac{\det(\tau_l/\mu^2)}{\det(\tau_l^{\text{free}}/\mu^2)}\right], \tag{4.6.26}$$

we consider the zeta functions

$$\zeta(s|\tau) = \sum_{l=0}^{\infty} \deg(d,l)\, \zeta(s|\tau_l)\,, \tag{4.6.27}$$

$$\zeta\left(s|\tau^{\text{free}}\right) \coloneqq \sum_{l=0}^{\infty} \deg(d,l)\, \zeta\left(s|\tau_l^{\text{free}}\right). \tag{4.6.28}$$

Using the contour integral representation of the zeta functions we then have

$$\zeta(s|\tau) - \zeta\left(s|\tau^{\text{free}}\right) = \sum_{l=0}^{\infty} \deg(d,l)\, \frac{1}{2\pi i} \oint_C z^{-s} \frac{\mathrm{d}}{\mathrm{d}z} \ln(\det(F_l(z)))\, \mathrm{d}z\,. \tag{4.6.29}$$

It is well known[102, pp. 12] (originally due to Weyl[120], but it is in German) that this representation of the zeta functions converges only for $\mathrm{Re}(s) > d/2$. We are of

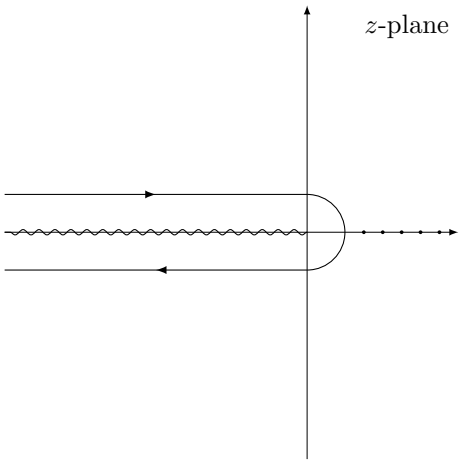


Figure 4.3: Deformed contour C.

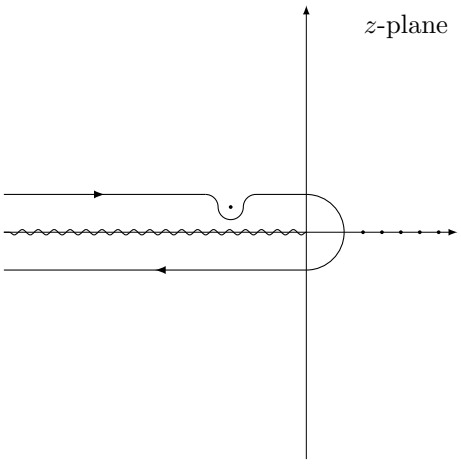


Figure 4.4: Deformed contour C with negative eigenvalue shifted off of the negative real axis.

course interested in the region around $s = 0$, so we need to analytically continue this expression.

We first deform the contour so that it encompasses the negative real z-axis. At this point we need to worry about any 0 or negative eigenvalues, since those would make it impossible for us to deform the contour in such a way that it includes the origin. For zero eigenvalues we can shift the spectrum by some small parameter $\epsilon > 0$: $F_l(z) \to F_l(z - \epsilon)$. The zero eigenvalues are then placed at ϵ, and we can deform the contour and take $\epsilon \to 0$ in the end (an algorithmic procedure for doing this is given in Section 4.8). If there is a negative eigenvalue at $z = -\omega^2$ than one would shift $F_l(z) \to F_l(z - i\epsilon)$, so that the contour can pass between the negative real axis and the negative mode (now at $\omega^2 + i\epsilon$).

Assuming there are no zero or negative eigenvalues we then proceed to shift the contour so that it passes just above the negative real z-axis, circles around the origin, and then passes just below the negative real z-axis as shown in Figure 4.3 and

Figure 4.4. The integration is done by including a small imaginary piece to z:

$$\text{above cut}: \qquad \int_{-\infty}^{0} (x+i\epsilon)^{-s} \frac{\mathrm{d}}{\mathrm{d}x} \ln(\det(F_l(x+i\epsilon)))\,\mathrm{d}x\,, \tag{4.6.30}$$

$$\text{below cut}: \qquad \int_{0}^{-\infty} (x-i\epsilon)^{-s} \frac{\mathrm{d}}{\mathrm{d}x} \ln(\det(F_l(x-i\epsilon)))\,\mathrm{d}x \tag{4.6.31}$$

We then make a change of variables to $x \equiv -\lambda$, and being careful with the terms

$$\lim_{\epsilon\to 0} (-\lambda+i\epsilon)^{-s} = \lambda^{-s} e^{-i\pi s}, \qquad \lim_{\epsilon\to 0} (-\lambda-i\epsilon)^{-s} = \lambda^{-s} e^{i\pi s},$$

yields

$$\zeta(s|\tau) - \zeta\Big(s|\tau^{\text{free}}\Big) = \sum_{l=0}^{\infty} \deg(d,l)\, \frac{\sin(\pi s)}{\pi} \int_0^{\infty} \lambda^{-s} \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln(\det(F_l(-\lambda)))\,\mathrm{d}\lambda\,. \tag{4.6.32}$$

If we assumed that this representation converged for $s = 0$ we could take the derivative with respect to s to find

$$\zeta'(0|\tau) - \zeta'\Big(0|\tau^{\text{free}}\Big) = -\sum_{l=0}^{\infty} \deg(d,l) \ln(\det(F_l(0))).$$

This is the Gel'fand-Yaglom result for $d = 1$. Unfortunately this result is divergent for $d > 1$, because the large l behavior of the Jost matrix function does not approach the identity matrix quickly enough. In the next section we show that the large l behavior of the Jost matrix function is $F_l(z) \sim \mathbb{1} + \mathcal{O}\Big(\frac{1}{l}\Big)$. In order to regulate the zeta functions we then add and subtract the asymptotic behavior of the Jost matrix functions

$$\zeta(s|\tau) - \zeta\Big(s|\tau^{\text{free}}\Big) = \zeta_{\text{finite}}(s) + \zeta_{\text{asymp}}(s)\,, \tag{4.6.33}$$

where

$$\zeta_{\text{finite}}(s) \equiv \sum_{l=0}^{\infty} \deg(d,l)\, \frac{\sin(\pi s)}{\pi} \int_0^{\infty} \lambda^{-s} \frac{\mathrm{d}}{\mathrm{d}\lambda} \operatorname{tr}\big[\ln(F_l(-\lambda)) - \ln(F_l^{\text{asymp}}(-\lambda))\big]\, \mathrm{d}\lambda \tag{4.6.34}$$

$$\zeta_{\text{asymp}}(s) \equiv \sum_{l=0}^{\infty} \deg(d,l)\, \frac{\sin(\pi s)}{\pi} \int_0^{\infty} \lambda^{-s} \frac{\mathrm{d}}{\mathrm{d}\lambda} \operatorname{tr}\big[\ln(F_l^{\text{asymp}}(-\lambda))\big]\, \mathrm{d}\lambda\,. \tag{4.6.35}$$

This adding and subtracting of the asymptotic behavior of the Jost matrix function is valid, since for sufficiently large s the series converges. We can then define the asymptotic Jost matrix function so that the series $\zeta_{\text{finite}}(s)$ converges for $s = 0$. The term $\zeta_{\text{asymp}}(s)$ is then analytically continued to $s = 0$ using the Riemann zeta function, which has a unique analytic continuation.

One very satisfying aspect of this regularization scheme is that there are no counter terms. This is in contrast to other regularization schemes in QFT, which usually require the addition of formally divergent counter terms to cancel the divergences coming from perturbation theory. One may argue that the counter terms in zeta function regularization have simply been swept into the Riemann zeta function (an implicit subtraction scheme), which to some extent is true. However, because the Riemann zeta function has a *unique* analytic continuation to the complex plane we see that these divergent counter terms are in fact relics of our representation of the propagator (the divergent sum over l in $\zeta(s|\tau)$ and $\zeta\Big(s|\tau^{\text{free}}\Big)$).

Most physicists are probably more familiar with dimensional regularization or a cutoff regularization scheme, which are most often used in scattering problems. For this reason we begin the next section with a brief review of regularization schemes, and how to translate between different schemes. The reader can then use our results,

derived using zeta function regularization, and easily translate them to their favorite regularization scheme quite easily.

4.7 Regularization and Renormalization

4.7.1 Introduction

There are several methods to regulate and renormalize the functional determinant of a self-adjoint operator. A particularly useful class of regularization techniques go by the name generalized proper-time, or Schwinger, regularizations.

$$\ln(\det(A))(\epsilon) = -\int_0^\infty \mathrm{d}t\, t^{-1}\, g_\epsilon(t)\, \mathrm{tr}\Big[e^{-tA}\Big], \tag{4.7.1}$$

where $g_\epsilon(t)$ is a suitable regularizing function used to control the small t (ultraviolet) divergences of $\mathrm{tr}\Big[e^{-tA}\Big]$. The quantity $\mathrm{tr}\Big[e^{-tA}\Big]$ is referred to as the *global heat kernel*, and is often written with respect to its local counterpart

$$\begin{aligned} K(t|A) &\equiv \mathrm{tr}\Big[e^{-tA}\Big] \\ &= \int_{\mathcal{M}} \mathrm{d}x\, \mathrm{tr}[K(x,x;t|A)]. \end{aligned} \tag{4.7.2}$$

The *local heat kernel* $K(x,x';t|A)$ is the fundamental solution of the heat equation[102]

$$\left(\frac{\partial}{\partial t} + A\right) K(x,x';t|A) = 0, \tag{4.7.3}$$

$$\mathcal{B}\, K(x,x';t|A)\Big|_{x\in\partial\mathcal{M}} = 0, \tag{4.7.4}$$

$$\lim_{t\to 0} K(x,x';t|A) = \delta(x,x')\,. \tag{4.7.5}$$

For A a strongly elliptic second-order differential operator on a smooth compact Riemannian manifold with a smooth boundary and local boundary conditions the global

heat kernel has the following asymptotic expansion[102]

$$K(t|A) \sim \sum_{n=0}^{\infty} K_n(A)\, t^{\frac{n-d}{2}}, \quad (t \to 0). \tag{4.7.6}$$

This small t behavior generically results in divergences that must be regulated in order to construct a meaningful quantity for the functional determinant. To see this we break the integral into two parts:

$$\int_0^\infty \mathrm{d}t\, t^{-1}\, K(t|A) = \int_0^1 \mathrm{d}t\, t^{-1}\, K(t|A) + \int_1^\infty \mathrm{d}t\, t^{-1}\, K(t|A)\,. \tag{4.7.7}$$

The integral over small values of t then results in

$$\int_0^1 \mathrm{d}t\, t^{-1}\, K(t|A) \sim \int_0^1 \mathrm{d}t \sum_{n=0}^{\infty} K_n(A)\, t^{\frac{n-d-2}{2}}, \quad (t \to 0). \tag{4.7.8}$$

Interchanging the order of summation and integration the integral is divergent for all $d > 0$. A commonly used trick is to let $d \to d - 2\epsilon$, and evaluate the integral for sufficiently large ϵ where the integral is convergent, then analytically continue to $\epsilon \to 0$ at the end. This is clearly equivalent to choosing a regulator $g_\epsilon(t) = t^\epsilon$ in (4.7.1), which defines the *analytic regularization scheme* (more commonly referred to in perturbation theory as *dimensional regularization*, or more briefly *dim reg*). This regularization scheme generically leads to the well known $1/\epsilon$ poles of perturbation theory. These divergences are then subtracted by introducing local counter terms with the same divergence but of opposite sign.

For A a nonnegative operator we use the Mellin transform of A^{-s},

$$A^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1} e^{-tA}, \tag{4.7.9}$$

to write the zeta function of the operator as

$$\zeta(s|A) = \frac{1}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1}\, \mathrm{tr}\Big[e^{-tA}\Big]. \tag{4.7.10}$$

We should also include a scale parameter μ with mass dimension 1, so that the argument of the exponent in the global heat kernel is dimensionless (we make the same substitution in (4.7.1)).

$$\begin{aligned}\zeta\Big(s|A/\mu^2\Big) &= \frac{1}{\Gamma(s)}\int_0^\infty \mathrm{d}t\, t^{s-1}\,\mathrm{tr}\Big[e^{-t\mu^{-2}A}\Big] \\ &= \frac{\mu^{2s}}{\Gamma(s)}\int_0^\infty \mathrm{d}x\, x^{s-1}\,\mathrm{tr}\Big[e^{-xA}\Big] \\ &= \mu^{2s}\,\zeta(s|A)\,.\end{aligned} \tag{4.7.11}$$

This integral representation of the zeta function is also valid only for $\mathrm{Re}(s) > d/2$, which follows immediately from the small t asymptotic expansion of the global heat kernel (4.7.6). However, what is now a standard argument[119] leads to a meromorphic extension of the zeta function for all complex s:

$$\Gamma(s)\,\zeta(s|A) = \sum_{n=0}^{\infty}\frac{K_n(A)}{s+\frac{n-d}{2}} + J(s)\,, \tag{4.7.12}$$

where $J(s)$ is a purely analytic function of s. The zeta function is then finite at $s=0$, and its value is

$$\zeta(0|A) = K_d(A)\,. \tag{4.7.13}$$

The derivative of the zeta function at $s=0$ then also exists and is finite.

Choosing analytic regularization in (4.7.1), i.e. $g_\epsilon(t) = t^\epsilon$, we then have

$$\begin{aligned}\ln\Big(\det\Big(A/\mu^2\Big)\Big)(\epsilon) &= -\,\Gamma(\epsilon)\,\zeta\Big(\epsilon|A/\mu^2\Big) \\ &\sim -\left(\frac{1}{\epsilon}-\gamma+2\ln(\mu)\right)\zeta(0|A) - \zeta'(0|A)\,, \quad (\epsilon\to 0).\end{aligned} \tag{4.7.14}$$

The $1/\epsilon$ term is the familiar logarithmic divergence that occurs in the renormalization of perturbation theory, and which is removed by introducing local counter terms.

Another important subclass of regularization schemes are those for which the regularization function $g_\epsilon(t)$ admits a Mellin transform:

$$\hat{g}_\epsilon(s) = \int_0^\infty \mathrm{d}t\, t^{s-1}\, g_\epsilon(t)\,, \tag{4.7.15}$$

$$g_\epsilon(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \mathrm{d}s\, t^{-s}\, \hat{g}_\epsilon(s)\,. \tag{4.7.16}$$

One can then write (4.7.1) as a complex integral involving $\hat{g}_\epsilon(s)$ and the Mellin transform of $\mathrm{tr}\Big[e^{-tA}\Big]$.

$$\ln\Big(\det\Big(A/\mu^2\Big)\Big)(\epsilon) = -\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \mathrm{d}s\, \hat{g}_\epsilon(-s)\, \mu^{2s}\, \Gamma(s)\, \zeta(s|A)\,. \tag{4.7.17}$$

Of these the most common is the *ultraviolet cutoff regularization scheme*, defined by $g_\epsilon(t) = \Theta(t-\epsilon)$. After a small amount of work one finds poles of the form $\ln(\epsilon), \epsilon^{-1}, \ldots, \epsilon^{-d/2}$, which correspond to the higher divergences in perturbation theory when regulating the theory with a ultraviolet cutoff, e.g. Pauli-Villars. We will not make use of these regularization schemes, as they are less common then analytic regularization.

Perhaps the most natural regularization scheme makes important use of the observation that the zeta function is analytic in a neigborhood of $s = 0$. The choice of regulator

$$g_\epsilon(t) = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\frac{t^\epsilon}{\Gamma(\epsilon)}, \tag{4.7.18}$$

defines the *zeta function regularization* scheme. With this choice we find

$$\begin{aligned}
\ln\Big(\det\Big(A/\mu^2\Big)\Big)(\epsilon) &= -\int_0^\infty \mathrm{d}t\, t^{-1}\frac{\mathrm{d}}{\mathrm{d}\epsilon}\frac{t^\epsilon}{\Gamma(\epsilon)}\,\mathrm{tr}\Big[e^{-t\mu^{-2}A}\Big] \\
&= -\frac{\mathrm{d}}{\mathrm{d}\epsilon}\,\zeta\Big(\epsilon|A/\mu^2\Big) \\
&\sim -\zeta'(0|A) - \ln\Big(\mu^2\Big)\,\zeta(0|A)\,, \quad (\epsilon\to 0).
\end{aligned} \tag{4.7.19}$$

Comparing the zeta function regularization scheme to the analytic regularization scheme we see that

$$\Big[\ln\Big(\det\Big(A/\mu^2\Big)\Big)(\epsilon)\Big]_{\text{zeta}} - \Big[\ln\Big(\det\Big(A/\mu^2\Big)\Big)(\epsilon)\Big]_{\text{analytic}} \sim \left(\frac{1}{\epsilon} - \gamma\right)\zeta(0|A)\,, \quad (\epsilon \to 0). \tag{4.7.20}$$

The remaining terms vanish in the limit $\epsilon \to 0$. We can then easily translate between the zeta function regularization scheme and the analytic regularization scheme by introducing local counter terms of the form

$$\delta S_{\text{ct}} = \left(\frac{1}{\epsilon} - \gamma\right)\zeta(0|A)\,. \tag{4.7.21}$$

In perturbation theory this corresponds to a modified minimal subtraction scheme with dimensional regularization. The relation to other subtraction schemes is then immediate, since these differ only by including additional finite contributions to (4.7.21). One recovers the MS scheme by letting $m^2_{\text{zeta}} = \mu^2_{\text{MS}} e^{\gamma}$ and the $\overline{\text{MS}}$ scheme by letting $\mu^2_{\text{zeta}} = 4\pi\mu^2_{\overline{\text{MS}}}$.

4.7.2 Zeta Function Regularization

Having included sufficiently many terms in the asymptotic expansion of the Jost matrix function the zeta function $\zeta_{\text{finite}}(s)$ is convergent in the neighborhood of $s = 0$. The remaining term, $\zeta_{\text{asymp}}(s)$, is determined by reduction to Riemann zeta

functions. The asymptotic Jost matrix function is defined as (in dimensions $d \leq 4$)

$$\begin{aligned}\ln\bigl(\det\bigl(F_l^{\text{asymp}}(-\lambda)\bigr)\bigr) &= \frac{1}{2\nu}\sum_{i=1}^{n}\int_0^\infty \frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}} \\ &\quad + \frac{1}{16\nu^3}\sum_{i=1}^{n}\int_0^\infty \left[1-\frac{6}{1+\frac{k_i^2r^2}{\nu^2}}+\frac{5}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^2}\right]\frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{3/2}} \\ &\quad - \frac{1}{4\nu^3}\sum_{i,j=1}^{n}\int_0^\infty \frac{V_{ij}(r)\,V_{ji}(r)\,r^3\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}+\left[1+\frac{k_j^2r^2}{\nu^2}\right]\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}},\end{aligned} \tag{4.7.22}$$

where $k_i \equiv \sqrt{\lambda+m_i^2}$. For each term in the sums we compute the integrals over λ by first making a change of variables to $k=\sqrt{\lambda+m_i^2}$ and using

$$\int_m^\infty \left(k^2-m^2\right)^{-s}\frac{\mathrm{d}}{\mathrm{d}k}\left[1+\frac{k^2r^2}{\nu^2}\right]^{-p/2}\mathrm{d}k = \frac{s\,\Gamma(-s)\,\Gamma\left(\frac{p}{2}+s\right)}{\Gamma\left(\frac{p}{2}\right)}\frac{r^{2s}}{\nu^{2s}\left[1+\frac{m^2r^2}{\nu^2}\right]^{\frac{p}{2}+s}}. \tag{4.7.23}$$

We organize the calculation into several pieces, as it is going to get rather complicated. The last term in (4.7.22) needs to be massaged a little before we can perform the integration over λ. Choose i and j such that $m_i \neq m_j$, we then have

$$\begin{aligned}&\frac{V_{ij}(r)\,V_{ji}(r)}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}+\left[1+\frac{k_j^2r^2}{\nu^2}\right]\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}} \\ &= \frac{V_{ij}(r)\,V_{ji}(r)}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}}\frac{1}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}+\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}} \\ &= \frac{\nu^2\,V_{ij}(r)\,V_{ji}(r)}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}}\frac{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}-\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}}{\left(m_i^2-m_j^2\right)r^2} \\ &= \frac{\nu^2\,V_{ij}(r)\,V_{ji}(r)}{\left(m_i^2-m_j^2\right)r^2\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}}-\frac{\nu^2\,V_{ij}(r)\,V_{ji}(r)}{\left(m_i^2-m_j^2\right)r^2\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}}\end{aligned} \tag{4.7.24}$$

When performing the sum over i and j these terms simply add together. Then denote the set $\sigma = \{(i,j) \mid m_i = m_j\}$ and its complement $\bar{\sigma} = \{(i,j) \mid i \in \{1,\dots,n\}, j \in \{1,\dots,n\}\} \setminus \sigma$. We then write (4.7.22) as

$$\begin{aligned}\ln\bigl(\det\bigl(F_l^{\text{asymp}}(-\lambda)\bigr)\bigr) = {}& \frac{1}{2\nu}\sum_{i=1}^{n}\int_0^\infty \frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}} \\ & + \frac{1}{16\nu^3}\sum_{i=1}^{n}\int_0^\infty \left[1-\frac{6}{1+\frac{k_i^2r^2}{\nu^2}}+\frac{5}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^2}\right]\frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{3/2}} \\ & - \frac{1}{8\nu^3}\sum_{(i,j)\in\sigma}\int_0^\infty \frac{V_{ij}(r)\,V_{ji}(r)\,r^3\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{3/2}}, \\ & - \frac{1}{2\nu}\sum_{(i,j)\in\bar{\sigma}}\int_0^\infty \frac{V_{ij}(r)\,V_{ji}(r)\,r\,\mathrm{d}r}{\left(m_i^2-m_j^2\right)\left[1+\frac{k_j^2r^2}{\nu^2}\right]^{1/2}}, \end{aligned} \tag{4.7.25}$$

