Analysis of Regge poles in non-relativistic quantum mechanics

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Abstract

Regge poles—the name given to poles of the scattering amplitude in the complex angular momentum plane—are of utmost importance in atomic and molecular scattering. We investigate various aspects of non-relativistic Regge pole theory, namely, their behaviour at low energy, cardinality, and sensitivity to boundary conditions. Upon investigation of the former, we find the long-standing conjecture that Regge poles become stable bound states for ultra low energy to be true; the proof is achieved for a potential satisfying the first moment condition at infinity and whose product with the radial variable is bounded near the origin, with the proviso that singular behaviour of the Regge poles may occur. It is known that for an analytic potential V with $r^2|V(r)|$ bounded at the origin and at infinity, there are finitely many Regge poles; we demonstrate that this is still the case for a compactly supported potential which is not as singular as the Coulomb interaction at the origin. This begs the question of whether or not it is possible to explicitly count Regge poles. Not only is this a difficult and interesting mathematical problem, but it also has implications in atomic physics where total cross-sections are often calculated using summations over Regge pole contributions. The author's attempt at counting Regge poles has revealed an unexpected effect on the Regge poles due to boundary conditions: we show that infinitely many Regge poles go to infinity under nothing more than a change of boundary condition, at least for the free particle case.

This work was supported financially by the Engineering and Physical Sciences Research Council (EPSRC) between October 2007 and April 2011.

Acknowledgements

This thesis would not have been possible without the invaluable contributions of numerous individuals. First and foremost, I would like to deeply and sincerely thank my supervisors Prof. Marco Marletta and Prof. Malcolm Brown. It is absolutely certain that I would not have attained any of these results without their guidance and encouragement—sustained, as it was, over periods during which my progress was difficult to discern. I would especially like to thank Marco for so much of his time during the work on Chapter 4, and I look forward to hopefully continuing this collaboration in the future.

I am indebted to Dr. Robert L. Warnock for bringing to my attention an incomplete proof; this has relieved the mind of uncertainty. My research has drawn on a great many published sources, which are recognized at various places throughout the text. However, I must mention the remarkable book on special functions by Prof. Frank W. J. Olver, without which, Chapter 4 would have been many orders of magnitude more difficult; moreover, I would like to thank Prof. Olver for several helpful e-mail correspondences. I am also very grateful to Dr. Karl Michael Schmidt, not only for his help over the last few years, but also for some interesting conversations about physics.

Last, but by no means least, I would like to thank all of my family and friends for all their kindness and support. In particular, I thank my wife Jenny for all her love and understanding, and for shielding me from real life when I needed it.

Contents

CHAPTER 1

Introduction

In quantum field theory, quantum chromodynamics (QCD) describes precisely all particle interactions at sufficiently short separation distances, whilst Regge (pole) theory continues to highlight our lack of dynamical understanding of the strong nuclear force at long distances [Cox, 1998, p. 9]. However, it is of fundamental importance to be able to derive Regge behaviour within the QCD framework, since the theory of Regge poles illuminates the deep connection between very energetic scattering and the spectrum of particles and resonances [Kaidalov, 2001]. Despite this, the topic of Regge theory has largely been abandoned in high energy particle physics; however, various phenomena in atomic and molecular physics have generated substantial interest in the (non-relativistic) Regge pole method [Felfli et al., 2008a,b, Sokolovski et al., 2007]. In particular, there has been a surge in research into low energy scattering, which has probably been instigated by certain physical processes such as cold electron collisions occurring in terrestrial and stellar atmospheres [Msezane et al., 2008]; the discovery of superconductivity in several of the heavy fermion compounds; and the appearance of a Bose-Einstein condensation of Ytterbium [Msezane et al., 2009]. Although this list is certainly incomplete, the fact remains that an understanding of these processes requires a complete kinematical knowledge of very low energy elastic scattering.

The theoretical aspects of low energy elastic scattering are best studied using Regge poles since they provide a rigorous definition of resonances. The Regge pole methodology is particularly suited to gaining insights into the formation of temporary anion states during electron attachment, and this is fundamental to the mechanism by which the scattering process deposits energy [Felfli et al., 2008b]. Moreover, the imaginary part of the orbital angular momentum can be used to distinguish between the shape resonances and the stable bound states of the anions formed as Regge poles in the electron-atom scattering, whereby this imaginary part is vastly smaller for the stable bound states [Msezane et al., 2009]. We will show that low energy bound state formation of the Regge poles found in experiment is theoretically consistent by proving that as the energy tends to zero, the Regge poles approach the angular momentum eigenvalues of the associated self-adjoint Schrödinger operator with zero energy. Original work on the low energy behaviour of Regge trajectories was carried out by Macek et al. [2004] and Ovchinnikov et al. [2006], in which oscillations in the total cross-sections for proton scattering are studied.

More precisely, we demonstrate this low energy behaviour of Regge poles described above for a radial potential with finite first moment at infinity, whose product with the radial variable is bounded near the origin. The proof, which uses a re-characterization of Regge poles in terms of the zeros of a Wronskian determinant, will be achieved in stages since each new case yields results which are used in subsequent generalizations. In presenting the theory this way, it becomes clear where the difficulties lie and what methods we are to use. Therefore, we initially consider the finite spherical well and then generalize to a compactly supported potential. The proof of the former merely uses various standard small energy asymptotics, whilst the latter implements an argument involving resolvent operators. Consequently, we will be in a position to prove our most general result regarding potentials for which $r|V(r)|$ is bounded in a neighbourhood of the origin and integrable at infinity. To do this we employ an integral equation method inspired by Shubova [1989], which allows us to write down recursive relations for the solutions; it is then possible to study the small energy limit of these solutions and their first derivative. Finally, with a diagonal sequence argument, the existence of such limits is established and we conclude that for our general potential, the associated Regge poles will either approach the angular momentum eigenvalues of the zero energy self-adjoint problem, or tend to infinity.

We also consider the issue addressed by Barut and Dilley [1963] of counting Regge poles. It was found that for a potential which can be analytically continued into the right-half radial plane, with the property that $r^2|V(r)|$ is bounded for $r = 0$ and $r = \infty$, there are only finitely many Regge poles. An example of such a potential is the so-called rational Thomas-Fermi potential, which is given by

$$V_{\text{RTF}}(r) = \frac{-2Z}{r(1 + aZ^{1/3}r)(1 + bZ^{2/3}r^2)} \tag{1.1}$$

where Z is the nuclear charge and a, b are physical constants. The analytic properties of the exact Thomas-Fermi potential are notoriously complicated, and so V_{RTF} is most often used in practice [Belov et al., 2004]. The Thomas-Fermi model was among the earliest attempts to study the behaviour of atoms with multiple electrons; it made the electron density, not the wavefunction, play the central role in atomic theory. This approach is important because it underpins the description of all neutral atoms [Spruch, 1991] and yields good predictions, even under the most blunt approximations [Broyles, 1961].

We investigate whether there are finitely many or infinitely many Regge poles associated with a compactly supported potential, whose absolute value has finite integral. In short, we find that for large complex angular momentum (CAM) there are no Regge poles, from which we can deduce that in total, there are only finitely many. The idea of the proof is to show that the solution with potential is well approximated by the free solution for sufficently large CAM; as we shall see, this will suffice only if the asymptotics are locally uniform in spatial variable. To achieve this we recycle the idea of using a recursive formula for the solution on the support of the potential, and we again take limits. However, we will now require fixed energy large CAM asymptotics, and this is not a straightforward problem. The complications will essentially arise from Bessel function theory, namely, their bounds and asymptotics for complex order.

With the various cardinality results in mind, it is desirable to be able to actually count Regge poles. Work has been done to this end, see, for example, the excellent book by Newton [1964]. In particular, estimates of Regge poles is discussed for analytic potentials and for potentials of Yukawa (or screened Coulomb, see bottom of p. 19) type. For our 'non-analytic' purposes, the candidate method for achieving an estimate is as follows: let us introduce a parameter $\gamma \in [0,1]$ into the boundary condition at infintity such that the Regge pole problem corresponds to setting $\gamma = 1$. The idea is to establish a correspondence between the Regge poles ($\gamma = 1$) and the eigenvalues of the self-adjoint problem associated with $\gamma = 0$, and hence count the Regge poles by counting these eigenvalues. However, it will transpire that there are infinitely many eigenvalues when $\gamma \in [0,1)$, which is bad news for our proposed approach to counting Regge poles. We do, however, discover the remarkable sensitivity of Regge poles to boundary conditions: we prove that for the identically zero potential, infinitely many Regge poles come from infinity when the value of γ is changed, by any amount, away from unity. This boundary condition phenomenon serves as a good illustration of just how 'non-self-adjoint' the Regge pole problem is.

Let us describe the organization of this thesis. Chapter 2 provides an in-depth review of non-relativistic Regge theory; this begins with a discussion of the radial Schrödinger equation, and continues with the following topics: the scattering amplitude, partial wave analysis, the S-matrix, complex angular momentum, Coulomb scattering, the integral form of the scattering amplitude, and a re-characterization of Regge poles in terms of a Wronskian determinant alluded to above. In Chapter 3, we provide a more detailed account of the paper Hiscox et al. [2010] in which we study the behaviour of Regge poles in the very low energy limit. Chapter 4 is concerned with the cardinality of Regge poles associated with a compactly supported potential, and Chapter 5 details the sensitivity of Regge poles to boundary conditions. Finally, Chapter 6 provides a summary of the work and discusses possible directions for future research; in particular, we consider the importance of acquiring explicit estimates on the number of Regge poles for a given potential energy function. In addition, certain non-standard—at least in the case of complex analysis—results used in this thesis are discussed at length in the various Appendices; these are results which I believe are important to expatiate, but their inclusion in the main body of text would only break the flow.

CHAPTER 2

Regge Theory

The emergence of quantum physics is typically placed in 1900 with the discovery by Max Planck that the energy absorbed or emitted by matter is quantized. More precisely, Planck observed that the radiation an object emits is proportional to the vibrational frequency of that object, with constant of proportionality being a new fundamental quantity called Planck's constant, which is denoted by h. It was subsequently found that this 'lumpy' nature of energy is not constrained to the absorption and emission by matter, but is a much more general law of nature. In 1905 Albert Einstein proposed that electromagnetic energy also comes in discrete packets—or quanta—of energy, called photons. Using Planck's results he was able to explain the photoelectric effect, namely, that the energy of the electrons knocked off a metal surface is proportional to the frequency ν of the incident light, i.e. $E = h\nu = \hbar\omega$ where $\hbar = h/2\pi$ and $\omega = 2\pi\nu$. The most persuasive evidence that light is indeed corpuscular emerges from the investigations of Arthur Compton (1922). It was found that x-rays scattered off a block of paraffin by less than $\pi/2$ radians possessed a greater wavelength than the incident radiation; this phenomenon is called the Compton effect and is readily explained in terms of an elastic collision between two particles, namely, a photon and an electron [Born, 1969, p. 87].

The quantized nature of light is not the only reason for the development of quantum theory, there were problems with Rutherford's picture of the atom in which the negatively charged electrons orbit, at any distance, the positively charged nucleus. If the electrons were orbiting a central nucleus then they would be accelerating, and thus according to classical electrodynamics they would radiate energy. The result of this loss of energy would be electrons that spiral into the nucleus in a time of the order 10^{-10} seconds [Bransden and Joachain, 1983, p. 27]. From common experience, this is clearly not the case and so classical electrodynamics cannot account for the stability of matter. Furthermore, this model does not account for the discrete frequencies of radiation emitted by atoms codified in their so-called spectral lines [Davies and Betts, 2002, p. 4]. These problems were partially solved in 1912 by Niels Bohr. With a blend of classical and quantum reasoning, Bohr proposed that electrons in an atom can only occupy certain 'allowed' orbits at discrete distances from the nucleus with specific energies. Moreover, Bohr conjectured that there is no continuous radiation of energy from the electrons, but only transitions between these discrete orbits can give rise to radiation. If a photon of frequency ν is absorbed by an atom, then by Einstein's formula and the conservation of energy we have Bohr's frequency relation $h\nu = E_f - E_i$, where E_i and E_f are the initial and final energies of the atom respectively and clearly, $E_i < E_f$. On the other hand, if the atom changes its state from an energy E_f to an energy E_i, then a photon is emitted with frequency determined by Bohr's frequency relation [Bransden and Joachain, 1983, p. 30].

However, there is still the question of how and why this occurs. To answer this a new mechanics is required—quantum mechanics. Quantum mechanics stems from the inescapable fact that all particles have wavelike properties. In 1924 Louis de Broglie suggested that all matter has an associated wave, a de Broglie wave with wavelength $\lambda = h/p$ where p is the magnitude of the momentum vector. This was essentially taken from the formulae concerning light: from classical electrodynamics we have $E = pc$ where c is the speed of light, but since we also have from Einstein that $E = h\nu$, then $p = h/\lambda$. Furthermore, a particle's wavelike propagation induces an intrinsic uncertainty in the behaviour of the particle, namely, if the particle is restricted to some region in space then it has an ill-defined momentum; this is a consequence of the fact that a confined classical wave cannot have a unique wavelength—the connection to the momentum of a particle being provided by de Broglie's formula $\lambda = h/p$. The precise statement is called the position-momentum uncertainty relation, and was first enunciated by Werner Heisenberg in 1927 [French and Taylor, 1978, p. 327]. It states that

$$\Delta x \Delta p_x \gtrsim \hbar \tag{2.1}$$

where we write p_x to specify the direction; in words, the product of the uncertainty in the position and the uncertainty in the momentum is greater than or approximately equal to $\hbar$. This is summarized in the famous book by Gamow [1993]: 'any body in an enclosed space possesses a certain motion, we physicists call it zero-point motion, such as, for example, the motion of electrons in any atom'. For instance, in a Hydrogen atom the electron is constrained to a region of (Bohr) radius $\approx 10^{-10}$ metres, and since $\hbar \approx 10^{-34}$ joule-seconds, then by equation (2.1) we have $\Delta p = m_{\text{electron}}\Delta v \gtrsim 10^{-24}$ kilogram-metres per second, where $m_{\text{electron}} \approx 10^{-30}$ kilograms and Δv is the uncertainty in the velocity. The velocity of the electron in a Hydrogen atom is thus undetermined by an amount $\Delta v \gtrsim 10^6$ metres per second, which is about $0.\dot{3}\%$ of the speed of light. Hence, the electron has motion solely because of the fact that it is confined. To be clear, the concept of exact position and exact momentum together has no meaning in nature.

2.1 The Radial Schrödinger Equation

The central postulate in the theory of quantum mechanics is that the associated de Broglie wave—or wavefunction—of a quantum-mechanical particle of mass m, satisfies the following wave equation proposed by Erwin Schrödinger in 1926:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{2.2}$$

where the potential energy V and the wavefunction Ψ are functions of $\boldsymbol{r} = (x, y, z) \in \mathbb{R}^3$ and $t \in \mathbb{R}$. Equation (2.2) is called the time-dependent Schrödinger equation. Although there is still much philosophical debate over how Ψ should be interpreted, the statistical interpretation due to Max Born is of fundamental importance in the application of quantum mechanics. In short, this statistical interpretation of Born says that the de Broglie waves are not waves of substance but are probability waves, and $|\Psi(\boldsymbol{r},t)|^2$ is proportional to the probability density for the particle to have position $\boldsymbol{r}$ at time t. Hence, $C|\Psi(\boldsymbol{r},t)|^2 \mathrm{d}\Omega$ is the probability that the particle will be inside the infinitesimal volume $\mathrm{d}\Omega$ at time t, where C is some constant independent of Ω. This is a postulate and cannot be derived, but it relates the uncertainty in our knowledge of the particle and the existence of the associated de Broglie wave [Davies and Betts, 2002, p. 12]. Since the particle must be somewhere in space we have

$$C\int_{\mathbb{R}^3} |\Psi(\boldsymbol{r},t)|^2 \mathrm{d}^3\boldsymbol{r} = 1, \tag{2.3}$$

and we call Ψ a normalizable state if the integral on the left side of equation (2.3) is finite for some time $t \in \mathbb{R}$. A normalizable state Ψ can always be multiplied by some non-zero constant to obtain a normalized state—and once normalized for some time t, it remains normalized for all time since the Schrödinger equation has the property of being normalization preserving; we do not need to renormalize [Griffiths, 2005, p. 13]—meaning

$$\int_{\mathbb{R}^3} |\Psi(\boldsymbol{r},t)|^2 \mathrm{d}^3\boldsymbol{r} = 1.$$

For a normalized quantum state Ψ, $\int_\Omega |\Psi(\boldsymbol{r},t)|^2 \mathrm{d}^3\boldsymbol{r}$ is the probability that the particle will be inside the volume Ω at time t. The value of this integral will clearly change with time since some of the wave associated with the particle flows in and out of Ω, along with the probability [Davies and Betts, 2002, p. 13]. Thus, taking the time derivative of the integral leads to the definition of probability current density

$$j(\boldsymbol{r},t) \equiv -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*), \tag{2.4}$$

which is the total flux into Ω.

If the potential is independent of time t, then by using the method of separation of variables on (2.2) there will be a general solution of the form

$$\Psi(\boldsymbol{r},t) = \sum_{n=1}^{\infty} c_n \psi_n(\boldsymbol{r}) \mathrm{e}^{-iE_n t/\hbar}, \tag{2.5}$$

where E is the separation constant, chosen since every measurement of the total energy is certain to return the value E. The spatial wavefunction ψ_n (strictly speaking this is not true; the wavefunction always has the time-dependent exponential factor but we shall continue to use such language) satisfies the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi. \tag{2.6}$$

In many situations the potential energy function is radial, i.e. depends only upon the distance from the origin. Under these circumstances it is an obvious choice to use spherical polar coordinates (r,ϑ,ϕ). Spherical polar coordinates give a one-to-one description of points in $\mathbb{R}^3 \setminus \{(0,0,z) : z \in \mathbb{R}\}$, and in this system (2.6) becomes

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial\psi}{\partial r} + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\sin\vartheta\frac{\partial\psi}{\partial\vartheta} + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2\psi}{\partial\phi^2}\right] + V(r)\psi = E\psi. \tag{2.7}$$

To separate out r we put $\psi(r,\vartheta,\phi) = R(r)Y(\vartheta,\phi)$ into (2.7), which results in the following two equations:

$$\sin\vartheta\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)\sin^2\vartheta Y \tag{2.8}$$

and

$$\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E) = \ell(\ell+1), \tag{2.9}$$

where we have labelled the separation constant by $\ell(\ell+1)$; there is no loss of generality here since at this point ℓ could be any number. We again separate variables and look for solutions Y such that $Y(\vartheta,\phi) = \Theta(\vartheta)\Phi(\phi)$. Thus, equation (2.8) splits into

$$\frac{1}{\Theta}\sin\vartheta\frac{\mathrm{d}}{\mathrm{d}\vartheta}\left(\sin\vartheta\frac{\mathrm{d}\Theta}{\mathrm{d}\vartheta}\right) + \ell(\ell+1)\sin^2\vartheta = m^2 \tag{2.10}$$

and

$$\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = -m^2, \tag{2.11}$$

where m^2 is the separation constant (again, no loss of generality). The solution to (2.11) is clearly $\Phi(\phi) = \mathrm{e}^{im\phi}$ (both solutions are included by letting m be negative). Notice that in spherical coordinates $\phi + 2\pi$ is the same point in space as ϕ, and so $\mathrm{e}^{im(\phi+2\pi)} = \mathrm{e}^{im\phi}$ or $\mathrm{e}^{2\pi im} = 1$. It follows that $m \in \mathbb{Z}$. For (2.10), the physically acceptable solution is famously given by

$$\Theta(\vartheta) = AP_\ell^m(\cos\vartheta) \tag{2.12}$$

where P_ℓ^m is the associated Legendre function

$$P_\ell^m(x) = (1-x^2)^{|m|/2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{|m|} P_\ell(x), \tag{2.13}$$

and $P_\ell(x)$ is the ℓ-th Legendre polynomial defined by the Rodrigues formula

$$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{\ell} (x^2-1)^\ell. \tag{2.14}$$

It is important to note that $P_\ell(x)$ is a polynomial of degree ℓ in x but $P_\ell^m(x)$ is, in general, not. However, we require $P_\ell^m(\cos\vartheta)$ and since $\sqrt{1-\cos^2\vartheta} = \sin\vartheta$, $P_\ell^m(\cos\vartheta)$ is always a polynomial in $\cos\vartheta$, multiplied by $\sin\vartheta$ when m is odd. In view of (2.14), ℓ must be a non-negative integer. In addition, since P_ℓ is of degree ℓ, equation (2.13) stipulates that if $|m| > \ell$ then $P_\ell^m = 0$. Thus, for a given value of ℓ there are $2\ell+1$ possible values for m, namely, $-\ell, -\ell+1, \dots, -1, 0, 1, \dots, \ell-1, \ell$. The normalized angular wavefunctions are called spherical harmonics and are given by [Griffiths, 2005, p. 139]

$$Y_\ell^m(\vartheta,\phi) = \varepsilon\sqrt{\frac{(2\ell+1)(\ell-|m|)!}{4\pi(\ell+|m|)!}}\mathrm{e}^{im\phi}P_\ell^m(\cos\vartheta) \tag{2.15}$$

where

$$\varepsilon = \begin{cases} (-1)^m & \text{if} \quad m \geq 0, \\ 1 & \text{if} \quad m \leq 0. \end{cases}$$

It is customary to call m the magnetic quantum number and ℓ the orbital angular momentum quantum number. These quantum numbers are related to the orbital angular momentum L—henceforth we drop the word orbital since we will not need to distinguish from spin angular momentum, which is not to be discussed in this thesis. In particular, Y_ℓ^m is an eigenfunction, or determinate state, of the square of the total orbital angular momentum L^2, with eigenvalue $\hbar^2\ell(\ell+1)$. In other words, a measurement of L^2 in such a state is certain to yield the 'allowed' values $\hbar^2\ell(\ell+1)$.[1]

The potential $V(r)$ affects only the radial part of the wave equation. On putting $u(r) = rR(r)$ in the R-equation (2.9), we acquire the radial equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = Eu. \tag{2.16}$$

This equation is nearly identical to the one-dimensional time-independent equation (2.6), except that the effective potential $V_{\text{eff}} = V + \hbar^2\ell(\ell+1)/2mr^2$ now entails the so-called

[1]For a particle in state Ψ, the expectation of an observable Q is $\langle Q\rangle = \int \Psi^* Q\Psi = \langle\Psi|Q\Psi\rangle$, and since the outcome of a measurement must be real: $\langle Q\rangle = \langle Q\rangle^*$; in other words, observables are represented by Hermitian operators. In a determinate state, i.e. a state in which $\langle Q\rangle = q$, the standard deviation ΔQ of an observable Q has to be zero. Thus, $(\Delta Q)^2 \equiv \langle(Q-\langle Q\rangle)^2\rangle = \langle\Psi|(Q-q)^2\Psi\rangle = \langle(Q-q)\Psi|(Q-q)\Psi\rangle = 0$, which implies that $Q\Psi = q\Psi$ [Griffiths, 2005, p. 99].

centrifugal term. This extra term tends to force the particle radially outward.