The integrals over λ can then be done:

$$\int_{m_i}^\infty \left(k_i^2-m_i^2\right)^{-s}\frac{\mathrm{d}}{\mathrm{d}k_i}\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{-1/2} = \frac{1}{\sqrt{\pi}}\frac{s\,\Gamma(-s)\,\Gamma\left(s+\frac{1}{2}\right)}{\left[1+\frac{m_i^2r^2}{\nu^2}\right]^{s+\frac{1}{2}}}\left(\frac{r}{\nu}\right)^{2s}, \tag{4.7.26a}$$

$$\int_{m_i}^\infty \left(k_i^2-m_i^2\right)^{-s}\frac{\mathrm{d}}{\mathrm{d}k_i}\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{-3/2} = \frac{2}{\sqrt{\pi}}\frac{s\,\Gamma(-s)\,\Gamma\left(s+\frac{3}{2}\right)}{\left[1+\frac{m_i^2r^2}{\nu^2}\right]^{s+\frac{3}{2}}}\left(\frac{r}{\nu}\right)^{2s}, \tag{4.7.26b}$$

$$\int_{m_i}^\infty \left(k_i^2-m_i^2\right)^{-s}\frac{\mathrm{d}}{\mathrm{d}k_i}\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{-5/2} = \frac{4}{3\sqrt{\pi}}\frac{s\,\Gamma(-s)\,\Gamma\left(s+\frac{5}{2}\right)}{\left[1+\frac{m_i^2r^2}{\nu^2}\right]^{s+\frac{5}{2}}}\left(\frac{r}{\nu}\right)^{2s}, \tag{4.7.26c}$$

$$\int_{m_i}^\infty \left(k_i^2-m_i^2\right)^{-s}\frac{\mathrm{d}}{\mathrm{d}k_i}\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{-7/2} = \frac{8}{15\sqrt{\pi}}\frac{s\,\Gamma(-s)\,\Gamma\left(s+\frac{7}{2}\right)}{\left[1+\frac{m_i^2r^2}{\nu^2}\right]^{s+\frac{7}{2}}}\left(\frac{r}{\nu}\right)^{2s}. \tag{4.7.26d}$$

The resulting expression for $\zeta_{\text{asymp}}(s)$ is

$$\begin{aligned}
\zeta_{\text{asymp}}(s) &= \sum_{l=0}^{\infty} \deg(d,l)\, \frac{\sin(\pi s)}{\pi} \int_0^{\infty} \lambda^{-s} \frac{\mathrm{d}}{\mathrm{d}\lambda} \operatorname{tr}\big[\ln\big(F_l^{\text{asymp}}(-\lambda)\big)\big]\, \mathrm{d}\lambda \\
&= \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+\frac{1}{2}\Big)}{2\pi^{3/2}} \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+1}} \sum_{i=1}^{n} \int_0^{\infty} \frac{V_{ii}(r)\, r^{2s+1}\, \mathrm{d}r}{\Big[1+\frac{m_i^2 r^2}{\nu^2}\Big]^{s+\frac{1}{2}}} \\
&+ \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+\frac{3}{2}\Big)}{8\pi^{3/2}} \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+3}} \sum_{i=1}^{n} \int_0^{\infty} \frac{V_{ii}(r)\, r^{2s+1}\, \mathrm{d}r}{\Big[1+\frac{m_i^2 r^2}{\nu^2}\Big]^{s+\frac{3}{2}}} \\
&- \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+\frac{5}{2}\Big)}{2\pi^{3/2}} \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+3}} \sum_{i=1}^{n} \int_0^{\infty} \frac{V_{ii}(r)\, r^{2s+1}\, \mathrm{d}r}{\Big[1+\frac{m_i^2 r^2}{\nu^2}\Big]^{s+\frac{5}{2}}} \\
&+ \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+\frac{7}{2}\Big)}{6\pi^{3/2}} \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+3}} \sum_{i=1}^{n} \int_0^{\infty} \frac{V_{ii}(r)\, r^{2s+1}\, \mathrm{d}r}{\Big[1+\frac{m_i^2 r^2}{\nu^2}\Big]^{s+\frac{7}{2}}} \\
&- \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+\frac{3}{2}\Big)}{4\pi^{3/2}} \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+3}} \sum_{(i,j)\in\sigma} \int_0^{\infty} \frac{|V_{ij}(r)|^2 r^{2s+3}\, \mathrm{d}r}{\Big[1+\frac{m_i^2 r^2}{\nu^2}\Big]^{s+\frac{3}{2}}} \\
&- \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+\frac{1}{2}\Big)}{2\pi^{3/2}} \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+1}} \sum_{(i,j)\in\bar{\sigma}} \int_0^{\infty} \frac{|V_{ij}(r)|^2 r^{2s+1}\, \mathrm{d}r}{\Big(m_i^2-m_j^2\Big)\Big[1+\frac{m_j^2 r^2}{\nu^2}\Big]^{s+\frac{1}{2}}}
\end{aligned} \tag{4.7.27}$$

Taking s to be sufficiently large so that the sums converge we can interchange the order of summation and integration. We do this in a similar fashion as how we have regulated the convergent part of the zeta function, by simultaneously adding and subtracting the large l behavior. It is convenient to first introduce some notation:

$$\Sigma_i^{N,p}(s,r) \equiv \sum_{l=0}^{\infty} \frac{\deg(d,l)}{\nu^{2s+2N+1}} \left[1+\frac{m_i^2 r^2}{\nu^2}\right]^{-s-p-\frac{1}{2}}, \tag{4.7.28}$$

$$A_p(s,r) \equiv \frac{\sin(\pi s) s\, \Gamma(-s)\, \Gamma\Big(s+p+\frac{1}{2}\Big)}{\pi^{3/2}} r^{2s}. \tag{4.7.29}$$

Contained in these functions is all of the s dependence of the asymptotic zeta function. The asymptotic zeta function can then be written in a slightly more compact form:

$$\begin{aligned}
\zeta_{\text{asymp}}(s) = &\frac{1}{2}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\,A_0(s,r)\,\Sigma_i^{0,0}(s,r)\,r\,\mathrm{d}r \\
&+\frac{1}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\,A_1(s,r)\,\Sigma_i^{1,1}(s,r)\,r\,\mathrm{d}r \\
&-\frac{1}{2}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\,A_2(s,r)\,\Sigma_i^{1,2}(s,r)\,r\,\mathrm{d}r \\
&+\frac{1}{6}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\,A_3(s,r)\,\Sigma_i^{1,3}(s,r)\,r\,\mathrm{d}r \\
&-\frac{1}{4}\sum_{(i,j)\in\sigma}\int_0^\infty |V_{ij}(r)|^2\,A_1(s,r)\,\Sigma_i^{1,1}(s,r)\,r^3\,\mathrm{d}r \\
&+\frac{1}{2}\sum_{(i,j)\in\bar{\sigma}}\int_0^\infty \frac{|V_{ij}(r)|^2}{m_i^2-m_j^2}\,A_0(s,r)\,\Sigma_i^{0,0}(s,r)\,r\,\mathrm{d}r\,.
\end{aligned} \tag{4.7.30}$$

Renormalizing the sum over l will depend on the dimension d, which we do by explicitly setting $d = 2, 3, 4$:

$\underline{d = 2}$:

The degeneracy factor is 1 if $l = 0$ and 2 if $l > 0$ and the order parameter $\nu = l$. When subtracting the asymptotic expansion of the Jost matrix function we do not include the $l = 0$ term, essentially setting $F_0^{\text{asymp}}(-\lambda) = \mathbb{1}$. Only the $N = p = 0$ sum needs to be

analytically continued.

$$\Sigma_i^{0,0}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+1}} \left[\left(1 + \frac{m_i^2 r^2}{l^2} \right)^{-s-\frac{1}{2}} - 1 \right] + 2\,\zeta_{\mathrm{R}}\left(2s+1\right), \tag{4.7.31a}$$

$$\Sigma_i^{1,1}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+3}} \left[1 + \frac{m_i^2 r^2}{l^2} \right]^{-s-\frac{3}{2}}, \tag{4.7.31b}$$

$$\Sigma_i^{1,2}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+3}} \left[1 + \frac{m_i^2 r^2}{l^2} \right]^{-s-\frac{5}{2}}, \tag{4.7.31c}$$

$$\Sigma_i^{1,3}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+3}} \left[1 + \frac{m_i^2 r^2}{l^2} \right]^{-s-\frac{7}{2}}. \tag{4.7.31d}$$

<u>$d = 3$:</u>

The degeneracy factor is $2l+1$ and the order parameter $\nu = l + \frac{1}{2}$. Again, we only need to analytically continue the $N = p = 0$ sum.

$$\Sigma_i^{0,0}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+1}} \left[\left(1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right)^{-s-\frac{1}{2}} - 1 \right] + 2\Big(2^{2s}-1\Big)\,\zeta_{\mathrm{R}}\left(2s\right), \tag{4.7.32a}$$

$$\Sigma_i^{1,1}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+3}} \left[1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right]^{-s-\frac{3}{2}}, \tag{4.7.32b}$$

$$\Sigma_i^{1,2}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+3}} \left[1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right]^{-s-\frac{5}{2}}, \tag{4.7.32c}$$

$$\Sigma_i^{1,3}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+3}} \left[1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right]^{-s-\frac{7}{2}}. \tag{4.7.32d}$$

<u>$d = 4$:</u>

The degeneracy factor is $(l+1)^2$ and the order parameter $\nu = l + 1$. In this case every

sum needs to be analytically continued. There will be a great deal of cancellation in the end though.

$$\Sigma_i^{0,0}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+1}} \left[\left(1 + \frac{m_i^2 r^2}{(l+1)^2}\right)^{-s-\frac{1}{2}} - 1 + \left(s+\tfrac{1}{2}\right) \frac{m_i^2 r^2}{(l+1)^2} \right] \tag{4.7.33a}$$

$$+ \zeta_{\mathrm{R}}(2s-1) - \left(s+\tfrac{1}{2}\right) m_i^2 r^2 \, \zeta_{\mathrm{R}}(2s+1),$$

$$\Sigma_i^{1,1}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+3}} \left[\left(1 + \frac{m_i^2 r^2}{\nu^2}\right)^{-s-\frac{3}{2}} - 1 \right] + \zeta_{\mathrm{R}}(2s+1), \tag{4.7.33b}$$

$$\Sigma_i^{1,2}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+3}} \left[\left(1 + \frac{m_i^2 r^2}{\nu^2}\right)^{-s-\frac{5}{2}} - 1 \right] + \zeta_{\mathrm{R}}(2s+1), \tag{4.7.33c}$$

$$\Sigma_i^{1,3}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+3}} \left[\left(1 + \frac{m_i^2 r^2}{\nu^2}\right)^{-s-\frac{7}{2}} - 1 \right] + \zeta_{\mathrm{R}}(2s+1). \tag{4.7.33d}$$

The remaining sums over l are all convergent and finite as $s \to 0$ for all $d \leq 4$.

The prefactor term has the asymptotic behavior

$$A_p(s,r) \sim -\frac{\Gamma\left(p+\frac{1}{2}\right)}{\sqrt{\pi}} s, \quad (s \to 0). \tag{4.7.34}$$

Therefore, it is sufficient set $s = 0$ everywhere in $\Sigma_i^{N,p}(s,r)$ except the terms containing factors of $\zeta_{\mathrm{R}}(2s+1)$, because this Riemann zeta function has a pole as $s \to 0$:

$$\zeta_{\mathrm{R}}(2s+1) \sim \frac{1}{2s} + \gamma, \quad (s \to 0). \tag{4.7.35}$$

It is convenient to factor off this pole term with

$$\Sigma_i^{N,p}(s,r) = \Sigma_{\mathrm{pole},i}^{N,p}(s,r) + \Sigma_{\mathrm{f},i}^{N,p}(s,r). \tag{4.7.36}$$

The factored sums are then given by

$\underline{d=2}$:

$$\Sigma_{\mathrm{pole},i}^{0,0}(s,r) = \frac{1}{s}, \qquad \Sigma_{\mathrm{pole},i}^{1,1}(s,r) = \Sigma_{\mathrm{pole},i}^{1,2}(s,r) = \Sigma_{\mathrm{pole},i}^{1,3}(s,r) = 0, \tag{4.7.37}$$

$$\Sigma^{0,0}_{\mathrm{f},i}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+1}} \left[\left(1 + \frac{m_i^2 r^2}{l^2} \right)^{-s-\frac{1}{2}} - 1 \right] + 2\,\zeta_{\mathrm{R}}\left(2s+1\right) - \frac{1}{s}, \tag{4.7.38a}$$

$$\Sigma^{1,1}_{\mathrm{f},i}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+3}} \left[1 + \frac{m_i^2 r^2}{l^2} \right]^{-s-\frac{3}{2}}, \tag{4.7.38b}$$

$$\Sigma^{1,2}_{\mathrm{f},i}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+3}} \left[1 + \frac{m_i^2 r^2}{l^2} \right]^{-s-\frac{5}{2}}, \tag{4.7.38c}$$

$$\Sigma^{1,3}_{\mathrm{f},i}(s,r) = \sum_{l=1}^{\infty} \frac{2}{l^{2s+3}} \left[1 + \frac{m_i^2 r^2}{l^2} \right]^{-s-\frac{7}{2}}. \tag{4.7.38d}$$

$\underline{d=3}$:

$$\Sigma^{0,0}_{\mathrm{pole},i}(s,r) = \Sigma^{1,1}_{\mathrm{pole},i}(s,r) = \Sigma^{1,2}_{\mathrm{pole},i}(s,r) = \Sigma^{1,3}_{\mathrm{pole},i}(s,r) = 0, \tag{4.7.39}$$

$$\Sigma^{0,0}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+1}} \left[\left(1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right)^{-s-\frac{1}{2}} - 1 \right] + 2\Big(2^{2s}-1\Big)\,\zeta_{\mathrm{R}}\left(2s\right), \tag{4.7.40a}$$

$$\Sigma^{1,1}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+3}} \left[1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right]^{-s-\frac{3}{2}}, \tag{4.7.40b}$$

$$\Sigma^{1,2}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+3}} \left[1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right]^{-s-\frac{5}{2}}, \tag{4.7.40c}$$

$$\Sigma^{1,3}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{2l+1}{\left(l+\frac{1}{2}\right)^{2s+3}} \left[1 + \frac{m_i^2 r^2}{\left(l+\frac{1}{2}\right)^2} \right]^{-s-\frac{7}{2}}. \tag{4.7.40d}$$

$\underline{d=4}$:

$$\Sigma^{0,0}_{\mathrm{pole},i}(s,r) = -\frac{m_i^2 r^2}{4s}, \qquad \Sigma^{1,1}_{\mathrm{pole},i}(s,r) = \Sigma^{1,2}_{\mathrm{pole},i}(s,r) = \Sigma^{1,3}_{\mathrm{pole},i}(s,r) = \frac{1}{2s}, \tag{4.7.41}$$

$$\Sigma^{0,0}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+1}} \left[\left(1 + \frac{m_i^2 r^2}{(l+1)^2}\right)^{-s-\frac{1}{2}} - 1 + \left(s+\tfrac{1}{2}\right) + \frac{m_i^2 r^2}{(l+1)^2} \right] \tag{4.7.42a}$$

$$+ \zeta_{\mathrm{R}}(2s-1) - \left(s+\tfrac{1}{2}\right) m_i^2 r^2\, \zeta_{\mathrm{R}}(2s+1) + \frac{m_i^2 r^2}{4s},$$

$$\Sigma^{1,1}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+3}} \left[\left(1 + \frac{m_i^2 r^2}{\nu^2}\right)^{-s-\frac{3}{2}} - 1 \right] + \zeta_{\mathrm{R}}(2s+1) - \frac{1}{2s}, \tag{4.7.42b}$$

$$\Sigma^{1,2}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+3}} \left[\left(1 + \frac{m_i^2 r^2}{\nu^2}\right)^{-s-\frac{5}{2}} - 1 \right] + \zeta_{\mathrm{R}}(2s+1) - \frac{1}{2s}, \tag{4.7.42c}$$

$$\Sigma^{1,3}_{\mathrm{f},i}(s,r) = \sum_{l=0}^{\infty} \frac{(l+1)^2}{(l+1)^{2s+3}} \left[\left(1 + \frac{m_i^2 r^2}{\nu^2}\right)^{-s-\frac{7}{2}} - 1 \right] + \zeta_{\mathrm{R}}(2s+1) - \frac{1}{2s}. \tag{4.7.42d}$$

By construction, the sum over l in $\zeta_{\mathrm{finite}}(s)$ converges for $s = 0$. Because of the $\sin(\pi s)$ prefactor we then have $\zeta_{\mathrm{finite}}(0) = 0$. The contribution to the renormalized zeta function then comes entirely from $\zeta_{\mathrm{asymp}}(0)$, which itself comes only from the pole terms. Expanding the prefactor to one higher order

$$A_p(s,r) \sim -\frac{\Gamma\left(p+\frac{1}{2}\right) s}{\sqrt{\pi}} \left[1 + \left(\ln\left(r^2\right) + H_{p-\frac{1}{2}}\right) s\right], \quad (s \to 0), \tag{4.7.43}$$

where H_N is the N^{th} *harmonic number*. We then have

$$A_p(r,s)\, \Sigma^{N,p}_{\mathrm{f},i}(r,s) \sim -\frac{\Gamma\left(p+\frac{1}{2}\right)}{\sqrt{\pi}} s\, \Sigma^{N,p}_{\mathrm{f},i}(r,0), \quad (s \to 0). \tag{4.7.44}$$

This holds in any dimension d.

Next we calculate the pole terms for $d = 2, 3, 4$:

$\underline{d=2}$:

$$A_0(s,r)\,\Sigma^{0,0}_{\text{pole},i}(s,r) \sim -1 - 2\ln\left(\frac{r}{2}\right)s, \qquad (s\to 0), \tag{4.7.45a}$$

$$A_1(s,r)\,\Sigma^{1,1}_{\text{pole},i}(s,r) = 0, \tag{4.7.45b}$$

$$A_2(s,r)\,\Sigma^{1,2}_{\text{pole},i}(s,r) = 0, \tag{4.7.45c}$$

$$A_3(s,r)\,\Sigma^{1,3}_{\text{pole},i}(s,r) = 0. \tag{4.7.45d}$$

$\underline{d=3}$:

$$A_p(s,r)\,\Sigma^{N,p}_{\text{pole},i}(s,r) = 0. \tag{4.7.46}$$

$\underline{d=4}$:

$$A_0(s,r)\,\Sigma^{0,0}_{\text{pole},i}(s,r) \sim \frac{m_i^2 r^2}{4}\left[1 + 2\ln\left(\frac{r}{2}\right)s\right], \tag{4.7.47a}$$

$$A_1(s,r)\,\Sigma^{1,1}_{\text{pole},i}(s,r) \sim -\frac{1}{4}\left[1 + 2\left(\ln\left(\frac{r}{2}\right) + 1\right)s\right], \tag{4.7.47b}$$

$$A_2(s,r)\,\Sigma^{1,2}_{\text{pole},i}(s,r) \sim -\frac{3}{8}\left[1 + 2\left(\ln\left(\frac{r}{2}\right) + \frac{4}{3}\right)s\right], \tag{4.7.47c}$$

$$A_3(s,r)\,\Sigma^{1,3}_{\text{pole},i}(s,r) \sim -\frac{15}{16}\left[1 + 2\left(\ln\left(\frac{r}{2}\right) + \frac{23}{15}\right)s\right], \tag{4.7.47d}$$

Finally, for $d = 2, 3, 4$ we substitute the small s asymptotic behavior of $A_p(s,r)\,\Sigma_i^{N,p}(s,r)$ into (4.7.30).

$\underline{d=2}$:

$$\begin{aligned}
\zeta_{\text{asymp}}(s) \sim & -\frac{1}{2}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\, r\,\mathrm{d}r - s\sum_{i=1}^{\infty}\int_0^\infty V_{ii}(r)\left[\gamma+\ln\left(\frac{r}{2}\right)\right] r\,\mathrm{d}r \\
& - s\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=1}^{\infty}\frac{1}{l}\left[\left(1+\frac{m_i^2r^2}{l^2}\right)^{-\frac{1}{2}}-1\right] r\,\mathrm{d}r \\
& - \frac{s}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=1}^{\infty}\frac{1}{l^3}\left[1+\frac{m_i^2r^2}{l^2}\right]^{-\frac{3}{2}} r\,\mathrm{d}r \\
& + \frac{3s}{4}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=1}^{\infty}\frac{1}{l^3}\left[1+\frac{m_i^2r^2}{l^2}\right]^{-\frac{5}{2}} r\,\mathrm{d}r \\
& - \frac{5s}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=1}^{\infty}\frac{1}{l^3}\left[1+\frac{m_i^2r^2}{l^2}\right]^{-\frac{7}{2}} r\,\mathrm{d}r \\
& + \frac{s}{4}\sum_{(i,j)\in\sigma}\int_0^\infty |V_{ij}(r)|^2\sum_{l=1}^{\infty}\frac{1}{l^3}\left[1+\frac{m_i^2r^2}{l^2}\right]^{-\frac{3}{2}} r^3\,\mathrm{d}r \\
& - s\sum_{(i,j)\in\bar{\sigma}}\int_0^\infty \frac{|V_{ij}(r)|^2}{m_i^2-m_j^2}\sum_{l=1}^{\infty}\frac{1}{l}\left[\left(1+\frac{m_i^2r^2}{l^2}\right)^{-\frac{1}{2}}-1\right] r\,\mathrm{d}r\,.
\end{aligned} \tag{4.7.48}$$

$\underline{d=3}$:

$$\begin{aligned}
\zeta_{\text{asymp}}(s) \sim & -s\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\left[\left(1+\frac{m_i^2r^2}{\left(l+\frac{1}{2}\right)^2}\right)^{-\frac{1}{2}}-1\right]r\,\mathrm{d}r \\
& -\frac{s}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\frac{1}{\left(l+\frac{1}{2}\right)^2}\left[1+\frac{m_i^2r^2}{\left(l+\frac{1}{2}\right)^2}\right]^{-\frac{3}{2}}r\,\mathrm{d}r \\
& +\frac{3s}{4}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\frac{1}{\left(l+\frac{1}{2}\right)^2}\left[1+\frac{m_i^2r^2}{\left(l+\frac{1}{2}\right)^2}\right]^{-\frac{5}{2}}r\,\mathrm{d}r \\
& -\frac{5s}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\frac{1}{\left(l+\frac{1}{2}\right)^2}\left[1+\frac{m_i^2r^2}{\left(l+\frac{1}{2}\right)^2}\right]^{-\frac{7}{2}}r\,\mathrm{d}r \\
& +\frac{s}{4}\sum_{(i,j)\in\sigma}\int_0^\infty |V_{ij}(r)|^2\sum_{l=0}^{\infty}\frac{1}{\left(l+\frac{1}{2}\right)^2}\left[1+\frac{m_i^2r^2}{\left(l+\frac{1}{2}\right)^2}\right]^{-\frac{3}{2}}r^3\,\mathrm{d}r \\
& -s\sum_{(i,j)\in\bar{\sigma}}\int_0^\infty \frac{|V_{ij}(r)|^2}{m_i^2-m_j^2}\sum_{l=0}^{\infty}\left[\left(1+\frac{m_i^2r^2}{\left(l+\frac{1}{2}\right)^2}\right)^{-\frac{1}{2}}-1\right]r\,\mathrm{d}r\,.
\end{aligned} \tag{4.7.49}$$