In order to express the normalization condition in spherical polar coordinates, we require the volume element $\mathrm{d}^3\boldsymbol{r}$ in spherical coordinates. An infinitesimal displacement in the $\hat{\boldsymbol{r}}$ direction is $\mathrm{d}r$ and an infinitesimal element of length in the $\hat{\boldsymbol{\vartheta}}$ direction is $r\mathrm{d}\vartheta$, whilst an infinitesimal element of length in the $\hat{\boldsymbol{\phi}}$ direction is $r\sin\vartheta\mathrm{d}\phi$. Thus, the volume element in these coordinates is given by $\mathrm{d}^3\boldsymbol{r} = r^2\sin\vartheta\mathrm{d}r\mathrm{d}\vartheta\mathrm{d}\phi$, which means that the normalization condition in spherical coordinates is

$$\begin{aligned}1 &= \int |\psi|^2 r^2 \sin\vartheta \mathrm{d}r\mathrm{d}\vartheta\mathrm{d}\phi \\ &= \int_0^{2\pi}\int_0^{\pi} |Y|^2 \sin\vartheta\mathrm{d}\vartheta\mathrm{d}\phi = \int_0^{\infty} |R|^2 r^2 \mathrm{d}r,\end{aligned}$$

which in turn means that the normalization condition for $u(r)$ is

$$\int_0^{\infty} |u|^2 \mathrm{d}r = 1. \tag{2.17}$$

2.2 The Scattering Amplitude

Classically, a particle incident on some scattering centre arrives with an energy E and leaves at some angle ϑ. Particles incident within some infinitesimal area $\mathrm{d}\sigma$ will scatter into a corresponding infinitesimal solid angle $\mathrm{d}\Omega$.[2] Clearly, the larger $\mathrm{d}\sigma$, the larger $\mathrm{d}\Omega$; this leads to the definition of a quantity called the differential cross-section $D(\vartheta) \equiv \mathrm{d}\sigma/\mathrm{d}\Omega$, which is just the proportionality factor. Moreover, the total cross-section σ is defined as the integral of the differential cross-section over all solid angles, i.e.

$$\sigma = \int D(\vartheta)\mathrm{d}\Omega \tag{2.18}$$

and is the total area of incident beam scattered by the target. In a typical scattering experiment, a uniform beam of particles with flux of J particles per unit area per second is incident onto a scattering centre. Let $\mathrm{d}N$ be the number of particles per second that are scattered into an element of solid angle $\mathrm{d}\Omega$ about the polar angles ϑ and ϕ. We expect that $\mathrm{d}N$ will be proportional to J and to the size of $\mathrm{d}\sigma$. This is summarized by

$$D(\vartheta) = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{J}\frac{\mathrm{d}N}{\mathrm{d}\Omega}. \tag{2.19}$$

In quantum scattering, an incident beam traveling in the z-direction, represented by a plane wave $\psi_{\mathrm{inc}}(z) = A\mathrm{e}^{ikz}$ where $k \equiv \sqrt{2mE}/\hbar$ is the quantum wave number, encounters a force at the scattering centre; this results in a distortion of ψ_{inc}, which we describe in

[2]The solid angle is the generalization of the planar angle to three dimensions. Just as planar angles correspond to sectors of a circle, solid angles correspond to cone-shaped segments of a sphere. More precisely, planar angles are measured by dividing the arc length by the radius. Similarly, solid angles are given by the surface area $\mathrm{d}A$ of a projection of an object onto the inside of a sphere centred at that point, divided by the square of the sphere's radius R.

terms of a perturbation. This perturbation takes the form of an additional scattered wave ψ_{sc} (Figure 2.1), whose amplitude depends upon the angle ϑ through a quantity $f(\vartheta, \phi)$ called the scattering amplitude [Davies and Betts, 2002, p. 55]. We study this problem by

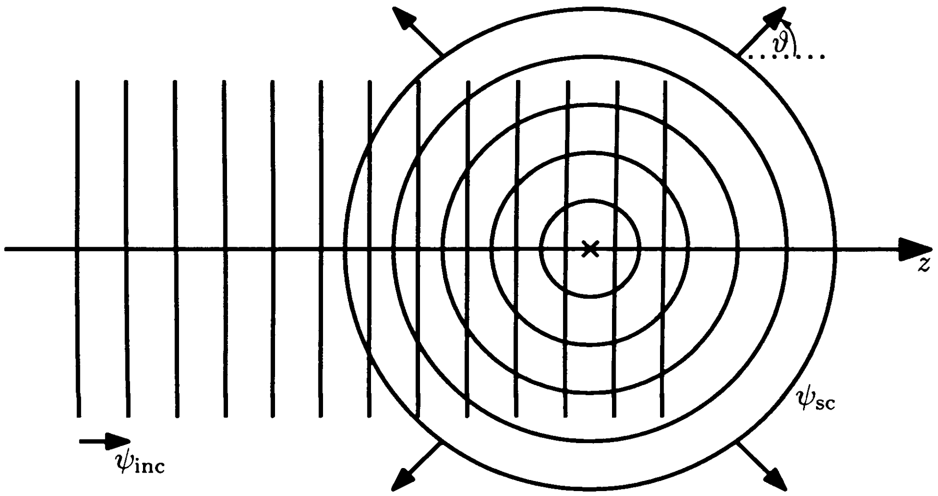

Figure 2.1: The scattering of a plane wave incident on a scattering centre ×.

solving the time-independent Schrödinger equation (2.6), and we do this for a spherically symmetric potential. As a consequence of the spherical symmetry, we will not need the azimuthal angle ϕ corresponding to rotations about the path of the incident beam, we only need ϑ to describe the post-collision trajectory. Therefore, we search for solutions satisfying $\psi(r, \vartheta) = \psi_{inc}(z) + \psi_{sc}(r, \vartheta)$. Although the exact details of ψ_{sc} depend upon the potential, we know that for a localized potential[3], ψ_{sc} satisfies [Mandl, 1992, p. 235]

$$\psi_{sc}(r, \vartheta) \sim f(\vartheta)\frac{e^{ikr}}{r}, \quad r \to \infty. \tag{2.20}$$

Localization of the potential is natural if we expect the beam to be scattered—an assumption that we uphold throughout this chapter, unless stated otherwise. Although this form of ψ_{sc} is true only for large r, it is satisfactory since we are interested in the wavefunction after the scattering event. Therefore, we have

$$\psi(r, \vartheta) \sim e^{ikz} + f(\vartheta)\frac{e^{ikr}}{r}, \quad r \to \infty. \tag{2.21}$$

By using (2.4) for the scattered wave defined by (2.20), we find that the number of particles scattered into $d\Omega$ per second is $(\hbar k/m)|f(\vartheta)|^2 d\Omega$. Similarly for ψ_{inc} we find that the number of particles incident per unit area per second is $\hbar k/m$. Hence, by using the definition of the differential cross-section (2.19) it follows that

$$D(\vartheta) = |f(\vartheta)|^2. \tag{2.22}$$

[3]A localized potential is a potential with a relatively short range, more precisely, it has the property that $rV(r) \to 0$ as $r \to \infty$. Note that this rules out the Coulomb potential, but the following analysis can be applied to the so-called 'screened' Coulomb (or Yukawa) potential—this is defined in §2.5.

The fundamental problem in scattering theory then, is to calculate the scattering amplitude, since this quantity gives the probability of scattering in any given direction ϑ. We now describe a particular method for determining the scattering amplitude, which is especially useful when the incident particle has a low speed.

2.3 Partial Wave Analysis

The Schrödinger equation for a spherically symmetric potential admits solutions of the form $\psi(r, \vartheta, \phi) = R(r)Y_\ell^m(\vartheta, \phi)$, where $u(r) = rR(r)$ satisfies (2.16). Due to the azimuthal symmetry we may take the magnetic quantum number to be zero in equation (2.15)—this is a common 'approximation' in the literature; see, for example, Taylor [1970] p. 183. Therefore, the wavefunction reduces to (for a particular ℓ)

$$\psi(r, \vartheta) = R(r)\sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\vartheta).$$

This also means that the scattering amplitude f depends only upon ϑ (the explicit dependence on the energy is traditionally omitted). Since the Legendre polynomials form a complete orthogonal set on $[-1, 1]$, we may write [Arfken and Weber, 2005, p. 757]

$$f(\vartheta) = \sum_{\ell=0}^{\infty} a_\ell(k)P_\ell(\cos\vartheta) \tag{2.23}$$

where a_ℓ is called the ℓ-th partial wave amplitude. The problem with which we are faced is as follows: given a potential $V(r)$, we need to determine the partial wave amplitudes $a_\ell(k)$. Firstly, consider the free particle. On writing the incident wave e^{ikz} as a Fourier-Legendre series we have [Taylor, 1970, p. 183]

$$\mathrm{e}^{ikz} = \mathrm{e}^{ikr\cos\vartheta} = \sum_{\ell=0}^{\infty} b_\ell P_\ell(\cos\vartheta). \tag{2.24}$$

To find b_ℓ, multiply equation (2.24) by $P_m(\cos\vartheta)$ and integrate:

$$\int_{-1}^{1} P_m(\cos\vartheta)\mathrm{e}^{ikr\cos\vartheta}\mathrm{d}\cos\vartheta = b_m\int_{-1}^{1} P_m(\cos\vartheta)P_m(\cos\vartheta)\mathrm{d}\cos\vartheta.$$

A standard result [Arfken and Weber, 2005, p. 757] states that

$$\int_{-1}^{1} P_\ell(x)P_m(x)\mathrm{d}x = \frac{2\delta_{\ell m}}{2\ell+1},$$

whence

$$b_\ell = \frac{2\ell+1}{2}\int_{-1}^{1} P_\ell(x)\mathrm{e}^{ikrx}\mathrm{d}x. \tag{2.25}$$

We may evaluate the integral in equation (2.25) simply by parts: since $P_\ell(1) = 1$ and $P_\ell(-x) = (-1)^\ell P_\ell(x)$, $\ell = 0, 1, 2, \ldots$ [Arfken and Weber, 2005, pp. 752–753], the boundary terms of the integration are given by

$$\begin{aligned}\frac{1}{ikr}(\mathrm{e}^{ikr} - (-1)^\ell \mathrm{e}^{-ikr}) &= \frac{1}{ikr}\left[\mathrm{e}^{ikr} - \mathrm{e}^{-i(kr-\ell\pi)}\right] \\ &= \frac{i^\ell}{ikr}\left[\mathrm{e}^{i(kr-\ell\pi/2)} - \mathrm{e}^{-i(kr-\ell\pi/2)}\right] \\ &= \frac{2i^\ell}{kr}\sin(kr - \ell\pi/2).\end{aligned}$$

For large r the integral remaining after integration by parts goes to zero, and thus

$$b_\ell = \frac{i^\ell}{kr}(2\ell+1)\sin(kr - \ell\pi/2) \tag{2.26}$$

for large r. Hence, as $r \to \infty$,

$$\mathrm{e}^{ikz} \sim \frac{1}{2ikr}\sum_{\ell=0}^{\infty}(2\ell+1)\left[\mathrm{e}^{ikr} - \mathrm{e}^{-i(kr-\ell\pi)}\right]P_\ell(\cos\vartheta). \tag{2.27}$$

In summary, this means that at each angular momentum quantum number, we have incoming and outgoing waves of the same amplitude but with different phases. Their phases differ by $\ell\pi$ due to the centrifugal term, which is present for all $\ell \neq 0$, even for a free particle [Shankar, 1994, p. 546].

Let us now turn on a localized potential. For large r, we must have $R(r)$ asymptotically equal to the free radial wavefunction, although we may encounter a phase shift (appearing in the scattering amplitude) due to the potential [Shankar, 1994, p. 546]. Therefore, we have as $r \to \infty$ that

$$R(r) \sim \frac{c_\ell}{kr}\sin(kr - \ell\pi/2 + \delta_\ell(k))$$

where δ_ℓ is called the phase shift of the ℓ-th partial wave, and c_ℓ is some constant yet to be determined. Therefore, the total wavefunction as $r \to \infty$ is

$$\psi(r,\vartheta) \sim \sum_{\ell=0}^{\infty}\frac{c_\ell}{kr}\left[\mathrm{e}^{i(kr-\ell\pi/2+\delta_\ell)} - \mathrm{e}^{-i(kr-\ell\pi/2+\delta_\ell)}\right]P_\ell(\cos\vartheta). \tag{2.28}$$

The potential produces an outgoing wave only, and so the incoming waves must be the same for e^{ikz} and ψ; on comparing coefficients of e^{-ikr}/kr in (2.27) and (2.28), we get that $c_\ell = (2\ell+1)\mathrm{e}^{i(\ell\pi/2+\delta_\ell)}/2i$ [Shankar, 1994, p. 547]. Whence,

$$\psi(r,\vartheta) \sim \frac{1}{kr}\sum_{\ell=0}^{\infty}\frac{2\ell+1}{2i}\left[\mathrm{e}^{2i\delta_\ell}\mathrm{e}^{ikr} - \mathrm{e}^{-i(kr-\ell\pi)}\right]P_\ell(\cos\vartheta) \tag{2.29}$$

$$= \mathrm{e}^{ikz} + \left[\sum_{\ell=0}^{\infty}(2\ell+1)\frac{\mathrm{e}^{2i\delta_\ell}-1}{2ik}P_\ell(\cos\vartheta)\right]\frac{\mathrm{e}^{ikr}}{r} \tag{2.30}$$

in the limit $r \to \infty$. Comparing equations (2.30) and (2.21) we have

$$a_\ell = (2\ell+1)\frac{e^{2i\delta_\ell}-1}{2ik}, \tag{2.31}$$

and so to calculate a_ℓ we must first find δ_ℓ. Thus, the effect of a potential is to attach a phase factor $e^{2i\delta_\ell}$ to the outgoing wave; this phase factor is denoted by $S_\ell(k)$, and we call $S_\ell(k)$ the S-matrix for angular momentum ℓ—or S-matrix. Moreover, in putting (2.31) into (2.23) we have the following partial wave representation of the scattering amplitude:

$$f(\vartheta) = \frac{1}{k}\sum_\ell (2\ell+1)P_\ell(\cos\vartheta)e^{i\delta_\ell}\sin\delta_\ell. \tag{2.32}$$

The phase shift approach is elegant since it illuminates the physics: the conservation of probability[4] means that the potential can only shift the phase of the outgoing wave. Using equation (2.22), we have from (2.32) that $D(\vartheta) = k^{-2}|\sum_\ell(2\ell+1)P_\ell(\cos\vartheta)e^{i\delta_\ell}\sin\delta_\ell|^2$; so

$$\begin{aligned}\sigma &= \frac{1}{k^2}\int d\Omega\left|\sum_\ell(2\ell+1)P_\ell(\cos\vartheta)e^{i\delta_\ell}\sin\delta_\ell\right|^2\\ &= \frac{1}{k^2}\int d\Omega\sum_{\ell,m}(2\ell+1)(2m+1)P_\ell(\cos\vartheta)P_m(\cos\vartheta)e^{-i\delta_\ell}\sin\delta_\ell e^{i\delta_m}\sin\delta_m\\ &= \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)^2\sin^2\delta_\ell.\end{aligned}$$

Therefore, $\sigma = \sum_\ell \sigma_\ell$ where

$$\sigma_\ell \equiv \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell. \tag{2.33}$$

The σ_ℓ are called the partial cross-sections at each angular momentum ℓ.

It is instructive to consider an exactly soluble example; for this purpose we take the case of the so-called hard sphere [Shankar, 1994, p. 549]

$$V(r) = \begin{cases}\infty & \text{if } r \le r_0,\\ 0 & \text{if } r > r_0.\end{cases}$$

We need to solve (2.9) and from the solution's large r asymptotics, identify the phase shift δ_ℓ. For $r \le r_0$ we must have $R(r) = 0$, since the probability of finding the particle in this region is zero. When $r > r_0$ we require the solution to the free particle R-equation

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}E = \ell(\ell+1). \tag{2.34}$$

[4] In elastic scattering the incoming and outgoing flow of probability must be equal.

To solve this we digress and consider Bessel's differential equation (BDE)

$$x^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + x\frac{\mathrm{d}y}{\mathrm{d}x} + [x^2 - \nu^2]y = 0. \tag{2.35}$$

The general solution of BDE is [Abramowitz and Stegun, 1965, p. 358]

$$y(x) = AJ_\nu(x) + BN_\nu(x) \tag{2.36}$$

where $J_\nu(x)$ is the Bessel function of order ν and $N_\nu(x)$ is the Neumann function of order ν. If we let $x = kr$ in (2.35), then BDE reads

$$r^2\frac{\mathrm{d}^2y}{\mathrm{d}r^2} + r\frac{\mathrm{d}y}{\mathrm{d}r} + [k^2r^2 - \nu^2]y = 0 \tag{2.37}$$

where $y = y(kr)$. The R-equation (2.34) in which the potential is identically zero can be written in the following form:

$$r^2\frac{\mathrm{d}^2R}{\mathrm{d}r^2} + 2r\frac{\mathrm{d}R}{\mathrm{d}r} + [k^2r^2 - \ell(\ell+1)]R = 0 \tag{2.38}$$

where k is the quantum wave number. Let us define a new function

$$w(kr) = \sqrt{kr}R(r) \tag{2.39}$$

in which case, (2.38) becomes

$$r^2\frac{\mathrm{d}^2w}{\mathrm{d}r^2} + r\frac{\mathrm{d}w}{\mathrm{d}r} + [k^2r^2 - (\ell+1/2)^2]w = 0. \tag{2.40}$$

By comparing (2.35) and (2.40) and recalling (2.36), it is clear that

$$w(kr) = AJ_\nu(kr) + BN_\nu(kr). \tag{2.41}$$

We note that here, the order of the Bessel and Neumann functions is $\nu = \ell + 1/2$. Now, from equation (2.39), $R(r) = w(kr)/\sqrt{kr}$ and thus

$$R(r) = \frac{A}{\sqrt{kr}}J_\nu(kr) + \frac{B}{\sqrt{kr}}N_\nu(kr). \tag{2.42}$$

It is convenient to recast $R(r)$ in terms of the spherical Bessel functions j_ℓ and n_ℓ, which are defined as follows [Arfken and Weber, 2005, p. 726]:

$$j_\ell(x) \equiv \sqrt{\frac{\pi}{2x}}J_{\ell+1/2}(x) \quad \text{and} \quad n_\ell(x) \equiv \sqrt{\frac{\pi}{2x}}N_{\ell+1/2}(x).$$

Hence, $R(r) = A_\ell j_\ell(kr) + B_\ell n_\ell(kr)$; we have made the addition of ℓ subscripts in order to emphasize the dependence of the normalization constants on the angular momentum quantum number. Matching the solutions continuously at r_0 stipulates that $R(r_0) = 0$, or equivalently

$$\frac{B_\ell}{A_\ell} = -\frac{j_\ell(kr_0)}{n_\ell(kr_0)}. \tag{2.43}$$

By standard large argument asymptotics for the spherical Bessel functions [Arfken and Weber, 2005, p. 729], the radial part of the wavefunction for large r satisfies

$$R(r) \sim \frac{1}{kr}[A_\ell \sin(kr - \ell\pi/2) - B_\ell \cos(kr - \ell\pi/2)].$$

We digress further in order to express R in a cleaner form. To achieve this, it would be useful to find an expression for $\sin(\arctan(x))$: let $y = \arctan(x)$ so that $\tan(y) = x$. Then we have $\sin^2(y) = x^2 \cos^2(y)$ or

$$\sin^2(\arctan(x)) = \frac{x^2}{1 + x^2}, \tag{2.44}$$

which yields $\sin(\arctan(-B_\ell/A_\ell)) = -B_\ell(A_\ell^2 + B_\ell^2)^{-1/2}$. Similar calculations for cosine show that $\cos(\arctan(B_\ell/A_\ell)) = A_\ell(A_\ell^2 + B_\ell^2)^{-1/2}$. Moreover,

$$\begin{aligned} \sin(kr - \ell\pi/2 + \arctan(-B_\ell/A_\ell)) &= \sin(kr - \ell\pi/2)\cos(\arctan(-B_\ell/A_\ell)) \\ &\quad + \cos(kr - \ell\pi/2)\sin(\arctan(-B_\ell/A_\ell)) \\ &= \frac{1}{\sqrt{A_\ell^2 + B_\ell^2}}[A_\ell \sin(kr - \ell\pi/2) - B_\ell \cos(kr - \ell\pi/2)]. \end{aligned}$$

Therefore, far from the scattering centre we have

$$R(r) \sim \frac{\sqrt{A_\ell^2 + B_\ell^2}}{kr} \sin(kr - \ell\pi/2 + \delta_\ell(k)), \tag{2.45}$$

where

$$\delta_\ell(k) = \arctan\left[-\frac{B_\ell}{A_\ell}\right] = \arctan\left[\frac{j_\ell(kr_0)}{n_\ell(kr_0)}\right]. \tag{2.46}$$

Note that we have used the matching condition (2.43) for the second equality in (2.46). For $\ell = 0$ we have s-wave scattering, so-called because of the sharp or s-orbitals of an atom, whose shape is dictated by the spherical harmonics. In our hard sphere example, we have [Arfken and Weber, 2005, p. 728]

$$\delta_0 = \arctan\left[-\frac{\sin(kr_0)/kr_0}{\cos(kr_0)/kr_0}\right] = -kr_0.$$

The interpretation of this is that the hard sphere pushes out the wavefunction, imposing sinusoidal oscillations at $r = r_0$ rather than at $r = 0$.

2.4 The S-Matrix

The partial cross-sections σ_ℓ are usually small for low energy; for example, in the case of the hard sphere potential we have

$$\tan\delta_\ell \sim \delta_\ell \sim (\text{const.})(kr_0)^{2\ell+1}$$

for small k, which follows from the standard small argument asymptotics for the spherical Bessel and Neumann functions, i.e. [Arfken and Weber, 2005, p. 729]

$$j_\ell(x) \sim \frac{x^\ell}{(2\ell+1)!!} \quad \text{and} \quad n_\ell(x) \sim -x^{-(\ell+1)}(2\ell-1)!!, \quad x \to 0.$$

This is to be expected. At low energies there should be negligible scattering for high angular momentum states [Shankar, 1994, p. 550]. However, the partial cross-section is capable of a myriad of behaviours as a function of the energy; in particular, we have the appearance of a sharp peak against a smooth background as the phase shift passes through $\pi/2$ [Ballentine, 1998, p. 458]. In order for δ_ℓ to achieve the value of $\pi/2$, the denominator inside the arctan must vanish, and so for energies $E \approx E_{\text{res}}$ we write

$$\delta_\ell = \arctan\left[\frac{\Gamma/2}{E_{\text{res}} - E}\right] \tag{2.47}$$

where Γ is a constant which depends on the energy. From equations (2.33) and (2.44), the associated partial cross-section for $E \approx E_{\text{res}}$ is

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\frac{(\Gamma/2)^2}{(E_{\text{res}} - E)^2 + (\Gamma/2)^2}.$$

Hence, σ_ℓ is given by a bell-shaped curve called the Breit-Wigner form; it has a maximum height $\sigma_\ell^{\max} = 4\pi(2\ell+1)/k^2$ and half-width $\Gamma/2$ [Shankar, 1994, p. 551]. When this occurs, we say that we have a resonance. As we will soon appreciate, it is most helpful to study resonances from the S-matrix perspective. Near a resonance, the S-matrix takes on a particularly simple form [Shankar, 1994, p. 551]:

$$\begin{aligned} S_\ell(k) &= \mathrm{e}^{2i\delta_\ell} \\ &= \frac{\cos\delta_\ell + i\sin\delta_\ell}{\cos\delta_\ell - i\sin\delta_\ell} \\ &= \frac{1 + i\tan\delta_\ell}{1 - i\tan\delta_\ell} \\ &= \frac{1 + i(\Gamma/2)/(E_{\text{res}} - E)}{1 - i(\Gamma/2)/(E_{\text{res}} - E)} \\ &= \frac{E - E_{\text{res}} - i\Gamma/2}{E - E_{\text{res}} + i\Gamma/2}. \end{aligned} \tag{2.48}$$

If we analytically continue the wavefunction to complex energy, and in particular to the energy $E = E_{\text{res}} - i\Gamma/2$, then we find from equation (2.48) that a resonance corresponds to a pole of the S-matrix near the positive real axis of the complex E-plane. For real and positive energy we know that

$$R(r) \sim \frac{1}{r}(A\mathrm{e}^{ikr} + B\mathrm{e}^{-ikr})$$

for sufficiently large r, and so from equation (2.29) we have

$$S_\ell(k) = \frac{A}{B} \tag{2.49}$$

up to multiplication by $i^{2\ell}$. Thus, we may define the S-matrix for any complex k as follows: first solve the R-equation for $k \in \mathbb{C}$, find the large r asymptotics, and then compute the ratio of the outgoing and incoming wave amplitudes [Shankar, 1994, p. 552]. If $k = i\kappa$, which corresponds to $E = \hbar^2 k^2/2m$ being negative, then

$$R(r) \sim \frac{1}{r}(A\mathrm{e}^{-\kappa r} + B\mathrm{e}^{\kappa r}).$$

Hence, for k such that $B = 0$, or equivalently $S_\ell(i\kappa) = \infty$, we have a bound state. Therefore, we may characterize bound states as poles of the S-matrix on the negative real energy axis [Taylor, 1970, p. 193]. This means that a resonance, which is a pole near the positive real axis, must be some kind of bound state. To appreciate this, consider the time dependence of the wavefunction: from equation (2.5), the time dependence for such a particle is given by $\mathrm{e}^{-iE_{\text{res}}t/\hbar}\mathrm{e}^{-\Gamma t/2\hbar}$ where we see that Γ must be positive. This also shows that the particle has a lifetime of order $\hbar/\Gamma$, and so a resonance describes some kind of semi-bound state with energy E_{res}—but not exactly this energy due to the uncertainty principle[5]. A large Γ describes a short-lived particle which is associated with a broad peak in the energy variation of the total cross-section; whilst a pole near the positive real axis, i.e. with a small Γ, describes a long-lived more stable particle with a corresponding sharp peak in the energy variation of the total cross-section [Taylor, 1970, pp. 194–195].

2.5 Complex Angular Momentum (CAM)

The notion of CAM was conceived by Watson [1918] in order to study the diffraction and scattering of short-length electromagnetic waves [Connor, 1990]. This CAM approach was resurrected with vigour when in 1959, Italian physicist Tullio Regge used the theory in the context of quantum mechanics. Regge showed that when considering solutions of the Schrödinger equation for non-relativistic scattering by a screened Coulomb (Yukawa) potential, $V(r) = -g^2\mathrm{e}^{-mr}/r$ [Eden, 1971], it is useful to regard the angular momentum quantum number ℓ, as a complex valued parameter [Collins, 1977].

[5]We refer here to the energy-time uncertainty principle $\Delta t \Delta E \gtrsim \hbar$ where Δt is the amount of time it takes the expectation of some observable Q to change by one standard deviation [Griffiths, 2005, p. 114].

To discuss Regge's considerations we rewrite the radial Schrödinger equation (2.16) for a quantum-mechanical particle of mass m in a potential field V as

$$-u'' + \left(\frac{\ell(\ell+1)}{r^2} + U(r) - k^2\right)u = 0, \quad r \in (0, \infty) \tag{2.50}$$

where $U(r) \equiv (2m/\hbar^2)V(r)$ is the so-called reduced potential energy function and, of course, $k = \sqrt{2mE}/\hbar$ is the quantum wave number. Let us make clear the properties we wish the solutions to have: we look for the solution satisfying

$$u(r) \sim r^\alpha, \quad r \to 0, \tag{2.51}$$

and so according to equation (2.50), where we assume that r^{-2} dominates $U(r)$ for small r, we must have $\alpha = \ell + 1$ or $\alpha = -\ell$ in (2.51). We choose the regular solution at the origin by taking $\alpha = \ell + 1$, thus we obtain the asymptotic behaviour

$$u(r) \sim r^{\ell+1}, \quad r \to 0. \tag{2.52}$$

This choice bestows a restriction on the values that ℓ can take. The general solution for small r is $c_1 r^{\ell+1} + c_2 r^{-\ell}$.[6] To eliminate the second term, $r^{-\ell}$ must dominate $r^{\ell+1}$ as $r \to 0$; this implies that $\mathrm{Re}(\ell) > -1/2$ [Landau and Lifshitz, 1977, p. 589]. Moreover, we look for a purely outgoing wave at large distances (we assume that the potential is such that such solutions exist):

$$u(r) \sim \mathrm{e}^{ikr}, \quad r \to \infty. \tag{2.53}$$

Consider the summand—ignoring the Legendre polynomial since we are only interested in the radial part—in (2.29), which gives the total wavefunction's asymptotics; with some rearrangment, this is equal to $(2\ell+1)(2i)^{-1}\mathrm{e}^{i\pi\ell/2}[\mathrm{e}^{-i\pi\ell/2}\mathrm{e}^{2i\delta_\ell}\mathrm{e}^{ikr} - \mathrm{e}^{i\pi\ell/2}\mathrm{e}^{-ikr}]$. Therefore, above threshold ($k^2 > 0$), the radial wavefunction u has asymptotic behaviour

$$u \sim N_\ell\Big[\mathrm{e}^{-i(kr-\pi\ell/2)} - S\mathrm{e}^{i(kr-\pi\ell/2)}\Big], \quad r \to \infty \tag{2.54}$$

where $S = \mathrm{e}^{2i\delta_\ell(k)}$ and N_ℓ is a normalization constant. At a pole of S, the second term in equation (2.54) receives an infinite boost and a purely outgoing wave results. Below threshold ($k^2 < 0$), at $k = i|k|$ say, we have

$$u \sim N_\ell\Big[\mathrm{e}^{|k|r+i\pi\ell/2} - S\mathrm{e}^{-|k|r-i\pi\ell/2}\Big], \quad r \to \infty. \tag{2.55}$$

In this case, a pole of S yields a normalizable bound state. Out of interest we mention that below threshold we can also have a bound state at $k = -i|k|$, which is provided by a zero of S; for each bound state, both the zero and the pole occur since the radial Schrödinger

[6] By letting $r = \mathrm{e}^{-t}$ and constructing a first order system, the Levinson Theorem tells us that $\int_0^{r_0} r(V(r) - k^2)\mathrm{d}r < \infty$, $r_0 > 0$ is sufficient for the existence of solutions with these asymptotics.

equation is invariant under the mapping $k \mapsto -k$ [Frautschi, 1963, p. 4]. Therefore, the S-matrix for $\ell = 0$ has a pole as a function of the energy; in general, a family of bound states with increasing $\ell \in \mathbb{Z}^+$ is represented by a family of energy poles of S.

However, there is no *a priori* reason why ℓ has to be a non-negative integer in the radial Schrödinger equation, this requirement stems from properties of the spherical harmonics. Below threshold, the so-called bound state condition $u \sim \mathrm{e}^{-|k|r}$ for large r—we are only interested in the poles of S here—defines a whole family of solutions, where, as ℓ increases continuously, these solutions interpolate smoothly between the bound states at physical values of angular momentum ℓ [Frautschi, 1963, p. 103]. Thus, the whole family of solutions satisfying the bound state condition can be described by the continuous movement of an ℓ-plane pole of the S-matrix; the motion of the pole being a result of varying the energy $E \in \mathbb{R}$. The physical bound states then correspond to this moving pole passing through non-negative integer values of ℓ [Frautschi, 1963, p. 103]. Therefore, regarding ℓ as being complex is certainly not just a mathematical frivolity.

In other words, the notion of CAM provides a way of unifying bound states and resonances as properties of a so-called trajectory function $\alpha(E)$. The trajectory function is defined such that if an energy E forces $\alpha(E)$ to equal a non-negative integer, L say, then a bound state will exist at that energy E with angular momentum L. Thus, instead of considering bound states at a given angular momentum $\ell = 0$ with energy E_0, and then at $\ell = 1$ with energy E_1 and so on (as described above), we now simply look at a single entity $\alpha(E)$ [Leader, 1978]. Therefore, making ℓ complex achieved what making the energy complex achieved. Namely, just as the scattering amplitude $f_L(E)$ has a pole at the energy E for which a bound state of angular momentum $\ell = L$ exists, $f(\ell, E)$ has a pole whenever E is such that $\alpha(E)$ equals ℓ [Leader, 1978]. The Regge trajectory function indicates the existence of bound states and resonances on the occasion that it passes through integer values; an illustrative example—assuming that the potential is such that there are no embedded eigenvalues—is shown in Figure 2.2.

It is possible to ascertain the location of the ℓ-plane poles of S using quite a general argument found in Frautschi [1963] pp. 103–104. For real energy and real potential function, consider the radial Schrödinger equation (2.50) and its complex conjugate

$$-\frac{\mathrm{d}^2 u^*}{\mathrm{d}r^2} + \left(\frac{\ell^*(\ell^*+1)}{r^2} + U(r) - k^2\right)u^* = 0. \tag{2.56}$$

Subtracting u multiplied by (2.56) from (2.50) multiplied by u^* gives

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}r^2}u^* + u\frac{\mathrm{d}^2 u^*}{\mathrm{d}r^2} + \frac{\ell(\ell+1) - \ell^*(\ell^*+1)}{r^2}|u|^2 = 0$$

or, with $\ell = \ell_R + i\ell_I$, this is

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(u\frac{\mathrm{d}u^*}{\mathrm{d}r} - \frac{\mathrm{d}u}{\mathrm{d}r}u^*\right) + 2i\ell_I(2\ell_R + 1)\frac{|u|^2}{r^2} = 0. \tag{2.57}$$

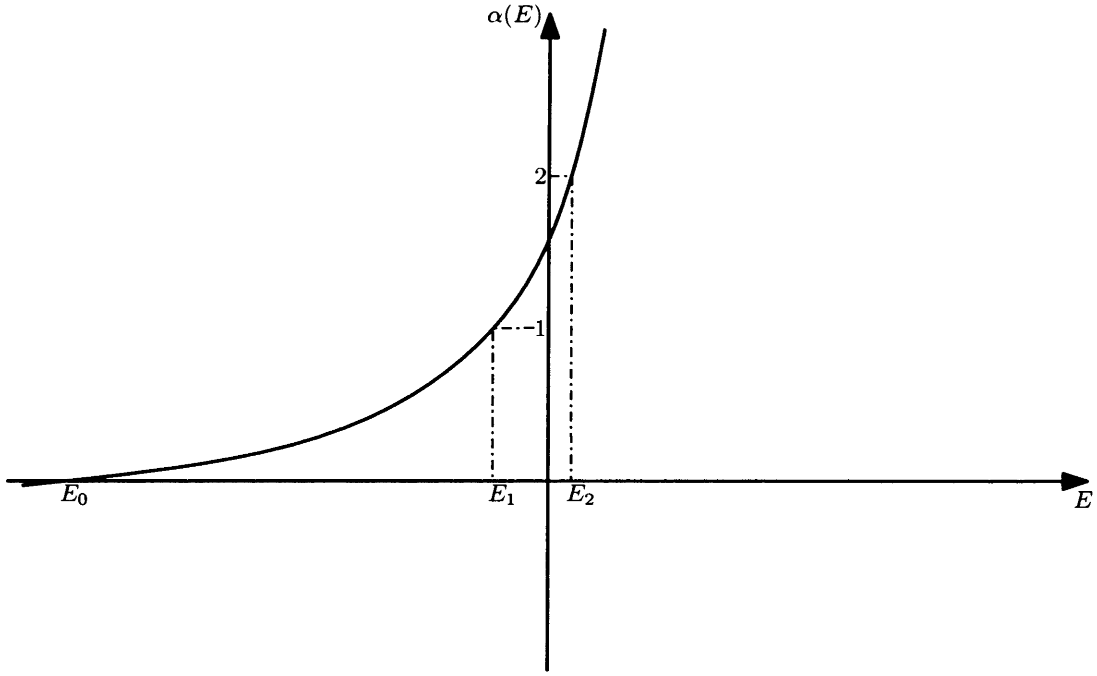

Figure 2.2: Bound states at E_0, E_1, and a resonance at E_2.

Integrating (2.57) yields

$$\left[u\frac{\mathrm{d}u^*}{\mathrm{d}r} - \frac{\mathrm{d}u}{\mathrm{d}r}u^*\right]_0^\infty + 2i\ell_I(2\ell_R + 1)\int_0^\infty \frac{|u|^2}{r^2}\mathrm{d}r = 0. \tag{2.58}$$

Below threshold, $u \sim r^{\ell+1}$ as $r \to 0$ and $u \sim \mathrm{e}^{-|q|r}$ as $r \to \infty$, which means that the first term in (2.58) vanishes for $\mathrm{Re}(\ell) > -1/2$. Moreover, the integral is positive and thus for a bound state (and pole of S), $\mathrm{Im}(\ell)$ must vanish. Above threshold, the outgoing wave condition for a pole of S gives $u \sim \mathrm{e}^{ikr}$ and $u^* \sim \mathrm{e}^{-ikr}$ as $r \to \infty$. Since the small r asymptotics are unchanged, equation (2.58) becomes

$$-2ik + 2i\ell_I(2\ell_R + 1)\int_0^\infty \frac{|u|^2}{r^2}\mathrm{d}r = 0,$$

which implies that $\mathrm{Im}(\ell)$ is positive. To summarize: below threshold, the poles of S at $\mathrm{Re}(\ell) > -1/2$ lie on the real axis; whereas above threshold, the poles are situated above the real axis. Therefore, there are no poles in the forth quadrant of the CAM plane—this is true more generally [Bottino et al., 1962]. Regge proved that for a variety of potentials, including the screened Coulomb potential, the only singularities of the scattering amplitude at $\mathrm{Re}(\ell) > -1/2$ are poles [Regge, 1959] or as they are now called, Regge poles.

2.5.1 Coulomb Scattering

As an example, let us consider the attractive Coulomb potential, $V(r) = -e^2/r$ where e^2 is the coupling constant of the Coulomb field. In order to find δ_ℓ, we need to calculate the large r asymptotics of the solution to the R-equation (2.9); to begin with, we rewrite the R-equation in the more tractable form

$$R'' + \frac{2}{r}R' + \left[-\frac{2m}{\hbar^2}(V - E) - \frac{\ell(\ell+1)}{r^2} \right] R = 0.$$

We wish to use atomic units, this is formally obtained by putting $e = m = \hbar = 1$ [Landau and Lifshitz, 1977, p. 118, footnote]. Thus, the equation we must solve is

$$R'' + \frac{2}{r}R' + \left[2E + \frac{2}{r} - \frac{\ell(\ell+1)}{r^2} \right] R = 0. \tag{2.59}$$

Introducing the new notation [Landau and Lifshitz, 1977, p. 118] $n \equiv (-2E)^{-1/2}$ and $\rho \equiv 2r/n$ into equation (2.59) yields

$$\frac{4}{n^2}\frac{\mathrm{d}^2R}{\mathrm{d}\rho^2} + \frac{8}{n^2\rho}\frac{\mathrm{d}R}{\mathrm{d}\rho} + \left[-\frac{1}{n^2} + \frac{4}{n\rho} - \frac{4\ell(\ell+1)}{n^2\rho^2} \right] R = 0,$$

or

$$\frac{\mathrm{d}^2R}{\mathrm{d}\rho^2} + \frac{2}{\rho}\frac{\mathrm{d}R}{\mathrm{d}\rho} + \left[-\frac{1}{4} + \frac{n}{\rho} - \frac{\ell(\ell+1)}{\rho^2} \right] R = 0. \tag{2.60}$$

Requiring regularity at the origin means we must stipulate that $R \sim \rho^\ell$ as $\rho \to 0$. On the other hand, for large ρ we acquire the equation [Landau and Lifshitz, 1977, p. 118]

$$R'' = \frac{1}{4}R,$$

from which we get $R = \mathrm{e}^{\pm\rho/2}$; but, since we seek the physically acceptable solution[7] we take $R \sim \mathrm{e}^{-\rho/2}$ as our large ρ asymptotic condition. Thus, peeling off the asymptotic behaviour we introduce the function $y(\rho)$ such that $R = \rho^\ell \mathrm{e}^{-\rho/2} y(\rho)$. We must now find the equation satisfied by y. So,

$$\begin{aligned}\frac{\mathrm{d}R}{\mathrm{d}\rho} &= (\ell\rho^{\ell-1}\mathrm{e}^{-\rho/2} - \rho^\ell \mathrm{e}^{-\rho/2}/2)y + \rho^\ell \mathrm{e}^{-\rho/2}y' \\ &= \rho^\ell \mathrm{e}^{-\rho/2}y' + \rho^{\ell-1}\mathrm{e}^{-\rho/2}y(\ell - \rho/2)\end{aligned}$$

[7]Corresponding to the classical notions of bound states and scattering states (and assuming that the potential has definite limits at $\pm\infty$), there are two kinds of solution to the Schrödinger equation. Due to quantum tunneling—the phenomenon in which there is a non-zero probability that a particle will 'tunnel' through any finite potential barrier—all that counts is the behaviour of the potential at infinity: if the total energy is less than the potential at $-\infty$ and $+\infty$ then we have a bound state, whilst if the total energy is greater than the potential at $-\infty$ or $+\infty$ then we have a scattering state. However, since in practice most potentials decay at infinity, we have that $E < 0$ corresponds to bound states whereas $E > 0$ yields scattering states [Griffiths, 2005, p. 68]. Therefore, for the physically acceptable solution here, we require $E < 0$ which makes ρ positive.

and thus the second derivative is given by

$$\frac{\mathrm{d}^2R}{\mathrm{d}\rho^2} = \rho^\ell \mathrm{e}^{-\rho/2}y'' + \rho^{\ell-1}\mathrm{e}^{-\rho/2}y'(\ell-\rho/2)$$
$$+ [\rho^{\ell-1}\mathrm{e}^{-\rho/2}y' + \rho^{\ell-2}\mathrm{e}^{-\rho/2}y(\ell-1-\rho/2)](\ell-\rho/2) - \rho^{\ell-1}\mathrm{e}^{-\rho/2}y/2.$$

Hence, putting $R = \rho^\ell \mathrm{e}^{-\rho/2}y(\rho)$ into equation (2.60) yields

$$\{\rho^\ell y'' + \ell\rho^{\ell-1}y' - \rho^\ell y'/2 + \ell\rho^{\ell-1}y' - \rho^\ell y'/2 + \ell(\ell-1)\rho^{\ell-2}y - (\ell-1)\rho^{\ell-1}y/2 - \ell\rho^{\ell-1}y/2$$
$$+ \rho^\ell y/4 - \rho^{\ell-1}y/2\} + \{2\rho^{\ell-1}y' + 2\ell\rho^{\ell-2}y - \rho^{\ell-1}y\} + [-1/4 + n/\rho - \ell(\ell+1)/\rho^2]\rho^\ell y = 0$$

or

$$\rho^2 y'' + (2\ell\rho - \rho^2 + 2\rho)y' + [\ell(\ell-1) - \ell\rho + 2\ell - \rho + n\rho - \ell(\ell+1)]y = 0.$$

This results in the equation

$$\rho y'' + (2\ell + 2 - \rho)y' - (\ell + 1 - n)y = 0, \tag{2.61}$$

which is the confluent hypergeometric equation. The solution of (2.61) satisfying the requirements of regularity at the origin, with an acceptable rate of divergence at infinity is given by the confluent hypergeometric function [Arfken and Weber, 2005, p. 864]

$$y(\rho) = F(\ell + 1 - n; 2\ell + 2; \rho). \tag{2.62}$$

The confluent hypergeometric series

$$F(\alpha;\beta;z) \equiv \sum_{j=0}^{\infty} \frac{\Gamma(\alpha+j)\Gamma(\beta)}{\Gamma(\alpha)\Gamma(\beta+j)}\frac{z^j}{j!}$$

is well-defined for any α and $\beta \notin \mathbb{Z}^- \cup \{0\}$ [Messiah, 1999, p. 480]. Here, $\Gamma(z)$ is Euler's gamma function, which is the generalization of the factorial function.

For scattering, as we have already discussed, we are required to consider positive energies $E > 0$; this means that our adopted notation becomes $n = -i/\sqrt{2E} = -i/k$ and $\rho = 2ikr$. Therefore, by equation (2.62) we obtain

$$R_{k\ell}(r) = C_{k\ell}(2ikr)^\ell \mathrm{e}^{-ikr}F(\ell + 1 + i/k; 2\ell + 2; 2ikr) \tag{2.63}$$

where $C_{k\ell}$ is a normalization factor. For large r, the solutions $R_{k\ell}$ defined by (2.63) take the following asymptotic form [Landau and Lifshitz, 1977, pp. 122 and 662]:

$$R_{k\ell}(r) = \frac{2}{r}|\Gamma(\ell+1-i/k)|\mathrm{Re}\left\{\frac{\mathrm{e}^{-i(kr-\pi(\ell+1)/2+\log(kr)/k)}}{\Gamma(\ell+1-i/k)}G(\ell+1+i/k, i/k-\ell, -2ikr)\right\} \tag{2.64}$$

where for G we have the asymptotic series

$$G(\alpha,\beta,z) = 1 + \frac{\alpha\beta}{1!z} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{2!z^2} + \cdots.$$

Taking the first term in (2.64) (with $\Gamma(\ell+1-i/k)^*/\Gamma(\ell+1-i/k)^*$ in the braces) gives

$$R_{k\ell}(r) \sim \frac{2}{r}\frac{1}{|\Gamma(\ell+1-i/k)|}\mathrm{Re}\{\mathrm{e}^{-i(kr-\pi(\ell+1)/2+\log(kr)/k)}\Gamma(\ell+1-i/k)^*\},$$

and from the calculations leading to equations (2.45) and (2.46) we have

$$\begin{aligned}\mathrm{Re}\{i\mathrm{e}^{-i\xi}\Gamma(\ell+1-i/k)^*\} &= \sin(\xi)\mathrm{Re}\{\Gamma(\ell+1-i/k)^*\} - \cos(\xi)\mathrm{Im}\{\Gamma(\ell+1-i/k)^*\}\\ &= |\Gamma(\ell+1-i/k)^*|\sin\left(\xi + \arctan\left[-\frac{\mathrm{Im}\{\Gamma(\ell+1-i/k)^*\}}{\mathrm{Re}\{\Gamma(\ell+1-i/k)^*\}}\right]\right)\\ &= |\Gamma(\ell+1-i/k)|\sin\left(\xi + \arctan\left[\frac{\mathrm{Im}\{\Gamma(\ell+1-i/k)\}}{\mathrm{Re}\{\Gamma(\ell+1-i/k)\}}\right]\right)\end{aligned}$$

where $\xi \equiv kr - \pi\ell/2 + \log(kr)/k$. Therefore,

$$R_{k\ell}(r) \sim \frac{2}{r}\sin(kr - \pi\ell/2 + \log(kr)/k + \delta_\ell) \tag{2.65}$$

where

$$\delta_\ell = \arg\{\Gamma(\ell+1-i/k)\}. \tag{2.66}$$

Equation (2.65) illustrates the stark difference between the Coulomb interaction and shorter range potentials: the logarithmic term means that even at the largest distances, the radial part of the scattered wave never tends to e^{ikr}/r [Messiah, 1999, p. 423].

In terms of the S-matrix $S_\ell(k) = \mathrm{e}^{2i\delta_\ell} = \mathrm{e}^{i\delta_\ell}/\mathrm{e}^{-i\delta_\ell}$, we have from the polar form definition of complex numbers and equation (2.66) that[8]

$$S_\ell(k) = \frac{\Gamma(\ell+1-i/k)}{\Gamma(\ell^*+1+i/k)}. \tag{2.67}$$

To arrive at the formula (2.67) we used the well-known conjugation formula $\Gamma(z)^* = \Gamma(z^*)$ found in, for example, Abramowitz and Stegun [1965] p. 256. For our purposes, the appearance of $\Gamma(\ell^*+1+i/k)$ in the denominator of equation (2.67) is of no consequence since $\Gamma(z)$ is without zeros [Olver, 1974, p. 35]. This means that the ℓ-plane singularities of the S-matrix occur at the singularites of the numerator. However, the only singularities of $\Gamma(z)$ are simple poles at $z = 0, -1, -2, -3, \ldots$ [Olver, 1974, p. 32]. Therefore, for Coulomb scattering the j-th Regge pole position is given by

$$\ell_j + 1 - \frac{i}{k} = -j, \quad j = 0, 1, 2, \ldots,$$

[8]Equation (2.67) is obtained for $E \geq 0$ and $\mathrm{Re}(\ell) > -1/2$, i.e. where the wavefunction is normalizable, and then continued for $E < 0$ and $\mathrm{Re}(\ell) \leq -1/2$ [Frautschi, 1963, p. 120].

or in the language of trajectories

$$\alpha_j(E) = -j - 1 + \frac{i}{\sqrt{2E}} \tag{2.68}$$

since, in atomic units, the quantum wave number becomes simply $k = \sqrt{2E}$. The Coulomb trajectory described by equation (2.68) is the result reported in Frautschi [1963] p. 121, which is where we will also take its interpretation from. Consider varying the energy. As $E \to -\infty$, the j-th Regge pole tends to $\ell = -j-1$. Let $\varepsilon > 0$ be small; as the energy winds up to $-\varepsilon$ from $-\infty$, the poles reside on the real ℓ-axis and move incrementally toward the point $\text{Re}(\ell) = +\infty$, $\text{Im}(\ell) = 0$. Equating $\alpha_j(E)$ to a non-negative integer $\ell = 0, 1, 2, 3, \ldots$ yields the famous formula for the bound states of a Bohr atom:

$$E_{j\ell} = -\frac{1}{2(j+\ell+1)^2}.$$

Hence, at this energy $E_{j\ell}$, the j-th Regge pole crosses the physically meaningful values of ℓ. For $E \to +\varepsilon$, the j-th Regge pole jumps to the straight line described by $\text{Re}(\ell) = -j-1$ and tends to $\ell = -j-1$ as $E \to +\infty$. The Coulomb trajectory described here is illustrated in Figure 2.3. It is a peculiarity of the Coulomb attraction that states of arbitrarily

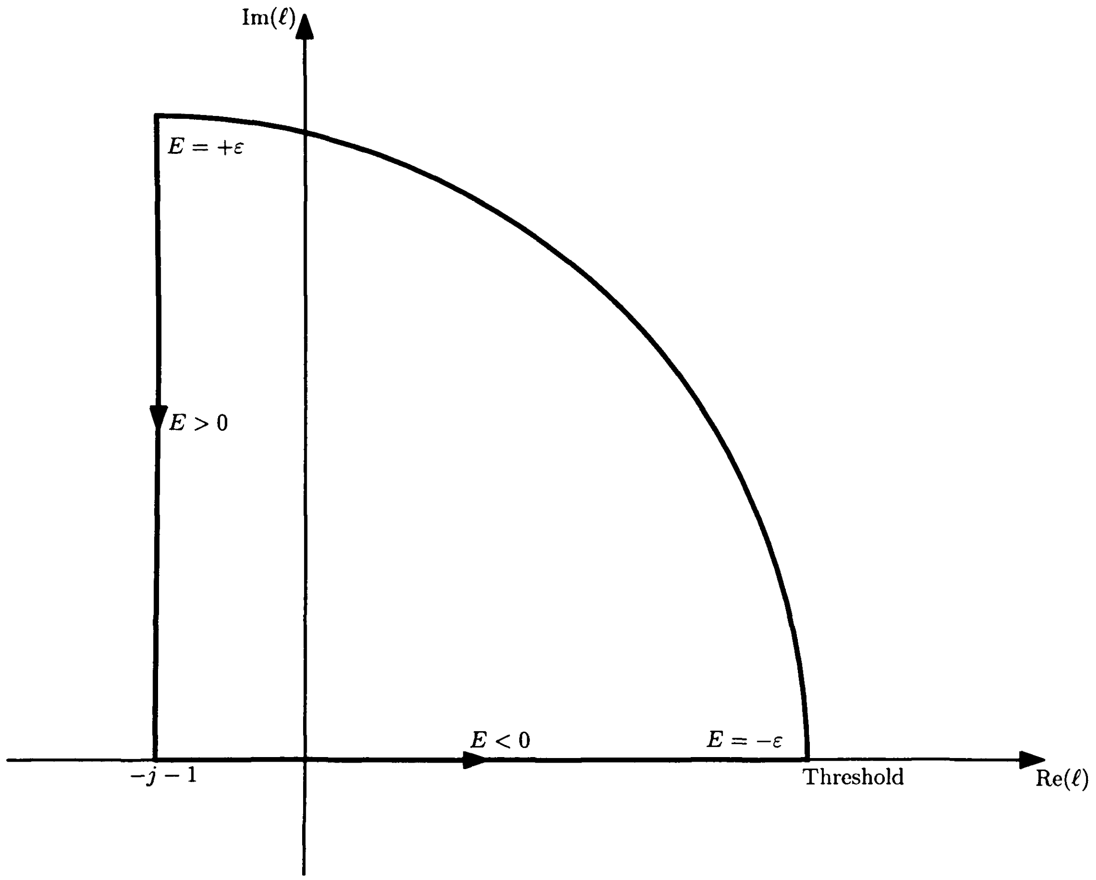

Figure 2.3: Regge trajectory moving to the right from $-j-1$ for the attractive Coulomb potential; schematic taken from Frautschi [1963] p. 127.

high angular momentum quantum number can be bound. Compare this to shorter range potentials $e^{-\mu r}/r$, $\mu \neq 0$; in these cases the centrifugal term dominates for all r when ℓ is sufficiently large, and so the Regge trajectories do not normally extend all of the way to the right [Frautschi, 1963, p. 122]. We also notice the jump in the Coulomb trajectory at threshold; for shorter range potentials it is expected that the trajectories are continuous at threshold. In fact, mathematical proof of this expectation is the topic of Chapter 3.