$\underline{d=4}$:

$$\begin{aligned}
\zeta_{\text{asymp}}(s) \sim{}& \frac{1}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\, m_i^2 r^3\,\mathrm{d}r + \frac{1}{16}\sum_{i,j=1}^{n}\int^\infty |V_{ij}(r)|^2 r^3\,\mathrm{d}r \\
&+ \frac{s}{4}\sum_{i=1}^{\infty}\int_0^\infty V_{ii}(r)\, m_i^2\left[1+\gamma+\ln\left(\frac{r}{2}\right)\right] r^3\,\mathrm{d}r \\
&+ \frac{s}{8}\sum_{i,j=1}^{n}\int_0^\infty |V_{ij}(r)|^2\left[1+\gamma+\ln\left(\frac{r}{2}\right)\right] r^3\,\mathrm{d}r\,, \\
&- \frac{s}{2}\sum_{i=1}^{\infty}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}(l+1)\left[\left(1+\frac{m_i^2 r^2}{(l+1)^2}\right)^{-\frac{1}{2}} - 1 + \frac{m_i^2 r^2}{2(l+1)^2}\right] r\,\mathrm{d}r \\
&- \frac{s}{16}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\frac{1}{l+1}\left[\left(1+\frac{m_i^2 r^2}{(l+1)^2}\right)^{-\frac{3}{2}} - 1\right] r\,\mathrm{d}r \\
&+ \frac{3s}{8}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\frac{1}{l+1}\left[\left(1+\frac{m_i^2 r^2}{(l+1)^2}\right)^{-\frac{5}{2}} - 1\right] r\,\mathrm{d}r \\
&- \frac{5s}{16}\sum_{i=1}^{n}\int_0^\infty V_{ii}(r)\sum_{l=0}^{\infty}\frac{1}{l+1}\left[\left(1+\frac{m_i^2 r^2}{(l+1)^2}\right)^{-\frac{7}{2}} - 1\right] r\,\mathrm{d}r \\
&+ \frac{s}{8}\sum_{(i,j)\in\sigma}\int_0^\infty |V_{ij}(r)|^2\sum_{l=0}^{\infty}\frac{1}{l+1}\left[\left(1+\frac{m_i^2 r^2}{(l+1)^2}\right)^{-\frac{3}{2}} - 1\right] r^3\,\mathrm{d}r \\
&- \frac{s}{2}\sum_{(i,j)\in\bar{\sigma}}\int_0^\infty \frac{|V_{ij}(r)|^2}{m_i^2-m_j^2}\sum_{l=0}^{\infty}(l+1)\left[\left(1+\frac{m_i^2 r^2}{(l+1)^2}\right)^{-\frac{1}{2}} - 1 + \frac{m_i^2 r^2}{2(l+1)^2}\right] r\,\mathrm{d}r
\end{aligned} \tag{4.7.50}$$

We then have the results

$$\zeta(0|\tau) - \zeta\Big(0|\tau^{\text{free}}\Big)\Big|_{d=2} = -\frac{1}{2}\int_0^\infty \mathrm{tr}[V(r)] r\,\mathrm{d}r\,, \tag{4.7.51}$$

$$\zeta(0|\tau) - \zeta\Big(0|\tau^{\text{free}}\Big)\Big|_{d=3} = 0, \tag{4.7.52}$$

$$\zeta(0|\tau) - \zeta\Big(0|\tau^{\text{free}}\Big)\Big|_{d=4} = \frac{1}{16}\int_0^\infty \mathrm{tr}\Big[V^2(r) + 2\,V(r)\,M^2\Big] r^3\,\mathrm{d}r\,. \tag{4.7.53}$$

The derivatives are also easily calculated. We first note that because $\zeta_{\text{finite}}(s)$ is regular at $s = 0$ we immediately have

$$\begin{aligned}\zeta'_{\text{finite}}(0) &= \sum_{l=0}^{\infty} \deg(d,l) \int_0^{\infty} \frac{\mathrm{d}}{\mathrm{d}\lambda} \operatorname{tr}\big[\ln(F_l(-\lambda)) - \ln\big(F_l^{\text{asymp}}(-\lambda)\big)\big]\, \mathrm{d}\lambda \\ &= -\sum_{l=0}^{\infty} \deg(d,l) \operatorname{tr}\big[\ln(F_l(0)) - \ln\big(F_l^{\text{asymp}}(0)\big)\big].\end{aligned} \tag{4.7.54}$$

We then see that, in $\zeta'_{\text{finite}}(0)$, every term coming from $\operatorname{tr}\big[\ln\big(F_l^{\text{asymp}}(0)\big)\big]$ cancels with an identical term in $\zeta'_{\text{asymp}}(0)$. After cancelling all of these terms we have the result for the derivative of the zeta functions:

$\underline{d = 2}$:

$$\begin{aligned}\zeta'(0|\tau) - \zeta'\Big(0|\tau^{\text{free}}\Big) = &- \operatorname{tr}[\ln(F_0(0))] - 2\sum_{l=1}^{\infty} \operatorname{tr}\bigg[\ln(F_l(0)) - \frac{1}{2l}\int_0^{\infty} V(r)\, r\, \mathrm{d}r\bigg] \\ &- \int_0^{\infty} \operatorname{tr}[V(r)]\bigg[\gamma + \ln\Big(\frac{r}{2}\Big)\bigg] r\, \mathrm{d}r\,.\end{aligned} \tag{4.7.55}$$

$\underline{d = 3}$:

$$\zeta'(0|\tau) - \zeta'\Big(0|\tau^{\text{free}}\Big) = -\sum_{l=0}^{\infty} (2l+1) \operatorname{tr}\left[\ln(F_l(0)) - \frac{1}{2\Big(l+\frac{1}{2}\Big)}\int_0^{\infty} V(r)\, r\, \mathrm{d}r\right]. \tag{4.7.56}$$

$\underline{d = 4}$:

$$\begin{aligned}\zeta'(0|\tau) - \zeta'\Big(0|\tau^{\text{free}}\Big) = -\sum_{l=0}^{\infty} (l+1)^2 \operatorname{tr}\bigg[&\ln(F_l(0)) - \frac{1}{2(l+1)}\int_0^{\infty} V(r)\, r\, \mathrm{d}r \\ &+ \frac{1}{8(l+1)^3}\int_0^{\infty} V(r)\Big[V(r) + 2M^2\Big] r^3\, \mathrm{d}r\bigg] \\ &+ \frac{1}{8}\int_0^{\infty} \operatorname{tr}\Big[V^2(r) + M^2\, V(r)\Big]\bigg[1 + \gamma + \ln\Big(\frac{r}{2}\Big)\bigg] r^3\, \mathrm{d}r\,.\end{aligned} \tag{4.7.57}$$

Finally, combining the above expressions with the renormalization involving $\zeta_{\text{asymp}}(0)$ yields the results in Theorem 4.1.1. We also note that since

$$F_l(z) = \lim_{r\to\infty} \Big[U_{0,l}^{\text{free}}(r;z)\Big]^{-1} U_{0,l}(r;z)\,,$$

we can just as easily define

$$T_l(r;z) \equiv \left[U_{0,l}^{\text{free}}(r;z)\right]^{-1} U_{0,l}(r;z)\,, \tag{4.7.58}$$

and then have

$$F_l(z) = \lim_{r\to\infty} T_l(r;z)\,. \tag{4.7.59}$$

Setting $z = 0$, it is not difficult to show that this matrix function $T_l(r)$ obeys (4.1.18). Because both $U_{0,l}^{\text{free}}(r)$ and $U_{0,l}(r)$ grow exponentially fast as $r \to \infty$, it is better to numerically solve for $T_l(r)$, rather than the principal solutions $U_{0,l}(r)$. The proof of Theorem 4.1.1 is now complete.

4.8 Zero Modes

In many physical applications the functional determinant contains zero modes. Specifically, for some angular momentum quantum number the unregulated functional determinant

$$\frac{\det(\tau_l)}{\det(\tau_l^{\text{free}})} = 0.$$

For instance, in vacuum-to-vacuum transition amplitude calculations such as bubble nucleation rates, sphaleron rates, and instanton tunnelling amplitudes, zero modes occur due to the background field configuration breaking translation invariance. These zero modes are not eigenvalues of the Hamiltonian of the quantum system, instead they are artifacts that result from fixing the coordinate system when solving for the background configuration. When expanding the classical action around a soliton or soliton-like background configuration we typically choose the soliton to be centered at the origin. In the

path integral formulation of QFT however, we are instructed to (functionally) integrate over all field configurations, so we must also integrate over the collective coordinates that defines the center of soliton. This integration over collective coordinates results in a prefactor in the transition rate proportional to some power of the classical action, and formally removes the zero modes (we have indicated the removal of zero modes in the functional determinant with a prime).

A naive application of our Gel'fand-Yaglom formula still results in zero modes for the above mentioned scenarios, because constructing the matrix potential $V(r)$ necessarily involves fixing the center of the soliton-like background configuration. We therefore must remove these zero modes by hand, and we devote this section to developing a general procedure for doing so in arbitrary dimensions d and coupled equations n.

First, we note that for the case being considered the manifold $\mathcal{M} = \mathbb{R}^d$, and the degeneracy of the $l = 1$ partial wave is

$$\deg(1, d) = \begin{cases} 0 & d = 1 \\ d & d > 1 \end{cases}. \tag{4.8.1}$$

With the exception of the $d = 1$ case (where exact analytic results can be determined anyways) the degeneracy of the partial wave components exactly matches the number of broken symmetries of a soliton-like background (d broken symmetries from broken translation invariance in d dimensions). Therefore, in most cases the $l = 1$ partial wave component of the functional determinant saturates the number of broken symmetries. Translated into our Gel'fand-Yaglom formalism this corresponds to the Jost matrix function

$$F_l(0) = \lim_{R\to\infty} T_l(R)$$

having one, and only one, column of zeros in some basis. In this case it is obvious that shifting the differential operator by some small factor k^2 results in

$$\frac{\det\left(\tau_l + k^2\right)}{\det\left(\tau_l^{\text{free}} + k^2\right)} \sim k^2 \frac{\det'(\tau_l)}{\det\left(\tau_l^{\text{free}}\right)}, \quad \Big(k^2 \to 0\Big). \tag{4.8.2}$$

This simply shifts the eigenvalue of the zero mode to $-k^2$. If more than one zero mode exists in the l^{th} partial wave component than one simply expands around small k^2 until a nonvanishing term is found. For us, we will assume there is only one zero mode (multiplied by the degeneracy factor of the l^{th} partial wave). Taylor expanding our Gel'fand-Yaglom formula around small k^2 then yields

$$\frac{\det\left(\tau_l + k^2\right)}{\det\left(\tau_l^{\text{free}} + k^2\right)} \sim \lim_{R\to\infty} \det(T_l(R)) + k^2 \frac{\mathrm{d}}{\mathrm{d}k^2} \det\Big(T_l\Big(R; -k^2\Big)\Big)\Big|_{k^2\to 0}, \quad \Big(k^2 \to 0\Big). \tag{4.8.3}$$

We can then use Jacobi's formula for the derivative of a finite dimensional determinant

$$\frac{\mathrm{d}}{\mathrm{d}t} \det(A(t)) = \mathrm{tr}\Big[\mathrm{adj}(A(t)) \frac{\mathrm{d}\,A(t)}{\mathrm{d}t}\Big], \tag{4.8.4}$$

and the definition of the matrix function $T_l(r; z)$,

$$T_l(r; z) = \Big[U_{0,l}^{\text{free}}(r; z)\Big]^{-1} U_{0,l}(r; z)\,,$$

to write the asymptotic behavior of the zero mode determinant as

$$\frac{\det\left(\tau_l + k^2\right)}{\det\left(\tau_l^{\text{free}} + k^2\right)} \sim \lim_{R\to\infty} k^2 \frac{1}{\det\Big(U_{0,l}^{\text{free}}(R)\Big)} \times \mathrm{tr}\Big[\mathrm{adj}(U_{0,l}(R)) \frac{\mathrm{d}}{\mathrm{d}k^2} U_{0,l}\Big(R; -k^2\Big)\Big]\Big|_{k^2=0}, \quad \Big(k^2 \to 0\Big). \tag{4.8.5}$$

Here, $\mathrm{adj}(M)$ is the adjugate matrix of the matrix M and we have ignored the derivatives of $U_{0,l}^{\text{free}}(R; -k^2)$ because they vanish. We then use a Volterra integral representation of

the interacting solutions to expand around small k^2:

$$U_{0,l}\Big(r;-k^2\Big) = U_{0,l}(r) \\ \times\left[\mathbb{1} + k^2\int_0^r\int_t^r \Big[U_{0,l}^\dagger(s)\,U_{0,l}(s)\Big]^{-1} U_{0,l}^\dagger(t)\,U_{0,l}\Big(t;-k^2\Big)\,s^{1-d}t^{d-1}\,\mathrm{d}s\,\mathrm{d}t\right], \quad (4.8.6)$$

which is valid because $U_{0,l}(r)$ is a principal solution near $r=0$ (note that this integral representation of the solution differs from that of (4.3.45), specifically there is no reference to the free solutions or the matrix potential $V(r)$). This can be solved iteratively for small k^2, taking only the leading order and next to leading order terms yields

$$U_{0,l}\Big(r;-k^2\Big) \sim U_{0,l}(r) \\ \times\left[\mathbb{1} + k^2\int_0^r\int_t^r \Big[U_{0,l}^\dagger(s)\,U_{0,l}(s)\Big]^{-1} U_{0,l}^\dagger(t)\,U_{0,l}(t)\,s^{1-d}t^{d-1}\,\mathrm{d}s\,\mathrm{d}t\right], \quad \Big(k^2\to 0\Big). \quad (4.8.7)$$

We can then approximate the determinant ratio for small k^2 as

$$\frac{\det(\tau_l+k^2)}{\det(\tau_l^{\text{free}}+k^2)} \sim \lim_{R\to\infty} k^2 \frac{\det(U_{0,l}(R))}{\det\Big(U_{0,l}^{\text{free}}(R)\Big)} \\ \times \mathrm{tr}\left[\int_0^R\int_t^R \Big[U_{0,l}^\dagger(s)\,U_{0,l}(s)\Big]^{-1} U_{0,l}^\dagger(t)\,U_{0,l}(t)\,s^{1-d}t^{d-1}\,\mathrm{d}s\,\mathrm{d}t\right], \quad \Big(k^2\to 0\Big). \quad (4.8.8)$$

We see that the small k^2 behavior of the determinant ratio is a modified version of the $k^2=0$ determinant ratio. Since we have assumed that this partial wave component has a zero mode, the prefactor term

$$\lim_{R\to\infty}\frac{\det(U_{0,l}(R))}{\det\Big(U_{0,l}^{\text{free}}(R)\Big)} = 0.$$

The trace term in (4.8.8) must then contain a piece that diverges as $R\to\infty$ that balances the decay of the $k^2=0$ determinant ratio. To simplify the integral in (4.8.8) we

use the matrix identities (4.3.31). After a substantial amount of algebra, and dropping terms that vanish, we find

$$\frac{\det(\tau_l + k^2)}{\det(\tau_l^{\text{free}} + k^2)} \sim -k^2 \lim_{R\to\infty} \frac{\operatorname{tr}\Big[\operatorname{adj}(U_{0,l}(R))\, U_{\infty,l}(R) \int_0^R U_{0,l}^\dagger(t)\, U_{0,l}(t)\, t^{d-1}\, \mathrm{d}t\Big]}{\det\Big(U_{0,l}^{\text{free}}(R)\Big)},$$

$$\Big(k^2 \to 0\Big). \quad (4.8.9)$$

In order to proceed we must specify the components of $U_{0,l}(r)$ which satisfy the Friedrichs boundary conditions. We construct a complete set of vector solutions as

$$f_l^{(i)}(r) \coloneqq U_{0,l}(r)\, \zeta_i, \qquad \bar{f}_l^{(i)}(r) \coloneqq U_{\infty,l}(r)\, \zeta_i, \quad (4.8.10)$$

where the ζ_i form a complete basis on $\mathbb{C}^n$. Without loss of generality we can assume that the ζ_i are real and orthonormal:

$$\langle \zeta_i, \zeta_j \rangle = \zeta_i^\dagger \zeta_j = \delta_j^i. \quad (4.8.11)$$

We then further assume that

$$f_l^{(1)}(r) = U_{0,l}(r)\, \zeta_1$$

is the only solution that satisfies the Friedrichs boundary conditions. This solution is easily found by using standard numerical methods to solve the boundary value problem

$$\left[-r^{1-d}\frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} + \frac{l(l+d-2)}{r^2} + M^2 + V(r)\right] f_l^{(1)}(r) = 0. \quad (4.8.12)$$

The unit vector ζ_1 is then determined uniquely by

$$\zeta_1 = \lim_{r\to 0} r^{-l}\, f_l^{(1)}(r)\,. \quad (4.8.13)$$

The remaining ζ_i can then be constructed arbitrarily, with the requirement that $\langle \zeta_i, \zeta_j \rangle = \delta_j^i$.

We then expand the trace term in (4.8.9) in this ζ-basis:

$$\mathrm{tr}\Big[\mathrm{adj}(U_{0,l}(r))\,U_{\infty,l}(r)\int_0^r U_{0,l}^\dagger(t)\,U_{0,l}(t)\,t^{d-1}\,\mathrm{d}t\Big]$$
$$=\sum_{i=1}^n\sum_{j=1}^n \zeta_i^\dagger \mathrm{adj}(U_{0,l}(r))\,U_{\infty,l}(r)\,\zeta_j\int_0^r \zeta_j^\dagger\,U_{0,l}^\dagger(t)\,U_{0,l}(t)\,\zeta_i t^{d-1}\,\mathrm{d}t\,. \quad (4.8.14)$$

This can be rewritten in terms of the vector solutions $f_l^{(i)}(r)$ and $\bar{f}_l^{(i)}(r)$

$$\mathrm{tr}\Big[\mathrm{adj}(U_{0,l}(r))\,U_{\infty,l}(r)\int_0^r U_{0,l}^\dagger(t)\,U_{0,l}(t)\,t^{d-1}\,\mathrm{d}t\Big]$$
$$=\sum_{i=1}^n\sum_{j=1}^n \zeta_i^\dagger \mathrm{adj}(U_{0,l}(r))\,\bar{f}_l^{(j)}(r)\int_0^r f_l^{(j)\dagger}(t)\,f_l^{(i)}(t)\,t^{d-1}\,\mathrm{d}t\,. \quad (4.8.15)$$

Because of the factor of $\det\Big(U_{0,l}^{\mathrm{free}}(R)\Big)$ in the denominator of (4.8.9), which diverges in the limit that $R\to\infty$, we only need to keep the terms that diverge in the large r limit in (4.8.15). The only term in the sum that satisfies this requirement is the $i=j=1$ term, therefore

$$\frac{\det(\tau_l+k^2)}{\det(\tau_l^{\mathrm{free}}+k^2)}\sim -k^2\lim_{R\to\infty}\frac{\zeta_1^\dagger\mathrm{adj}(U_{0,l}(R))\,\bar{f}_l^{(1)}(R)\int_0^R f_l^{(1)\dagger}(t)\,f_l^{(1)}(t)\,t^{d-1}\,\mathrm{d}t}{\det\Big(U_{0,l}^{\mathrm{free}}(R)\Big)},$$
$$\Big(k^2\to 0\Big). \quad (4.8.16)$$

We can further simplify this by introducing a new matrix function $H_l^+(r)$ through

$$H_l^+(r)\,\zeta_1 \coloneqq \bar{f}_l^{(1)}(r)\,,\qquad H_l^+(r)\,\zeta_i \coloneqq f_l^{(i)}(r)\,,\qquad i\neq 1. \quad (4.8.17)$$

This matrix function has a simple interpretation: its columns in the ζ-basis are just the columns of $U_{0,l}(r)$, with the first column replaced by $\bar{f}_l^{(1)}(r)$ (in $U_{0,l}(r)$ the first column in the ζ-basis is the zero mode solution $f_l^{(1)}(r)$). The adjugate term can then be written (this is a simple relationship found from the definition of the adjugate matrix)

$$\zeta_1^\dagger\mathrm{adj}(U_{0,l}(r))\,\bar{f}_l^{(1)}(r)=\det\Big(H_l^+(r)\Big). \quad (4.8.18)$$

The asymptotic behavior of this matrix function is immediately apparent:

$$H_l^+(r) \sim U_{0,l}^{\text{free}}(r)\,\mathbb{H}_l^+, \quad (r \to \infty), \tag{4.8.19}$$

where the constant matrix $\mathbb{H}_l^+$ is guaranteed to be nonsingular, since by assumption the zero mode solution $f_l^{(1)}(r)$ is not contained in $H_l^+(r)$ and the columns of $H_l^+(r)$ are linearly independent. The zero mode determinant ratio has now been simplified substantially to

$$\frac{\det(\tau_l + k^2)}{\det(\tau_l^{\text{free}} + k^2)} \sim -k^2 \lim_{R\to\infty} \frac{\det\Big(H_l^+(R)\Big)}{\det\Big(U_{0,l}^{\text{free}}(R)\Big)} \int_0^R f_l^{(1)\dagger}(t)\, f_l^{(1)}(t)\, t^{d-1}\,\mathrm{d}t\,, \quad \Big(k^2 \to 0\Big). \tag{4.8.20}$$

The determinant ratio with zero modes removed then follows immediately from (4.8.2):

$$\frac{\det'(\tau_l)}{\det(\tau_l^{\text{free}})} = -\det\Big(\mathbb{H}_l^+\Big) \int_0^\infty f_l^{(1)\dagger}(r)\, f_l^{(1)}(r)\, r^{d-1}\,\mathrm{d}r\,. \tag{4.8.21}$$

We still need to determine the constant matrix $\mathbb{H}_l^+$, which fortunately is not difficult given the zero mode solution $f_l^{(1)}(r)$ and the matrix solution $T_l(r)$, which we assume have been determined numerically or by some other means. We begin by constructing an orthogonal matrix Ω from the unit vectors ζ_i:

$$\mathbf{e}_i^\dagger \Omega \mathbf{e}_j = [\zeta_j]_i, \tag{4.8.22}$$

where the $\mathbf{e}_i$ are the standard unit vectors on $\mathbb{R}^n$:

$$[\mathbf{e}_i]_j = \delta_{ij}. \tag{4.8.23}$$

In plain language the columns of Ω in the $\mathbf{e}$-basis are simply the units vectors ζ_i. We

can then write two matrix solutions (written in block diagonal notation)

$$H_l^+(r) = U_{0,l}(r)\,\Omega \begin{pmatrix} 0 & \\ & \mathbb{1} \end{pmatrix} \Omega^\intercal + U_{\infty,l}(r)\,\Omega \begin{pmatrix} 1 & \\ & \mathbb{0} \end{pmatrix} \Omega^\intercal, \tag{4.8.24a}$$

$$H_l^-(r) = U_{0,l}(r)\,\Omega \begin{pmatrix} 1 & \\ & \mathbb{0} \end{pmatrix} \Omega^\intercal + U_{\infty,l}(r)\,\Omega \begin{pmatrix} 0 & \\ & \mathbb{1} \end{pmatrix} \Omega^\intercal, \tag{4.8.24b}$$

where $H_l^+(r)$ is the same matrix function we have already introduced.