2.5.2 Regge Representation of the Scattering Amplitude

Recall the partial wave representation of the scattering amplitude (2.32); rewriting the $\sin \delta_\ell$ in terms of exponentials we have

$$f(k, \vartheta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1)(S_\ell - 1) P_\ell(\cos \vartheta). \tag{2.69}$$

By using the Sommerfeld-Watson transformation [Connor, 1990], Regge rewrote the partial wave sum given in (2.69) as a contour integral where each term in the partial wave sum is the residue of a pole in the integrand. In this section, we will derive this contour integral but first, let us adopt in the spirit of Regge [1959], the notion of generalized CAM, which is denoted by $\lambda \equiv \ell + 1/2$. Define the function $F(\lambda) = -\pi f(\lambda)/\cos(\pi\lambda)$, where we assume that f (not the f of (2.69)) is an analytic function of λ in a region close to the real λ-axis. Then F has simple poles at $\lambda = 1/2, 3/2, 5/2, \ldots$ where its residue is

$$\text{Res}(F, \lambda) = \frac{f(\lambda)}{\sin(\pi\lambda)} = (-1)^{\lambda - 1/2} f(\lambda).$$

Hence, through the Sommerfeld-Watson method we have the relation

$$\sum_{\ell=0}^{\infty} (-1)^\ell f(\ell + 1/2) = \frac{1}{2i} \int_\gamma \frac{f(\lambda)}{\cos(\pi\lambda)} \mathrm{d}\lambda \tag{2.70}$$

where the contour γ encloses the physical angular momentum quantum numbers—the positive half-integers—in a clockwise sense (Figure 2.4). Assuming that the S-matrix is an analytic function of ℓ, and hence of the generalized CAM λ in the vicinity of the positive real λ-axis, we have by applying equation (2.70) to the partial wave series form of the scattering amplitude (2.69) that

$$\begin{aligned} \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1)(S_\ell - 1)(-1)^\ell P_\ell(\cos \vartheta) &= \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1)(S_\ell - 1) P_\ell(-\cos \vartheta) \\ &= -\frac{1}{4k} \int_\gamma \frac{2\lambda (S_{\lambda-1/2} - 1) P_{\lambda - 1/2}(-\cos \vartheta)}{\cos(\pi\lambda)} \end{aligned} \tag{2.71}$$

where we have used, for the second time, the formula $(-1)^\ell P_\ell(\cos \vartheta) = P_\ell(-\cos \vartheta)$. For this analysis to work, it is important to note that $P_\ell(-\cos \vartheta)$ is free from singularities

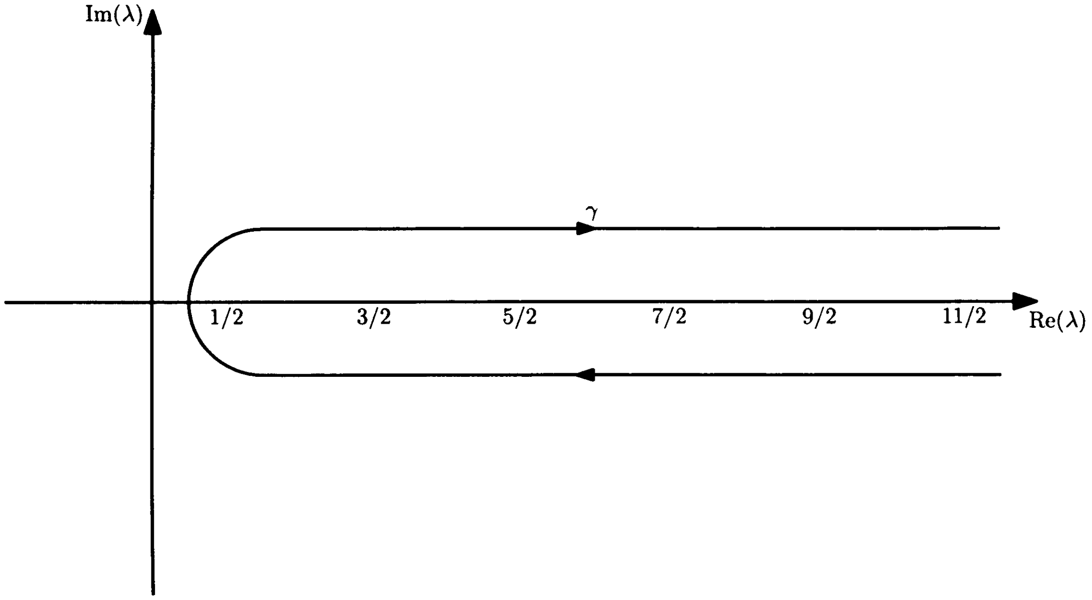

Figure 2.4: The contour γ used in the Sommerfeld-Watson transformation.

at any finite ℓ [Frautschi, 1963, p. 109], and thus only the Regge pole singularities of S remain. We also note that $P_{\lambda-1/2}(-\cos\vartheta)$, which appears in equation (2.71), is no longer a polynomial, but a Legendre function of complex degree $\lambda-1/2$ [Connor, 1990]. Therefore, by (2.69) and (2.71) we have (with $z\equiv\cos\vartheta$) the integral form of (2.69):

$$f(\vartheta) = -\frac{1}{2k}\int_{\gamma}\frac{\lambda(S_{\lambda-1/2}-1)P_{\lambda-1/2}(-z)}{\cos(\pi\lambda)}\mathrm{d}\lambda. \tag{2.72}$$

Assuming the integrand in (2.72) is well-behaved for large $|\lambda|$, we may deform the contour γ away from the real axis into a new contour, $\tilde{\gamma}$ say. Deforming γ this way results in f picking up contributions from poles of the S-matrix in the first quadrant; this yields the Regge representation of the scattering amplitude [Connor, 1990]:

$$f(\vartheta) = -\frac{1}{2k}\int_{\tilde{\gamma}}\frac{\lambda(S_{\lambda-1/2}-1)P_{\lambda-1/2}(-z)}{\cos(\pi\lambda)}\mathrm{d}\lambda - \frac{i\pi}{k}\sum_{n=0}^{\infty}\frac{\lambda_n r_n}{\cos(\pi\lambda_n)}P_{\lambda_n-1/2}(-z), \tag{2.73}$$

where λ_n and r_n are the Regge pole positions and residues respectively. The Regge representation of the scattering amplitude (2.73) is very important, for if we knew of a class of potentials in which there were a relatively small number of associated Regge poles, then the sum over the contributions from a small number of Regge poles would offer significant simplicity compared to the sum over a large number of partial waves. In §2.5.1 we learned that there are infinitely many Regge poles of the Coulomb scattering matrix (2.67), and therefore the Regge representation of the scattering amplitude offers little advantage in this case. However, even if there are many poles for a particular class of potentials, the residues may decrease rapidly thus negating the need to use them all.

2.6 The Wronskian Characterization of Regge Poles

The Wronskian condition for Regge poles was derived and used by Regge himself; it is the characterization that is adopted in this thesis. Suppose $u_0(r,k,\lambda)$ is the well-behaved solution at the origin of the radial Schrödinger equation

$$-u'' + \left(\frac{\lambda^2 - 1/4}{r^2} + U(r) - k^2\right)u = 0, \quad r \in (0,\infty). \tag{2.74}$$

Since (2.74) is a second order equation we must have a relation of the form

$$u_0(r,k,\lambda) = A(\lambda)u_\infty(r,k,\lambda) + B(\lambda)\tilde{u}_\infty(r,k,\lambda) \tag{2.75}$$

where u_∞ and $\tilde{u}_\infty$ are linearly independent solutions of (2.74) with $u_\infty(r,k,\lambda) \sim e^{ikr}$ and $\tilde{u}_\infty(r,k,\lambda) \sim e^{-ikr}$ far from the origin. We can write (2.75) as

$$\begin{aligned} u_0(r,k,\lambda) &= A(\lambda)[u_\infty(r,k,\lambda) + (A(\lambda)/B(\lambda))^{-1}\tilde{u}_\infty(r,k,\lambda)] \\ &= A(\lambda)[u_\infty(r,k,\lambda) + S(\lambda)^{-1}\tilde{u}_\infty(r,k,\lambda)] \end{aligned}$$

where $S(\lambda) = A(\lambda)/B(\lambda)$ is the scattering matrix. The Wronskian of $u_0(r,k,\lambda)$ and $u_\infty(r,k,\lambda)$, denoted $\mathscr{W}(u_0(r,k,\lambda), u_\infty(r,k,\lambda))$, is defined by

$$\mathscr{W}(u_0(r,k,\lambda), u_\infty(r,k,\lambda)) \equiv \begin{vmatrix} u_0(r,k,\lambda) & u_\infty(r,k,\lambda) \\ u_0'(r,k,\lambda) & u_\infty'(r,k,\lambda) \end{vmatrix}. \tag{2.76}$$

The Wronskian can be used to determine whether a set of differentiable functions are linearly independent over a given interval. More precisely, if the Wronskian of two differentiable functions is non-zero at some point on the interval, then those two functions are linearly independent over that interval. Relaxing the dependency on r, k, and λ for the moment, and introducing (2.75) into (2.76), we have

$$\begin{aligned} \mathscr{W}(u_0, u_\infty) &= A(\lambda)\mathscr{W}(u_\infty, u_\infty) + B(\lambda)\mathscr{W}(u_\infty, \tilde{u}_\infty) \\ &= B(\lambda)\mathscr{W}(u_\infty, \tilde{u}_\infty). \end{aligned}$$

Since u_∞ and $\tilde{u}_\infty$ are linearly independent, their Wronskian $\mathscr{W}(u_\infty(r,k,\lambda), \tilde{u}_\infty(r,k,\lambda))$ is non-zero for some $r > 0$; in fact, it is non-zero for all $r > 0$ since the Wronskian of two solutions of a homogeneous second order ordinary differential equation is independent of r [Simmons, 1972, p. 78]. Therefore, $\mathscr{W}(u_0(r,k,\lambda), u_\infty(r,k,\lambda))$ is zero if and only if $B(\lambda) = 0$, i.e. when the scattering matrix $S(\lambda)$ has a pole.

CHAPTER 3

Low Energy

3.1 Notation and Introduction

Consider the radial Schrödinger equation in the generalized CAM form with reduced potential given by (2.74), and suppose $r_0 > 0$ is some finite and fixed number; our notation for the present chapter is as follows: denote by $u_0(r, k, \lambda)$ the solution for $r \leq r_0$, which is well-behaved in a neighbourhood of the origin, i.e. the solution satisfying

$$u_0(r, k, \lambda) \sim r^{\lambda+1/2}, \quad r \to 0. \tag{3.1}$$

Let $u_\infty(r, k, \lambda)$ be the solution for $r > r_0$ satisfying the usual scattering condition of an outgoing wave at distances far from the origin, i.e.

$$u_\infty(r, k, \lambda) \sim \mathrm{e}^{ikr}, \quad r \to \infty. \tag{3.2}$$

Recall that e^{-ikr} does not represent an outgoing wave, which is the reason for (3.2). Moreover, we will let $u_\infty(r, 0, \lambda)$ identify the unique (up to multiplication by a non-zero constant) $k = 0$ solution in $\mathcal{L}^2(r_0, \infty; r^{-2})$—this will become clear in due course.

We note at the outset that it is difficult—but not impossible—to solve the low energy Regge pole problem using operator theoretic methods; this is because the scattering condition required at infinity depends upon the very parameter that we are sending to zero, namely, k. Hence, the domain of any operator that we define in order to analyse the problem will also change. Therefore, we will take a different, arguably more direct, approach to studying the threshold continuity of Regge trajectories. The approach we take is to study the small k pointwise limit of the Regge pole condition, which we will now discuss. In view of the Wronskian characterization of Regge poles introduced in §2.6, the condition on λ to be a Regge pole can be written as

$$\frac{u_0'(r,k,\lambda)}{u_0(r,k,\lambda)} = \frac{u_\infty'(r,k,\lambda)}{u_\infty(r,k,\lambda)} \tag{3.3}$$

where $r = r_0 > 0$ is fixed. For the remainder of this chapter, and indeed for the next chapter, r will always be identified with some fixed $r_0 > 0$ unless stated otherwise. We are interested in what happens to the Regge poles as $k \to 0$, and thus we study the equation

$$\lim_{k\to 0}\left\{\frac{u_0'(r,k,\lambda)}{u_0(r,k,\lambda)}\right\} = \lim_{k\to 0}\left\{\frac{u_\infty'(r,k,\lambda)}{u_\infty(r,k,\lambda)}\right\} \tag{3.4}$$

locally uniformly in λ.

The local uniform convergence in λ for this problem is very important: suppose we have a sequence $(k_n)_{n\in\mathbb{N}}$ with $k_n \to 0$ as $n \to \infty$, and $f_n(\cdot) \equiv f(\cdot, k_n)$ such that $f_n(\lambda_n) = 0$ for all $n \in \mathbb{N}$ (where $\lambda_n = \lambda(k_n)$). Also assume that $f_n \to f$ as $n \to \infty$. Then denoting by (λ_{n_j}) a convergent subsequence of (λ_n) with limit λ_∞, it may not be the case that $f(\lambda_\infty) = 0$. This is only guaranteed if the convergence $f_n \to f$ is locally uniform in λ.

We illustrate this with a simple example. Let us construct a sequence of functions $(f_n)_{n\in\mathbb{N}}$ with the following properties:

1. $f_n(0) = -1$ for all $n \in \mathbb{N}$,
2. $f_n(\lambda) \to -1$ as $n \to \infty$ for all $\lambda \neq 0$,
3. $f_n(\lambda_n) = 0$ where $\lambda_n \to 0$ as $n \to \infty$.

The sequence of functions given by

$$f_n(\lambda) = \frac{-(\lambda + \varepsilon_n)}{(1 + 1/n)\lambda + \varepsilon_n}$$

where $\varepsilon_n \to 0$ as $n \to \infty$, satisfies the properties 1–3 if we have $\lambda_n = -\varepsilon_n$. Retaining the above notation, we do not have $f(\lambda_\infty) = 0$. In this example f_n has a pole at

$$\lambda = -\frac{\varepsilon}{(1 + 1/n)},$$

and consequently f_n is not uniformly bounded in λ violating the hypotheses of Montel's Theorem.[1] We will invoke this extremely useful result in due course to ensure that the convergence in the low energy Regge pole problem is locally uniform in λ.

As we discussed in Chapter 1, our strategy for proving the expected continuity of Regge trajectories at threshold begins with the finite spherical well. This is a relatively simple spherically symmetric potential—unencumbered by obfuscating details, it will be an invaluable example which brings out the core of the argument.

[1]This is proved in Appendix C, the result can be found in Conway [1978] p. 153, for example.

3.2 Finite Spherical Well

Consider the soft sphere scattering problem, i.e. we must solve equation (2.74) in which the potential is given by

$$U(r) = \begin{cases} -U_0 & \text{if} \quad r \leq r_0, \\ 0 & \text{if} \quad r > r_0 \end{cases} \tag{3.5}$$

and $U_0, r_0 > 0$. The well-behaved solution at the origin $u_0(r, k, \lambda)$ may be found using the Frobenius method, and so we are able to rewrite equation (3.4) as

$$\frac{u_0'(r, 0, \lambda)}{u_0(r, 0, \lambda)} = \lim_{k \to 0} \left\{ \frac{u_\infty'(r, k, \lambda)}{u_\infty(r, k, \lambda)} \right\}, \tag{3.6}$$

where we choose the matching point to be at $r = r_0$. Therefore, we only need to calculate the limit of the ratio concerning u_∞. We have already encountered the free R-solutions: they are given by equation (2.42) and since $u(r) = rR(r)$,

$$u_\infty(r, k, \lambda) = A\sqrt{\frac{r}{k}} J_\lambda(kr) + B\sqrt{\frac{r}{k}} N_\lambda(kr) \tag{3.7}$$

where we have used the established notation $\lambda = \ell + 1/2$. However, neither $J_\lambda(kr)$ nor $N_\lambda(kr)$ represents an outgoing (or incoming for that matter) wave. For this purpose, we introduce the Hankel functions of the first and second kind, $H_\lambda^{(1)}$ and $H_\lambda^{(2)}$ respectively; these are defined as follows [Arfken and Weber, 2005, p. 707]:

$$H_\lambda^{(1)}(x) \equiv J_\lambda(x) + iN_\lambda(x) \quad \text{and} \quad H_\lambda^{(2)}(x) \equiv J_\lambda(x) - iN_\lambda(x).$$

For large r, $H_\lambda^{(1)}(kr)$ is asymptotically proportional to $\mathrm{e}^{ikr}/\sqrt{r}$, whilst $H_\lambda^{(2)}(kr)$ behaves like $\mathrm{e}^{-ikr}/\sqrt{r}$ [Abramowitz and Stegun, 1965, p. 364]. They are linearly independent solutions but we only require the former, and so absorbing the normalization constant we have from equation (3.7) that

$$u_\infty(r, k, \lambda) = \sqrt{\frac{r}{k}} H_\lambda^{(1)}(kr). \tag{3.8}$$

This means that since $r = r_0$ is fixed, the problem of calculating the limit

$$\lim_{k \to 0} \left\{ \frac{u_\infty'(r, k, \lambda)}{u_\infty(r, k, \lambda)} \right\}, \tag{3.9}$$

simplifies to calculating small argument asymptotics of the Hankel function of the first kind and its first derivative with respect to spatial variable. These are quite standard, and we perform the necessary calculations in the next section; upon applying these asymptotics in order to compute the limit (3.9), it is straightforward to establish the required result.

3.2.1 Hankel Function Asymptotics

We need to compute the small argument asymptotics of $H^{(1)}_\lambda(kr)$, but also of its first derivative with respect to r, evaluated at $r = r_0$—this can be taken as the definition of the notation $'$ for the remainder of this chapter. First of all, we have from Abramowitz and Stegun [1965] p. 360 the standard series definition of the Bessel function

$$J_\nu(z) \equiv \left(\frac{z}{2}\right)^\nu \sum_{j=0}^{\infty} \frac{(-z^2/4)^j}{j!\Gamma(\nu+j+1)}, \tag{3.10}$$

where $\Gamma(z)$ is Euler's gamma function. Equation (3.10) yields

$$J_{-\lambda}(kr) = \left(\frac{kr}{2}\right)^{-\lambda} \sum_{j=0}^{\infty} \frac{(-(kr)^2/4)^j}{j!\Gamma(j-\lambda+1)} \tag{3.11}$$

and

$$\{J_{-\lambda}(kr)\}' = -\frac{\lambda}{r}\left(\frac{kr}{2}\right)^{-\lambda} \sum_{j=0}^{\infty} \frac{(-(kr)^2/4)^j}{j!\Gamma(j-\lambda+1)} + \frac{2}{r}\left(\frac{kr}{2}\right)^{-\lambda} \sum_{j=0}^{\infty} \frac{j(-(kr)^2/4)^j}{j!\Gamma(j-\lambda+1)}. \tag{3.12}$$

Moreover, from the well-known recurrence formula for differentiating Hankel functions, namely, $2H'_\nu(r) = H_{(\nu-1)}(r) - H_{(\nu+1)}(r)$ [Arfken and Weber, 2005, p. 708], we have

$$\{H^{(1)}_\lambda(kr)\}' = \frac{k}{2}(H^{(1)}_{(\lambda-1)}(kr) - H^{(1)}_{(\lambda+1)}(kr)). \tag{3.13}$$

It follows from standard relations in Bessel function theory, all readily found in the book of Arfken and Weber [2005], that

$$\begin{aligned}
&H^{(1)}_{(\lambda-1)}(kr) - H^{(1)}_{(\lambda+1)}(kr) = J_{(\lambda-1)}(kr) + iN_{(\lambda-1)}(kr) - \{J_{(\lambda+1)}(kr) + iN_{(\lambda+1)}(kr)\} \\
&= J_{(\lambda-1)}(kr) + i(\cot(\lambda-1)\pi J_{(\lambda-1)}(kr) - \csc(\lambda-1)\pi J_{(-\lambda+1)}(kr)) - \{J_{(\lambda+1)}(kr) \\
&\qquad + i(\cot(\lambda+1)\pi J_{(\lambda+1)}(kr) - \csc(\lambda+1)\pi J_{(-\lambda-1)}(kr))\} \\
&= \frac{2}{k}\{J_\lambda(kr)\}' + i\cot(\lambda-1)\pi(J_{(\lambda-1)}(kr) - J_{(\lambda+1)}(kr)) + i\csc(\lambda-1)\pi(J_{(-\lambda-1)}(kr) \\
&\qquad - J_{(-\lambda+1)}(kr)) \\
&= \frac{2}{k}(1 + i\cot(\lambda-1)\pi)\{J_\lambda(kr)\}' + \frac{2i}{k}\csc(\lambda-1)\pi\{J_{-\lambda}(kr)\}'.
\end{aligned}$$

Therefore, by equations (3.12) and (3.13) the dominant part of $\{H^{(1)}_\lambda(kr)\}'$, for small k, is $i\csc(\lambda-1)\pi\{J_{-\lambda}(kr)\}'$. Also, $H^{(1)}_\lambda(kr) = J_\lambda(kr) + i(\cot\lambda\pi J_\lambda(kr) - \csc\lambda\pi J_{-\lambda}(kr))$, of which the dominant part is $-i\csc\lambda\pi J_{-\lambda}(kr)$, as can be seen from (3.11). Performing analogous calculations for $H_\lambda^{(2)}(kr)$ yields that

$$\begin{aligned} H_{(\lambda-1)}^{(2)}(kr) - H_{(\lambda+1)}^{(2)}(kr) &= J_{(\lambda-1)}(kr) - iN_{(\lambda-1)}(kr) - \{J_{(\lambda+1)}(kr) - iN_{(\lambda+1)}(kr)\} \\ &= \frac{2}{k}(1 - i\cot(\lambda-1)\pi)\{J_\lambda(kr)\}' - \frac{2i}{k}\csc(\lambda-1)\pi\{J_{-\lambda}(kr)\}', \end{aligned}$$

and therefore the dominant part of $\{H_\lambda^{(2)}(kr)\}'$ is $-i\csc(\lambda-1)\pi\{J_{-\lambda}(kr)\}'$. Finally, we also have that the dominant part of $H_\lambda^{(2)}(kr)$, for small argument, is $i\csc\lambda\pi J_{-\lambda}(kr)$. Taking only the leading terms in (3.11) and (3.12) gives

$$H_\lambda^{(1)}(kr) \sim \frac{-i\csc\lambda\pi(kr/2)^{-\lambda}}{\Gamma(-\lambda+1)} \quad \text{and} \quad \{H_\lambda^{(1)}(kr)\}' \sim \frac{-\lambda i\csc(\lambda-1)\pi(kr/2)^{-\lambda}}{r\Gamma(-\lambda+1)} \tag{3.14}$$

for small k. From (3.8) it follows that

$$u'_\infty(r,k,\lambda) = \sqrt{\frac{r}{k}}\{H_\lambda^{(1)}(kr)\}' + \frac{1}{2\sqrt{kr}}H_\lambda^{(1)}(kr) \tag{3.15}$$

whence

$$\frac{u'_\infty(r,k,\lambda)}{u_\infty(r,k,\lambda)} = \frac{\{H_\lambda^{(1)}(kr)\}'}{H_\lambda^{(1)}(kr)} + \frac{1}{2r}. \tag{3.16}$$

Consequently, for fixed $r = r_0$ equation (3.14) yields

$$\frac{u'_\infty(r,k,\lambda)}{u_\infty(r,k,\lambda)} \sim \frac{-\lambda}{r} + \frac{1}{2r}, \quad k \to 0. \tag{3.17}$$

If we write $u'_{\text{lim}}(r,\lambda) \equiv \lim_{k\to 0} u'_\infty(r,k,\lambda)$ and $u_{\text{lim}}(r,\lambda) \equiv \lim_{k\to 0} u_\infty(r,k,\lambda)$, then from (3.17) we have

$$\frac{u'_{\text{lim}}(r,\lambda)}{u_{\text{lim}}(r,\lambda)} = \frac{-\lambda+1/2}{r}; \tag{3.18}$$

a consequence of the fact that only the irregular part of u_∞ should be taken into account when calculating the logarithmic derivative. Recall that $u_0(r,0,\lambda)$ satisfies the equation

$$-u''_0(r,0,\lambda) + \left(- U_0 + \frac{\lambda^2 - 1/4}{r^2}\right) u_0(r,0,\lambda) = 0 \tag{3.19}$$

and furthermore, the function $u_{\text{lim}}(r,\lambda) = r^{-\lambda+1/2}$ satisfies the limiting equation (3.18) at $r = r_0$. It also satisfies

$$-u''_{\text{lim}}(r,\lambda) + \left(\frac{\lambda^2 - 1/4}{r^2}\right) u_{\text{lim}}(r,\lambda) = 0, \tag{3.20}$$

which means that $u_{\text{lim}}(r,\lambda) = u_\infty(r,0,\lambda)$. Rewriting (3.20) as

$$-u''_\infty(r,0,\lambda) + \left(\frac{\lambda^2 - 1/4}{r^2}\right) u_\infty(r,0,\lambda) = 0, \tag{3.21}$$

we can combine equations (3.19) and (3.21) to get

$$-u'' + \left(U(r) + \frac{\lambda^2 - 1/4}{r^2}\right)u = 0, \tag{3.22}$$

which is precisely equation (2.74) with finite spherical well potential (3.5) and k set to zero. Equation (3.22) is self-adjoint since there is at most one square integrable solution at each singular endpoint.[2] Equivalently, we have shown the equations

$$\lim_{k\to 0}\left\{\frac{u_0'(r,k,\lambda)}{u_0(r,k,\lambda)}\right\} = \frac{u_0'(r,0,\lambda)}{u_0(r,0,\lambda)} \tag{3.23}$$

and

$$\lim_{k\to 0}\left\{\frac{u_\infty'(r,k,\lambda)}{u_\infty(r,k,\lambda)}\right\} = \frac{u_\infty'(r,0,\lambda)}{u_\infty(r,0,\lambda)} \tag{3.24}$$

to be true, which by the Regge pole condition (3.4) means that we have

$$\frac{u_0'(r,0,\lambda)}{u_0(r,0,\lambda)} = \frac{u_\infty'(r,0,\lambda)}{u_\infty(r,0,\lambda)}, \tag{3.25}$$

and (3.25) is the condition on the wavefunctions in order to have an eigenvalue.

An alternative viewpoint on the Regge pole condition is to consider, for example, the time-independent Schrödinger equation in which the potential is attractive and decays sufficiently fast as $x \to \pm\infty$. If we restrict our consideration to bound states then we require that the solution $\psi(x) \to 0$ as $x \to \pm\infty$, which we know is possible only for certain discrete values of the energy E. Let us label by 1 and 3 the regions where $E < V(x)$ for all x and by 2 the region in which $E > V(x)$. In region 2, $\psi(x)$ oscillates whilst in regions 1 and 3 there are two linearly independent solutions—one physical and one unphysical. We must take the physically acceptable solution in both regions 1 and 3, which is possible only for certain 'allowed' energies. The technique for finding these energies E is the so-called shooting method. The idea of the shooting method is to start in region 1 and integrate into region 2, which results in some function $\psi_{\text{left}}(x)$. Similarly, we acquire a function $\psi_{\text{right}}(x)$ by starting in region 3 and integrating backwards into region 2. The wavefunction and its first derivative must be continuous, and thus we stipulate $\psi_{\text{left}}(x) = \psi_{\text{right}}(x)$ and $\psi_{\text{left}}'(x) = \psi_{\text{right}}'(x)$ in region 2. This can be combined into a single matching condition by multiplying by an appropriate constant, which is valid since the Schrödinger equation is linear. Therefore, we could take the condition to be $\psi_{\text{left}}'(x)/\psi_{\text{left}}(x) = \psi_{\text{right}}'(x)/\psi_{\text{right}}(x)$, and this can be tested at a given value of x. Adjustments of the energy E are then done until this condition is satisfied. In any case, we have shown the following:

Theorem 1. *In the limit as the energy tends to zero, the Regge poles associated with a finite spherical well tend to the angular momentum eigenvalues of the self-adjoint problem formed when the energy is identically zero.*

[2]This result—Theorem A.12—is developed in detail in Appendix A.3.

The finite spherical well may not be the most realistic model—although it is quite useful for the scattering of sub-nuclear particles [Taylor, 1970, p. 187]—but it usually proves, as in many quantum mechanical problems, to be an instructive example. Naturally, the sequel will be concerned with a compactly supported integrable potential, for which it will be shown that Theorem 1 still holds. The integrability condition on the potential just ensures that the differential equation has solutions.

3.3 Compactly Supported Potential

Suppose that U is any integrable potential such that $U(r) = 0$ for $r > r_0$. Guided by the method used in §3.2 for the finite spherical well, we need to demonstrate that equations (3.23) and (3.24) still hold. It is clear that equation (3.24) is satisfied since the potential is identically zero for $r > r_0$; however, it is unclear whether equation (3.23) is true. We certainly know that $u_0(r, k, \lambda)$ satisfies

$$-u_0''(r,k,\lambda) + \left(U(r) + \frac{\lambda^2 - 1/4}{r^2} - k^2\right)u_0(r,k,\lambda) = 0, \quad r \leq r_0. \tag{3.26}$$

Suppose we choose the well-behaved solution $u_0(r, k, \lambda)$ at the origin, i.e. the solution for $r \leq r_0$ such that $u_0(r, k, \lambda) \sim r^{\lambda+1/2}$ as $r \to 0$, then we have $u_0(r, k, \lambda) \to 0$ as $r \to 0$ provided $\mathrm{Re}(\lambda) > 0$. Thus, we are free to use the normalization $u_0(r_0, k, \lambda) = 1$. Define

$$\phi(r,k,\lambda) \equiv u_0(r,k,\lambda) - u_0(r,0,\lambda) \tag{3.27}$$

so that ϕ satisfies

$$-\phi''(r,k,\lambda) + \left(U(r) + \frac{\lambda^2 - 1/4}{r^2} - k^2\right)\phi(r,k,\lambda) = k^2 u_0(r,0,\lambda), \quad r \leq r_0 \tag{3.28}$$

and $\phi(r, k, \lambda) \to 0$ as $r \to 0$. Also, by our normalization of $u_0(r_0, k, \lambda)$, $\phi(r_0, k, \lambda) = 0$. Furthermore, define an operator

$$T \equiv -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \left(U(r) + \frac{\lambda^2 - 1/4}{r^2}\right) \tag{3.29}$$

with domain given by

$$\mathscr{D}(T) = \{f \in \mathcal{L}^2(0,r_0) : Tf \in \mathcal{L}^2(0,r_0), f(r_0) = 0\}. \tag{3.30}$$

Then

$$\phi(r,k,\lambda) = (T - k^2)^{-1} k^2 u_0(r,0,\lambda), \tag{3.31}$$

where $(T-k^2)^{-1}u_0$ is analytic in k. Therefore, $\phi \to 0$ as $k \to 0$, i.e. $u_0(r, k, \lambda) \to u_0(r, 0, \lambda)$ as $k \to 0$ in $\mathcal{L}^2$. With regard to (3.23), we also need to consider the first derivative of ϕ

with respect to r, ϕ'. Multiplying (3.28) by ϕ^* and integrating by parts we have

$$\int_0^{r_0} |\phi'|^2 \mathrm{d}r + \int_0^{r_0} U(r)|\phi|^2 \mathrm{d}r + (\lambda^2 - 1/4)\int_0^{r_0} \left|\frac{1}{r}\phi\right|^2 \mathrm{d}r = k^2\left[\int_0^{r_0} |\phi|^2 \mathrm{d}r + \int_0^{r_0} u_0(r,0,\lambda)\phi^* \mathrm{d}r\right]. \quad (3.32)$$

For small k, $\phi = T^{-1}k^2 u_0(r,0,\lambda)$ (since $(T-k^2)^{-1} - T^{-1} = k^2 T^{-1}(T-k^2)^{-1}$ by the Hilbert identity and T^{-1} is bounded, as we shall see). Thus, for $\phi' \to 0$ as $k \to 0$ in the $\mathcal{L}^2$ norm, we require that the operator $(1/r)T^{-1}$ be bounded in $\mathcal{L}^2(0, r_0)$ and the term involving the potential vanishes as $k \to 0$. For the former, consider the operator $T_0 \equiv T - U$ and write

$$\begin{aligned}\frac{1}{r}T^{-1} &= \frac{1}{r}(T_0 + UT_0^{-1}T_0)^{-1} \\ &= \frac{1}{r}T_0^{-1}(\mathbf{1} + UT_0^{-1})^{-1}. \end{aligned} \quad (3.33)$$

In order to demonstrate the boundedness of the operator $(1/r)T^{-1}$ we need only consider the boundedness of $(1/r)T_0^{-1}$ and UT_0^{-1}; we will see that the boundedness of the latter implies that the term in (3.32) involving the potential is also bounded. To obtain an explicit expression for T_0^{-1}, we must solve the inhomogeneous problem

$$-y'' + (\lambda^2 - 1/4)r^{-2}y = g, \quad g \in \mathcal{L}^2(0, r_0).$$

The solution $y_1(r,\lambda) = r^{\lambda+1/2}$ satisfies the boundary condition at zero, whilst the second solution $y_2(r,\lambda) = r_0^{2\lambda}r^{-\lambda+1/2} - r^{\lambda+1/2}$ satisfies the boundary condition at r_0. Moreover, their Wronskian is given by $2\lambda r_0^{2\lambda}$. Therefore,

$$\begin{aligned}(T_0^{-1}g)(r) &= \frac{1}{\mathscr{W}(y_1,y_2)}\left[\int_0^r y_2(r)y_1(s)g(s)\mathrm{d}s + \int_r^{r_0} y_1(r)y_2(s)g(s)\mathrm{d}s\right] \\ &= \frac{1}{2\lambda}\left[\int_0^r \sqrt{rs}\left(\left(\frac{s}{r}\right)^\lambda - \left(\frac{rs}{r_0^2}\right)^\lambda\right)g(s)\mathrm{d}s + \int_r^{r_0} \sqrt{rs}\left(\left(\frac{r}{s}\right)^\lambda - \left(\frac{rs}{r_0^2}\right)^\lambda\right)g(s)\mathrm{d}s\right]. \end{aligned} \quad (3.34)$$

Consequently, we have from equation (3.34) that

$$\left(\frac{1}{r}T_0^{-1}g\right)(r) = \frac{1}{2\lambda}\left[\int_0^r \sqrt{\frac{s}{r}}\left(\left(\frac{s}{r}\right)^\lambda - \left(\frac{rs}{r_0^2}\right)^\lambda\right)g(s)\mathrm{d}s + \int_r^{r_0}\left(\frac{r}{s}\right)^{\lambda-1/2}\left(1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right)g(s)\mathrm{d}s\right]. \quad (3.35)$$

The first integral in equation (3.35) is clearly bounded: note that $s \le r$ and so each term involving s/r can be bounded by 1, then the Cauchy-Schwarz inequality gives the result since $g \in \mathcal{L}^2(0, r_0)$ and our range of intergration is finite; but, the boundedness of the second integral is not so clear and thus it will require further work. For convenience, let us denote the second integral in equation (3.35) by $\mathscr{I}(r)$. Since the Lebesgue space $\mathcal{L}^2$ is its own dual, we can use for bounding $\mathscr{I}$ the norm given by[3]

$$\|\mathscr{I}\|_{\mathcal{L}^2(0,r_0)} = \sup_{h\in\mathcal{L}^2(0,r_0)} \frac{|\langle h|\mathscr{I}\rangle|}{\|h\|_{\mathcal{L}^2(0,r_0)}}. \tag{3.36}$$

By first changing the order of integration and then twice applying the Cauchy-Schwarz inequality, we have

$$\begin{aligned}
|\langle h|\mathscr{I}\rangle| &= \left| \int_0^{r_0} h(r) \left[\int_r^{r_0} \left(\frac{r}{s}\right)^{\lambda-1/2} \left(1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right) g(s)\mathrm{d}s \right] \mathrm{d}r \right| \\
&= \left| \int_0^{r_0} s^{-\lambda+1/2} \left(1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right) g(s) \left[\int_0^s h(r) r^{\lambda-1/2} \mathrm{d}r \right] \mathrm{d}s \right| \\
&\leq \|h\|_{\mathcal{L}^2(0,r_0)} \int_0^{r_0} \left|s^{-\lambda+1/2}\right| \left|1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right| |g(s)| \left| \int_0^s r^{2\lambda-1}\mathrm{d}r \right|^{1/2} \mathrm{d}s \\
&= \|h\|_{\mathcal{L}^2(0,r_0)} \int_0^{r_0} s^{-\mathrm{Re}(\lambda)}\sqrt{s} \left|1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right| |g(s)| \frac{\left|s^{2\lambda}\right|^{1/2}}{\sqrt{2|\lambda|}} \mathrm{d}s \\
&= \frac{1}{\sqrt{2|\lambda|}} \|h\|_{\mathcal{L}^2(0,r_0)} \int_0^{r_0} \sqrt{s} \left|1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right| |g(s)|\mathrm{d}s \\
&\leq \frac{1}{\sqrt{2|\lambda|}} \|h\|_{\mathcal{L}^2(0,r_0)} \|g\|_{\mathcal{L}^2(0,r_0)} \left[\int_0^{r_0} s \left|1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right|^2 \mathrm{d}s \right]^{1/2}.
\end{aligned}$$

On dividing by $\|h\|_{\mathcal{L}^2(0,r_0)}$ (which is finite and positive) and taking the supremum over all $h \in \mathcal{L}^2(0, r_0)$, we find from (3.36) that

$$\|\mathscr{I}\|_{\mathcal{L}^2(0,r_0)} \leq \frac{1}{\sqrt{2|\lambda|}} \|g\|_{\mathcal{L}^2(0,r_0)} \left[\int_0^{r_0} s \left|1 - \left(\frac{s}{r_0}\right)^{2\lambda}\right|^2 \mathrm{d}s \right]^{1/2} < \infty.$$

Therefore, $(1/r)T_0^{-1}$ is a bounded operator in $\mathcal{L}^2(0, r_0)$. Recall that we also require UT_0^{-1} to be bounded in $\mathcal{L}^2(0, r_0)$; this follows if we add a further restriction to the potential. The extra condition that we need is illuminated when we write $UT_0^{-1} = rU(1/r)T_0^{-1}$, namely, we must also make sure that the potential is such that $rU(r)$ is supremum-norm bounded in a neighbourhood of the origin. This neither strengthens nor weakens the integrability condition, but it does allow Coulombic behaviour of the potential at the origin. Note that as soon as we are away from the origin, integrabililty of the potential alone will suffice. Concerning the term in (3.32) involving the potential, we write $U|\phi|^2$ as $UT^{-1}k^2u_0(T^{-1}k^2u_0)^*$. To see that this will vanish as $k \to 0$ we notice that since T_0^{-1} is bounded from (3.34) then T^{-1} is bounded from (3.33). Equation (3.33) also yields that

[3] $\mathcal{L}^2$ is a Hilbert space and every Hilbert space is self-dual. More precisely, there is an antilinear bijection between $\mathscr{H}$ and its dual $\mathscr{H}^*$ which is norm preserving, and so it is usual to identify $\mathscr{H}$ with $\mathscr{H}^*$ in the sense of correspondence under the isometric anti-isomorphism described by the Riesz representation Theorem [Weidmann, 1980, p. 61]. Moreover, when a norm $\|g\|$ in $\mathscr{E}$ is given so that $\mathscr{E}$ becomes a normed space, $\mathscr{E}^*$ is also a normed space with norm defined by $\|f\| \equiv \sup_{0\neq g\in\mathscr{E}} |\langle f|g\rangle|/\|g\|$ [Kato, 1966, p. 13].

UT^{-1} is bounded since we have already noted that UT_0^{-1} is bounded. We conclude that $(1/r)T^{-1}$ is a bounded operator in $\mathcal{L}^2(0, r_0)$ and thus $\phi/r \to 0$ as $k \to 0$ in the $\mathcal{L}^2$ norm. Finally, the right side of (3.32) tends to zero since $u_0(r, 0, \lambda) \in \mathcal{L}^2(0, r_0)$, and as we know T^{-1} is bounded. Thus, it must be the case that $\phi' \to 0$ as $k \to 0$ in the $\mathcal{L}^2$ norm.

In light of (3.23) we actually require pointwise convergence of the wavefunctions, whilst we have convergence in $\mathcal{L}^2(0, r_0)$. However, recycling the arguments just made, it is clear from the differential equation (3.28) that ϕ'' will also go to zero in the $\mathcal{L}^2$ norm. Therefore, we have shown that $\int_0^{r_0}(|\phi|^2 + |\phi'|^2 + |\phi''|^2)\mathrm{d}r \to 0$ as $k \to 0$, i.e. that $\phi \to 0$ as $k \to 0$ in the Sobolev space H^2 norm. Hence, by a Sobolev Embedding Theorem[4], both ϕ and ϕ' vanish pointwise as $k \to 0$. The convergence is locally uniform in $\lambda \in K$ by Montel's Theorem, where K is a compact set in the first quadrant bounded away from zero: T_0^{-1}/r is uniformly bounded in $\lambda \in K$, and this means that ϕ is uniformly bounded in $\lambda \in K$ because $r \le r_0$. We can state what we have found as follows:

Theorem 2. *In the limit as the energy tends to zero, the Regge poles associated with a compactly supported integrable potential U in which $r|U(r)|$ is bounded in a neighbourhood of the origin, tend to the angular momentum eigenvalues of the self-adjoint problem formed when the energy is identically zero.*

We will now see that losing the compactly supported property produces a number of complications, of which, the most fundamental is how to formulate the right side of equation (3.4). In §3.2 we were able to explicitly calculate this limit simply because we could write down the solution and its derivative. To compensate for this, we will be reduced to expressing the solution recursively using integral equations [Shubova, 1989].

3.4 The General Potential

For the left-hand solution, we have already seen that for an integrable potential which forms a bounded product with the spatial variable near the origin, (3.23) holds. Thus, for the general potential (with finite first moment for $r > r_0$) we need only prove (3.24):

$$\lim_{k\to 0}\left\{\frac{u'_\infty(r,k,\lambda)}{u_\infty(r,k,\lambda)}\right\} = \frac{u'_\infty(r,0,\lambda)}{u_\infty(r,0,\lambda)}$$

for some fixed $r = r_0 > 0$. We reiterate that $u_\infty(r, k, \lambda)$ is the solution of (2.74) for $r > r_0$ such that $u'_\infty(r, k, \lambda)/u_\infty(r, k, \lambda) \sim ik$ as $r \to \infty$, $u_\infty(r, 0, \lambda)$ is the unique (up to a scalar multiple) $\mathcal{L}^2(r_0, \infty; r^{-2})$ solution of (2.74) with $k = 0$, and the symbol $'$ denotes differentiation with respect to r evaluated at $r = r_0$. Also, we know from §3.2 that the functions $\mathring{u}_\infty(r, k, \lambda) \equiv \sqrt{r/k}H_\lambda^{(1)}(kr)$ and $\tilde{u}_\infty(r, k, \lambda) \equiv \sqrt{r/k}H_\lambda^{(2)}(kr)$ are two linearly independent free solutions. As alluded to above, the idea is to formulate an integral

[4]See, for example, Sobolev [1963] p. 56. The required result is essentially given by the following line of reasoning: $|f(x) - f(y)| = |\int_y^x f'(s)\mathrm{d}s| \le |x-y|^{1/2}(\int_y^x |f'(s)|^2\mathrm{d}s)^{1/2} \le |x-y|^{1/2}\|f\|_{\mathrm{H}^2(\mathbf{R})}$, where the first inequality is just an application of Cauchy-Schwarz.

equation for the solution $u_\infty(r,k,\lambda)$. More precisely, we claim that any solution of[5]

$$u_\infty(r,k,\lambda) = \mathring{u}_\infty(r,k,\lambda) + \frac{1}{\mathscr{W}_\infty}\int_r^\infty \Theta(r,s,k)U(s)u_\infty(s,k,\lambda)\mathrm{d}s, \tag{3.37}$$

where $\mathscr{W}_\infty$ is the Wronskian of $\mathring{u}_\infty$ and $\tilde{u}_\infty$, and

$$\begin{aligned}\Theta(r,s,k) &\equiv \mathring{u}_\infty(r,k,\lambda)\tilde{u}_\infty(s,k,\lambda) - \tilde{u}_\infty(r,k,\lambda)\mathring{u}_\infty(s,k,\lambda)\\ &= \frac{\sqrt{rs}}{k}[H_\lambda^{(1)}(kr)H_\lambda^{(2)}(ks) - H_\lambda^{(1)}(ks)H_\lambda^{(2)}(kr)],\end{aligned} \tag{3.38}$$

is a solution of (2.74). To justify this claim we compute

$$\begin{aligned}u'_\infty(r,k,\lambda) &= \mathring{u}'_\infty(r,k,\lambda) + \frac{1}{\mathscr{W}_\infty}\Bigg[\mathring{u}'_\infty(r,k,\lambda)\int_r^\infty \tilde{u}_\infty(s,k,\lambda)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\\ &\quad - \mathring{u}_\infty(r,k,\lambda)\tilde{u}_\infty(r,k,\lambda)U(r)u_\infty(r,k,\lambda) + \tilde{u}_\infty(r,k,\lambda)\mathring{u}_\infty(r,k,\lambda)U(r)u_\infty(r,k,\lambda)\\ &\quad - \tilde{u}'_\infty(r,k,\lambda)\int_r^\infty \mathring{u}_\infty(s,k,\lambda)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\Bigg]\\ &= \mathring{u}'_\infty(r,k,\lambda) + \frac{1}{\mathscr{W}_\infty}\Bigg[\mathring{u}'_\infty(r,k,\lambda)\int_r^\infty \tilde{u}_\infty(s,k,\lambda)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\\ &\quad - \tilde{u}'_\infty(r,k,\lambda)\int_r^\infty \mathring{u}_\infty(s,k,\lambda)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\Bigg],\end{aligned}$$

which means that

$$\begin{aligned}u''_\infty(r,k,\lambda) &= \mathring{u}''_\infty(r,k,\lambda) + \frac{1}{\mathscr{W}_\infty}\Bigg[\mathring{u}''_\infty(r,k,\lambda)\int_r^\infty \tilde{u}_\infty(s,k,\lambda)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\\ &\quad + \mathring{u}'_\infty(r,k,\lambda)\tilde{u}_\infty(r,k,\lambda)U(r)u_\infty(r,k,\lambda) - \tilde{u}'_\infty(r,k,\lambda)\mathring{u}_\infty(r,k,\lambda)U(r)u_\infty(r,k,\lambda)\\ &\quad - \tilde{u}''_\infty(r,k,\lambda)\int_r^\infty \mathring{u}_\infty(s,k,\lambda)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\Bigg].\end{aligned} \tag{3.39}$$

Using the definition of $\mathring{u}_\infty(r,k,\lambda)$ and equation (3.37), it follows from (3.39) that

$$\begin{aligned}u''_\infty(r,k,\lambda) &= \left(\frac{\lambda^2-1/4}{r^2}-k^2\right)\mathring{u}_\infty(r,k,\lambda) + \frac{1}{\mathscr{W}_\infty}\Bigg[\mathscr{W}_\infty U(r)u_\infty(r,k,\lambda)\\ &\quad + \left(\frac{\lambda^2-1/4}{r^2}-k^2\right)(u_\infty(r,k,\lambda)-\mathring{u}_\infty(r,k,\lambda))\mathscr{W}_\infty\Bigg]\\ &= \left(\frac{\lambda^2-1/4}{r^2}-k^2\right)u_\infty(r,k,\lambda) + U(r)u_\infty(r,k,\lambda).\end{aligned}$$

[5]For a potential with finite first moment and bounded kernel this integral equation makes sense, but as we shall see this kernel is in fact unbounded, and so the equation will have to be modified.