Theorem 4.8.1. *The large r asymptotic behavior of the matrix solutions $H_l^+(r)$ and $H_l^-(r)$ is given by*

$$H_l^+(r) \sim U_{0,l}^{\text{free}}(r)\,\mathbb{H}_l^+, \qquad (r \to \infty), \tag{4.8.25}$$

$$H_l^-(r) \sim U_{\infty,l}^{\text{free}}(r)\,\mathbb{H}_l^-, \qquad (r \to \infty), \tag{4.8.26}$$

for some nonsingular matrices $\mathbb{H}_l^+$ and $\mathbb{H}_l^-$.

Proof. From (4.3.31) we have

$$\zeta_i^\dagger \{Y_{\infty,l}, Y_{0,l}\} \zeta_j = r^{d-1} \left[\frac{\partial f^{(i)\dagger}}{\partial r} \bar{f}_l^{(j)} - f_l^{(i)\dagger} \frac{\partial \bar{f}^{(j)}}{\partial r} \right] = \delta_{ij}. \tag{4.8.27}$$

For $i \neq 1$ the vector solutions $f_l^{(i)}(r)$ are regular at $r = 0$, but cannot be square integrable, since by assumption $f_l^{(1)}(r)$ is the only zero mode. These solutions must then have the asymptotic behavior

$$f_l^{(i)}(r) \sim U_{0,l}^{\text{free}}(r; z)\,\mathbf{a}_i, \qquad i \neq 1, \qquad (r \to \infty), \tag{4.8.28}$$

for some constant nonvanishing vectors $\mathbf{a}_i$. The complementary vector solution to the zero mode has to be some linear combination of the free solutions as $r \to \infty$:

$$\bar{f}_l^{(1)}(r) \sim U_{0,l}^{\text{free}}(r)\,\mathbf{b}_1 + U_{\infty,l}^{\text{free}}(r)\,\mathbf{c}_1, \qquad (r \to \infty). \tag{4.8.29}$$

The zero mode must have asymptotic behavior

$$f_l^{(1)}(r) \sim U_{\infty,l}^{\text{free}}(r)\,\mathbf{a}_1, \qquad\qquad (r \to \infty), \tag{4.8.30}$$

since this solution is square integrable by assumption. But then (4.8.27) shows that

$$\mathbf{a}_1^\dagger \mathbf{b}_1 = -1, \tag{4.8.31}$$

so $\mathbf{b}_1$ cannot vanish. Then, from (4.8.24a)

$$\bar{f}_l^{(1)}(r) = H_l^+(r)\,\zeta_1, \qquad f_l^{(i)}(r) = H_l^+(r)\,\zeta_i, \qquad i \neq 1, \tag{4.8.32}$$

we have the following asyptotic behavior for $H_l^+(r)$:

$$H_l^+(r)\,\zeta_1 \sim U_{0,l}^{\text{free}}(r)\,\mathbf{b}_1, \qquad H_l^+(r)\,\zeta_i \sim U_{0,l}^{\text{free}}(r)\,\mathbf{a}_i, \qquad i \neq 1, \tag{4.8.33}$$

Because the unit vectors ζ_i form a complete basis this shows that $\mathbb{H}_l^+$ must be nonsingular, since neither $\mathbf{b}_1$ nor any of the $\mathbf{a}_i$ can be zero for $i \neq 1$.

Defining the $2n \times n$ first order system matrix solutions $Y_l^+(r)$ and $Y_l^-(r)$ as

$$Y_l^+(r) \coloneqq \begin{pmatrix} H_l^+(r) \\ r^{d-1}\frac{\partial}{\partial r} H_l^+(r) \end{pmatrix}, \tag{4.8.34a}$$

$$Y_l^-(r) \coloneqq \begin{pmatrix} H_l^-(r) \\ r^{d-1}\frac{\partial}{\partial r} H_l^-(r) \end{pmatrix}, \tag{4.8.34b}$$

we have the constant matrix

$$\left\{Y_l^+, Y_l^-\right\} = r^{d-1}\left[\frac{\partial H_l^{-\dagger}}{\partial r} H_l^+ - H_l^{-\dagger}\frac{\partial H_l^+}{\partial r}\right] = \Omega \begin{pmatrix} 1 & \\ & -\mathbb{1} \end{pmatrix} \Omega^\intercal. \tag{4.8.35}$$

The matrix solution $H_l^-(r)$ must be some linear combination of the free solutions as $r \to \infty$:

$$H_l^-(r) \sim U_{0,l}^{\text{free}}(r)\,A + U_{\infty,l}^{\text{free}}(r)\,\mathbb{H}_l^-, \quad (r \to \infty). \tag{4.8.36}$$

But then taking the limit $r \to \infty$ of (4.8.35) shows that

$$\mathbb{H}_l^{-\dagger}\mathbb{H}_l^{+} = \Omega \begin{pmatrix} -1 & \\ & \mathbb{1} \end{pmatrix} \Omega^{\intercal}. \tag{4.8.37}$$

Since $\mathbb{H}_l^{+}$ has already been shown to be nonsingular we can invert it to give

$$\mathbb{H}_l^{-\dagger} = \Omega \begin{pmatrix} -1 & \\ & \mathbb{1} \end{pmatrix} \Omega^{\intercal} \left[\mathbb{H}_l^{+}\right]^{-1}. \tag{4.8.38}$$

Taking the determinant of $\mathbb{H}_l^{-}$ then completes the proof, since

$$\det\left(\mathbb{H}_l^{-\dagger}\right) = \det\left(\Omega \begin{pmatrix} -1 & \\ & \mathbb{1} \end{pmatrix} \Omega^{\intercal} \left[\mathbb{H}_l^{+}\right]^{-1}\right) = -\frac{1}{\det\left(\mathbb{H}_l^{+}\right)} \neq 0. \tag{4.8.39}$$

□

We can now explicitly construct the ratio of determinants with the zero modes removed. To do so we introduce a new set of vectors from the results of Theorem 4.8.1:

$$\xi_i \coloneqq \mathbb{H}_l^{+}\zeta_i, \qquad\qquad \bar{\xi}_i \coloneqq \mathbb{H}_l^{-}\zeta_i. \tag{4.8.40}$$

These ξ_i also form a complete basis on $\mathbb{R}^n$, since

$$\sum_{i=1}^{n} \xi_i \xi_i^{\dagger} = \mathbb{H}_l^{+} \sum_{i=1}^{n} \zeta_i \zeta_i^{\dagger} \mathbb{H}_l^{+\dagger} = \mathbb{H}_l^{+}\mathbb{H}_l^{+\dagger}. \tag{4.8.41}$$

From Theorem 4.8.1 we have $\det\left(\mathbb{H}_l^{+}\right) \neq 0$, so

$$\det\left(\xi_i \xi_i^{\dagger}\right) \neq 0, \tag{4.8.42}$$

therefore the $n \times n$ constant matrix $\xi_i \xi_i^{\dagger}$ must be full rank, immediately implying that the ξ_i are all linearly independent. If we can determine these vectors we will immediately have the result, since

$$\det\left(\mathbb{H}_l^{+}\right) = \det\left(\Omega^{\intercal}\mathbb{H}_l^{+}\Omega\right), \tag{4.8.43}$$

and the components of this transformed matrix are

$$\left[\Omega^{\intercal}\mathbb{H}_l^{+}\Omega\right]_{ij} = \mathbf{e}_i^{\dagger}\Omega^{\intercal}\mathbb{H}_l^{+}\Omega\mathbf{e}_j = \zeta_i^{\dagger}\xi_j. \tag{4.8.44}$$

Assuming we have already solved for the matrix solution $T_l(r)$ a numerically stable way of determining the ξ_i comes from

$$\xi_i = \lim_{r\to\infty} T_l(r)\,\zeta_i, \quad i \neq 1. \tag{4.8.45}$$

However, we cannot determine ξ_1 in this manner since

$$\lim_{r\to\infty} T_l(r)\,\zeta_1 = \lim_{r\to\infty}\left[U_{0,l}^{\text{free}}(r)\right]^{-1} U_{0,l}(r)\,\zeta_1 = \lim_{r\to\infty}\left[U_{0,l}^{\text{free}}(r)\right]^{-1} U_{\infty,l}^{\text{free}}(r)\,\bar{\xi}_1 = 0. \tag{4.8.46}$$

Instead, we can determine $\bar{\xi}_1$ and hope that we can determine ξ_1 from this knowledge. In this case it is better to first numerically solve for the zero mode $f_l^{(1)}(r)$, and then use

$$\bar{\xi}_1 = \lim_{r\to\infty}\left[U_{\infty,l}^{\text{free}}(r)\right]^{-1} f_l^{(1)}(r)\,. \tag{4.8.47}$$

Then, from (4.8.35) we have the following relationship:

$$\bar{\xi}_i^{\dagger}\xi_j = \begin{cases} -1 & \text{if } i=j=1 \\ \delta_{ij} & \text{else} \end{cases}. \tag{4.8.48}$$

We can then write ξ_1 as

$$\xi_1 = -\frac{\bar{\xi}_1}{\left\|\bar{\xi}_1\right\|^2} + v_{\perp}, \tag{4.8.49}$$

where $v_{\perp}$ is some vector in $\mathbb{R}^n$ such that $\bar{\xi}_1^{\dagger}v_{\perp} = 0$. But since the ξ_i form a complete basis this vector $v_{\perp}$ can be written as

$$v_{\perp} = \sum_{i=1}^{n} c_i\xi_i. \tag{4.8.50}$$

Then again using (4.8.48) it is trivial to show the $c_i = 0$ for all i. The full set of vectors is then

$$\xi_1 = -\frac{\bar{\xi}_1}{\left\|\bar{\xi}_1\right\|^2}, \tag{4.8.51a}$$

$$\xi_i \lim_{r\to\infty} T_l(r)\,\zeta_i, \qquad\qquad i \neq 1. \tag{4.8.51b}$$

We state the final result in the following theorem:

Theorem 4.8.2. *Assume that there exists one solution of $\tau_l u = 0$ that obeys the Friedrichs boundary conditions in the l^{th} partial wave expansion. The ratio of functional determinants for this mode with zero mode removed is given by*

$$\frac{\det'(\tau_l)}{\det(\tau_l^{\text{free}})} = -\det\left(\mathbb{H}_l^+\right)\int_0^\infty f_l^{(1)\dagger}(r)\, f_l^{(1)}(r)\, r^{d-1}\,\mathrm{d}r\,, \tag{4.8.52}$$

where $f_l^{(1)}(r)$ is the square integrable solution of

$$\tau_l\, f_l^{(1)}(r) = 0,$$

which obeys the Friedrichs boundary conditions and the constant matrix $\mathbb{H}_l^+$ has components equal to

$$\left[\Omega^\intercal \mathbb{H}_l^+ \Omega\right]_j^i = \zeta_i^\dagger \xi_j.$$

The orthonormal unit vectors ζ_i are constructed from the zero mode solution by

$$\zeta_1 = \lim_{r\to 0} r^{-l}\, f_l^{(1)}(r)\,,$$

$$\zeta_i^\dagger \zeta_j = \delta_{ij},$$

which further defines the orthogonal transformation matrix Ω through

$$\Omega_j^i = [\zeta_j]_i.$$

Finally, the vectors ξ_i are constructed from

$$\bar{\xi}_1 = \lim_{r\to\infty} \left[U^{\text{free}}_{\infty,l}(r)\right]^{-1} f^{(1)}_l(r)\,,$$

$$\xi_1 = -\frac{\bar{\xi}_1}{\left\|\bar{\xi}_1\right\|^2},$$

$$\xi_i = \lim_{r\to\infty} T_l(r)\,\zeta_i, \qquad\qquad i \neq 1,$$

where $T_l(r)$ is the matrix solution of

$$\frac{\mathrm{d}^2 T_l}{\mathrm{d}r^2} + \left[\frac{d-1}{r} + 2\left[U^{\text{free}}_{0,l}(r)\right]^{-1}\frac{\mathrm{d}\,U^{\text{free}}_{0,l}(r)}{\mathrm{d}r}\right]\frac{\mathrm{d}T_l}{\mathrm{d}r} - \left[U^{\text{free}}_{0,l}(r)\right]^{-1} V(r)\,U^{\text{free}}_{0,l}(r)\,T_l = 0,$$

$$T_l(0) = \mathbb{1}, \quad \left.\frac{\mathrm{d}\,T_l(r)}{\mathrm{d}r}\right|_{r=0} = \mathbb{0}$$

4.9 Conclusion

Our results are summarized in Theorem 4.1.1, with an additional algorithm for removing zero modes given by Theorem 4.8.2. Our results generalize some special cases previously found for functional determinants of radial operators[104–106]. What has been derived is a Gel'fand-Yaglom formula for spherically symmetric matrix elliptic operators in 2, 3, and 4 dimensions. We have regulated and renormalized the theory using zeta function regularization, and given a translation to other regularization schemes (most notably dimensional regularization) in Section 4.7.

Our results are important because they allow one to calculate functional determinants for field theories with arbitrarily many interacting particles. The matrix structure of the operators considered also allows one to calculate functional determinants of fermionic operators, of which we are aware of no other general results (excepting cases where the background potential matrix function takes a simple analytic form, e.g.

the BPST instanton[37]). The brute force method of numerically calculating the entire spectrum of eigenvalues is extremely computationally intensive, and can suffer greatly from rounding errors. Our method effectively skips this step, by computing the *product* of all of the eigenvalues without having to directly compute any eigenvalues.

Areas where this research may be of use are in vacuum-to-vacuum transition amplitude calculations, such as bubble nucleation and sphaleron rates. Our results could also be used to determine one-loop approximations of Casimir energies, for instance the mass energy of a soliton configuration.

Future work could be directed towards extending these results to the case where one or more of the particles in the theory is massless. In this case there are infrared divergences that also need to be regulated. It would also not be too difficult to derive similar results in dimensions greater than 4, but this may be somewhat tedious. Finally, the sums over the angular momentum quantum number l are convergent, but only barely. The partial sums converge like $1/l^2$ for $d = 2, 4$ and $1/l$ for $d = 3$. To achieve very precise results one needs to calculate an unreasonably large number of terms. In theory, one can accelerate the convergence using standard techniques (such as Richardson extrapolation), but we have found from numerical experiments this can be unstable. Using Richardson extrapolation one needs to calculate each term to much higher precision than one ultimately desires, since the cancellation of the higher order corrections fails if the error is dominated by precision losses.

Closing remarks

> A group of villagers heard that a strange animal, called an elephant, had been brought to the town in the night, but none of them were aware of its shape and form. Out of curiosity, they said: "We must inspect and know it by touch, as this night is too dark for us to see". So, they sought it out, and when they found it they groped about it. The first person, whose hand landed on the trunk, said, "This being is like a thick snake". For another one whose hand reached its ear, it seemed like a kind of fan. As for another person, whose hand was upon its leg, said, the elephant is a pillar like a tree-trunk. The person who placed their hand upon its side said the elephant, "is a wall". Another who felt its tail, described it as a rope. The last felt its tusk, stating the elephant is that which is hard, smooth and like a spear.
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> ---

The results presented in this thesis may seem at times disjoint, and to be fair, they are in some regards. This has been more of a collection of different research projects, rather than a single line of reasoning with a logical beginning and end. The final Chapter 4 was originally intended as the first step in a more ambitious project: to calculate the sphaleron rate in BSM scenarios. The aim was to provide constraints on models using the observed baryon excess, since sphalerons tend to push the universe towards $B + L = 0$. The sphaleron rate cannot be too large in the broken symmetry phase, otherwise the excess baryons are converted into antileptons, thus providing a new phenomenological tool for BSM searches. Even with the development of the the Gel'fand-Yaglom formalism in Chapter 4, this is a difficult computational task. The sphaleron configuration is a solution of a nonlinear boundary value problem, and can only be known numerically. I developed a set of numerical tools to determine this sphaleron profile, which were successful, but unfortunately took a great deal of time. I would like to continue this research, which at this point is technically feasible as all of the necessary tools have been developed and tested. It is now simply a matter of application

and execution (I say simply here, but this is meant only in the theoretical sense. In practice this would still be very difficult and require a great amount of computational resources and time).

There is also the question of first order phase transitions and baryogenesis, which Chapter 4 is also meant to provide tools for. An extension of the scalar sector of the SM is one avenue of generating the observed baryon excess. The SM alone is incapable of generating a baryon excess because the large mass of the Higgs results in a smooth transition from the unbroken phase to the broken phase. There is no latent heat released during this transition, and consequently it happens at near thermal equilibrium. Any process that generates a net increase in baryon number is countered by a similar process that reduces the overall baryon number, since thermal equilibrium implies that the baryon chemical potential and antibaryon chemical potentials are equal and opposite, and thus these processes occur at equal rates. Augmenting the scalar sector of the SM could fix this by introducing additional intermediate vacuum states, such that a first order phase transition occurs during some epoch between the end of inflation and our current matter dominated epoch.

A major difficulty in applying the results of Chapter 4 is that the sum over angular momentum modes is barely convergent. Convergence acceleration techniques, such as Richardson extrapolation, can be used to arrive at a more precise result while calculating fewer terms. However, after some numerical experiments I found these convergence acceleration techniques to be unstable and prone to error, likely due to the finite precision of floating point types and compounded rounding errors. Future work could be directed towards making the numerical determination of the angular

momentum modes more stable, or simply calculating higher order corrections to the Jost matrix function (an outline for this procedure is given in Appendix D.1.1).

Chapter 1 outlined some heuristic arguments in favor of a nonperturbative approach to scattering with large numbers of particles. Whether such a scenario has any implications for phenomenology has yet to be truly determined, but what we can say for certain is that the first few terms of the asymptotic expansion in small coupling are not representative of the physical scattering process. In regions of space-time where many wavepackets overlap the dominant contribution to the path integral is shifted significantly away from the free field configuration. This might suggest that a systematic analysis of scattering with large numbers of particles is more akin to a dilute instanton gas calculation than it is to a perturbative scattering amplitude calculation. This is purely speculative, but it would be interesting to know if a more rigorous treatment can be done.

My hope is that the research I have presented in this thesis is (1) of practical importance to the physics community, either as a set of tools for phenomenological searches, or to better understand the structure of quantum field theory, (2) useful for the development of new theories, and (3) interesting. A major goal in physics, since the days of Newton, has been to unify the disparate sub-fields into a grand unified theory. Progress towards this goal has been made incrementally over the past 400 years, punctuated by periods of rapid advancement between intervals where the field seems to languish, not dead, but instead writhing, twisted and knotted, grasping for something that might lead us out and onto the next horizon. It is true that these phases of accelerated expansion usually occur on the heels of some new development in

experimental physics, either new evidence or a novel technique or tool; but is equally true that advancements in pure and applied mathematics has allowed us to understand, construct, or actually use our theories.

I would argue that progress in science is the result of a combination of several ingredients, including observations, mathematical structure, and methods of analysis. In hindsight it is easy to see which essential component was missing before the last great thrust of scientific endeavour, but it is much more difficult for us to see what we do not already know. There are some problems, such as baryogenesis and dark matter, that I feel might be solved by extending the particle content of the standard model, buoyed by ever more precise data from astronomy and particle detectors. There are others, such as quantum gravity, the heirarchy problem, and the Yang-Mills mass gap that I suspect will require advances in theory and mathematical methods.

Critically, these unresolved questions are not independent of one another. Progress towards answering any one may result in progress towards answering another. I have enjoyed working on several projects that are not, or at least don't immediately seem, directly related. In this regard I am especially interested in applying nonperturbative methods as they apply to resurgence in the context of quantum field theories. This is a relatively recent development, and I am interested to see what comes out of it. In any case, I feel optimistic. Perhaps soon, a passing light might briefly illuminate the connective tissue between two ideas we thought were extraneous, and allow us to form a better picture of the whole.

Appendices

Appendix A

Behavior of Cross Sections for Large Numbers of Particles

A.1 Diagram Counting

In the case of $\lambda\phi^4$ theory we have the generating function, in 0 dimensions:

$$Z(\lambda, j) \coloneqq \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\phi \exp\Big(-\frac{1}{2}\phi^2 - \frac{\lambda}{4}\phi^4 + j\phi\Big), \tag{A.1.1}$$

where we have set $m = 1$ for simplicity and included an external source term. Expanded to order λ^n, the generating function simply counts the number of graphs (defined as the number of Wick contractions) at each order. For general λ, this can be studied as an ordinary integral.

The generating function for graphs with N external legs is then

$$\begin{aligned} Z^{(N)}(\lambda) \coloneqq & \frac{\mathrm{d}^N}{\mathrm{d}j^N} Z(\lambda, j)\Big|_{j=0}, \\ =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\phi\, \phi^N \exp\Big(-\frac{1}{2}\phi^2 - \frac{\lambda}{4}\phi^4\Big). \end{aligned} \tag{A.1.2}$$

This integral vanishes for odd N, so we let $N \equiv 2n$ so that we may consider only the non zero components. One can expand around small λ. After exchanging the order of integration and summation we find:

$$\begin{aligned} Z^{(2n)}(\lambda) \sim & \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k\, 2^{2k+n+1/2}\, \Gamma\Big(2k+n+\frac{1}{2}\Big)}{k!} \left(\frac{\lambda}{4}\right)^k, \quad (\lambda \to 0)\,, \\ \sim & \sum_{k=0}^{\infty} \frac{(-1)^k\, (4k+2n-1)!!}{k!} \left(\frac{\lambda}{4}\right)^k, \quad (\lambda \to 0)\,. \end{aligned} \tag{A.1.3}$$

The total number of graphs at each order k is the absolute value of each coefficient after factoring out the $k!$ in the denominator:

$$\eta_{2n,k} = (4k + 2n - 1)!!. \tag{A.1.4}$$

The integral (A.1.2) can be expressed as a sum of modified Bessel functions. The rapid growth of the coefficients means the series is asymptotic, with a radius of convergence of 0. We are interested, in particular, in the subset of these graphs which are fully connected. One may wonder if removing the vacuum and disconnected graphs might reduce the factorial growth of the coefficients in (A.1.3). The connected diagram generating function is related to the full generating function via

$$W(\lambda, j) \coloneqq -\ln\left(\frac{Z(\lambda, j)}{Z(\lambda, 0)}\right). \tag{A.1.5}$$

To determine the behavior of W at leading order we employ the Schwinger-Dyson equations (reintroducing $\hbar$ as a loop counting parameter).

$$\left[-\hbar\frac{\mathrm{d}}{\mathrm{d}j} - \lambda\hbar^3\frac{\mathrm{d}^3}{\mathrm{d}j^3} + j\right] Z(\lambda, j) = 0. \tag{A.1.6}$$

Substituting (A.1.5) into (A.1.6):

$$\frac{\mathrm{d}\,W(\lambda,j)}{\mathrm{d}j} + \lambda\left(\frac{\mathrm{d}\,W(\lambda,j)}{\mathrm{d}j}\right)^3 - 3\lambda\hbar\frac{\mathrm{d}\,W(\lambda,j)}{\mathrm{d}j}\frac{\mathrm{d}^2\,W(\lambda,j)}{\mathrm{d}j^2} + \lambda\hbar^2\frac{\mathrm{d}^3\,W(\lambda,j)}{\mathrm{d}j^3} + j = 0. \tag{A.1.7}$$

Taking $\hbar \to 0$ in (A.1.7) results in the loop expansion of Feynman diagrams. The leading order (or tree-level) term, W_0, is the solution of a simple cubic equation. The real root is easily solved for using Cardano's formula for depressed cubics. One then integrates the cubic equation and applies the boundary condition $W(0) = 0$. Expanding the solution for $j \to 0$ yields an asymptotic series whose coefficients give the number of connected graphs at tree-level with $2n$ external legs:

$$W_0(\lambda, j) = \sum_{n=0}^{\infty} \frac{(-1)^n\, 4^{n-1}\,\Gamma(3n-2)}{\Gamma(2n+1)\,\Gamma(n)}\left(\frac{\lambda}{4}\right)^{n-1} j^{2n} - \frac{1}{6\lambda}. \tag{A.1.8}$$

We can compare this with the corresponding behavior of $Z^{(2n)}(\lambda)$. The tree-level connected graphs arise at order

$$k = n - 1. \tag{A.1.9}$$

Calculating the coefficient of $Z^{(2n)}(\lambda)$ at this order by inserting (A.1.9) into (A.1.4) we find that (reverting to $N = 2n$),

$$z_{n-1} \sim N! \sim \left.\frac{\mathrm{d}^N W_0}{\mathrm{d}j^N}\right|_{j=0}, \quad (N \to \infty), \tag{A.1.10}$$

where $Z^{(2n)}(\lambda) = \sum z_k(\lambda/4)^k$. As we noted in the text, the similarities in the behavior of the full and connected Green's functions are expected for large N.