In view of equation (3.24), we also require the first derivative of $u_\infty(r,k,\lambda)$. This was calculated above and so is given by

$$u'_\infty(r,k,\lambda) = \mathring{u}'_\infty(r,k,\lambda) + \frac{1}{\mathscr{W}_\infty}\int_r^\infty \Theta'(r,s,k)U(s)u_\infty(s,k,\lambda)ds \tag{3.40}$$

where

$$\Theta'(r,s,k) \equiv \mathring{u}'_\infty(r,k,\lambda)\tilde{u}_\infty(s,k,\lambda) - \tilde{u}'_\infty(r,k,\lambda)\mathring{u}_\infty(s,k,\lambda). \tag{3.41}$$

Since we are under the very small energy regime, it is useful to note the following small argument asymptotics calculated in §3.2.1:

$$\mathring{u}_\infty(r,k,\lambda) \sim -k^{-1/2}\Big(\frac{k}{2}\Big)^{-\lambda}\frac{i\csc\lambda\pi}{\Gamma(-\lambda+1)}r^{-\lambda+1/2}, \quad k\to 0 \tag{3.42}$$

and

$$\tilde{u}_\infty(r,k,\lambda) \sim k^{-1/2}\Big(\frac{k}{2}\Big)^{-\lambda}\frac{i\csc\lambda\pi}{\Gamma(-\lambda+1)}r^{-\lambda+1/2}, \quad k\to 0. \tag{3.43}$$

Moreover, we have

$$\begin{aligned}\mathring{u}'_\infty(r,k,\lambda) &\sim i\sqrt{\frac{r}{k}}\csc(\lambda-1)\pi\{J_{-\lambda}(kr)\}' - \frac{i}{2\sqrt{kr}}\csc\lambda\pi J_{-\lambda}(kr)\\ &= -i\sqrt{\frac{r}{k}}\csc\lambda\pi\Big(\{J_{-\lambda}(kr)\}' + \frac{1}{r}J_\lambda(kr)\Big)\\ &\sim k^{-1/2}\Big(\frac{k}{2}\Big)^{-\lambda}\frac{i\csc\lambda\pi}{\Gamma(-\lambda+1)}r^{-(\lambda+1/2)}(\lambda-1), \quad k\to 0\end{aligned} \tag{3.44}$$

and similarly

$$\tilde{u}'_\infty(r,k,\lambda) \sim -k^{-1/2}\Big(\frac{k}{2}\Big)^{-\lambda}\frac{i\csc\lambda\pi}{\Gamma(-\lambda+1)}r^{-(\lambda+1/2)}(\lambda-1), \quad k\to 0. \tag{3.45}$$

We also need fixed r, small k asymptotics for Θ, which is given by (3.38). The only difference between Hankel functions of the first and second kind is the sign of the Neumann function $N_\nu(z)$, in the linear combination that defines the Hankel functions. Thus, in the kernel, only the mixed terms survive:

$$\Theta(r,s,k) = 2i\frac{\sqrt{rs}}{k}[J_\lambda(ks)N_\lambda(kr) - J_\lambda(kr)N_\lambda(ks)]. \tag{3.46}$$

Let $r = r_0$ be fixed and consider Θ for a chosen small k. Putting $s = 1/k$ we find that Θ is not, in general, bounded. This follows from the asymptotics given at the beginning of §2.4—$J_\lambda(1)$ is bounded, $N_\lambda(kr)$ will blow up, $J_\lambda(kr)$ is bounded at the origin and so is $N_\lambda(1)$. In light of this difficulty we consider the integral equation defining the solution $u_\infty(r,0,\lambda)$ of the $k=0$ radial Schrödinger equation, i.e.

$$-u'' + \left(U(r) + \frac{\lambda^2-1/4}{r^2}\right)u = 0. \tag{3.47}$$

3.4.1 The Zero Energy Case

Denote by $\mathring{u}_\infty(r,0,\lambda)$ and $\tilde{u}_\infty(r,0,\lambda)$ the two linearly independent free solutions of (3.47), i.e. $\mathring{u}_\infty(r,0,\lambda) = r^{-\lambda+1/2}$ and $\tilde{u}_\infty(r,0,\lambda) = r^{\lambda+1/2}$. Then any solution of

$$u_\infty(r,0,\lambda) = \mathring{u}_\infty(r,0,\lambda) + \frac{1}{\mathscr{W}_{\infty,k=0}} \int_r^\infty \Xi(r,s)U(s)u_\infty(s,0,\lambda)\mathrm{d}s, \tag{3.48}$$

where $\mathscr{W}_{\infty,k=0} = \mathscr{W}(\mathring{u}_\infty(r,0,\lambda), \tilde{u}_\infty(r,0,\lambda))$ and

$$\Xi(r,s) = \mathring{u}_\infty(r,0,\lambda)\tilde{u}_\infty(s,0,\lambda) - \mathring{u}_\infty(s,0,\lambda)\tilde{u}_\infty(r,0,\lambda),$$

is a solution of (3.47). Now, $\mathscr{W}_{\infty,k=0} = 2\lambda$ and the kernel is given by

$$\Xi(r,s) = \sqrt{rs}\left[\left(\frac{s}{r}\right)^\lambda - \left(\frac{r}{s}\right)^\lambda\right].$$

Thus, (3.48) becomes

$$u_\infty(r,0,\lambda) = r^{-\lambda+1/2} + \frac{1}{2\lambda}\int_r^\infty \sqrt{rs}\left[\left(\frac{s}{r}\right)^\lambda - \left(\frac{r}{s}\right)^\lambda\right]U(s)u_\infty(s,0,\lambda)\mathrm{d}s. \tag{3.49}$$

We prove that there is a bounded solution—with respect to an appropriate norm, which is yet to be introduced—of equation (3.49). The arguments used to achieve this will subsequently be applied to the non-zero energy case in order to address the unboundedness of the kernel Θ. Multiplying both sides of (3.49) by $r^{\lambda-1/2}$ we obtain

$$\begin{aligned} r^{\lambda-1/2}u_\infty(r,0,\lambda) &= 1 + \frac{1}{2\lambda}\int_r^\infty sU(s)(s^{\lambda-1/2}u_\infty(s,0,\lambda))\mathrm{d}s \\ &\quad - \frac{r^{2\lambda}}{2\lambda}\int_r^\infty s^{-2\lambda+1}U(s)(s^{\lambda-1/2}u_\infty(s,0,\lambda))\mathrm{d}s \\ &= 1 + \frac{1}{2\lambda}\int_r^\infty sU(s)(s^{\lambda-1/2}u_\infty(s,0,\lambda))\mathrm{d}s \\ &\quad - \frac{1}{2\lambda}\int_r^\infty \left(\frac{r}{s}\right)^{2\lambda} sU(s)(s^{\lambda-1/2}u_\infty(s,0,\lambda))\mathrm{d}s. \end{aligned} \tag{3.50}$$

Let us define the weighted Chebyshev norm

$$\|f(\cdot)\|_w \equiv \sup_{r>0}|wf(r)| \tag{3.51}$$

where the weight is given by $w \equiv 1/\mathring{u}_\infty$. We note that in general, w depends on r, k, and λ; moreover, we may on occasion refer to the norm (3.51) as the w-norm. Let us also make the identification

$$u_{\infty,w}(r,\cdot,\lambda) \equiv wu_\infty(r,\cdot,\lambda) \tag{3.52}$$

where, in this case, we have the weight $w = r^{\lambda-1/2}$. For absolute clarity, the weight is just the reciprocal of the associated $U = 0$ solution; this is the meaning of the above notation where w is defined initially. Hence, we write instead of (3.50) the following new integral equation, which is to be analysed for a bounded solution:

$$u_{\infty,w}(r,0,\lambda) = 1 + \frac{1}{2\lambda}\left[\int_r^\infty sUu_{\infty,w}(s,0,\lambda)\mathrm{d}s - \int_r^\infty \left(\frac{r}{s}\right)^{2\lambda} sUu_{\infty,w}(s,0,\lambda)\mathrm{d}s\right]. \quad (3.53)$$

We apply the method of successive approximations[6] to (3.53): to begin with, define the sequence $\{u^{(n)}_{\infty,w}(r,0,\lambda)\}$, $n \in \mathbb{N}$ by $u^{(1)}_{\infty,w}(r,0,\lambda) = 1$ and

$$u^{(n+1)}_{\infty,w}(r,0,\lambda) = 1 + \frac{1}{2\lambda}\int_r^\infty sUu^{(n)}_{\infty,w}(s,0,\lambda)\mathrm{d}s - \frac{1}{2\lambda}\int_r^\infty \left(\frac{r}{s}\right)^{2\lambda} sUu^{(n)}_{\infty,w}(s,0,\lambda)\mathrm{d}s. \quad (3.54)$$

Firstly, we demonstrate that $u^{(n)}_{\infty,w}(r,0,\lambda)$ is bounded by induction on n. Assume that $|u^{(n)}_{\infty,w}(r,0,\lambda)| \le C_n$ where C_n is some constant (which could depend on λ). By (3.54),

$$\begin{aligned} |u^{(n+1)}_{\infty,w}(r,0,\lambda)| &\le 1 + \frac{1}{2|\lambda|}\left[\int_r^\infty |sU(s)||u^{(n)}_{\infty,w}|\mathrm{d}s + \int_r^\infty \left|\frac{r}{s}\right|^{2\lambda}|sU(s)||u^{(n)}_{\infty,w}|\mathrm{d}s\right] \\ &\le 1 + \frac{C_n}{2|\lambda|}\int_r^\infty |sU(s)|\mathrm{d}s \end{aligned}$$

since $|r/s|^{2\lambda} \le 1$ for $\mathrm{Re}(\lambda) > 0$. By definition we have $u^{(1)}_{\infty,w}(r,0,\lambda) = 1$, and therefore the boundedness of $u^{(n)}_{\infty,w}(r,0,\lambda)$ for each n follows if we suppose that $sU(s)$ is integrable on (r,∞) for fixed $r = r_0$. We now prove that $u^{(n)}_{\infty,w}(r,0,\lambda)$ converges to a limit $u_{\infty,w}(r,0,\lambda)$. By noticing the following series of equations:

$$\begin{aligned} |u^{(n+1)}_{\infty,w}(r,0,\lambda) - u^{(n)}_{\infty,w}(r,0,\lambda)| &\le \frac{1}{2|\lambda|}\int_r^\infty |sU(s)||u^{(n)}_{\infty,w}(s,0,\lambda) - u^{(n-1)}_{\infty,w}(s,0,\lambda)|\mathrm{d}s, \\ |u^{(n)}_{\infty,w}(r,0,\lambda) - u^{(n-1)}_{\infty,w}(r,0,\lambda)| &\le \frac{1}{2|\lambda|}\int_r^\infty |sU(s)||u^{(n-1)}_{\infty,w}(s,0,\lambda) - u^{(n-2)}_{\infty,w}(s,0,\lambda)|\mathrm{d}s, \\ &\vdots \\ |u^{(3)}_{\infty,w}(r,0,\lambda) - u^{(2)}_{\infty,w}(r,0,\lambda)| &\le \frac{1}{2|\lambda|}\int_r^\infty |sU(s)||u^{(2)}_{\infty,w}(s,0,\lambda) - u^{(1)}_{\infty,w}(s,0,\lambda)|\mathrm{d}s, \\ |u^{(2)}_{\infty,w}(r,0,\lambda) - u^{(1)}_{\infty,w}(r,0,\lambda)| &\le \frac{1}{2|\lambda|}\int_r^\infty |sU(s)|\mathrm{d}s, \end{aligned}$$

we have by back substitution that

$$|u^{(n+1)}_{\infty,w}(r,0,\lambda) - u^{(n)}_{\infty,w}(r,0,\lambda)| \le \left(\frac{1}{2|\lambda|}\int_r^\infty |sU(s)|\mathrm{d}s\right)^n.$$

[6] This is completely analagous to the method used in the book of Eastham [1989] pp. 8–15 to prove Levinson's Theorem.

For a fixed $r = r_0$ let us suppose that

$$\frac{1}{2|\lambda|}\int_r^\infty |sU(s)|\mathrm{d}s < 1. \tag{3.55}$$

Then by comparison with a geometric series, $\sum\{u^{(n+1)}_{\infty,w}(r,0,\lambda) - u^{(n)}_{\infty,w}(r,0,\lambda)\}$ converges for a fixed $r = r_0$. Hence, we define

$$u_{\infty,w}(r,0,\lambda) = u^{(1)}_{\infty,w}(r,0,\lambda) + \sum_{j=1}^{\infty}\{u^{(j+1)}_{\infty,w}(r,0,\lambda) - u^{(j)}_{\infty,w}(r,0,\lambda)\} \equiv \lim_{n\to\infty} u^{(n)}_{\infty,w}(r,0,\lambda)$$

and so $u_{\infty,w}(r,0,\lambda)$ is bounded for a fixed $r = r_0$. Therefore, we conclude that if $sU(s)$ is integrable, then for a fixed $r = r_0 > 0$ satisfying the condition (3.55), there is a solution of (3.49) bounded in the norm $\|\cdot\|_w$—a well-defined norm in this case since $r = r_0 > 0$.

3.4.2 Normalizing the Non-Zero Energy Equation

Returning to the difficulty of unboundedness in the kernel Θ, we expect that control of this term will be achieved under the norm $\|\cdot\|_w$ with weight $w = 1/\mathring{u}_\infty$; we first need to ensure that this norm is well-defined. Now, the Hankel function of the first kind has infinitely many zeros as a function of its order [Magnus and Kotin, 1960], i.e. infinitely many λ-zeros; however, we also need to consider the r-zeros for $\mathrm{Re}(\lambda) > 0$. When λ is real, it suffices to note that the positive zeros of any two real cylinder functions of the same order are interlaced [Abramowitz and Stegun, 1965, p. 360]. On the other hand, when λ is such that $\arg(\lambda) \in (0, \pi/2)$ the argument is as follows: let χ denote any one of J_λ, N_λ, $H^{(1)}_\lambda$, or $H^{(2)}_\lambda$ and consider Bessel's differential equation (BDE)

$$r^2y'' + ry + (r^2 - \lambda^2)y = 0$$

with $y(r_1) = 0$ and $y(r_2) = 0$, where $0 < r_1 < r_2$ are two r-zeros of χ. Rewriting BDE in so-called self-adjoint form ($r > 0$) yields

$$(ry')' + (r - \nu/r)y = 0 \tag{3.56}$$

where $\nu \equiv \lambda^2$. Multiplying (3.56) by χ^* and multiplying the conjugate of (3.56) by χ, then taking the difference $\mathrm{d}|\chi|^2\,\mathrm{d}r =$ ultant equations and integrating yields

$$(\nu - \nu^*)\int_{r_1}^{r_2}\frac{|\chi|^2}{r}\mathrm{d}r = \int_{r_1}^{r_2}\left[\chi^*(r\chi')' - \chi(r(\chi^*)')'\right]\mathrm{d}r.$$

We may integrate the right side of this equation and this gives

$$(\nu - \nu^*)\int_{r_1}^{r_2}\frac{|\chi|^2}{r}\mathrm{d}r = \left[r\chi^*\chi' - r\chi(\chi^*)'\right]_{r_1}^{r_2} = 0,$$

and since $r^{-1} > 0$ in $[r_1, r_2]$, it must be that $\nu^* = \nu$ or λ^2 is real. Hence, for λ in the strict first quadrant, χ has at most one r-zero. Thus, for each fixed r, $H_\lambda^{(1)}(r)$ has infinitely many λ-zeros, but if you fix λ to be one of those zeros and vary r, we find that $r = \hat{r}$ is the only r-zero. We may therefore avoid any zeros by a suitable choice of λ and r.

To proceed we will also need an explicit expression for the Wronskian $\mathscr{W}_\infty$ appearing in our integral equation (3.37). It is useful to notice that

$$\mathscr{W}_\infty = \frac{r}{k}\left(H_\lambda^{(1)}(kr)\{H_\lambda^{(2)}(kr)\}' - H_\lambda^{(2)}(kr)\{H_\lambda^{(1)}(kr)\}'\right)$$

can be simplified by an application of the Wronskian formula for the Hankel functions given in Arfken and Weber [2005] p. 711; it follows that $1/\mathscr{W}_\infty = i\pi k/4$, and so along with utilizing (3.46), (3.37) becomes

$$u_\infty(r,k,\lambda) = \mathring{u}_\infty(r,k,\lambda) - \frac{\pi}{2}\left[\int_r^\infty \sqrt{rs}J_\lambda(ks)N_\lambda(kr)U(s)u_\infty(s,k,\lambda)\mathrm{d}s - \int_r^\infty \sqrt{rs}J_\lambda(kr)N_\lambda(ks)U(s)u_\infty(s,k,\lambda)\mathrm{d}s\right]. \tag{3.57}$$

Recall the notation (3.52), then multiplying (3.57) by $w = \mathring{u}_\infty^{-1}$ results in the equation

$$u_{\infty,w}(r,k,\lambda) = 1 - \frac{\pi}{2}\left[\int_r^\infty \sqrt{rs}\frac{J_\lambda(ks)}{w(s)}w(r)N_\lambda(kr)U(s)u_{\infty,w}(s,k,\lambda))\mathrm{d}s - \int_r^\infty \sqrt{rs}\frac{N_\lambda(ks)}{w(s)}w(r)J_\lambda(kr)U(s)u_{\infty,w}(s,k,\lambda))\mathrm{d}s\right]. \tag{3.58}$$

Equation (3.58) can be written in the more succinct form

$$u_{\infty,w}(r,k,\lambda) = 1 - \frac{\pi}{2}\int_r^\infty \mathscr{T}(r,s,k)sU(s)u_{\infty,w}(s,k,\lambda)\mathrm{d}s \tag{3.59}$$

where

$$\mathscr{T}(r,s,k) \equiv \frac{J_\lambda(ks)H_\lambda^{(1)}(ks)N_\lambda(kr)}{J_\lambda(kr)+iN_\lambda(kr)} - \frac{J_\lambda(kr)H_\lambda^{(1)}(ks)N_\lambda(ks)}{J_\lambda(kr)+iN_\lambda(kr)}. \tag{3.60}$$

We have accounted for the possibility of the denominator of $\mathscr{T}$ vanishing, but we should also note that since $J_\lambda(z)$ and $N_\lambda(z)$ are analytic functions of z throughout the z-plane cut along the negative real axis, $\mathscr{T}$ is analytic in r, s, and k. In light of what is to come, it would be prudent to list the small and large argument asymptotics of the Bessel functions, holding the order fixed: for small x we have [Abramowitz and Stegun, 1965, p. 360]

$$J_\lambda(x) \sim \frac{1}{\Gamma(\lambda+1)}(x/2)^\lambda \quad \text{and} \quad N_\lambda(x) \sim \frac{1}{\pi}\Gamma(\lambda)(x/2)^{-\lambda}. \tag{3.61}$$

Whilst for large x we have [Abramowitz and Stegun, 1965, p. 364]

$$J_\lambda(x) \sim \sqrt{\frac{2}{\pi x}}\cos(x - \pi\lambda/2 - \pi/4) \quad \text{and} \quad N_\lambda(x) \sim \sqrt{\frac{2}{\pi x}}\sin(x - \pi\lambda/2 - \pi/4). \tag{3.62}$$

Recall that we are to take $k \to 0$. Thus, we show uniform boundedness in k of $\mathscr{T}$ in order to use Lebesgue dominated convergence and interchange limit and integration. So, let $\sigma = ks$ and $\rho = kr$ such that $\sigma \geq \rho$, then consider the first term in (3.60):

$$[J_\lambda(\sigma)(J_\lambda(\sigma) + iN_\lambda(\sigma))]\left[\frac{N_\lambda(\rho)}{(J_\lambda(\rho) + iN_\lambda(\rho))}\right]. \tag{3.63}$$

In a neighbourhood of the origin, the first term in square brackets is bounded since $J_\lambda(\sigma)$ vanishes at the precise same rate as $N_\lambda(\sigma)$ blows up. Also, it is clear that the second term in square brackets is bounded at the origin. In principle, σ could be large but since we are interested in a finite fixed r, it will suffice to show that (3.63) is uniformly bounded for large σ and small ρ, which is obvious since both the Bessel and Neumann functions tend to zero at infinity. Similarly, for the second term in (3.60)

$$[J_\lambda(\rho)(J_\lambda(\sigma) + iN_\lambda(\sigma))]\left[\frac{N_\lambda(\sigma)}{(J_\lambda(\rho) + iN_\lambda(\rho))}\right], \tag{3.64}$$

we have boundedness at the origin of the first term in square brackets since $\sigma \geq \rho$ implies that $J_\lambda(\rho)$ vanishes faster than $N_\lambda(\sigma)$ blows up. The second square bracket term is bounded at the origin since $\sigma \geq \rho$ implies that $N_\lambda(\rho)$ blows up faster than $N_\lambda(\sigma)$. The argument for uniform boundedness when σ becomes large is unchanged from above. Thus, we can see heuristically that $\mathscr{T}$ is bounded for small σ and ρ, but for our purposes we require uniform boundedness in k and λ. So, to be more precise, write

$$\mathscr{T}(r,s,k) = \frac{H_\lambda^{(1)}(\sigma)J_\lambda(\sigma)N_\lambda(\rho) - H_\lambda^{(1)}(\sigma)J_\lambda(\rho)N_\lambda(\sigma)}{J_\lambda(\rho) + iN_\lambda(\rho)} \tag{3.65}$$

and consider small σ and ρ. We have from Arfken and Weber [2005] p. 709 that

$$H_\lambda^{(1)}(\sigma) = \frac{1}{\pi i}\int_\gamma \mathrm{e}^{\frac{\sigma}{2}(z-1/z)}\frac{\mathrm{d}z}{z^{\lambda+1}}, \quad \mathrm{Re}(\lambda) > 0 \tag{3.66}$$

where the contour $\gamma = \gamma_1 \cup \gamma_2$ (Figure 3.1) is chosen so as to have the integral given in equation (3.66) converge.

This particular choice of contour is justified as follows: let us rewrite the contour integral (3.66) into two contour integrals, namely,

$$H_\lambda^{(1)}(\sigma) = \frac{1}{\pi i}\int_{\gamma_1} \mathrm{e}^{\frac{\sigma}{2}(z-1/z)}\frac{\mathrm{d}z}{z^{\lambda+1}} + \frac{1}{\pi i}\int_{\gamma_2} \mathrm{e}^{\frac{\sigma}{2}(z-1/z)}\frac{\mathrm{d}z}{z^{\lambda+1}}. \tag{3.67}$$

For convergence of the first integral in (3.67) we would like $\mathrm{Re}(z-1/z) < 0$, where $z = p\mathrm{e}^{i\vartheta}$

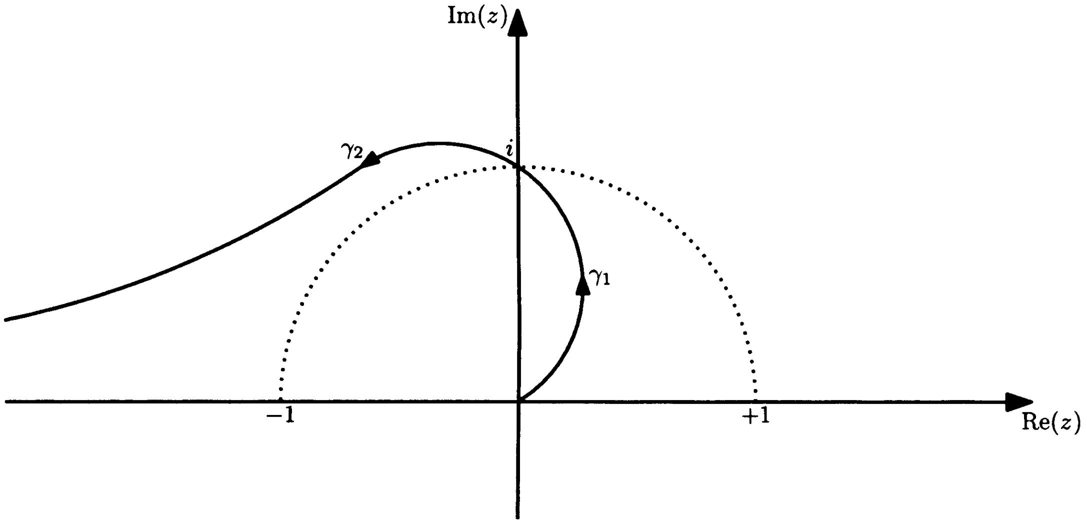

Figure 3.1: The contour $\gamma = \gamma_1 \cup \gamma_2$ chosen for (3.66).

with $\vartheta \in [0, \pi/2]$ and $p > 0$; thus, $p \cos\vartheta - (1/p)\cos\vartheta < 0$. This is equivalent to requiring $(p^2 - 1)\cos\vartheta < 0$, which implies that $p < 1$. Similarly, to gain convergence of the second integral in equation (3.67), we must have $\mathrm{Re}(z - 1/z) < 0$ where $z = pe^{i\vartheta}$, $\vartheta \in [\pi/2, \pi]$. It follows that $(p^2 - 1)\cos\vartheta < 0$ and so we need $p > 1$.

By making a change of variable $z = \sigma\xi$ in equation (3.66), we may rewrite the defining contour integral for the Hankel function as

$$H_\lambda^{(1)}(\sigma) = \frac{\sigma^{-\lambda}}{\pi i} \int_\gamma \mathrm{e}^{(\sigma^2\xi - 1/\xi)/2} \frac{\mathrm{d}\xi}{\xi^{\lambda+1}}.$$

Referring to equation (3.10) it is clear that $H_\lambda(\sigma)J_\lambda(x)$ is uniformly bounded in k and $\lambda \in K$, with the stipulation that $\sigma \geq x$. In particular, this means that both $H_\lambda(\sigma)J_\lambda(\sigma)$ and $H_\lambda(\sigma)J_\lambda(\rho)$ are uniformly bounded in k and $\lambda \in K$. Recall that ρ is fixed but can be arbitrarily small since we are interested in small k; thus, let ρ be such that $0 < \rho \leq \delta$ where δ is small, then we have that [Abramowitz and Stegun, 1965, p. 360]

$$J_\lambda(\rho) + iN_\lambda(\rho) \sim iN_\lambda(\rho), \tag{3.68}$$

λ fixed with $\mathrm{Re}(\lambda) > 0$. Hence, in considering the term

$$\left|\frac{H_\lambda(\sigma)J_\lambda(\sigma)N_\lambda(\rho)}{J_\lambda(\rho) + iN_\lambda(\rho)}\right| \sim |H_\lambda(\sigma)J_\lambda(\sigma)|, \tag{3.69}$$

we find that (3.69) is uniformly bounded in k and $\lambda \in K$. With regard to the term

$$\frac{H_\lambda(\sigma)J_\lambda(\rho)N_\lambda(\sigma)}{J_\lambda(\rho) + iN_\lambda(\rho)} \tag{3.70}$$

we use equation (3.68), and since we know $H_\lambda(\sigma)J_\lambda(\rho)$ is uniformly bounded in k and

$\lambda \in K$, it only remains to show the boundedness of $|N_\lambda(\sigma)/N_\lambda(\rho)|$. However, for the particular values of ρ being considered here (i.e., small) we have that

$$\left|\frac{N_\lambda(\sigma)}{N_\lambda(\rho)}\right| \leq \left|\frac{N_\lambda(\sigma)}{N_\lambda(\sigma)}\right| = 1 \tag{3.71}$$

for $\lambda \in K$ since $0 < \rho \leq \sigma$. Hence, (3.70) is uniformly bounded in k and $\lambda \in K$. Piecing together equations (3.69) and (3.70), we see that $\mathscr{T}(r, s, k)$ is uniformly bounded with respect to k and $\lambda \in K$. Thus, the proof that there is a bounded solution of (3.49) can readily be applied to (3.59); the only difference being in the explicit bounds on the respective kernels. Therefore, there is a uniformly bounded solution with respect to k and $\lambda \in K$ of (3.57) in the w-norm. Let us define

$$u_{\text{lim}}(r, \lambda) \equiv \lim_{k \to 0} u_{\infty,w}(r, k, \lambda), \tag{3.72}$$

where we suppose for now that this limit exists—the existence of such a limiting function will be discussed in §3.4.3. This means that for a fixed r defined by an analogous condition to (3.55) and $k \to 0$, we have by using Lebesgue dominated convergence on (3.59) that

$$\begin{aligned} u_{\text{lim}}(r, \lambda) = 1 + 2i\Big(\frac{i\pi}{4}\Big)\Bigg[\int_r^\infty &\left\{\frac{1}{\Gamma(\lambda+1)}\Big(\frac{ks}{2}\Big)^\lambda\right\}\left\{\frac{-\csc\lambda\pi}{\Gamma(-\lambda+1)}\Big(\frac{ks}{2}\Big)^{-\lambda}\right\} \\ &\times \left\{\frac{i\Gamma(-\lambda+1)}{\csc\lambda\pi}\Big(\frac{kr}{2}\Big)^\lambda\right\}\left\{\frac{-\csc\lambda\pi}{\Gamma(-\lambda+1)}\Big(\frac{kr}{2}\Big)^{-\lambda}\right\} sU(s)u_{\text{lim}}(s,\lambda)ds \\ - \int_r^\infty &\left\{\frac{-\csc\lambda\pi}{\Gamma(-\lambda+1)}\Big(\frac{ks}{2}\Big)^{-\lambda}\right\}\left\{\frac{-\csc\lambda\pi}{\Gamma(-\lambda+1)}\Big(\frac{ks}{2}\Big)^{-\lambda}\right\} \\ &\times \left\{\frac{i\Gamma(-\lambda+1)}{\csc\lambda\pi}\Big(\frac{kr}{2}\Big)^\lambda\right\}\left\{\frac{1}{\Gamma(\lambda+1)}\Big(\frac{kr}{2}\Big)^{\lambda}\right\} sU(s)u_{\text{lim}}(s,\lambda)ds\Bigg] \\ = 1 + \frac{\pi/(2\sin\pi\lambda)}{\Gamma(1-\lambda)\Gamma(\lambda+1)}&\left[\int_r^\infty sU(s)u_{\text{lim}}(s,\lambda)ds - \int_r^\infty \Big(\frac{r}{s}\Big)^{2\lambda} sU(s)u_{\text{lim}}(s,\lambda)ds\right] \end{aligned}$$

where we have used the asymptotics (3.14). This can be simplified using standard formulae for the gamma function; see, for example, Olver [1974] pp. 32–35:

$$\frac{1}{\Gamma(1-\lambda)\Gamma(\lambda+1)} = \frac{1}{\Gamma(1-\lambda)\Gamma(\lambda)\lambda} = \frac{\sin\pi\lambda}{\pi\lambda}. \tag{3.73}$$

Therefore, from equation (3.73) we have

$$u_{\text{lim}}(r, \lambda) = 1 + \frac{1}{2\lambda}\left[\int_r^\infty sU(s)u_{\text{lim}}(s,\lambda)ds - \int_r^\infty \Big(\frac{r}{s}\Big)^{2\lambda} sU(s)u_{\text{lim}}(s,\lambda)ds\right], \tag{3.74}$$

which is precisely the integral equation (3.53) in the $k = 0$ case. In summary, we have formally shown that if u_{lim} exists, then it will have the exact form (3.53) that is required.