Appendix B

Asymptotic Analysis of the Boltzmann Equation for Dark Matter Relic Abundance

B.1 Numerical Determination of α

To aid in the application of our approximation in cases where the thermally averaged cross section is quite complicated (as in the case of coannihilations) we present in this appendix a simple and straightforward method of computing the relic density with little knowledge of the analytic behavior of the thermally averaged cross section. For large x we will assume the asymptotic form for the thermally averaged cross section:

$$\langle \sigma v_{\text{Møl}} \rangle \sim x^{\beta} e^{-\alpha x} \ln(x)^{\gamma}, \quad (x \to \infty). \tag{B.1.1}$$

The arbitrary coefficients α, β, and γ are generally domain dependent. Without precise knowledge of the analytic behavior of the thermally averaged cross section it may be difficult to know these parameters *a priori*, so we give a brief explanation of how to estimate them from a numerical analysis of the thermally averaged cross section. We are really only interested in the coefficient α in the vacinity of freeze-out, the other coefficients are automatically taken into account in our analysis. Hence we calculate

$$\frac{\mathrm{d}^2}{\mathrm{d}\ln(x)^2} \ln(\langle \sigma v_{\text{Møl}} \rangle) = -\alpha x - \frac{\gamma}{\ln(x)^2}, \quad (x \to \infty). \tag{B.1.2}$$

For large x the second term on the right is negligible, provided α is not identically 0. We can therefore approximate α in the freeze-out region via

$$\alpha \sim -\frac{1}{x_{\mathrm{f}}} \frac{\mathrm{d}^2}{\mathrm{d}\ln(x)^2} \ln(\langle \sigma v_{\text{Møl}} \rangle) \bigg|_{x=x_{\mathrm{f}}}, \quad (x_{\mathrm{f}} \to \infty). \tag{B.1.3}$$

Figure B.1 illustrates this numerical procedure for determining α. The lower plot shows the coefficient of the exponent behaves much like a step function for large x, with a large negative spike where the coefficient in the exponent transitions. Using (B.1.3) we find $\alpha \doteqdot 0.3549$. Because the exponential behavior is due to the Boltzmann

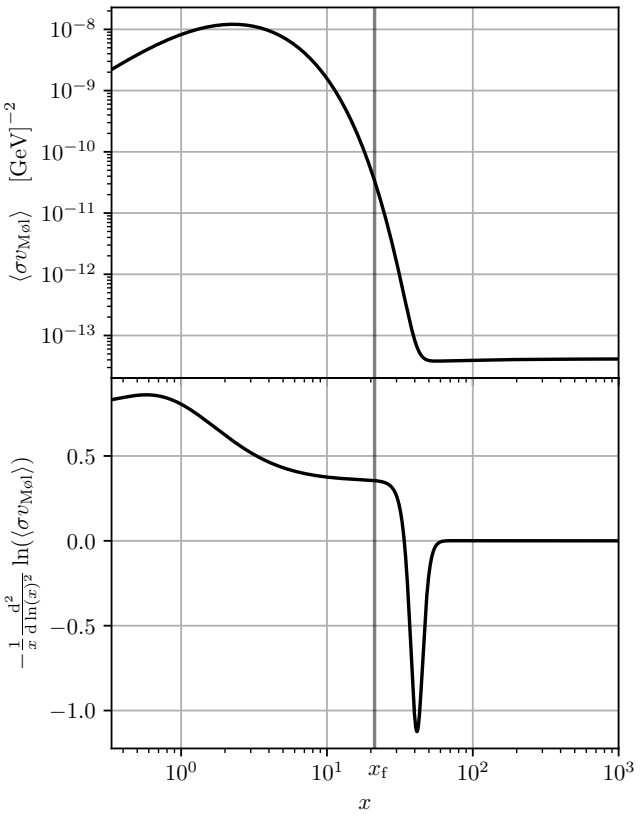

Figure B.1: Numerical determination of α using the benchmark model in Section 2.5 with $M_V = 1$ TeV, $m_\chi = 850$ GeV, $g = 1$, and $\epsilon = 10^{-3}$. The freeze-out temperature $x_f \doteqdot 21.2132$ is indicated by a vertical line. The top plot shows the thermally averaged cross section, while the bottom plot shows (B.1.3) evaluated at x.

suppressed $\chi\chi \to VV$ annihilation channel, (2.2.8b) gives $\alpha = 2(M_V - m_\chi)/m_\chi \doteqdot 0.3529$.

Determining α in this way only requires a numerical knowledge of the thermally averaged cross section, where the derivatives can be evaluated by finite differences (or a similar method). In addition, this definition selects the appropriate domain for the estimation of α. However, if x_f is very near a domain boundary (the negative spike in the lower plot of Figure B.1), where the leading order behavior of $\langle \sigma v_{\text{Møl}} \rangle$ is transitioning, this estimate will likely fail.

B.2 Boundary Layer Analysis

In this appendix we elaborate on some comments we make in the main body of the text concerning the boundary layer analysis in [76]. We will label Region I as the thermal-equilibrium region, Region II as the freeze-out region, and Region III as the

post-freeze-out region. The rest of the notation follows that in [76]. Assuming that

$$f(x) \sim x^{-n-2}, \quad (x \to \infty),$$

we attempt to approximate the solutions of (2.1.6) in the following form

$$Y'(x) = -\lambda x^{-n-2}\Big[Y^2(x) - Y_{\rm eq}^2(x)\Big]. \tag{B.2.1}$$

We begin by deriving the preliminary results in [76]. In the thermal equilibrium region (I) we approximate the solutions as a series expansion in powers of λ^{-1}.

$$Y^{\rm I}(x) \sim \sum_{k=0}^{\infty} \lambda^{-k}\, Y_k^{\rm I}(x)\,, \quad (\lambda \to \infty). \tag{B.2.2}$$

Solving for the first two terms and applying the boundary condition we get

$$Y_0^{\rm I}(x) = Y_{\rm eq}(x)\,, \tag{B.2.3a}$$

$$Y_1^{\rm I}(x) = -\frac{1}{2}x^{n+2}\frac{\rm d}{{\rm d}x}\ln(Y_{\rm eq}(x)). \tag{B.2.3b}$$

Using the large x approximation of the equilibrium abundance the two leading order terms have the asymptotic behavior

$$Y_0^{\rm I}(x) \sim \sqrt{\frac{\pi}{2}} A x^{3/2} e^{-x}, \qquad (x \to \infty) \tag{B.2.4a}$$

$$Y_1^{\rm I}(x) \sim \frac{x^{n+2}}{2}, \qquad (x \to \infty) \tag{B.2.4b}$$

Note that our definition of A differs from that in [76] by a factor of $\sqrt{\pi/2}$. When the next to leading order term is comparable to the leading order term the asymptotic approximation fails. We denote this value of x as $x_{\rm f}$, and define it by the transcendental equation

$$x_{\rm f} \sim \ln\Big(\sqrt{2\pi}\lambda A\Big) - \Big(n + \tfrac{1}{2}\Big)\ln(x_{\rm f}), \quad (\lambda \to \infty). \tag{B.2.5}$$

In the post-freeze-out region (III) the solution of (B.2.1) is easily approximated by dropping the equilibrium abundance. Thus, we place a small parameter ϵ in front of the equilibrium abundance

$$Y'(x) = -\lambda x^{-n-2}\Big[Y^2(x) - \epsilon\, Y_{\rm eq}^2(x)\Big],$$

and assume a solution in the form of a series in small ϵ.

$$Y^{\rm III}(x) \sim \sum_{k=0}^{\infty} Y_k^{\rm III}(x)\,\epsilon^k, \quad (\epsilon \to 0). \tag{B.2.6}$$

The leading order solution is easily found:

$$Y_0^{\rm III}(x) = \frac{C_0(n+1)x^{n+1}}{(n+1)x^{n+1} - C_0\lambda}. \tag{B.2.7}$$

The order ϵ term is slightly more complicated, but it is solvable. We will not need this solution, but we quote the result for completeness:

$$Y_1^{\mathrm{III}}(x) \sim \frac{C_1 x^{2n+2}}{\left[(n+1)x^{n+1} - C_0\lambda\right]^2} - \frac{\pi\lambda A^2}{4} x^{-n+1} e^{-2x}, \quad (x \to \infty). \tag{B.2.8}$$

In the freeze-out region (II) we find a new expansion parameter by letting $x \equiv x_{\mathrm{f}} + \kappa X$, where κ represents the width of the boundary region and should vanish as $\lambda \to \infty$. Assuming x_{f} is itself quite large we can approximate (B.2.1) by

$$\frac{1}{\kappa}\frac{\mathrm{d}Y^{\mathrm{II}}}{\mathrm{d}X} \sim -\frac{\lambda x_{\mathrm{f}}^{-n-2}}{\left(1+\frac{\kappa X}{x_{\mathrm{f}}}\right)^{n+2}}\left[\left(Y^{\mathrm{II}}\right)^2 - \frac{x_{\mathrm{f}}^{2n+4}}{4\lambda^2} e^{-2\kappa X}\right], \tag{B.2.9}$$

where we have used the definition of x_{f} to simplify the second term on the right. Dominant balance is achieved by letting $\kappa = x_{\mathrm{f}}^{n+2}/\lambda$. The second term on the right is of order κ^2, and can be ignored at leading order. We then assume a series solution of the form

$$Y^{\mathrm{II}}(X) \sim \sum_{k=0}^{\infty} Y_k^{\mathrm{II}}(X)\,\kappa^k, \quad (\kappa \to 0). \tag{B.2.10}$$

The first two terms are easily found

$$Y_0^{\mathrm{II}}(X) = \frac{1}{D_0 + X}, \tag{B.2.11a}$$

$$Y_1^{\mathrm{II}}(X) = \frac{1}{(D_0+X)^2}\left[D_1 + \frac{(n+1)X^2}{2x_{\mathrm{f}}(D_0+X)}\right] \tag{B.2.11b}$$

where D_0 and D_1 are arbitrary integration constants.

In order to asymptotically match the region I and region II solutions we expand the region I solution around $x = x_{\mathrm{f}} + \kappa X$, letting $x_{\mathrm{f}} \to \infty$, $X \to -\infty$, $\kappa \to 0$, and $\kappa X \to 0$, keeping only the leading order term.

$$\begin{aligned} Y^{\mathrm{I}}(X) &\sim Y_0^{\mathrm{I}}(x_{\mathrm{f}} + \kappa X) + \frac{1}{\lambda} Y_1^{\mathrm{I}}(x_{\mathrm{f}} + \kappa X) \\ &\sim \frac{\kappa}{2} e^{-\kappa X} + \frac{\kappa}{2}, \\ &\sim \kappa, \quad (\kappa \to 0). \end{aligned} \tag{B.2.12}$$

We have retained only the first two terms in the large λ expansion, but as is noted in [76], every term in the region I approximation is order κ near $x = x_{\mathrm{f}}$.

$$Y_k^{\mathrm{I}}(x) \sim \frac{(-1)^k x^{\frac{2kn+k+3}{2}} e^{(k-1)x}}{2^{(k+1)/2}\pi^{(k-1)/2}A^{k-1}}\alpha_k, \quad (x \to \infty), \tag{B.2.13}$$

where the α_k satisfy the recursion relation

$$\alpha_{k+1} = (k-1)\alpha_k - \frac{1}{2}\sum_{j=1}^{k} \alpha_j \alpha_{k-j+1}, \qquad \alpha_0 = 1. \tag{B.2.14}$$

Evaluating this near x_f yields

$$Y_k^\mathrm{I}(x_\mathrm{f})\,\lambda^{-k} = \frac{\kappa}{2}(-1)^k \alpha_k, \quad (x_\mathrm{f} \to \infty). \tag{B.2.15}$$

So in order to construct a highly precise approximation one must perform a resummation of every term in this series (which is divergent). Using Borel summation we find that we should replace κ in (B.2.12) with $c\kappa$, where $c \doteqdot 0.68995$ is a numerical correction. For simplicity we will not make this replacement.

It is clear that (B.2.12) cannot be asymptotically matched onto the region II solution (B.2.11a) for finite D_0 as is done in [76], because (B.2.12) and (B.2.11a) behave quite differently for large X. Therefore, we must choose $D_0 = \infty$. We then have $Y_0^\mathrm{II} = 0$, which seems to imply that Y_1^II is also vanishing. However, we can freely choose $D_1 = DD_0^2$ so that $Y_1^\mathrm{II} = D$ when setting $D_0 = \infty$. The region II solution is then approximated by

$$Y^\mathrm{II}(X) \sim \kappa D, \quad (\kappa \to 0). \tag{B.2.16}$$

We now have an exact asymptotic match to the region I solution by letting $D = 1$ (or $D = c$ if we include the numerical correction).

Next, approximating the region III solution with $\kappa \to 0$, $X \to \infty$, $\kappa X \to 0$ we find

$$Y^\mathrm{III}(X) \sim \frac{1}{\frac{1}{C_0} - \frac{\lambda x_\mathrm{f}^{-n-1}}{n+1} + X}, \quad (\kappa \to 0). \tag{B.2.17}$$

This does not appear to match to the region II solution. However, we know from matching regions I and II that the solution must be order κ, so we include a factor of κ in both the numerator and denominator.

$$Y^\mathrm{III}(X) \sim \frac{\kappa}{\frac{\kappa}{C_0} - \frac{x_\mathrm{f}}{n+1} + \kappa X}, \quad (\kappa \to 0), \tag{B.2.18}$$

where we have used $\kappa = x_\mathrm{f}^{n+2}/\lambda$. We see that the κX term in the denominator is negligible compared to the constant term $x_\mathrm{f}/(n+1)$. Therefore, we have

$$Y^\mathrm{III}(X) \sim \frac{\kappa}{\frac{\kappa}{C_0} - \frac{x_\mathrm{f}}{n+1}}, \quad (\kappa \to 0). \tag{B.2.19}$$

Solving for C_0 by comparing (B.2.16) with $D = 1$ and (B.2.18) then yields the final result:

$$\begin{aligned} C_0 &\sim \frac{(n+1)\kappa}{n+1+x_\mathrm{f}}, \quad (\kappa \to 0), \\ &\sim \frac{(n+1)x_\mathrm{f}^{n+2}}{\lambda(n+1+x_\mathrm{f})}, \quad (\kappa \to 0). \end{aligned} \tag{B.2.20}$$

This is the result often found in the literature. In [76] a spurious factor of 2 is inserted in the region I approximation, and the asymptotic matching is done at leading order so that the result comes out correct. However, the solutions cannot be matched at leading order, since in the limit $\lambda \to \infty$ the relic abundance should also vanish. One should also include the higher order corrections to the function $f(x)$, since these will contribute $\mathcal{O}(1)$ terms in the denominator of (B.2.20).

Appendix C

Lowest Dimensional Portals to SU(N) Exotics

C.1 Roots, Weights, and Representations

In this appendix we briefly cover some basic concepts in representation theory and a few common representations of SU(N), stating some necessary definitions.

Definition 16 (Representations of Groups)**.** A representation ρ of a group G is a linear mapping of the elements of the group to the automorphisms of some vector space V that preserves the group multiplication.

$$\begin{aligned} \rho\colon G &\to \mathrm{GL}(V), \\ g &\mapsto \rho(g), \quad g \in G, \\ \rho(g)\cdot\rho(h) &= \rho(g\circ h) \quad \forall g,h \in G, \end{aligned} \tag{C.1.1}$$

where $\circ$ is the multiplication on G and $\cdot$ is the multiplication on GL(V). If the representation space V is finite dimensional then $\cdot$ is matrix multiplication between $\dim(V)\times\dim(V)$ matrices.

The fundamental representation of SU(N) is defined by the mapping

$$\rho_F\colon \mathrm{SU}(N) \to \mathrm{GL}(\mathbb{C}^N), \tag{C.1.2}$$

i.e. we choose $V=\mathbb{C}^N$. We can then choose a basis $\{\mathbf{e}_a\}$ on $\mathbb{C}^N$:

$$\psi = T^a\mathbf{e}_a, \quad T^a \in \mathbb{C}, \forall\psi \in V. \tag{C.1.3}$$

Definition 17 (Dual Vector Space)**.** The **dual** vector space to V, which we denote V^*, is the vector space consisting of linear functionals of V to the base field of V.

$$V^*\colon V \to K, \tag{C.1.4}$$

where K is the field underlying the vector space V.

Definition 18 (Dual Basis of the Dual Space)**.** A choice of basis on V induces a natural basis on V^*,

$$\xi = T_a \mathbf{e}^a, \quad T_a \in \mathbb{C}, \ \forall \xi \in V^*. \tag{C.1.5}$$

where the $\{\mathbf{e}^a\}$ form the **dual basis of the dual space**, i.e. $\mathbf{e}^b(\mathbf{e}_a) = \delta^b_a$.

Because V is finite dimensional V^* is isomorphic to V as a vector space.

Definition 19. Dual Representation Take G to be a group and ρ to be a representation of G on the vector space V. Then the dual representation, ρ^*, is a representation of G on the dual vector space V^*:

$$\forall g \in G, \ \rho^*(g) = \rho(g^{-1})^\intercal, \tag{C.1.6}$$

where $\intercal$ denotes the transpose.

We need to make a distinction between *dual vector space* and *dual representation*. For a finite dimensional vector space, V, the dual vector space V^* is isomorphic to V. For representations this is usually not the case, a representation ρ is generally not isomorphic to its dual, ρ^*.

Definition 20 (Adjoint Representation)**.** The adjoint representation of $\mathrm{SU}(N)$, denoted Ad, is a map from the group into the automorphisms of the associated Lie algebra:

$$\begin{aligned} \mathrm{Ad}\colon \mathrm{SU}(N) &\to \mathrm{Aut}(\mathfrak{su}(N)) \\ g &\mapsto \mathrm{Ad}_g, \quad g \in \mathrm{SU}(N). \end{aligned} \tag{C.1.7}$$

The group action on a vector in the adjoint representation is

$$\mathrm{Ad}_g(\eta) = g\eta g^{-1}, \quad \eta \in \mathfrak{su}(N). \tag{C.1.8}$$

Because $SU(N)$ is a closed subgroup of the general linear group the above hold for all $g \in SU(N)$ and all $\eta \in \mathfrak{su}(N)$. Thus, we have the basis for adjoint representation

$$A = T^a_b \mathbf{e}_a \otimes \mathbf{e}^b, \quad A \in \mathfrak{su}(N), \ T^a_b \in \mathbb{R}, \tag{C.1.9}$$

with

$$T^a_a = 0. \tag{C.1.10}$$

We have introduced the tensor product notation, which we now explain. A tensor is a generalization of the notion of the dual vector space. It is a multilinear functional that takes some copies of the vector spaces V and V^* and maps them to the base field.

$$T^r_s V\colon \underbrace{V \times \ldots \times V}_{r} \times \underbrace{V^* \times \ldots \times V^*}_{s} \to K, \tag{C.1.11}$$

where K is the base field underlying the vector space V and $\times$ is the usual Cartesian product. With the previous choice of basis we write

$$\begin{aligned} T &= T^{a_1 \ldots a_r}_{b_1 \ldots b_s} \mathbf{e}_{a_1} \otimes \ldots \otimes \mathbf{e}_{a_r} \otimes \mathbf{e}^{b_1} \otimes \ldots \otimes \mathbf{e}^{b_s}, \\ T &\in T^r_s V. \end{aligned} \tag{C.1.12}$$

For example, $v \otimes u$ is just a multilinear map. The $\otimes$ here is not an operation, but just part of the symbol used to denote the map. However, we can inherit the addition and scalar multiplication induced by V, making $T^r_s V$ a $\dim(V)^{r+s}$ vector space over the field K. It is then clear that the $\mathbf{e}_{a_1} \otimes \ldots \otimes \mathbf{e}_{a_r} \otimes \mathbf{e}^{b_1} \otimes \ldots \otimes \mathbf{e}^{b_2}$ constitutes a basis on $T^r_s V$. We then can define the abstract tensor product of vector spaces $V \otimes W$. A vector $\psi \otimes \xi \in V \otimes W$ is then an equivalence class $[(\psi, \xi)]$ with representative (ψ, ξ), where $\psi \in V$ and $\xi \in W$. Generally the space $V \otimes W$ is much larger than the space spanned by vectors of the form $\psi \otimes \xi$, it will also include linear combinations of vectors. We use the same symbol, $\otimes$, to represent the tensor product between *vector spaces* ($\otimes$) and *vectors* ($\otimes$), as is common in the literature, because the usage is clear from context.

Definition 21 (Root Vectors)**.** For a complex semisimple Lie algebra $\mathfrak{g}$ with a Cartan subalgebra $\mathfrak{h}$ the **root vectors** are elements of $\mathfrak{h}^*$, i.e. the dual of the Cartan subalgebra.