3.4.3 Existence of the Limiting Wavefunction

To show the existence of $u_{\lim}$ we will implement the following argument involving a diagonal sequence: take an increasing sequence $(r_j)_{j=1}^{\infty}$ with $r_j > r = r_0$ for all $j \in \mathbb{N}$ and $r_j \to \infty$ as $j \to \infty$. Choose another sequence $(k_p)_{p=1}^{\infty}$ with $k_p \to 0$ as $p \to \infty$ such that the sequence of functions $(f_{p,1})_{p=1}^{\infty}$ defined by

$$f_{p,1}(\cdot) = u_{\infty,w}(\cdot, k_p), \quad p \in \mathbb{N}, \tag{3.75}$$

converges uniformly on $[r, r_1]$. This sequence is uniformly bounded with the same bound as the original family of functions $u_{\infty,w}(\cdot, k)$, $k > 0$, and (as we will show) equicontinuous on $[r, \infty)$. Thus, by the Arzelá-Ascoli Theorem [Kato, 1966, p. 157] we can extract a subsequence from $(f_{p,1})$ which converges uniformly on $[r, r_2]$; denote it by $(f_{p,2})_{p=1}^{\infty}$. In general, we have $(f_{p,j})_{p=1}^{\infty}$ uniformly convergent on $[r, r_j]$, and uniformly bounded and equicontinuous on $[r, \infty)$. Hence, we can extract a subsequence $(f_{p,j+1})_{p=1}^{\infty}$ from $(f_{p,j})$ which converges uniformly on $[r, r_{j+1}]$. Thus, on each fixed interval $[r, r_n]$, the diagonal sequence $f_{1,1}, f_{2,2}, f_{3,3}, \ldots$ is a subsequence of the original uniformly convergent and uniformly bounded sequence defined in (3.75). It follows that the diagonal sequence is uniformly convergent on any compact subset of $[r, \infty)$, and is uniformly bounded. This means that provided we can show equicontinuity of the family of functions $u_{\infty,w}(\cdot, k)$, $k > 0$, the limiting wavefunction $u_{\lim}$ exists along a subsequence, namely, the diagonal sequence $(f_{n,n})_{n=1}^{\infty}$. However, on $[r, r_n]$ with $p > n$, $f_{pp}(\cdot) = u_{\infty,w}(\cdot, k_p)$ does not depend on n. Furthermore, $\lim_{p\to\infty} f_{pp}(\cdot)$ depends only upon (k_p), which is an arbitrary sequence with limit zero. Therefore, any convergent subsequence converges to $u_{\lim}$.

A standard result states that if the family of functions $u_{\infty,w}(\cdot, k)$, $k > 0$ has a bounded first derivative, then the family is equicontinuous by the Mean Value Theorem. Consider the first derivative of $u_{\infty,w}(r, k, \lambda)$, which by the notation in (3.52) and the integral equations (3.37) and (3.40) is

$$\begin{aligned}
u'_{\infty,w}(r,k,\lambda) &= w(r)u'_{\infty}(r,k,\lambda) + w'(r)u_{\infty}(r,k,\lambda) \\
&= w(r)\left[\mathring{u}'_{\infty}(r,k,\lambda) + \frac{1}{\mathscr{W}_{\infty}}\int_r^{\infty} \Theta'(r,s,k)U(s)u_{\infty}(s,k,\lambda)\mathrm{d}s\right] \\
&\quad + w'(r)\left[\mathring{u}_{\infty}(r,k,\lambda) + \frac{1}{\mathscr{W}_{\infty}}\int_r^{\infty} \Theta(r,s,k)U(s)u_{\infty}(s,k,\lambda)\mathrm{d}s\right] \\
&= \frac{1}{\mathscr{W}_{\infty}}\int_r^{\infty}\left[\frac{w(r)\Theta'(r,s,k) + w'(r)\Theta(r,s,k)}{w(s)}\right]U(s)w(s)u_{\infty}(s,k,\lambda)\mathrm{d}s \\
&\quad + [w(r)\mathring{u}_{\infty}(r,k,\lambda)]' \\
&= \frac{1}{\mathscr{W}_{\infty}}\int_r^{\infty}\left[\frac{w(r)\Theta'(r,s,k) + w'(r)\Theta(r,s,k)}{w(s)}\right]U(s)u_{\infty,w}(s,k,\lambda)\mathrm{d}s
\end{aligned}$$

by definition (3.51) of $w(r)$. Whence

$$u'_{\infty,w}(r,k,\lambda) = \frac{1}{\mathscr{W}_\infty}\int_r^\infty \frac{[w(r)\Theta(r,s,k)]'}{w(s)} U(s)u_{\infty,w}(s,k,\lambda)\mathrm{d}s. \tag{3.76}$$

We need to show that this is uniformly bounded in k. Now, by (3.38) we have

$$\begin{aligned}
[w(r)\Theta(r,s,k)]' &= \sqrt{\frac{s}{k}}\left[\frac{1}{H_\lambda^{(1)}(kr)}\left(H_\lambda^{(1)}(kr)H_\lambda^{(2)}(ks) - H_\lambda^{(2)}(kr)H_\lambda^{(1)}(ks)\right)\right]' \\
&= \sqrt{\frac{s}{k}}\left[H_\lambda^{(2)}(ks) - \frac{H_\lambda^{(1)}(ks)(J_\lambda(kr) - iN_\lambda(kr))}{J_\lambda(kr) + iN_\lambda(kr)}\right]' \\
&= -\sqrt{\frac{s}{k}}H_\lambda^{(1)}(ks)\Big[(J_\lambda(kr) + iN_\lambda(kr))(\{J_\lambda(kr)\}' - i\{N_\lambda(kr)\}') \\
&\quad - (J_\lambda(kr) - iN_\lambda(kr))(\{J_\lambda(kr)\}' + i\{N_\lambda(kr)\}')\Big]/(H_\lambda^{(1)}(kr))^2 \\
&= 2i\sqrt{\frac{s}{k}}\frac{H_\lambda^{(1)}(ks)}{(H_\lambda^{(1)}(kr))^2}\Big[J_\lambda(kr)\{N_\lambda(kr)\}' - \{J_\lambda(kr)\}'N_\lambda(kr)\Big] \\
&= 2ik\sqrt{\frac{s}{k}}\frac{H_\lambda^{(1)}(ks)}{(H_\lambda^{(1)}(kr))^2}\Big[J_\lambda(kr)N'_\lambda(kr) - J'_\lambda(kr)N_\lambda(kr)\Big].
\end{aligned} \tag{3.77}$$

If we use the Wronskian formula $J_\nu(z)N'_\nu(z) - J'_\nu(z)N_\nu(z) = 2/\pi z$ for the Bessel and Neumann functions [Arfken and Weber, 2005, p. 705] in equation (3.77), then on dividing by $w(s)$ we obtain

$$\frac{[w(r)\Theta(r,s,k)]'}{w(s)} = 2ik\frac{s}{k}\left[\frac{H_\lambda^{(1)}(ks)}{H_\lambda^{(1)}(kr)}\right]^2\frac{2}{\pi kr} = \frac{4i}{\pi k}\frac{s}{r}\left[\frac{H_\lambda^{(1)}(ks)}{H_\lambda^{(1)}(kr)}\right]^2.$$

Using our calculation for $1/\mathscr{W}_\infty$, the derivative is thus given by

$$u'_{\infty,w}(r,k,\lambda) = -\int_r^\infty \frac{1}{r}\left[\frac{H_\lambda^{(1)}(ks)}{H_\lambda^{(1)}(kr)}\right]^2 sU(s)u_{\infty,w}(s,k,\lambda)\mathrm{d}s, \tag{3.78}$$

and hence it follows from (3.71) that (modulo a constant)

$$|u'_{\infty,w}(r,k,\lambda)| \le \frac{1}{r}\int_r^\infty s|U(s)||u_{\infty,w}(s,k,\lambda)|\mathrm{d}s. \tag{3.79}$$

Since r is defined by (3.55) and an analogous condition for the $k \neq 0$ case—we can just take r to be the maximum of each value satisfying each integral condition—it is clearly finite. Also, $sU(s)$ is integrable and we know from §3.4.2 that $u_{\infty,w}(r,k,\lambda)$ is uniformly bounded. Thus, the family $u_{\infty,w}(\cdot,k)$, $k > 0$ is equicontinuous. This therefore means that $u_\infty(r,k,\lambda) \to u_\infty(r,0,\lambda)$ as $k \to 0$ in the w-norm.

Recall that we also require $u'_\infty(r,k,\lambda) \to u'_\infty(r,0,\lambda)$ as $k \to 0$ in the norm $\|\cdot\|_w$. We see from (3.79) that $u'_\infty(r,k,\lambda)$ is uniformly bounded with respect to k in the w-norm; thus, if we had equicontinuity of the family $u'_\infty(r,k,\lambda)$, $k>0$, then by the diagonal sequence argument described in §3.4.3, the limit $\lim_{k\to 0} u'_\infty(r,k,\lambda)$ would exist. Therefore, we only need to prove that $u''_\infty(r,k,\lambda)$ is uniformly bounded with respect to k in the w-norm. However, we notice that this is given by the differential equation (2.74), and indeed we see that $u''_\infty(r,k,\lambda)$ is uniformly bounded with respect to k in the norm $\|\cdot\|_w$. Finally, to show that $\lim_{k\to 0} u'_\infty(r,k,\lambda)$ is of the required form, we first calculate $u'_{\infty,w}(r,0,\lambda)$. Since $sU(s)$ is integrable, we have from equation (3.53) that

$$\begin{aligned} u'_{\infty,w}(r,0,\lambda) &= \frac{1}{2\lambda}\Bigg[- rU(r)u_{\infty,w}(r,0,\lambda) - \frac{2\lambda}{r}\int_r^\infty \left(\frac{r}{s}\right)^{2\lambda} sU(s)u_{\infty,w}(s,0,\lambda)\mathrm{d}s \\ &\qquad - r^{2\lambda}\left(- \frac{1}{r^{2\lambda}} rU(r)u_{\infty,w}(r,0,\lambda)\right)\Bigg] \\ &= -\frac{1}{r}\int_r^\infty \left(\frac{r}{s}\right)^{2\lambda} sU(s)u_{\infty,w}(s,0,\lambda)\mathrm{d}s. \end{aligned} \tag{3.80}$$

On the other hand, defining the notation $u'_{\lim}(r,\lambda) \equiv \lim_{k\to 0} u'_{\infty,w}(r,k,\lambda)$, the formal limit of equation (3.78) as $k\to 0$ is given by

$$u'_{\lim}(r,\lambda) = -\frac{1}{r}\int_r^\infty \left(\frac{r}{s}\right)^{2\lambda} sU(s)u_{\lim}(s,\lambda)\mathrm{d}s$$

where we have used the asymptotics given by (3.14) and the small energy convergence result $\lim_{k\to 0} u_{\infty,w}(r,k,\lambda) = u_{\lim}(r,\lambda)$ established earlier. Note that we can interchange limit and integration, as we have done before, using Lebesgue dominated convergence since the integrand in equation (3.78) is uniformly bounded in k. We conclude that $u'_\infty(r,k,\lambda) \to u'_\infty(r,0,\lambda)$ as $k\to 0$ in the w-norm.

Note that convergence of the $k>0$ Wronksian to the $k=0$ Wronskian is along any convergent subsequence (see §3.4.3). A general fact about analytic functions is that if $f_n(z)$ tends to $f(z)$ as $n\to\infty$, and if the convergence is uniform on compact sets, then the zeros of f_n can only either: escape from any compact set, i.e. tend to infinity, or tend to the zeros of f. Since these Wronskians (whose zeros are the Regge poles) are analytic as functions of λ, and the convergence is locally uniform in λ (as guaranteed by Montel's Theorem), we cannot rule out the possibility of Regge poles tending to infinity.

Under the hypothesis that the potential has finite first moment for $r>r_0$, we have shown equation (3.24) to be true. Amalgamating this with the compactly supported result, we have a two-part condition on the potential; namely, that it is integrable for $r\le r_0$ with $r|U(r)|$ bounded in a neighbourhood of the origin, and has finite first moment for $r>r_0$. We combine these hypotheses and state that we have shown the following result:

Theorem 3. *In the limit as the energy goes to zero, the Regge poles associated with a potential U such that $(1+r)U(r)$ is integrable and $r|U(r)|$ is bounded in a neighbourhood of the origin, tend either to the angular momentum eigenvalues of the self-adjoint problem formed when the energy is identically zero, or they diverge to infinity.*

CHAPTER 4

Regge Pole Cardinality

In this chapter we consider Regge poles residing far out in the first quadrant of the CAM plane; in particular, we demonstrate that outside some compact set there are no Regge poles associated with a compactly supported potential. To achieve this, we use the integral equation strategy of Chapter 3. This approach has the advantage of not requiring analyticity of the potential, which has hitherto been a central assumption; see, for example, Barut and Dilley [1963]. We must first return to the Regge pole condition; we will find it enormously helpful to think of this condition in a way that avoids derivatives.

4.1 Yet Another Characterization of Regge Poles

The Regge pole condition (3.3) may be expressed in an equivalent manner without derivatives. The reason for doing this was touched upon in Chapter 1: for a potential which vanishes when $r > r_0$ we wish to study the regular solution of (2.74) for large $|\lambda|$, and so in contrast to the previous chapter, λ is no longer a fixed parameter—or bounded to a compact set, as the case may be. This presents several complications on taking the limit as $|\lambda| \to \infty$ of the solution; chief among these is gaining uniform bounds in order to swap limit and integration in the integral equation which defines the solution recursively. As we have already encountered, the kernel in the integral equation is built out of the free solutions of (2.74), which in this case are Bessel functions. It is difficult enough to get bounds for the kernel itself, let alone its derivative. Thus motivated, consider the ideal matching condition (3.3); this is equivalent to requiring that

$$\frac{u_0(r+h,\lambda)}{u_0(r,\lambda)} = \frac{u_\infty(r+h,\lambda)}{u_\infty(r,\lambda)} \tag{4.1}$$

for fixed $r = r_0 > 0$ and for all small h.

Recall our notation from §3.1. Let us set $k = 1$ so that from equation (3.8) and the notation given at the start of §3.4, $u_\infty(r,\lambda) = \mathring{u}_\infty(r,\lambda) = \sqrt{r}H_\lambda^{(1)}(r)$. Moreover, let us denote by $\mathring{u}_0(r,\lambda)$ and $\tilde{u}_0(r,\lambda)$ two linearly independent free solutions for $r \leq r_0$, which in this case are proportional to $\sqrt{r}J_\lambda(r)$ and $\sqrt{r}N_\lambda(r)$ respectively. Observing that there are no Regge poles for a free particle—if there is no potential then there is no phase shift δ_ℓ and hence no Regge poles—we need only show that for large $|\lambda|$, $u_0(r,\lambda) \sim \mathring{u}_0(r,\lambda)$ locally uniformly in r. The stipulation that these large $|\lambda|$ asymptotics should be locally uniform in spatial variable ensures that the condition (4.1) is satisfied.

4.2 The Integral Equation for the Left-Hand Solution

As we have seen from Chapter 3, it is possible to formulate an implicit expression for the solutions of the radial Schrödinger equation (2.74). In this case, we have

$$u_0(r,\lambda) = \mathring{u}_0(r,\lambda) + \int_0^r K(r,s,\lambda)U(r)u_0(s,\lambda)\mathrm{d}s, \tag{4.2}$$

where

$$K(r,s,\lambda) = \frac{1}{\mathscr{W}}[\mathring{u}_0(r,\lambda)\tilde{u}_0(s,\lambda) - \mathring{u}_0(s,\lambda)\tilde{u}_0(r,\lambda)] \tag{4.3}$$

with $\mathscr{W}$ denoting the Wronskian of $\mathring{u}_0$ and $\tilde{u}_0$, and $U(r)$ is an integrable potential which vanishes for $r > r_0$. The kernel K is unbounded in λ and thus equation (4.2) fails to define a bounded solution, which is bad news if we are to take the limit as $|\lambda| \to \infty$. We deal with this as before and divide the integral equation by a suitable normalizer, the obvious candidate being $\mathring{u}_0(r,\lambda)$. However, we must ensure that division by zero is avoided.

4.2.1 The Zeros of the Bessel Function

Firstly, $J_\lambda(r)$ is an entire function of λ [Abramowitz and Stegun, 1965, p. 358], and for all sufficiently large λ in a cone excluding the negative real axis, it has no zeros; this is because $\mathring{u}_0(r,\lambda)$ is asymptotically $r^{\lambda+1/2}$—perhaps easiest to see from the radial Schrödinger equation. Thus, $J_\lambda(r)$ has finitely many λ-zeros by Theorem D.2 in Appendix D.1. In the situation where λ is real, we have the bound [Neuman, 2004]

$$\frac{(x/2)^\lambda}{\Gamma(\lambda+1)}\cos\left\{\frac{x}{\sqrt{2}(\lambda+1)}\right\} \leq J_\lambda(x), \quad \lambda > -1/2, \ |x| \leq \pi/2, \tag{4.4}$$

from which we conclude that $J_\lambda(r)$ is non-zero for $\lambda \geq 0$ and $0 < r \leq \pi/2$. Moreover, if λ is on the imaginary axis, $J_\lambda(r)^* = J_{\lambda^*}(r)$ is also a solution of Bessel's equation since the order appears squared; this of course means that $\mathrm{Re}\{J_\lambda(r)\}$ and $\mathrm{Im}\{J_\lambda(r)\}$ are also solutions. Hence, there are no r-zeros ($r > 0$, which is always the case) of the Bessel function for purely imaginary order since the real and imaginary parts of $J_\lambda(r)$ are solutions of the same Sturm-Liouville equation, and so they cannot share any zeros. In addition, if there are no r-zeros then there can be no λ-zeros also: if there were a λ-zero, say at $\lambda = \hat{\lambda}$, then we could legitimately view this as an r-zero for the fixed $\lambda = \hat{\lambda}$.

It is also apparent from §3.4.2 that $J_\lambda(r)$ has at most one r-zero for λ such that $\arg(\lambda) \in (0, \pi/2)$; we can, however, say more than this. Observe from (3.61) that

$$\frac{\mathring{u}_0(r,\lambda)}{\tilde{u}_0(r,\lambda)} = \frac{J_\lambda(r)}{N_\lambda(r)} \to 0 \quad \text{as} \quad r \to 0,$$

which shows $\mathring{u}_0$ to be a principal solution [Hartman, 2002, p. 355] since both the Bessel and Neumann functions have finitely many zeros for $r \leq \pi/2$—recall that $\mathring{u}_0$ and $\tilde{u}_0$ are free solutions and so in particular, the potential is real (being zero). Hence, by the machinery of the so-called Niessen-Zettl transformation [Niessen and Zettl, 1992] we may transform our singular problem into a regular one. The transformed equation is the Friedrichs extension whose domain entails a boundary condition at the singular endpoint(s). In our situation, we bestow on $\mathring{u}_0$ the Friedrichs boundary condition $\mathring{u}_0(0,\lambda) = 0$, or more precisely, $\lim_{r\to 0} \mathring{u}_0(r,\lambda) = 0$. If we assume that we have an r-zero of $\mathring{u}_0$, say at $r = \hat{r} > 0$, then we could place a Dirichlet boundary condition on $\mathring{u}_0$ at $\hat{r}$ and show, in parallel with the argument from §3.4.2, that λ^2 must be real. This reduces the number of r-zeros of the Bessel function from one down to zero. As we have already mentioned before, if there are no r-zeros then there can be no λ-zeros, or more succinctly: $J_\lambda(r)$ has no zeros for $0 < r \leq \pi/2$ and λ in the first quadrant. Thus, we may use $\mathring{u}_0(r,\lambda)$ as a normalizer.

4.2.2 Two Equivalent Kernels

Let $r \leq \pi/2$, then on dividing the integral equation (4.2) by $\mathring{u}_0(r,\lambda)$ we acquire the following normalized (in the sense that the leading term is unity) equation:

$$u_{0,w}(r,\lambda) = 1 + \int_0^r \mathscr{K}(r,s,\lambda)U(s)u_{0,w}(s,\lambda)\mathrm{d}s, \tag{4.5}$$

where

$$\mathscr{K}(r,s,\lambda) = \frac{\mathring{u}_0(s,\lambda)}{\mathring{u}_0(r,\lambda)}K(r,s,\lambda) \tag{4.6}$$

and recycling the notation (3.52) from the previous chapter, i.e.

$$u_{0,w}(\cdot,\lambda) \equiv w u_0(\cdot,\lambda), \quad w = \mathring{u}_0(\cdot,\lambda)^{-1}.$$

Note that $\mathscr{K}$ is entire in λ and analytic in r and s; this is because each of the Bessel functions are entire functions of their order for non-zero argument and analytic as functions of their argument z throughout the z-plane, cut along the negative real axis [Abramowitz and Stegun, 1965, p. 358]. Hence, in order to take the limit as $|\lambda| \to \infty$ inside the integral in (4.5), we only need to check boundedness of $\mathscr{K}$ for small r and s, and for $|\lambda|$ small and large; the boundedness of $\mathscr{K}$ also ensures that there is a bounded solution of (4.5).