Definition 22 (Root)**.** A $\alpha \in \mathfrak{h}^*$ is called a root of $\mathfrak{g}$ relative to $\mathfrak{h}$ if $\alpha \neq 0$ and there exists an $X \neq 0 \in \mathfrak{g}$ such that

$$[H, X] = \alpha(H)X, \quad \forall H \in \mathfrak{h}. \tag{C.1.13}$$

The Cartan subalgebra of $\mathfrak{su}(N)$ has $N-1$ generators that commute with all other elements of the algebra. Hence, $\mathfrak{h}$ is an $N-1$ dimensional vector space over $\mathbb{C}$ (in the complexified version of $\mathfrak{su}(N)$). It is, however, somewhat simpler to consider the generators of $\mathfrak{h}$ as elements of $\mathbb{R}^N$ with the restriction that the sum over all N components vanishes, that is

$$H_\lambda = \lambda^j \mathbf{e}_j, \quad \sum_{j=1}^{N} \lambda^j = 0, \tag{C.1.14}$$

where the $\{\mathbf{e}_j\}$ are the usual orthonormal basis vectors on $\mathbb{R}^N$. Since the roots α lie in the dual space to $\mathfrak{h}$, i.e. $\mathfrak{h}^*$, we can use the dual basis to write them as

$$\alpha^{jk} = \mathbf{e}^j - \mathbf{e}^k, \quad \mathbf{e}^j(H_\lambda) = \lambda^j, \quad j \neq k. \tag{C.1.15}$$

We then have

$$[H_\lambda, E_{jk}] = \left(\lambda^j - \lambda^k\right) E_{jk}, \tag{C.1.16}$$

where the E_{jk} are $N \times N$ matrices with a 1 in the $(j,k)^{\text{th}}$ position and zeros elsewhere in the fundamental representation (there is no sum over j and k).

Definition 23 (Simple Roots)**.** The simple roots of the algebra are given by

$$\alpha^j \coloneqq \alpha^{j\,j+1}. \tag{C.1.17}$$

All of the other roots can be constructed by linear combinations of the simple roots.

This root system is known as A_{N-1}, and we will denote the set of all roots as Δ. The simple roots are also vectors in $\mathbb{R}^N$ whose components sum to 0 due to

the isomorphism between a finite dimensional vector space and its dual. This is the *standard basis* (sometimes called the *orthogonal-basis*):

$$\begin{aligned}\alpha^1 &= (1,-1,\underbrace{0,\ldots,0}_{N-2}),\\ \alpha^j &= (\underbrace{0,\ldots,0}_{j-1},1,-1,\underbrace{0,\ldots,0}_{N-j-1}),\\ \alpha^{N-1} &= (\underbrace{0,\ldots,0}_{N-2},1,-1).\end{aligned} \tag{C.1.18}$$

The simple roots form a complete basis for the space of vectors in $\mathbb{R}^{N-1}$ whose components sum to 0, but they are not orthonormal. We can therefore express any vector in this space as a linear combination of the simple roots

$$v \in \mathbb{R}^{N-1} = v_i\alpha^i, \quad v_i \in \mathbb{R}. \tag{C.1.19}$$

This is referred to as the *α-basis*.

Definition 24 (Fundamental Weights)**.** The *fundamental weights*, ω^j, are defined by

$$\frac{2\left\langle \omega^j, \alpha^k \right\rangle}{\langle \alpha^k, \alpha^k \rangle} = \delta^k_j \tag{C.1.20}$$

where $\langle \cdot, \cdot \rangle$ is the usual inner product on $\mathbb{R}^N$.

The ω^j constitute the *ω-basis*, or *Dynkin-basis*.

Definition 25 (Cartan Matrix)**.** We can translate between the α-basis and ω-basis via

$$\alpha^j = \sum_{k=1}^{N-1} A^j_k \omega^k, \tag{C.1.21a}$$

$$\omega^j = \sum_{k=1}^{N-1} \left(A^{-1}\right)^j_k \alpha^k, \tag{C.1.21b}$$

where the *Cartan matrix* A is

$$A^j_k = \frac{2\left\langle \alpha^k, \alpha^j \right\rangle}{\langle \alpha^k, \alpha^k \rangle}. \tag{C.1.22}$$

As previously stated, for SU(N) the root system is A_{N-1}, and the Cartan matrix is

$$A^j_k = \begin{pmatrix} 2 & -1 & 0 & \ldots & 0 & 0 \\ -1 & 2 & -1 & \ldots & 0 & 0 \\ 0 & -1 & 2 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 2 & -1 \\ 0 & 0 & 0 & \ldots & -1 & 2 \end{pmatrix}. \tag{C.1.23}$$

Definition 26 (Coroot)**.** We can make the two basis dual by introducing the **coroot** $\alpha^{\vee jk}$:

$$\alpha^{\vee}_{jk} \coloneqq \frac{2\alpha^{jk}}{\langle \alpha^{jk}, \alpha^{jk} \rangle}. \tag{C.1.24}$$

This then gives

$$\left\langle \omega^j, \alpha^{\vee}_k \right\rangle = \delta^j_k, \tag{C.1.25}$$

where $\alpha^{\vee}_j$ is the coroot associated to the simple root α^j.

It then follows that a representation of a Lie algebra is a set of matrices that satisfy the same commutation relations as the abstract algebra. Each of the matrices can be labeled by a weight as follows: Let V be a representation of a Lie algebra $\mathfrak{g}$ over $\mathbb{C}$ and let λ be a linear functional on the Cartan subalgebra $\mathfrak{h}$.

Definition 27 (Weight Space)**.** The **weight space** of V with weight λ is

$$V_\lambda \coloneqq \{v \in V \mid \forall H \in \mathfrak{h},\ H \cdot v = \lambda(H)v\}. \tag{C.1.26}$$

Essentially, this generalizes the familiar ladder operators of $\mathfrak{su}(2)$. As a consequence of the root equation (C.1.13) if v is a weight vector with weight λ

$$\begin{aligned} H \cdot Xv &= X \cdot Hv + [H, X]v \\ &= [\lambda(H) + \alpha(H)]Xv, \quad \forall H \in \mathfrak{h}. \end{aligned} \tag{C.1.27}$$

Therefore Xv is either the zero vector or a weight vector with weight $\lambda + \alpha$.

Definition 28 (Algebraically Integral Weights)**.** Denote by $\mathfrak{h}^*_0$ the real subspace of the dual of the Cartan subalgebra $\mathfrak{h}^*$ generated by the roots of $\mathfrak{g}$. Then an element $\lambda \in \mathfrak{h}_0$ is said to be **algebraically integral** if

$$\left\langle \lambda, \alpha^{\vee}_{jk} \right\rangle \in \mathbb{Z}, \quad \forall \alpha^{\vee}_{jk} \in \mathfrak{h}^*_0. \tag{C.1.28}$$

The coroot $\alpha^{\vee}_{jk}$ can be identified with the H element in the X, Y, H basis of an $\mathfrak{sl}(2, \mathbb{C})$-subalgebra of $\mathfrak{g}$. The eigenvalues of $\alpha^{\vee}_{jk}$ in any finite dimensional representation of $\mathfrak{g}$ must then be an integer.

Definition 29 (Dominant Weights)**.** For an algebraically integral element λ we can write its components in the ω-basis

$$a_j = \left\langle \lambda, \alpha^{\vee}_j \right\rangle, \tag{C.1.29}$$

where the a_j are integers for every simple root. The smallest non-zero weights with $a_j \geq 0$ are the fundamental weights. We then refer to the a_j as the **Dynkin labels** of the weight. Therefore, an element λ is algebraically integral if and only if it is expressible as a combination of the fundamental weights with integer coefficients. A weight is called **dominant** if all of the $a_j \geq 0$.

Definition 30 (Partial Ordering of Weights)**.** The weights of a representation can be partially ordered. Consider the positive roots in Δ, denoted Δ^+, as the set of all α^{jk} with $j < k$. We then partially order the weights as

$$\lambda \succeq \mu \quad \text{if} \quad \lambda - \mu = \theta_{ij}\alpha^{ij}, \quad \theta_{ij} \in \mathbb{R}^+, \alpha^{ij} \in \Delta^+. \tag{C.1.30}$$

That is, λ is **higher** than μ if the difference $\lambda - \mu$ can be written as a linear combination of positive roots with non-negative real coefficients. A weight λ of a representation V of an algebra $\mathfrak{g}$ is then said to be the **highest weight** if every other weight of V is lower than λ. The **level** of a weight is the number of simple roots that must be subtracted from the highest weight in order to obtain it. The highest level of an irrep is call its **height**.

We can now state the following theorem:

Theorem C.1.1. *Theorem of the Highest Weight*

1. *Every irreducible (finite dimensional) representation has a highest weight,*
2. *the highest weight is always a dominant, algebraically integral element,*
3. *two irreps with the same highest weight are isomorphic, and*
4. *every dominant, algebraically integral element is the highest weight of an irrep.*

From Theorem C.1.1, the highest weight of an irrep uniquely determines the representation. When used in the context of a representation (as opposed to an individual weight) we use *Dynkin label* to refer to the Dynkin labels of the highest weight in the weight space of the representation.

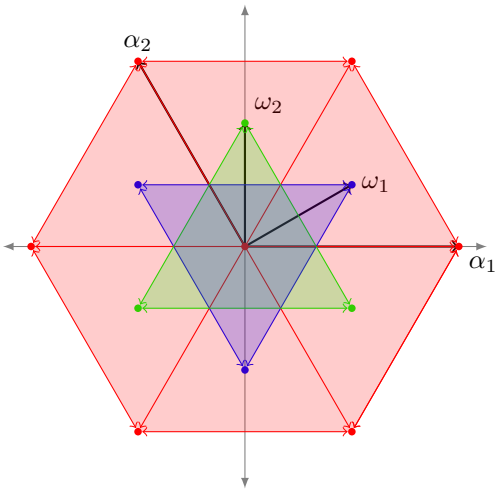

Figure C.1: Weight spaces for some irreps of SU(3). Shown are the fundamental (3), antifundamental ($\bar{3}$), and adjoint (8) representations in blue, green, and red respectively.

Finally, a finite-dimensional representation V of a semisimple Lie algebra $\mathfrak{g}$ is uniquely specified by a set of weights.

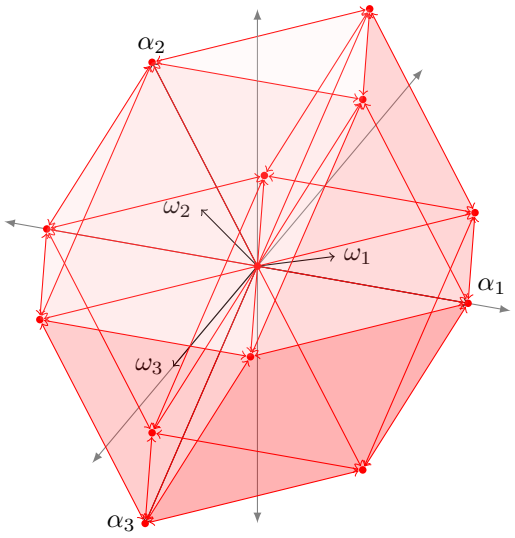

Figure C.2: Weight space of the adjoint representation of SU(4). Vertices indicate locations of the weights while red arrows indicate the Weyl group orbits.

Definition 31 (Highest-Weight-Module)**.** If V is generated by a $v \in V$ that is annihilated by the action of all positive root spaces in $\mathfrak{g}$ then V is called a **highest-weight module**.

It can be shown that every finite-dimensional highest-weight module is irreducible. A representation can then be decomposed into irreps by sorting the weights into weight spaces that correspond to the irreps. The dimension of a representation is just the number of weights in its weight space. Several examples of weights spaces are given in Fig. C.1 and Fig. C.2.

A *Young tableau* (plural, "tableaux") of a Ferrers diagram is obtained by placing the elements of some ordered set into each box of the diagram. The diagram itself must have rows of weakly decreasing length as traversed from top to bottom, with the number of boxes overhanging in each row corresponding to the Dynkin label of the irrep. A *standard* Young tableau has elements that form an increasing sequence when moving from left to right in each row and from top to bottom in each column. A *semistandard* Young tableau has nondecreasing elements along each row and increasing elements in each column. Young tableaux contain a great deal of information about an irrep. For instance, the dimension of the irrep can be calculated using the Hook length formula. As well, Young tableaux can be used to decompose a tensor product of two irreps into a direct sum of irreps. As a consequence of Theorem C.1.1 every Young tableau corresponds uniquely to an irrep of SU(N), and we make considerable use of this when deriving the results of Sections 3.2 and 3.3. For more information about Young tableaux see Ref. [98].

C.2 Adjoint Product Decomposition

The vector space of the adjoint representation of SU(N) is spanned by the generators of the algebra of $\mathfrak{su}(n)$. There are $N-1$ zero weights coming from the $N-1$ generators of the Cartan subalgebra, and $N(N-1)$ weights from the remaining generators with roots α^{jk}, giving the dimension of the adjoint representation as N^2-1 since there are N^2-1 weights. By Theorem C.1.1 there is a unique highest weight,

$$\bar{\lambda} = \alpha^{1N} = \sum_{j=1}^{N-1} \alpha^j = \omega^1 + \omega^{N-1}, \tag{C.2.1}$$

which we use to label the adjoint representation. Taking the tensor product of 2 copies of the adjoint we add all the weights of one copy of the adjoint to every weight of the second copy. This gives a set of $(N^2-1)(N^2-1)$ weights, many of them duplicates, that must be sorted in order to decompose the tensor product into a direct sum of irreps. Continuing to take the tensor product k times in total produces $(N^2-1)^k$ weights, and sorting all of these weights quickly becomes unreasonably tedious. For fixed k it can be done using Freudenthal's recursion formula for the multiplicities of the weight λ in the irrep with highest weight Λ:

$$(\langle \Lambda+\delta, \Lambda+\delta\rangle - \langle \lambda+\delta, \lambda+\delta\rangle) m_\Lambda(\lambda) = 2 \sum_{\alpha\in\Delta^+} \sum_{j\geq 1} \langle \lambda + j\alpha, \alpha\rangle \, m_\Lambda(\lambda + j\alpha), \tag{C.2.2}$$

where $\langle\cdot,\cdot\rangle$ is the usual inner product on $\mathbb{R}^N$, $\delta \coloneqq \sum_{j=1}^{N-1} \omega^j$ is the Weyl vector, $m_\Lambda(\lambda)$ is the multiplicity of the weight λ in the irrep with highest weight Λ, and the first sum is over all positive roots of the algebra. If k is left as a free parameter this formula becomes less useful, so we take a different approach based on Schur-Weyl duality.

The tensor product of any two irreps of SU(N), V_μ and V_ν, can be accomplished in the following way:

$$V_\mu \otimes V_\nu \cong \bigoplus_\lambda c^\lambda_{\mu\nu} V_\lambda, \tag{C.2.3}$$

where $c^\lambda_{\mu\nu}$ is the multiplicity of the irrep labeled by its highest weight λ in the tensor product and the sum is taken over all dominant weights λ. The multiplicities are given by the *Littlewood-Richardson rule*, which counts the number of Littlewood-Richardson tableau with skew shape λ/μ and content ν. They appear as the coefficients in the decomposition of the multiplication of Schur functions

$$s_\mu s_\nu = \sum_\lambda c^\lambda_{\mu\nu} s_\lambda. \tag{C.2.4}$$

This decomposition follows from the Weyl character formula for representations of a simple Lie algebra over a complex field[121]. In fact, the multiplicities can be calculated explicitly, without reference to Littlewood-Richardson tableau:

Theorem C.2.1. *Steinberg [121]*

$$c^\lambda_{\mu\nu} = \sum_{\sigma,\tau\in\mathfrak{S}_N} \det(\sigma\tau)\mathfrak{p}(\sigma(\mu+\delta) + \tau(\nu+\delta) - (\lambda+2\delta)), \tag{C.2.5}$$

where $\mathfrak{S}_N$ is the symmetric group of permutations acting on vectors with N elements, δ is the Weyl vector, and $\mathfrak{p}(v)$ is the Kostant partition function.

$$\mathfrak{p}(v) = \left| \left\{ n_\alpha \in \mathbb{R}^{N-1} \mid v = \sum_{\alpha \in \Delta^+} n_\alpha \alpha, n_\alpha \geq 0 \right\} \right|. \tag{C.2.6}$$

$\mathfrak{p}(v)$ counts the number of ways a vector v (weight) can be written as the sum of positive roots.

In particular, if we let μ and ν be either $(1, 0, \ldots, 0)$ or $(1, 1, \ldots, 1, 0, \ldots, 0)$ we have Pieri's formula:

$$s_\mu h_r = \sum_\lambda s_\lambda, \tag{C.2.7}$$

where h_r is a complete homogeneous symmetric polynomial and the sum is taken over all partitions λ obtained from μ by adding r boxes with no boxes in the same column. We also have the dual Pieri rule

$$s_\mu e_r = \sum_\lambda s_\lambda, \tag{C.2.8}$$

where e_r is an elementary symmetric polynomial and the sum is taken over all partitions λ obtained from μ by adding r boxes with no boxes in the same row. For these choices of the partitions μ and ν the Littlewood-Richardson coefficients are either 1 or 0.

Schur-Weyl duality comes from considering the k-fold tensor product of $\mathbb{C}^N$. The action of the symmetric group $\mathfrak{S}_k$ and the general linear group $G = \mathrm{GL}(\mathbb{C}^N)$ commute, and as an $\mathfrak{S}_k \times G$-module we have the decomposition

$$\left(\mathbb{C}^N\right)^{\otimes k} \cong \bigoplus_\lambda M_\lambda \otimes \mathbb{S}_\lambda \mathbb{C}^N, \tag{C.2.9}$$

where M_λ is an irrep of $\mathfrak{S}_N$ indexed by the partition λ and the Schur functor $\mathbb{S}_\lambda V$ is the image of the Young symmetrizer. The fundamental representation, V_F, of $\mathrm{SU}(N)$ is a G-module isomorphic to $\mathbb{C}^N$, hence we have

$$V_F^{\otimes k} \cong \bigoplus_\lambda V_\lambda^{\oplus m_\lambda}, \tag{C.2.10}$$

where $m_\lambda \equiv \dim(M_\lambda)$, and $V_\lambda \equiv \mathbb{S}_\lambda \mathbb{C}^N$ is an irrep of $\mathrm{SU}(N)$. The sum is over all partitions λ of the integer k. In addition, the dual representation to V_F, denoted V_F^*, is also isomorphic to $\mathbb{C}^N$, so we also have

$$(V_F^*)^{\otimes k} \cong \bigoplus_\lambda V_{\lambda^*}^{\oplus m_\lambda}, \tag{C.2.11}$$

where, again, the sum is over all partitions λ of the integer k and λ^* is the conjugate partition to λ.

Theorem C.2.2. *The k-fold tensor product of the adjoint representation of* $\mathrm{SU}(N)$*, G_N, decomposes into a direct sum of irreps*

$$\mathrm{G}_N^{\otimes k} \cong \bigoplus_{\lambda} V_\lambda^{m_\lambda(G_N)}, \tag{C.2.12}$$

where the sum over λ is over all dominant weights. The multiplicity, $m_\lambda(G_N)$, of the irrep V_λ in the sum is

$$m_\lambda(G_N) = \sum_{n=0}^{k} \sum_{\mu_n} \sum_{\nu_n} (-1)^{k-n} \binom{k}{n} m_{\mu_n} m_{\nu_n} c^{\lambda}_{\mu_n \nu_n^*}, \tag{C.2.13}$$

where the second and third sums are over all partitions μ_n and ν_n of the integer n and ν_n^* is the conjugate partition to ν_n.

Proof. Using Pieri's rule we can relate the adjoint representation to the fundamental and antifundamental representations of $\mathrm{SU}(N)$:

$$V_F \otimes V_F^* \cong G_N \oplus \mathbb{1}. \tag{C.2.14}$$

This then implies

$$(V_F \otimes V_F^*)^{\otimes k} \cong \bigoplus_{n=0}^{k} \binom{k}{n} G_N^{\otimes k-n}, \tag{C.2.15}$$

where $G_N^{\otimes 0} \coloneqq \mathbb{1}$. We can then simply invert (C.2.15) to solve for $G_N^{\otimes k}$:

$$\begin{aligned}
G_N^{\otimes k} &\cong (V_F \otimes V_F^* \ominus \mathbb{1})^{\otimes k} \\
&\cong \bigoplus_{n=0}^{k} (-1)^{k-n} \binom{k}{n} V_F^{\otimes n} \otimes (V_F^*)^{\otimes n} \\
&\cong \bigoplus_{n=0}^{k} (-1)^{k-n} \binom{k}{n} \bigoplus_{\mu_n} m_{\mu_n} V_{\mu_n} \bigoplus_{\nu_n} m_{\nu_n} V_{\nu^*} \\
&\cong \bigoplus_{\lambda} \bigoplus_{n=0}^{k} \bigoplus_{\mu_n} \bigoplus_{\nu_n} (-1)^{k-n} \binom{k}{n} m_{\mu_n} m_{\nu_n} c^{\lambda}_{\mu_n \nu_n^*} V_\lambda \\
&\cong \bigoplus_{\lambda} V_\lambda^{\oplus m_\lambda(G_N)}.
\end{aligned} \tag{C.2.16}$$

□

Theorem C.2.3. *The multiplicity of the irrep $V_\lambda \subset \mathrm{G}_N^{\otimes k}$ is non-vanishing for all dominant λ such that $\bar{\Lambda} \succeq \lambda$, where $\bar{\Lambda}$ is the highest weight of the highest irrep in $\mathrm{G}_N^{\otimes k}$.*

$$\lambda \text{ dominant} \wedge \bar{\Lambda} \succeq \lambda \implies m_\lambda(G_N) > 0. \tag{C.2.17}$$

Proof. From (C.2.15), we have the following implications

$$\forall n, k \in \mathbb{N}_0 \mid n \leq k \colon V_\lambda \subset G_N^{\otimes n} \implies V_\lambda \subset (V_F \otimes V_F^*)^{\otimes k}, \tag{C.2.18}$$

and

$$\forall k \in \mathbb{N}_0 \colon V_\lambda \subset (V_F \otimes V_F^*)^{\otimes k} \implies \exists\, n \in \mathbb{N}_0 \mid 0 \leq n \leq k \colon V_\lambda \subset G_N^{\otimes n}. \tag{C.2.19}$$

We then look at the tensor product of two copies of the adjoint:

$$G_N \otimes G_N \cong \bigoplus_\lambda c_{\lambda\bar{\lambda}}^{\lambda} V_\lambda, \tag{C.2.20}$$

where $\bar{\lambda} = (1, 0, \ldots, 0, 1)$ is the highest weight of G_N. Using Theorem C.2.1 we explicitly calculate the multiplicities

$$c_{\lambda\bar{\lambda}}^{\bar{\lambda}} = \begin{cases} 1 & N = 2 \\ 2 & N > 2 \end{cases}, \tag{C.2.21a}$$

$$c_{\lambda\bar{\lambda}}^{0} = 1. \tag{C.2.21b}$$

This shows that $G_N \subset G_N \otimes G_N$ and $\mathbb{1} \subset G_N \otimes G_N$. Therefore

$$\forall n \in \mathbb{N} \mid n > 1,\ G_N^{\otimes n-1} \subset G_N^{\otimes n}. \tag{C.2.22}$$

But then from (C.2.19) we find

$$\forall k \in \mathbb{N} \mid k > 1, V_\lambda \subset (V_F \otimes V_F^*)^{\otimes k} \implies V_\lambda \subset G_N^{\otimes k}. \tag{C.2.23}$$

Computing the tensor product of $(V_F \otimes V_F^*)^{\otimes k}$ directly gives

$$(V_F \otimes V_F^*)^{\otimes k} = \bigoplus_{\mu \in P_k} \bigoplus_{\nu \in P_k} \bigoplus_\lambda m_\mu m_\nu c_{\mu\nu^*}^{\lambda} V_\lambda, \tag{C.2.24}$$

where P_k is the set of all partitions of the integer k into no more than N parts. There exists no sufficient conditions for $c_{\mu\nu^*}^{\lambda} \neq 0$ (although there are necessary conditions, such as $|\lambda| = |\mu| + |\nu^*|$), so we instead construct the tableaux for the irreps V_λ in steps:

$$\begin{aligned} (V_F \otimes V_F^*)^{\otimes k} &= (V_F^*)^{\otimes k} \otimes \underbrace{V_F \otimes \ldots \otimes V_F}_{k} \\ &= \bigoplus_{\nu \in P_k} V_{\nu^*}^{\oplus m_\nu} \otimes \underbrace{V_F \otimes \ldots \otimes V_F}_{k} \end{aligned} \tag{C.2.25}$$

The multiplicity m_ν is non-vanishing for all partitions ν, so we can collect all possible V_{ν^*}, and then add k boxes in possible ways (there are no symmetry arguments to consider because each V_F is added individually). Begin with a rectangular tableau that has N rows and k columns. As a partition this is

$$\lambda_0 \coloneqq \underbrace{k + k + \ldots + k + k}_{N} \equiv (\underbrace{k, \ldots, k}_{N}), \tag{C.2.26}$$

where each component of λ_0 corresponds to the number of boxes in that row of the tableau (in this case they are all k). Then remove k boxes in all possible ways that results in a valid tableau. Write this partition as $\lambda_0 - r$, where

$$r \coloneqq (r_1, r_2, \ldots, r_{N-1}, r_N), \quad r_j \in \mathbb{N}_0, \tag{C.2.27a}$$

$$\sum_{j=1}^{N} r_j = k, \tag{C.2.27b}$$

$$r_i \leq r_j, \quad \text{if} \quad i < j. \tag{C.2.27c}$$

The first condition specifies that k boxes are to be removed, while the second condition is necessary so that $\lambda_0 - r$ remains a partition (the elements must be weakly decreasing). Finally, add k boxes in all possible ways and write this partition as $\lambda_0 - r + a$, where

$$a \coloneqq (a_1, a_2, \ldots, a_{N-1}, a_N), \quad a_j \in \mathbb{N}_0, \tag{C.2.28a}$$

$$\sum_{j=1}^{N} a_j = k, \tag{C.2.28b}$$

$$a_i - a_j \geq r_i - r_j, \quad \text{if} \quad i < j. \tag{C.2.28c}$$

Again, the first condition specifies that k boxes are to be added, while the second condition is necessary so that $\lambda_0 - r + a$ remain a partition. By construction, every λ that can be written as $\lambda_0 - r + a$ has nonzero multiplicity. Clearly, removing some number of boxes from a row and then adding the same number of boxes to the same row is redundant, so this procedure is not unique. We can remove the redundancy by defining:

$$\eta \equiv (\eta_1, \eta_2, \ldots, \eta_k), \quad \eta_j \coloneqq a_j - r_j \in \mathbb{Z}. \tag{C.2.29}$$

The components of this vector no longer need to be non-negative, but they satisfy

$$\sum_{j=1}^{N} \eta_j = 0 \tag{C.2.30a}$$

$$\eta_i \geq \eta_j, \quad \text{if} \quad i < j, \tag{C.2.30b}$$

$$|\eta_j| \leq k. \tag{C.2.30c}$$

which are direct consequences of (C.2.27) and (C.2.28). This η is a N component vector, where the sum of its components vanish, which implies it can be decomposed into a linear combination of the simple roots α^j of SU(N). In particular, we can calculate the Dynkin labels of $\lambda = \lambda_0 + \eta$:

$$\left\langle \lambda, \alpha_j^\vee \right\rangle = \left\langle \lambda_0, \alpha_j^\vee \right\rangle + \left\langle \eta, \alpha_j^\vee \right\rangle = \eta_j - \eta_{j+1}. \tag{C.2.31}$$

This immediately leads to the conclusion that all such λ are dominant since $\eta_j \geq \eta_{j+1}$. In addition, since $|\eta_j| \leq k$ there is one vector with $\eta_1 = k$ and $\eta_N = -k$ that is higher

than any other λ. Translating to the standard basis

$$\lambda = (\eta_j - \eta_{j+1})\Big(A^{-1}\Big)^j_k \alpha^k. \tag{C.2.32}$$

Then

$$\begin{aligned} k\alpha^{1N} - \lambda &= \sum_{i=1}^{N-1} \Big[k - (\eta_j - \eta_{j+1})\Big(A^{-1}\Big)^j_i\Big]\alpha^i, \\ &= \sum_{i=1}^{N-1} \theta_i \alpha^i, \end{aligned} \tag{C.2.33}$$

where the θ_i are necessarily non-negative real numbers, which follows from the definition of the Cartan matrix A. We then have

$$(\text{C.2.30}) \implies \lambda \text{ dominant} \wedge k\alpha^{1N} \succeq \lambda. \tag{C.2.34}$$

Going in the other direction, if we assume λ can be written as

$$\lambda = k\alpha^{1N} - \theta_{ij}\alpha^{ij}, \tag{C.2.35}$$

where

$$\theta_{ij} = 0 \quad \text{if} \quad i \geq j, \quad \theta_{ij} \geq 0 \quad \text{if} \quad i < j, \tag{C.2.36}$$

then such a vector has Dynkin labels

$$\Big\langle \lambda, \alpha_j^\vee \Big\rangle = k\delta^1_j + k\delta^N_{j+1} + \underbrace{\sum_{i=1}^{N} [\theta_{i\,j} - \theta_{j\,i}]}_{-m_j} - \underbrace{\sum_{i=1}^{N} [\theta_{i\,j+1} - \theta_{j+1\,i}]}_{-m_{j+1}}. \tag{C.2.37}$$

Requiring each component be a non-negative integer then gives

$$-m_j + m_{j+1} \in \mathbb{N}_0 \tag{C.2.38a}$$

$$m_1 - k \leq m_2 \tag{C.2.38b}$$

$$m_j \leq m_{j+1}, \quad 1 < j < N-1, \tag{C.2.38c}$$

$$m_{N-1} - k \leq m_N. \tag{C.2.38d}$$

It is no restriction to assume the m_j are themselves integers, since we can always add a vector of the form $c_j\omega^j$, where $c_j = c \in \mathbb{R}$, and get an identical representation. Setting $j = N$,

$$m_N = -\sum_{i=1}^{N} [\theta_{iN} - \theta_{Ni}] = -\sum_{i=1}^{N} \theta_{iN}, \tag{C.2.39}$$

implies $m_N \leq 0$, because the θ_{ij} are necessarily non-negative. Setting $j = 1$ yields

$$m_1 = -\sum_{i=1}^{N} [\theta_{i1} - \theta_{1i}] = \sum_{i=1}^{N} \theta_{1i}, \tag{C.2.40}$$

which implies $m_1 \geq 0$. In addition, we also have

$$\sum_{j=1}^{N} m_j = \sum_{j=1}^{N}\sum_{i=1}^{N} [\theta_{ij} - \theta_{ji}] = 0. \tag{C.2.41}$$

Then writing

$$\eta_i \equiv -m_i + k\delta_i^1 - k\delta_i^N, \tag{C.2.42}$$

gives $\lambda = (\eta_j - \eta_{j+1})\omega^j$, where the η_j satisfy (C.2.30). Therefore

$$\lambda \text{ dominant} \wedge k\alpha^{1N} \succeq \lambda \implies \text{(C.2.30)}. \tag{C.2.43}$$

We have then shown the implication in both directions, so together (C.2.34) and (C.2.43) are

$$\text{(C.2.30)} \iff \lambda \text{ dominant} \wedge k\alpha^{1N} \succeq \lambda, \tag{C.2.44}$$

and the conditions can be interchanged.

From Lemma 3.3.1 the highest weight of the highest irrep in $\mathrm{G}_N^{\otimes k}$ is $\bar{\Lambda} = k\alpha^{1N}$. We then have:

$$\forall \lambda \mid \lambda \text{ dominant} \wedge \bar{\Lambda} \succeq \lambda \colon V_\lambda \subset (V_F \otimes V_F^*)^{\otimes k}. \tag{C.2.45}$$

But then, from (C.2.23), this implies $V_\lambda \subset \mathrm{G}_N^{\otimes k}$, which proves the theorem. □

We can then think of the integers m_j as the number of boxes removed from row j of the tableau corresponding to the irrep with highest weight $\bar{\Lambda}$. Because the sum over all m_j is zero we clearly never remove any boxes from the tableau (unless we form a completed column). As well, because the m_j are weakly decreasing we can only move boxes from the upper rows of the tableau to the lower rows.

Theorem C.2.3 immediately leads to two new identities for the Littlewood-Richardson coefficients, which some may find useful.

Corollary C.2.3.1. *For λ a dominant partition of the integer Nk, such that*

$$\bar{\Lambda} - \lambda = \theta_{ij}\alpha^{ij}, \quad \theta_{ij} \in \mathbb{R}^+, \ \alpha^{ij} \in \Delta^+, \tag{C.2.46}$$

where $\bar{\Lambda}$ is the partition of the integer Nk:

$$\begin{aligned} \bar{\Lambda} &= 2k + \underbrace{k + \ldots + k}_{N-2}, \\ &\equiv k\alpha^{1N} \\ &\equiv k\omega^1 + k\omega^{N-1}, \end{aligned} \tag{C.2.47}$$

we have

$$\sum_{\mu \in P_k} \sum_{\nu \in P_k} c_{\lambda\nu}^{\mu} > 0, \tag{C.2.48}$$

and

$$\sum_{n=0}^{k} \sum_{\mu_n \in P_n} \sum_{\nu_n \in P_n} (-1)^{k-n} \binom{k}{n} m_{\mu_n} m_{\nu_n} c_{\lambda\nu}^{\mu} > 0. \tag{C.2.49}$$

C.3 User Manual for the `tessellation` code

The code can be easily installed by cloning the repository https://github.com/jaulbric/Tesselation. Alternatively, the package can be downloaded by issuing the following commands via a terminal:

bash:

```
# Get the version of the latest release
version=`curl -s
↪  https://api.github.com/repos/jaulbric/Tesselation/releases/latest \
| grep "tag_name" \
| cut -d ":" -f 2 \
| tr -d " "-\"-,`
# download and untar the package
wget https://github.com/jaulbric/Tesselation/archive/$version.tar.gz \
&& mkdir ~/Tesselation \
&& tar xvfz $version.tar.gz -C ~/Tesselation \
--strip-components 1 && rm $version.tar.gz
```

csh/tcsh:

```
# Get the version of the latest release
set version=`curl -s
↪  https://api.github.com/repos/jaulbric/Tesselation/releases/latest \
| grep "tag_name" \
| cut -d ":" -f 2 \
| tr -d " "-\"-,`
# download and untar the package
wget https://github.com/jaulbric/Tesselation/archive/$version.tar.gz \
&& mkdir ~/Tesselation \
&& tar xvfz $version.tar.gz -C ~/Tesselation \
--strip-components 1 && rm $version.tar.gz
```

Once downloaded the package can be installed with `pip install .` in the root directory of the repository (in the above examples `~/Tesselation`).

We now give an example of how to use the code by reproducing the results of Fig. 3.5.

```
import numpy as np
import tesselation as t

X1 = np.array([3, 0, 0, 1])
X2 = np.array([0, 2, 1, 0])
X3 = np.array([0, 0, 1, 1])
X4 = np.array([1, 3, 0, 0])
```

```
N = 5
i = N - t.Nality(X1) # This is 3 for all cases

idx = 1
for x in [X1, X2, X3, X4]:
    l1, l2 = t.l_pair(x, i) # Calculate l1 and l2
    fj = t.fj(x) # Calculate the Dynkin label
    kmin = t.kmin(x) # Calculate kmin
    print("X{0}:".format(idx))
    print("l1 = {0}, l2 = {1}".format(l1, l2))
    print("f = ({0}, {1}, {2}, {3})".format(*fj))
    print("kmin = {0}\n".format(kmin))
    idx += 1
```

The output of the above code is

```
X1:
l1 = 1, l2 = 4
f = (2, 0, 1, 0)
kmin = 2

X2:
l1 = 2, l2 = 3
f = (0, 1, 1, 0)
kmin = 2

X3:
l1 = 0, l2 = 3
f = (1, 0, 0, 1)
kmin = 1

X4:
l1 = 2, l2 = 5
f = (1, 2, 0, 0)
kmin = 3
```

There are four helper functions available to the user:

- `l_pair(p, i)`: Takes a Dynkin label (`list` or `numpy.ndarray`) and a `int` as input and outputs ℓ_1 and ℓ_2 as described in Section 3.3.1.
- `Nality(p)`: Takes a Dynkin label (`list` or `numpy.ndarray`) as an input and returns the N-ality of the representation, that is $\sum_{j=0}^{N-1} jp_j \mod N$.
- `fj(p)`: Takes a Dynkin label (`list` or `numpy.ndarray`) as an input and returns the Dynkin label of the irrep in $X \otimes Q_i$ that gives the smallest value of k_{min}.

- `kmin(p)`: Takes a Dynkin label (`list` or `numpy.ndarray`) as an input and returns the minimum number of copies of the adjoint representation required such that $\mathbb{1} \subset X \otimes Q_i \otimes G_N^{\otimes k_{\min}}$.

Appendix D

Functional Determinants in Quantum Field Theory

D.1 Jost Matrix Function Asymptotics

D.1.1 Large l

Using the Volterra integral representation of $U_{0,l}(r;z)$ (4.3.45) and the definition

$$T_l(r;z) = \left[U_{0,l}^{\text{free}}(r;z)\right]^{-1} U_{0,l}(r;z)$$

we find a Volterra integral representation of $T_l(r;z)$:

$$\begin{aligned} T_l(r;z) &= \mathbb{1} + \lambda \int_0^r U_{\infty,l}^{\text{free}}(t;z)\, V(t)\, U_{0,l}^{\text{free}}(t;z)\, T_l(t;z)\, t^{d-1}\, \mathrm{d}t \\ &\quad - \lambda \left[U_{0,l}^{\text{free}}(r;z)\right]^{-1} U_{\infty,l}^{\text{free}}(r;z) \int_0^r U_{0,l}^{\text{free}}(t;z)\, V(t)\, U_{0,l}^{\text{free}}(t;z)\, T_l(t;z)\, t^{d-1}\, \mathrm{d}t\,, \end{aligned} \tag{D.1.1}$$

where λ is a power counting parameter that will be set to 1 in the end. We then expand in powers of λ

$$T_l(r;z) \sim \sum_{k=0}^{\infty} \mathcal{T}_l^{(k)}(r;z)\, \lambda^k, \quad (\lambda \to 0). \tag{D.1.2}$$

Solving for each term order by order gives

$$\mathcal{T}_l^{(0)}(r;z) = \mathbb{1}, \tag{D.1.3}$$

$$\mathcal{T}_l^{(k+1)}(r;z) = \int_0^r \mathcal{U}_l(r,t;z)\, V(t)\, U_{0,l}^{\text{free}}(t;z)\, \mathcal{T}_l^{(k)}(t;z)\, t^{d-1}\, \mathrm{d}t\,, \tag{D.1.4}$$

where

$$\mathcal{U}_l(r,t;z) \equiv U_{\infty,l}^{\text{free}}(t;z) - \left[U_{0,l}^{\text{free}}(r;z)\right]^{-1} U_{\infty,l}^{\text{free}}(r;z)\, U_{0,l}^{\text{free}}(t;z)\,. \tag{D.1.5}$$

The first few terms are given explicitly as

$$\mathcal{T}_l^{(0)}(r;z) = \mathbb{1}, \tag{D.1.6}$$

$$\mathcal{T}_l^{(1)}(r;z) = \int_0^r \mathcal{U}_l(r,s;z)\, V(s)\, U_{0,l}^{\text{free}}(s;z)\, s^{d-1}\, \mathrm{d}s\,, \tag{D.1.7}$$

$$\begin{aligned}\mathcal{T}_l^{(2)}(r;z) = \int_0^r \mathcal{U}_l(r,s;z)\, V(s)\, U_{0,l}^{\text{free}}(s;z) \\ \times \int_0^s \mathcal{U}_l(s,t;z)\, V(t)\, U_{0,l}^{\text{free}}(t;z)\, t^{d-1}\, \mathrm{d}t\, s^{d-1}\, \mathrm{d}s\,.\end{aligned} \tag{D.1.8}$$

Higher order terms are given by

$$\mathcal{T}_l^{(k+1)}(r_{k+1};z) = \prod_{j=0}^{k} \left[\int_0^{r_{j+1}} \mathcal{U}_l(r_{j+1},r_j;z)\, V(r_j)\, U_{0,l}^{\text{free}}(r_j;z)\, r_j^{d-1}\, \mathrm{d}r_j\right]\mathbb{1}. \tag{D.1.9}$$

The ordering of the terms in (D.1.9) is important since these matrices generally don't commute. The convention is that higher terms in the product are prepended on the left.

Taking the trace of the logarithm of this matrix function then gives

$$\mathrm{tr}[\ln(T_l(r;z))] = \mathrm{tr}\left[\ln\left(\mathbb{1} + \sum_{k=1}^{\infty} \mathcal{T}_l^{(k)}(r;z)\,\lambda^k\right)\right]. \tag{D.1.10}$$

Because we know that the $\mathcal{T}_l^{(1)}(r;z)$ term is order ν^{-1} this series expansion in powers of λ is asymptotic in powers of ν^{-1}. We are usually interested in dimensions $d \leq 4$, where we only need to keep terms up to λ^2 in order to renormalize the functional determinant. However, the higher order corrections are useful in order to accelerate the convergence of the partial wave expansion, so we retain a few extra terms. Expanding the above in powers of λ we find (we will drop the explicit dependence on l, r, and z here)

$$\begin{aligned}\mathrm{tr}[\ln(T_l(r;z))] \sim \lambda\,\mathrm{tr}\left[\mathcal{T}^{(1)}\right] + \lambda^2\,\mathrm{tr}\left[\mathcal{T}^{(2)} - \frac{1}{2}\left(\mathcal{T}^{(1)}\right)^2\right] \\ + \lambda^3\,\mathrm{tr}\left[\mathcal{T}^{(3)} - \mathcal{T}^{(1)}\mathcal{T}^{(2)} + \frac{1}{3}\left(\mathcal{T}^{(1)}\right)^3\right] \\ + \lambda^4\,\mathrm{tr}\left[\mathcal{T}^{(4)} - \frac{1}{2}\left(\left(\mathcal{T}^{(2)}\right)^2 + 2\mathcal{T}^{(1)}\mathcal{T}^{(3)}\right) + \left(\mathcal{T}^{(1)}\right)^2\mathcal{T}^{(2)} - \frac{1}{4}\left(\mathcal{T}^{(1)}\right)^4\right],\end{aligned} \tag{D.1.11}$$

where we have used the cyclic property of the trace to rearrange a few terms. The Jost matrix is just the above expression in the limit that $r \to \infty$. Things are going to get a little messy though, so we introduce some notation:

$$\tilde{V}_{0,l}^{0}(r;z) \coloneqq U_{0,l}^{\text{free}}(r;z)\, V(r)\, U_{0,l}^{\text{free}}(r;z)\,, \tag{D.1.12}$$

$$\tilde{V}_{\infty,l}^{0}(r;z) \coloneqq U_{0,l}^{\text{free}}(r;z)\, V(r)\, U_{\infty,l}^{\text{free}}(r;z)\,, \tag{D.1.13}$$

$$\tilde{V}_{0,l}^{\infty}(r;z) \coloneqq U_{\infty,l}^{\text{free}}(r;z)\, V(r)\, U_{0,l}^{\text{free}}(r;z)\,, \tag{D.1.14}$$

$$\tilde{V}_{\infty,l}^{\infty}(r;z) \coloneqq U_{\infty,l}^{\text{free}}(r;z)\, V(r)\, U_{\infty,l}^{\text{free}}(r;z)\,. \tag{D.1.15}$$

Using this notation, we write the first few terms as

$$\lim_{R\to\infty} \mathcal{T}_l^{(1)}(r;z) = \int_0^\infty \tilde{V}_{0,l}^{\infty}(r;z)\, r^{d-1}\,\mathrm{d}r\,. \tag{D.1.16}$$

$$\begin{aligned}\lim_{R\to\infty} \mathcal{T}_l^{(2)}(r;z) = &\int_0^\infty \int_0^r \tilde{V}_{0,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{\infty}(t;z)\, t^{d-1}\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r \\ &- \int_0^\infty \int_0^r \tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{0}(t;z)\, t^{d-1}\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r\end{aligned} \tag{D.1.17}$$

$$\begin{aligned}\lim_{R\to\infty} \mathcal{T}_l^{(3)}(r;z) = &\int_0^\infty \int_0^r \int_0^t \tilde{V}_{0,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{\infty}(t;z)\, \tilde{V}_{0,l}^{\infty}(s;z)\, s^{d-1}\,\mathrm{d}s\, t^{d-1}\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r \\ &- \int_0^\infty \int_0^r \int_0^t \tilde{V}_{0,l}^{\infty}(r;z)\, \tilde{V}_{\infty,l}^{\infty}(t;z)\, \tilde{V}_{0,l}^{0}(s;z)\, s^{d-1}\,\mathrm{d}s\, t^{d-1}\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r \\ &- \int_0^\infty \int_0^r \int_0^t \tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{0}(t;z)\, \tilde{V}_{0,l}^{\infty}(s;z)\, s^{d-1}\,\mathrm{d}s\, t^{d-1}\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r \\ &+ \int_0^\infty \int_0^r \int_0^t \tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{\infty,l}^{0}(t;z)\, \tilde{V}_{0,l}^{0}(s;z)\, s^{d-1}\,\mathrm{d}s\, t^{d-1}\,\mathrm{d}t\, r^{d-1}\,\mathrm{d}r\end{aligned} \tag{D.1.18}$$

There will be a great deal of cancellation here. For instance, in the λ^2 term we have

$$\begin{aligned}&\lim_{R\to\infty} \operatorname{tr}\Big[\mathcal{T}^{(2)}(R;z) - \frac{1}{2}\Big(\mathcal{T}^{(1)}(R;z)\Big)^2\Big] \\ &\quad= \int_0^\infty \int_0^\infty \operatorname{tr}\Big[\tilde{V}_{0,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{\infty}(s;z)\Big]\, \Theta(r-s)\, s^{d-1}\,\mathrm{d}s\, r^{d-1}\,\mathrm{d}r \\ &\qquad- \int_0^\infty \int_0^r \operatorname{tr}\Big[\tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{0}(s;z)\Big] s^{d-1}\,\mathrm{d}s\, r^{d-1}\,\mathrm{d}r \\ &\qquad- \frac{1}{2}\int_0^\infty \int_0^\infty \operatorname{tr}\Big[\tilde{V}_{0,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{\infty}(s;z)\Big] r^{d-1} s^{d-1}\,\mathrm{d}r\,\mathrm{d}s \\ &\quad= -\int_0^\infty \int_0^r \operatorname{tr}\Big[\tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{0}(s;z)\Big] s^{d-1}\,\mathrm{d}s\, r^{d-1}\,\mathrm{d}r\end{aligned} \tag{D.1.19}$$

We have cancelled the first and last integrals by exchanging the integration variables and using the cyclic property of the trace. Similarly, the λ^3 term reduces to

$$\begin{aligned}&\lim_{R\to\infty} \operatorname{tr}\Big[\mathcal{T}^{(3)}(R;z) - \mathcal{T}^{(2)}(R;z)\,\mathcal{T}^{(1)}(R;z) + \frac{1}{3}\Big(\mathcal{T}^{(1)}(R;z)\Big)^3\Big] \\ &\quad= \int_0^\infty \int_0^r \int_s^r \operatorname{tr}\Big[\tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{0,l}^{0}(s;z)\, \tilde{V}_{0,l}^{\infty}(t;z)\Big] t^{d-1}\,\mathrm{d}t\, s^{d-1}\,\mathrm{d}s\, r^{d-1}\,\mathrm{d}r \\ &\qquad+ \int_0^\infty \int_0^r \int_0^s \operatorname{tr}\Big[\tilde{V}_{\infty,l}^{\infty}(r;z)\, \tilde{V}_{\infty,l}^{0}(s;z)\, \tilde{V}_{0,l}^{0}(t;z)\Big] t^{d-1}\,\mathrm{d}t\, s^{d-1}\,\mathrm{d}s\, r^{d-1}\,\mathrm{d}r\,.\end{aligned} \tag{D.1.20}$$

After deforming the contour integral of the zeta function we integrate over z from 0 to $-\infty$. Thus, z will always be negative, and the components of these potential matrices are

$$\Big[\tilde{V}^0_{0,l}(r;-z)\Big]^i_j = 2^{2\nu}\,\Gamma^2(\nu+1)\,r^{2-d}k_i^{-\nu}k_j^{-\nu}\,I_\nu(k_ir)\,I_\nu(k_jr)\,V_j^i(r)\,, \tag{D.1.21}$$

$$\Big[\tilde{V}^0_{\infty,l}(r;-z)\Big]^i_j = r^{2-d}k_i^{-\nu}k_j^{\nu}\,I_\nu(k_ir)\,K_\nu(k_jr)\,V_j^i(r)\,, \tag{D.1.22}$$

$$\Big[\tilde{V}^\infty_{0,l}(r;-z)\Big]^i_j = r^{2-d}k_i^{\nu}k_j^{-\nu}\,K_\nu(k_ir)\,I_\nu(k_jr)\,V_j^i(r)\,, \tag{D.1.23}$$

$$\Big[\tilde{V}^\infty_{\infty,l}(r;-z)\Big]^i_j = \frac{1}{2^{2\nu}\,\Gamma^2(\nu+1)}r^{2-d}k_i^{\nu}k_j^{\nu}\,K_\nu(k_ir)\,K_\nu(k_jr)\,V_j^i(r)\,, \tag{D.1.24}$$

where $k_i = \sqrt{m_i^2+z}$. To calculate the order λ term we then evaluate

$$\int_0^\infty K_\nu(k_ir)\,I_\nu(k_ir)\,V_i^i(r)\,r\,\mathrm{d}r\,.$$

To calculate the order λ^2 term we evaluate

$$\int_0^\infty\int_0^r K_\nu(k_ir)\,K_\nu(k_jr)\,I_\nu(k_js)\,I_\nu(k_is)\,V_j^i(r)\,V_i^j(s)\,s\,\mathrm{d}s\,r\,\mathrm{d}r\,.$$

To calculate the order λ^3 term we evaluate

$$\int_0^\infty\int_r^\infty\int_0^r K_\nu(k_ir)\,I_\nu(k_jr)\,K_\nu(k_js)\,K_\nu(k_ls)\,I_\nu(k_lt)\,I_\nu(k_it)$$
$$\times\Big[V_j^i(r)\,V_l^j(s)\,V_i^l(t)+V_j^{*i}(r)\,V_l^{*j}(s)\,V_i^{*l}(t)\Big]t\,\mathrm{d}t\,s\,\mathrm{d}s\,r\,\mathrm{d}r$$

Taking the limit $\nu\to\infty$, $k_i\to\infty$, while holding k_i/ν fixed we can then approximate the integrals using the uniform asymptotic approximations of the Bessel functions, and integration by parts. Let

$$\eta_i \equiv \sqrt{1+\frac{k_i^2r^2}{\nu^2}}+\ln\!\left(\frac{k_ir}{\nu}\right)-\ln\!\left(1+\sqrt{1+\frac{k_i^2r^2}{\nu^2}}\right),\qquad p_i\equiv\frac{1}{\sqrt{1+\frac{k_i^2r^2}{\nu^2}}}. \tag{D.1.25}$$

The uniform asymptotic expansion of the modified Bessel functions is

$$I_\nu(\nu z)\sim\frac{e^{\nu\eta}}{(2\pi\nu)^{1/2}(1+z^2)^{1/4}}\sum_{k=0}^\infty\frac{W_k(p)}{\nu^k},\qquad(\nu\to\infty), \tag{D.1.26}$$

$$K_\nu(\nu z)\sim\left(\frac{\pi}{2\nu}\right)^{1/2}\frac{e^{-\nu\eta}}{(1+z^2)^{1/4}}\sum_{k=0}^\infty(-1)^k\frac{W_k(p)}{\nu^k},\qquad(\nu\to\infty), \tag{D.1.27}$$

where the $W_k(p)$ are polynomials in p of degree $3k$, with $W_0(p)=1$ and

$$W_{k+1}(p)=\frac{1}{2}p^2\Big(1-p^2\Big)\,W_k'(p)+\frac{1}{8}\int_0^p\Big(1-5t^2\Big)\,W_k(t)\,\mathrm{d}t\,. \tag{D.1.28}$$

We will explicitly calculate only terms up to order ν^{-3}, as this is all that is needed to renormalize the functional determinant in $d = 4$ dimensions. Higher order terms can be calculated, but they quickly become quite tedious. It is not too hard to show that the λ^3 term is in fact order ν^{-5}, so we will not include this term. The leading order approximation to the λ^2 comes from approximating the intergal

$$\int_0^r I_\nu(k_j s)\, I_\nu(k_i s)\, V_i^j(s)\, s\, \mathrm{d}s$$

$$\sim \frac{1}{2\pi\nu} \int_0^r \frac{e^{\nu(\eta_j(s)+\eta_i(s))}}{\left(1+\frac{k_j^2 s^2}{\nu^2}\right)^{1/4}\left(1+\frac{k_i^2 s^2}{\nu^2}\right)^{1/4}} V_i^j(s)\, s\, \mathrm{d}s\,, \quad (\nu\to\infty). \quad \text{(D.1.29)}$$

Then writing the exponential term as

$$e^{\nu(\eta_j(s)+\eta_i(s))} = \frac{s}{\nu} \frac{\frac{\mathrm{d}}{\mathrm{d}s} e^{\nu(\eta_j(s)+\eta_i(s))}}{\sqrt{1+\frac{k_j^2 s^2}{\nu^2}}+\sqrt{1+\frac{k_j^2 s^2}{\nu^2}}}, \quad \text{(D.1.30)}$$

The integral is then approximated by

$$\int_0^r I_\nu(k_j s)\, I_\nu(k_i s)\, V_i^j(s)\, s\, \mathrm{d}s$$

$$\sim \frac{1}{2\pi\nu^2} \frac{e^{\nu(\eta_j(r)+\eta_i(r))}\, V_i^j(r)\, r^2}{\left(1+\frac{k_j^2 r^2}{\nu^2}\right)^{1/4}\left(1+\frac{k_i^2 r^2}{\nu^2}\right)^{1/4}\left[\sqrt{1+\frac{k_j^2 r^2}{\nu^2}}+\sqrt{1+\frac{k_j^2 r^2}{\nu^2}}\right]}, \quad (\nu\to\infty). \quad \text{(D.1.31)}$$

The leading contribution from the λ^2 term is then

$$\int_0^\infty \int_0^r K_\nu(k_i r)\, K_\nu(k_j r)\, I_\nu(k_j s)\, I_\nu(k_i s)\, V_j^i(r)\, V_i^j(s)\, s\, \mathrm{d}s\, r\, \mathrm{d}r$$

$$\sim \frac{1}{4\nu^3} \int_0^\infty \frac{V_j^i(r)\, V_i^j(r)\, r^3\, \mathrm{d}r}{\left(1+\frac{k_j^2 r^2}{\nu^2}\right)^{1/2}\left(1+\frac{k_i^2 r^2}{\nu^2}\right)^{1/2}\left[\sqrt{1+\frac{k_j^2 r^2}{\nu^2}}+\sqrt{1+\frac{k_j^2 r^2}{\nu^2}}\right]}, \quad (\nu\to\infty). \quad \text{(D.1.32)}$$

The λ term is even easier to approximate, since the exponential terms cancel immediately.

$$\int_0^\infty K_\nu(k_i r)\, I_\nu(k_i r)\, V_i^i(r)\, r\, \mathrm{d}r \sim \frac{1}{2\nu} \int_0^\infty \frac{V_{ii}(r)\, r\, \mathrm{d}r}{\left[1+\frac{k_i^2 r^2}{\nu^2}\right]^{1/2}}$$

$$+ \frac{1}{16\nu^3} \int_0^\infty \left[1 - \frac{6}{1+\frac{k_i^2 r^2}{\nu^2}} + \frac{5}{\left[1+\frac{k_i^2 r^2}{\nu^2}\right]^2}\right] \frac{V_i^i(r)\, r\, \mathrm{d}r}{\left[1+\frac{k_i^2 r^2}{\nu^2}\right]^{3/2}}, \quad (\nu\to\infty). \quad \text{(D.1.33)}$$

We then have the large l approximation of the Jost matrix function as

$$\begin{aligned}\operatorname{tr}[\ln(F_l(-z))] \sim{}& \frac{1}{2\nu}\int_0^\infty \frac{V_{ii}(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{1/2}} \\ &+\frac{1}{16\nu^3}\int_0^\infty \left[1-\frac{6}{1+\frac{k_i^2r^2}{\nu^2}}+\frac{5}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^2}\right]\frac{V_i^i(r)\,r\,\mathrm{d}r}{\left[1+\frac{k_i^2r^2}{\nu^2}\right]^{3/2}} \\ &+\frac{1}{4\nu^3}\int_0^\infty \frac{V_j^i(r)\,V_i^j(r)\,r^3\,\mathrm{d}r}{\left(1+\frac{k_j^2r^2}{\nu^2}\right)^{1/2}\left(1+\frac{k_i^2r^2}{\nu^2}\right)^{1/2}\left[\sqrt{1+\frac{k_j^2r^2}{\nu^2}}+\sqrt{1+\frac{k_j^2r^2}{\nu^2}}\right]}, \quad (\nu\to\infty),\end{aligned} \tag{D.1.34}$$

Higher order corrections can be obtained in a similar manner, but because of the integration by parts procedure used to determine the λ^2 term this becomes rather complicated. At first it would appear that there should be a contribution at the order of ν^{-4}, but numerical experiments show that this term vanishes.

D.1.2 Small r

The boundary conditions imply that the matrix function $T_l(r;z)$ has a valid Taylor series expansion at small r:

$$T_l(r;z)=\sum_{k=0}^{\infty} T_{l,k}(z)\,r^k. \tag{D.1.35}$$

The first two terms are easily found by iterating the integral representation of $T_l(r;z)$;

$$T_{l,0}(z)=\mathbb{1}, \qquad T_{l,1}(z)=\mathbf{0}. \tag{D.1.36}$$

Further expanding the matrix potential as a power series in small r

$$V(r)\sim V_0+V_1r+V_2r^2, \quad (r\to 0), \tag{D.1.37}$$

as well as the free solutions

$$U_{0,l}^{\text{free}}(r;z)\sim r^l\left(\mathbb{1}+k^2\frac{r^2}{2(2l+d)}\right), \qquad (r\to 0), \tag{D.1.38a}$$

$$\left[U_{0,l}^{\text{free}}(r;z)\right]^{-1}\sim r^{-l}\left(\mathbb{1}-k^2\frac{r^2}{2(2l+d)}\right), \qquad (r\to 0), \tag{D.1.38b}$$

where the matrix k is defined by

$$k_j^i\equiv\sqrt{m_i^2-z}\,\delta_j^i, \tag{D.1.39}$$

we can determine the higher order terms using the differential equation for $T_l(r;z)$. We retain terms up to r^2 and drop all higher order terms, and use

$$\frac{d-1}{r} + 2\Big[U_{0,l}^{\text{free}}(r;z)\Big]^{-1} \frac{\mathrm{d}}{\mathrm{d}r}\, U_{0,l}^{\text{free}}(r;z) \sim \frac{2l+d-1}{r} + 2k^2 \frac{r}{2l+d}, \tag{D.1.40a}$$

$$\Big[U_{0,l}^{\text{free}}(r;z)\Big]^{-1} V(r)\, U_{0,l}^{\text{free}}(r;z) \sim V_0 + V_1 r + \left\{V_2 + \frac{1}{2(2l+d)}\Big[V_0, k^2\Big]\right\} r^2. \tag{D.1.40b}$$

We then find the next two terms are

$$T_{l,2}(z) = \frac{1}{2(2l+d)}\, V(0)\,, \tag{D.1.41a}$$

$$T_{l,3}(z) = \frac{1}{3(2l+d+1)}\, \frac{\mathrm{d}}{\mathrm{d}r}\, V(r)\Big|_{r=0}. \tag{D.1.41b}$$

D.2 Numerical Solution of Jost Matrix Function

In this appendix we briefly describe a procedure to efficiently find the Jost matrix function numerically. The differential equation to be solved is (we set $z = 0$ and suppress the dependence on z)

$$\frac{\mathrm{d}^2 T_l}{\mathrm{d}r^2} + \left(\frac{d-1}{r} + 2\left[U_{0,l}^{\text{free}}(r)\right]^{-1} \frac{\mathrm{d}\, U_{0,l}^{\text{free}}(r)}{\mathrm{d}r}\right) \frac{\mathrm{d}T_l}{\mathrm{d}r} - \Big[U_{0,l}^{\text{free}}(r)\Big]^{-1} V(r)\, U_{0,l}^{\text{free}}(r)\, T_l = 0,$$

with boundary conditions

$$T_l(0) = \mathbb{1}, \qquad\qquad \frac{\mathrm{d}T_l}{\mathrm{d}r}\Big|_{r=0} = \mathbb{0}.$$

Most numerical integration routines require the differential equation be written in first-order form, so we define

$$Y_l(r) \coloneqq \begin{pmatrix} T_l(r) \\ \dfrac{\mathrm{d}\, T_l(r)}{\mathrm{d}r} \end{pmatrix}, \tag{D.2.1}$$

and the first order operator

$$F(r, Y_l(r)) \coloneqq \frac{\mathrm{d}\, Y_l(r)}{\mathrm{d}r}. \tag{D.2.2}$$

The first order system can then be written as

$$F(r, Y_l(r)) = \frac{1}{r} S\, Y_l(r) + f(r, Y_l(r))\,, \qquad\qquad Y_l(0) = \begin{pmatrix} \mathbb{1} \\ \mathbb{0} \end{pmatrix}, \tag{D.2.3}$$

where

$$S \equiv \begin{pmatrix} \mathbb{0} & \mathbb{0} \\ \mathbb{0} & -(2l+d-1)\mathbb{1} \end{pmatrix}, \tag{D.2.4}$$

and

$$f(r, Y_l(r)) = \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ \left[U^{\text{free}}_{0,l}(r)\right]^{-1} V(r)\, U^{\text{free}}_{0,l}(r) & \frac{2l}{r} - 2\left[U^{\text{free}}_{0,l}(r)\right]^{-1} \frac{\mathrm{d}U^{\text{free}}_{0,l}(r)}{\mathrm{d}r} \end{pmatrix} Y_l(r)\,. \quad \text{(D.2.5)}$$

The boundary conditions imply that the first order system is regular everywhere, but numerically the singular term results in $0/0$ when evaluating r at the origin. In order to improve the numerical analysis we convert this into an algebraic-differential equation in the spirit of [122], by treating the origin as a special point. Regularity at the origin requires

$$\lim_{r\to 0} \frac{1}{r} S\, Y_l(r) = S\, Y_l'(0)\,. \quad \text{(D.2.6)}$$

Thus, taking the limit $r \to 0$ in (D.2.2) then gives

$$F(0, Y_l(0)) = S\, F(0, Y_l(0)) + f(0, Y_l(0))\,. \quad \text{(D.2.7)}$$

Because the constant matrix S is singular we cannot invert it. Instead, we employ the Moore-Penrose inverse:

$$F(0, Y_l(0)) = (\mathbb{1} - S)^{+}\, f(0, Y_l(0))\,, \quad \text{(D.2.8)}$$

where

$$(\mathbb{1} - S)^{+} = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \frac{1}{2l+d}\mathbb{1} \end{pmatrix}. \quad \text{(D.2.9)}$$

We then have

$$F(0, Y_l(0)) = \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ \frac{1}{2l+d} V(0) & \mathbb{0} \end{pmatrix} Y_l(0)\,. \quad \text{(D.2.10)}$$

We can then readily solve the first order system using standard techniques (for instance, using an explicity Runge-Kutta method), using (D.2.2) for $r > 0$ and (D.2.10) for $r = 0$.

When l becomes very large the system can become stiff, resulting in very long integration times and loss of precision. Implicit integration routines typically require analytic Jacobians. Here, again, we will run into numerical difficulties using (D.2.2) when $r = 0$. The solutions will be found column-wise for the full matrix solution, so we let $Y_l(r)$ implicitly represent a fixed column of the full matrix solution and

$$[Y_l(r)]_i \equiv [Y_l(r)]_{ij},$$

suppressing the index j, since it will be fixed throughout the calculation. The Jacobian is given generally by

$$J_{ij}(r, Y_l(r)) = \frac{\partial\, F_i(r, Y_l(r))}{\partial [Y_l(r)]_j}. \quad \text{(D.2.11)}$$

For $r > 0$ this unambiguously gives

$$J_{ij}(r, Y_l(r)) = \frac{1}{r} S_{ij} + \frac{\partial\, f_i(r, Y_l(r))}{\partial [Y_l(r)]_j}, \quad r > 0. \quad \text{(D.2.12)}$$

When $r = 0$ however we should instead substitute (D.2.10) into (D.2.11), which yields

$$J(0, Y_l(0)) = \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ \frac{1}{2l+d} V(0) & \mathbb{0} \end{pmatrix}. \tag{D.2.13}$$

A popular class of stiff integrators are the Rosenbrock diagonally implicit Runge-Kutta methods. These methods are designed to solve autonomous systems. For non-autonomous systems one can transform the system to an autonomous one by including the independent variable r as an extra entry in the dependent vector $Y_l(r)$, essentially increasing the system size to $n + 1$. Popular Rosenbrock solvers do this resizing internally, but the user must further supply the integration routine with another partial derivative:

$$\frac{\partial F(r, Y_l(r))}{\partial r},$$

where the components of $Y_l(r)$ are treated as independent of r. For $r > 0$ we again encounter no difficulties, and using (D.2.2) we find

$$\frac{\partial F(r, Y_l(r))}{\partial r} = -\frac{1}{r^2} S\, Y_l(r) + \frac{\partial f(r, Y_l(r))}{\partial r}, \quad r > 0. \tag{D.2.14}$$

The above expression cannot be used for $r = 0$ because it diverges. Instead, we use the results of Appendix D.1.2 to write

$$\frac{\mathrm{d} F(r, Y_l(r))}{\mathrm{d} r} \sim \begin{pmatrix} \frac{1}{2l+d} V(0)\, \mathbf{e}_i \\ \frac{2}{2l+d+1} V'(0)\, \mathbf{e}_i \end{pmatrix}, \quad (r \to 0), \tag{D.2.15}$$

where $\mathbf{e}_i$ is the i^{th} unit vector in $\mathbb{R}^n$, which corresponds to solving for the i^{th} column of $Y_l(r)$. We can then write

$$\frac{\partial F(r, Y_l(r))}{\partial r} = \frac{\mathrm{d} F(r, Y_l(r))}{\mathrm{d} r} - J(r, Y_l(r)) \frac{\mathrm{d} Y_l(r)}{\mathrm{d} r}. \tag{D.2.16}$$

Taking the $r \to 0$ limit of the above and replacing $J(r, Y_l(r))$ and $F(r, Y_l(r))$ with their $r = 0$ definitions yields

$$\left.\frac{\partial F(r, Y_l(r))}{\partial r}\right|_{r=0} = \begin{pmatrix} \mathbb{0} \\ \frac{2}{2l+d+1} V'(0)\, \mathbf{e}_i \end{pmatrix}. \tag{D.2.17}$$

Using these definitions at $r = 0$ then allows one to integrate the first order system over the entire domain (or at least up to some very large r), which improves the precision and removes the computational effort of having to choose a suitable starting position.

There is one more simple thing we can do to increase the precision of the numerical integration routine. When r is very large the free solutions grow exponentially fast, since they are composed of modified Bessel functions of the first kind. For large r one should then use exponentially scaled modified Bessel functions:

$$Ie_\nu(z) \coloneqq e^{-z} I_\nu(z)\,. \tag{D.2.18}$$

The exponential growth then either completely cancels, or at least partially cancels, in the differential equations, reducing the chance of overflow errors. Similarly, when r is small and l is large the modified Bessel functions rapidly approach 0, which causes 0/0 issues due to the finite precision of floating point representations. This can be alleviated by using generalized hypergeometric functions:

$$I_\nu(z) = \frac{\left(\frac{z}{2}\right)^\nu}{\Gamma(\nu+1)}\,{}_0F_1\left(;\nu+1;\tfrac{1}{4}z^2\right). \tag{D.2.19}$$

The factors of z^ν then cancel when taking ratios of modified Bessel functions of the same order. Because the generalized hypergeometric functions tend to 1 as their argument approaches 0 along the real line the ratios of hypergeometric functions are more numerically stable than ratios of modified Bessel functions for very small arguments.

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