We will use the Phragmén-Lindelöf Principle to show the boundedness of $\mathscr{K}$ in λ. The Phragmén-Lindelöf Principle [Markushevich, 1965, p. 214] states that if a function f is analytic inside some sector of $\gamma\pi$ radians ($0 < \gamma \leq 2$) with the following properties: f is bounded by some constant for every point on the boundary of the sector, and f has growth order[1] less than $1/\gamma$ in the sector; then f is bounded by that same constant for all points in the sector. Roughly speaking, the maximum occurs on the boundary. For our purposes, the sector is defined by $\gamma = 1/2$ and we will need to show that the kernel is bounded on the real and imaginary λ-axes. We will find it convenient to switch between $N_\lambda(r)$ and $J_{-\lambda}(r)$ for the second solution $\tilde{u}_0$; however, this presents the following complication: when λ is integral, $J_\lambda(r)$ and $J_{-\lambda}(r)$ are not linearly independent [Arfken and Weber, 2005, p. 677], thus we must use the Neumann function on the real axis. We justify the switching of the second solution by showing that in fact, they yield the same kernel. Firstly,

$$\begin{aligned}
\mathscr{W}_J &\equiv \mathscr{W}(\sqrt{r}J_\lambda(r), \sqrt{r}J_{-\lambda}(r)) \\
&= \sqrt{r}J_\lambda(r)[\sqrt{r}J_{-\lambda}(r)]' - \sqrt{r}J_{-\lambda}(r)[\sqrt{r}J_\lambda(r)]' \\
&= \sqrt{r}J_\lambda(r)\left[\sqrt{r}J'_{-\lambda}(r) + \frac{1}{2\sqrt{r}}J_{-\lambda}(r)\right] - \sqrt{r}J_{-\lambda}(r)\left[\sqrt{r}J'_\lambda(r) + \frac{1}{2\sqrt{r}}J_\lambda(r)\right] \\
&= r[J_\lambda(r)J'_{-\lambda}(r) - J'_\lambda(r)J_{-\lambda}(r)] \\
&= r\left[\frac{-2\sin(\pi\lambda)}{\pi r}\right] \\
&= -\frac{2}{\pi}\sin(\pi\lambda)
\end{aligned} \tag{4.7}$$

where the penultimate line is given by a standard Wronskian formula [Arfken and Weber, 2005, p. 702]. Similarly,

$$\begin{aligned}
\mathscr{W}_N &\equiv \mathscr{W}(\sqrt{r}J_\lambda(r), \sqrt{r}N_\lambda(r)) \\
&= r[J_\lambda(r)N'_\lambda(r) - J'_\lambda(r)N_\lambda(r)] \\
&= 2/\pi
\end{aligned} \tag{4.8}$$

where again we have used a Wronskian formula [Arfken and Weber, 2005, p. 703]. If we continue the notation started here and write subscript N to refer to the kernel with $\tilde{u}_0(r,\lambda) = N_\lambda(r)$, and subscript J when $\tilde{u}_0(r,\lambda) = J_{-\lambda}(r)$, then from the definition of the Neumann function [Arfken and Weber, 2005, p. 699] and (4.3), we have

$$\begin{aligned}
(rs)^{-1/2}K_N &= \frac{\pi}{2}[J_\lambda(r)N_\lambda(s) - J_\lambda(s)N_\lambda(r)] \\
&= \frac{\pi}{2}\left[J_\lambda(r)\left\{\frac{\cos(\pi\lambda)}{\sin(\pi\lambda}J_\lambda(s) - \frac{J_{-\lambda}(s)}{\sin(\pi\lambda)}\right\} - J_\lambda(s)\left\{\frac{\cos(\pi\lambda)}{\sin(\pi\lambda}J_\lambda(r) - \frac{J_{-\lambda}(r)}{\sin(\pi\lambda)}\right\}\right] \\
&= -\frac{\pi}{2\sin(\pi\lambda)}[J_\lambda(r)J_{-\lambda}(s) - J_\lambda(s)J_{-\lambda}(r)] \\
&= (rs)^{-1/2}K_J,
\end{aligned}$$

[1] The growth order of an entire function is the subject of Appendix D.2.

which implies that the normalized kernels coincide, i.e. $\mathscr{K}_N = \mathscr{K}_J$. For convenience, the normalized kernels (see (4.6)) are given by

$$\frac{\mathscr{W}_N\mathscr{K}_N}{s} = J_\lambda(s)N_\lambda(s) - J_\lambda(s)N_\lambda(r)\frac{J_\lambda(s)}{J_\lambda(r)} \tag{4.9}$$

and

$$\frac{\mathscr{W}_J\mathscr{K}_J}{s} = J_\lambda(s)J_{-\lambda}(s) - J_\lambda(s)J_{-\lambda}(r)\frac{J_\lambda(s)}{J_\lambda(r)}. \tag{4.10}$$

4.3 Boundedness of the Normalized Kernel

For ease of reading we will consider each case of real axis, imaginary axis and interior growth order separately. Let us first consider bounding the kernel for real λ.

4.3.1 The Real Axis

To emphasize that λ is real, let us write $\lambda = \omega$, $\omega \geq 0$. On the real axis we will no doubt encounter ω as a non-negative integer, say n, and thus, as anticipated, we need to take the second solution to be the Neumann function. Moreover, because of the way in which the Neumann function is defined [Arfken and Weber, 2005, p. 699], it is imperative that this distinction between integer and non-integer order be sustained. Consider each term in equation (4.9) separately: observe that [Olver, 1974, p. 59]

$$|J_\omega(x)| \leq \frac{(x/2)^\omega}{\Gamma(\omega+1)}, \quad \omega \geq -1/2, \;\; x \geq 0. \tag{4.11}$$

It is prudent to note that the inequality (4.11) applies whether the order ω is integral or not. From Abramowitz and Stegun [1965] p. 360, we have

$$\begin{aligned} N_n(x) = &-\frac{1}{\pi}(x/2)^{-n}\sum_{j=0}^{n-1}\frac{(n-j-1)!}{j!}(x^2/4)^j + \frac{2}{\pi}\log(x/2)J_n(x) \\ &- \frac{1}{\pi}(x/2)^n\sum_{j=0}^{\infty}[\Psi(j+1)+\Psi(n+j+1)]\frac{(-x^2/4)^j}{j!(n+j)!} \end{aligned} \tag{4.12}$$

where $\Psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function. In absolute value, the first term of equation (4.12) may be bounded as follows:

$$\begin{aligned} \frac{1}{\pi}(x/2)^{-n}n!\sum_{j=0}^{n-1}\frac{(n-j-1)!}{j!n!}(x^2/4)^j &\leq \frac{1}{\pi}(x/2)^{-n}n!\sum_{j=0}^{n-1}\frac{(x^2/4)^j}{j!} \\ &\leq \frac{n!}{\pi}(x/2)^{-n}\exp(x^2/4), \end{aligned}$$

whilst the second term in absolute value is bounded by $(2/\pi)\log(x/2)$; note that we have used the inequality $|J_n(z)| \leq \exp\{\mathrm{Im}(z)\}$, $n \in \mathbb{Z}$ [Olver, 1974, p. 59]. Consider bounding the third term of $N_n(x)$. Since j and n are non-negative integers, we may make use of the identity $\Psi(j+1) + \Psi(n+j+1) = -C + \sum_{p=1}^{j} 1/p + \sum_{q=1}^{n+j} 1/q$ where C is some positive constant [Olver, 1974, p. 39]. This yields the bound $\Psi(j+1)+\Psi(n+j+1) \leq 2\log(j+1)$, from which we find that the third term in modulus is bounded by

$$\frac{2}{\pi}\sum_{j=0}^{\infty} \log(j+1)\frac{(x/2)^{n+2j}}{j!(n+j)!} \leq \frac{2}{\pi}(x/2)^n \exp(x^2/4).$$

Combining the estimates for these three terms yields the bound

$$|N_n(x)| \leq \frac{n!}{\pi}(x/2)^{-n}\exp(x^2/4) + \frac{2}{\pi}\log(x/2) + \frac{2}{\pi}(x/2)^n \exp(x^2/4). \tag{4.13}$$

Looking at (4.9), we also need to bound the ratio $J_\omega(s)/J_\omega(r)$ for $s \leq r \leq \pi/2$. From the inequalities (4.4) and (4.11) we have

$$\left|\frac{J_\omega(s)}{J_\omega(r)}\right| \leq (s/r)^\omega \sec\left\{\frac{r}{\sqrt{2}(\omega+1)}\right\} \leq 2, \quad r \leq 1. \tag{4.14}$$

We need not have placed the further restriction of $r \leq 1$, it has no effect in the greater scheme; however, it is cleaner and more transparent to work with, and so it is the assumption on the spatial variable for the remainder of this chapter. Therefore, for integer order we have from (4.11), (4.13), and (4.14) that

$$\begin{aligned}\left|\frac{\mathscr{W}_N\mathscr{K}_N}{s}\right| \leq \frac{\exp(s^2/4)}{\pi} + \frac{2\log(s/2)}{\pi\Gamma(n+1)}(s/2)^n + \frac{2\exp(s^2/4)}{\pi\Gamma(n+1)}(s/2)^{2n} \\ + \frac{2\exp(r^2/4)}{\pi}(s/r)^n + \frac{4\log(r/2)}{\pi\Gamma(n+1)}(s/2)^n + \frac{4\exp(r^2/4)}{\pi\Gamma(n+1)}(sr/4)^n,\end{aligned} \tag{4.15}$$

which is fine given that $s \leq r \leq 1$. Note that to acquire the bound (4.15), we have used the fact that the gamma function is the generalization of the factorial, i.e. $\Gamma(n) = (n-1)!$ for any natural number n [Olver, 1974, p. 32]. Also observe that when multiplication by s is performed to bound $\mathscr{K}_N$, the logarithmic terms will be dealt with.

We now turn our attention to ω, which is not in general integral. The biggest issue will be getting an expression for $N_\omega(x)$ so that we may bound it; this will be achieved using the following standard definitions [Abramowitz and Stegun, 1965, p. 360]:

$$\begin{aligned}N_\omega(x) &= \frac{\cos(\pi\omega)}{\sin(\pi\omega)}J_\omega(x) - \frac{1}{\sin(\pi\omega)}J_{-\omega}(x) \\ &= \frac{\cos(\pi\omega)}{\sin(\pi\omega)}(x/2)^\omega \sum_{j=0}^{\infty}\frac{(-x^2/4)^j}{j!\Gamma(\omega+j+1)} - \frac{1}{\sin(\pi\omega)}(x/2)^{-\omega}\sum_{j=0}^{\infty}\frac{(-x^2/4)^j}{j!\Gamma(-\omega+j+1)}.\end{aligned}$$

We aim to derive an expression for the Neumann function of real order which reduces to the integer order representation (4.12) as $\omega \to n$. So, let $\omega = n + \varepsilon$ where $n \in \mathbb{Z}^+$ and $\varepsilon \in [-1/2, 1/2)$. Now, $\Gamma(-n+j+1)$ blows up for $j = 0, 1, \ldots, n-1$ since $\Gamma(z)$ has simple poles at $z = 0, -1, -2, \dots$ [Olver, 1974, p. 32]; also recall that $\Gamma(z)$ has no zeros [Olver, 1974, p. 35]. Hence, we will regroup the terms in $N_\omega(x)$ accordingly to get

$$\begin{aligned}
N_\omega(x) = & -\frac{1}{\sin(\pi\omega)}(x/2)^{-\omega}\sum_{j=0}^{n-1}\frac{(-x^2/4)^j}{j!\Gamma(-\omega+j+1)} + \frac{\cos(\pi\omega)}{\sin(\pi\omega)}(x/2)^{\omega}\sum_{j=0}^{\infty}\frac{(-x^2/4)^j}{j!\Gamma(\omega+j+1)} \\
& -\frac{1}{\sin(\pi\omega)}(x/2)^{-\omega}\sum_{j=0}^{\infty}\frac{(-x^2/4)^{j+n}}{(j+n)!\Gamma(-\omega+j+n+1)} \\
= & -\frac{1}{\sin(\pi\omega)}\frac{1}{\Gamma(1-\omega)}(x/2)^{-\omega}\sum_{j=0}^{n-1}\frac{\Gamma(1-\omega)(-x^2/4)^j}{j!\Gamma(-\omega+j+1)} \\
& +\frac{\cos(\pi\omega)}{\sin(\pi\omega)}(x/2)^{\omega}\sum_{j=0}^{\infty}\frac{(-x^2/4)^j}{j!\Gamma(\omega+j+1)} \\
& -\frac{1}{\sin(\pi\omega)}(x/2)^{-\omega}\sum_{j=0}^{\infty}\frac{(-x^2/4)^{j+n}}{(j+n)!\Gamma(-\omega+j+n+1)}.
\end{aligned}$$

Using the well-known formula $\Gamma(1-z) = \pi/[\Gamma(z)\sin(\pi z)]$ given by (3.73), we have

$$\frac{\Gamma(1-\omega)}{\Gamma(1-(\omega-j))} = \frac{\Gamma(\omega-j)\sin\{\pi(\omega-j)\}}{\Gamma(\omega)\sin(\pi\omega)} = (-1)^j\frac{\Gamma(\omega-j)}{\Gamma(\omega)}. \tag{4.16}$$

Furthermore, since $\omega \approx n$ we may write $(x/2)^{\omega}(x^2/4)^j \approx (x/2)^{-\omega}(x^2/4)^{j+n}$, or

$$(x/2)^{-\omega}(x^2/4)^{j+n} = (x/2)^{\omega}(x^2/4)^j + R(\omega, j, x) \tag{4.17}$$

where $R(\omega, j, x)$ is some remainder term. If we notice that $\cos(\pi\omega) = (-1)^n\cos(\pi\varepsilon)$ and $\sin(\pi\omega) = (-1)^n\sin(\pi\varepsilon)$, then using equations (4.16) and (4.17) we get

$$\begin{aligned}
N_\omega(x) = & -\frac{1}{\pi}(x/2)^{-\omega}\sum_{j=0}^{n-1}\frac{\Gamma(\omega-j)}{j!}(x^2/4)^j + \frac{1}{\sin(\pi\varepsilon)}\left\{\sum_{j=0}^{\infty}\frac{(x/2)^{\omega}\cos(\pi\varepsilon)(-x^2/4)^j}{j!\Gamma(\omega+j+1)}\right. \\
& \left. -\sum_{j=0}^{\infty}\frac{(-1)^j[(x/2)^{\omega}(x^2/4)^j + R(\omega,j,x)]}{(j+n)!\Gamma(-\omega+j+n+1)}\right\} \\
= & -\frac{1}{\pi}(x/2)^{-\omega}\sum_{j=0}^{n-1}\frac{\Gamma(\omega-j)}{j!}(x^2/4)^j && (4.18) \\
& +\sum_{j=0}^{\infty}(x/2)^{\omega}(-x^2/4)^j\left[\frac{\cos(\pi\varepsilon)/\sin(\pi\varepsilon)}{j!\Gamma(j+1+n+\varepsilon)} - \frac{1/\sin(\pi\varepsilon)}{(j+n)!\Gamma(j+1-\varepsilon)}\right] && (4.19) \\
& -\sum_{j=0}^{\infty}(-1)^j\frac{R(\omega,j,x)/\sin(\pi\varepsilon)}{(j+n)!\Gamma(j+1-\varepsilon)}. && (4.20)
\end{aligned}$$

We need to check that this is the correct function, i.e. that this representation of $N_\omega(x)$ gives $N_n(x)$ in the limit as $\varepsilon \to 0$. The first term (4.18) tends to

$$-\frac{1}{\pi}(x/2)^{-n}\sum_{j=0}^{n-1}\frac{(n-j-1)!}{j!}(x^2/4)^j$$

as $\varepsilon \to 0$ since $\Gamma(z)$ is analytic save for poles at the non-positive integers; this is consistent with the corresponding term in $N_n(x)$. As for bounding this term we have

$$\begin{aligned}|(4.18)| &= \frac{\Gamma(\omega+1)}{\pi}(x/2)^{-\omega}\sum_{j=0}^{n-1}\frac{\Gamma(\omega-j)}{\Gamma(\omega+1)}\frac{(x^2/4)^j}{j!} \\ &\le a\Gamma(\omega+1)(x/2)^{-\omega}\exp(x^2/4) \qquad (4.21)\end{aligned}$$

for some constant a; this is essentially a consequence of $\Gamma(z)$ being monotone increasing for $z \gtrsim 1.46$ [Olver, 1974, p. 36, Fig. 1.1]—it is a property of the gamma function that we will use extensively in this chapter.

The second term (4.19) is not so straightforward. Let us begin with rewriting the contents of the square bracket in (4.19) as follows:

$$\frac{[\cos(\pi\varepsilon)-1]/\sin(\pi\varepsilon)}{j!\Gamma(\omega+j+1)}+\frac{1}{\sin(\pi\varepsilon)}\left[\frac{1}{j!\Gamma(j+1+n+\varepsilon)}-\frac{1}{(j+n)!\Gamma(j+1-\varepsilon)}\right]. \qquad (4.22)$$

It is clear that the first term in equation (4.22) vanishes as $\varepsilon \to 0$ by L'Hôpital's rule, since $[\cos(\pi\varepsilon)-1]'|_{\varepsilon=0} = 0$ and $[\sin(\pi\varepsilon)]'|_{\varepsilon=0} = \pi$. The second term of (4.22) is

$$\frac{1}{\sin(\pi\varepsilon)}\left[\frac{\Gamma(j+1-\varepsilon)(j+n)!-\Gamma(j+1+n+\varepsilon)j!}{j!(j+n)!\Gamma(j+1-\varepsilon)\Gamma(j+1+n+\varepsilon)}\right] \qquad (4.23)$$

of which we concentrate on the numerator divided by $\sin(\pi\varepsilon)$, i.e.

$$j!\Gamma(j+1-\varepsilon)\left\{\frac{1}{\sin(\pi\varepsilon)}\left[\frac{\Gamma(j+1+n)}{\Gamma(j+1)}-\frac{\Gamma(j+1+n+\varepsilon)}{\Gamma(j+1-\varepsilon)}\right]\right\}. \qquad (4.24)$$

We apply L'Hôpital's rule to the contents of the braces in (4.24). So,

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\frac{\Gamma(j+1+n)}{\Gamma(j+1)}-\frac{\Gamma(j+1+n+\varepsilon)}{\Gamma(j+1-\varepsilon)}\right] \\ &\quad= \frac{-\Gamma'(j+1-\varepsilon)\Gamma(j+1+n+\varepsilon)-\Gamma(j+1-\varepsilon)\Gamma'(j+1+n+\varepsilon)}{\Gamma(j+1-\varepsilon)^2} \\ &\quad= -\frac{\Gamma(j+1+n+\varepsilon)}{\Gamma(j+1-\varepsilon)}\left[\frac{\Gamma'(j+1+n+\varepsilon)}{\Gamma(j+1+n+\varepsilon)}+\frac{\Gamma'(j+1-\varepsilon)}{\Gamma(j+1-\varepsilon)}\right] \\ &\quad= -\frac{\Gamma(j+1+n+\varepsilon)}{\Gamma(j+1-\varepsilon)}[\Psi(j+1+n+\varepsilon)+\Psi(j+1-\varepsilon)],\end{aligned}$$

which yields

$$(4.23) \to -\frac{1}{\pi}\frac{\Psi(j+1+n)+\Psi(j+1)}{j!(j+n)!} \quad \text{as} \quad \varepsilon \to 0.$$

Therefore, the second term (4.19) tends to

$$-\frac{1}{\pi}(x/2)^n \sum_{j=0}^{\infty}[\Psi(j+1)+\Psi(n+j+1)]\frac{(-x^2/4)^j}{j!(n+j)!}$$

as $\varepsilon \to 0$, and this coincides with the corresponding term in $N_n(x)$. To bound (4.19) consider part of the summand given by equation (4.22): firstly,

$$\left|\frac{\cos(\pi\varepsilon)-1}{\sin(\pi\varepsilon)}\right| \leq b_1 \left|\frac{\varepsilon^2}{\varepsilon}\right| = b_1|\varepsilon| \tag{4.25}$$

for some constant b_1. Furthermore, $|1/\sin(\pi\varepsilon)| \leq |1/\varepsilon|$ since $\varepsilon \in [-1/2, 1/2)$, and hence let us consider bounding the numerator of (4.23) divided by ε, i.e. bounding

$$\begin{aligned}
&\left|\frac{\Gamma(j+1+n+\varepsilon)\Gamma(j+1)-\Gamma(j+1+n)\Gamma(j+1-\varepsilon)}{\varepsilon}\right| \\
&= \left|\left(\frac{\Gamma(j+1+n+\varepsilon)-\Gamma(j+1+n)}{\varepsilon}\right)\Gamma(j+1)\right. \\
&\qquad \left. - \left(\frac{\Gamma(j+1-\varepsilon)-\Gamma(j+1)}{\varepsilon}\right)\Gamma(j+1+n)\right| \\
&\leq \Gamma(j+1) \sup_{z\in[j+1/2+n,j+3/2+n]} |\Gamma'(z)| \\
&\qquad + \Gamma(j+1+n) \sup_{z\in[j+1/2,j+3/2]} |\Gamma'(z)|
\end{aligned} \tag{4.26}$$

by the Mean Value Theorem. Now, Binet's formula states [Olver, 1974, p. 295]

$$\log\Gamma(z) = \left(z-\frac{1}{2}\right)\log z - z + \frac{1}{2}\log(2\pi) + 2\int_0^{\infty}\frac{\arctan(y/z)}{\exp(2\pi y)-1}\mathrm{d}y, \tag{4.27}$$

where $|\arg(z)| < \pi/2$. Differentiating Binet's formula with respect to z yields the following formula for the logarithmic derivative of the gamma function:

$$\begin{aligned}
\frac{\Gamma'(z)}{\Gamma(z)} &= \log z + \frac{z-1/2}{z} - 1 + 2\int_0^{\infty}\frac{1}{1+y^2/z^2}\frac{-y/z^2}{\exp(2\pi y)-1}\mathrm{d}y \\
&= \log z - \frac{1}{2z} - 2\int_0^{\infty}\frac{y}{(y^2+z^2)(\exp(2\pi y)-1)}\mathrm{d}y.
\end{aligned}$$

Since

$$\left|\frac{y}{\exp(2\pi y)-1}\right| \leq \frac{1}{2\pi}$$

and for $z \geq 0$

$$\int_0^{\infty}\frac{\mathrm{d}y}{y^2+z^2} = \frac{1}{z}\arctan(y/z)\Big|_{y=0}^{y=\infty} = \frac{\pi}{2z},$$

we have

$$|\Gamma'(z)| \leq \Gamma(z)|\log z| + \frac{\Gamma(z)}{z}, \quad z \geq 0. \tag{4.28}$$

Thus, by applying the bound (4.28) to equation (4.26), and using the monotone increasing nature of the gamma function mentioned above, we get

$$\sup_{z\in[j+1+n-1/2,j+1+n+1/2]} |\Gamma'(z)| \leq b_2\Gamma(j+1+n+1/2)\left[\log(j+1+n+1/2)+\frac{1}{j+n+1/2}\right]$$

and

$$\sup_{z\in[j+1-1/2,j+1+1/2]} |\Gamma'(z)| \leq b_3\Gamma(j+1+1/2)\left[\log(j+1+1/2)+\frac{1}{j+1/2}\right]$$

for some constants b_2, b_3. These two inequalities give the bound

$$\begin{aligned}
&\left|\frac{\Gamma(j+1+n+\varepsilon)\Gamma(j+1)-\Gamma(j+1+n)\Gamma(j+1-\varepsilon)}{\varepsilon}\right| \\
&\quad\leq b_2\Gamma(j+1)\Gamma(j+1+n+1/2)\left[\log(j+1+n+1/2)+\frac{1}{j+n+1/2}\right] \\
&\quad\quad + b_3\Gamma(j+1+n)\Gamma(j+1+1/2)\left[\log(j+1+1/2)+\frac{1}{j+1/2}\right] \qquad (4.29)
\end{aligned}$$

and so

$$\begin{aligned}
|(4.23)| \leq\ & b_2\frac{\Gamma(j+1+n+1/2)[\log(j+1+n+1/2)+1/(j+n+1/2)]}{(j+n)!\Gamma(j+1-\varepsilon)\Gamma(j+1+n+\varepsilon)} \\
&+ b_3\frac{\Gamma(j+1+1/2)[\log(j+1+1/2)+1/(j+1/2)]}{j!\Gamma(j+1-\varepsilon)\Gamma(j+1+n+\varepsilon)}.
\end{aligned}$$

The fundamental recurrence formula $\Gamma(1+z) = z\Gamma(z)$ [Olver, 1974, p. 32] (this identity has been used previously, see equation (3.73) in the previous chapter) can be iterated to show that $\Gamma(j+z) = (j-1+z)(j-2+z)\cdots(2+z)(1+z)\Gamma(1+z)$, from which we have

$$\begin{aligned}
\frac{\Gamma(j+1+n+1/2)}{\Gamma(j+1+n+\varepsilon)} &\leq b_4\frac{\Gamma(j+1+n+1/2)}{\Gamma(j+1+n-1/2)} \\
&= b_4\frac{(j+n+1/2)(j+n-1/2)\cdots(5/2)(3/2)\Gamma(3/2)}{(j+n-1/2)(j+n-3/2)\cdots(3/2)(1/2)\Gamma(1/2)} \\
&= b_4(j+n+1/2)
\end{aligned}$$

for some constant b_4. Similarly, $\Gamma(j+1+1/2)/\Gamma(j+1-\varepsilon) \leq b_5(j+1/2)$ where b_5 is a constant. Hence, the bound becomes

$$\begin{aligned}
|(4.23)| \leq\ & b_6\frac{j+n+1/2}{(j+n-1)!\Gamma(j+1-\varepsilon)} + \frac{b_6}{(j+n)!\Gamma(j+1-\varepsilon)} \\
&+ b_7\frac{j+1/2}{(j-1)!\Gamma(j+1+n+\varepsilon)} + \frac{b_7}{j!\Gamma(j+1+n+\varepsilon)}
\end{aligned}$$

for b_6, b_7 constants. This can be simplified with the following string of observations: there is a constant b_8 such that $|1/\Gamma(j+1+n+\varepsilon)| \leq b_8$ for all $n \geq 0$ and $\varepsilon \in [-1/2, 1/2)$, which deals with the forth term. For the third term, we merely note that there is a constant b_9 such that $|j(j+1/2)/\Gamma(j+1+n+\varepsilon)| \leq b_9$ for all $n \geq 0$ and $\varepsilon \in [-1/2, 1/2)$. The second term is clearly bounded by some constant divided by $j!$. For the first term, the cases where $n = 0, 1$ are clear since they have already been dealt with; however, the cases $n \geq 2$ require investigation: let us expand the denominator as follows:

$$\frac{j+n+1/2}{(j+n-1)!\Gamma(j+1-\varepsilon)} = \frac{j+n+1/2}{j!(j+1)\cdots(j+n-1)\Gamma(j+1-\varepsilon)}$$

and observe that

$$\left|\frac{p+1/2}{p-1}\right| \leq \frac{5}{2}, \quad p \in \{2, 3, 4, \ldots\},$$

whence the first term is bounded by a constant over $j!$. Our bound on (4.23) therefore simplifies to

$$\left|\frac{\Gamma(j+1-\varepsilon)(j+n)! - \Gamma(j+1+n+\varepsilon)j!}{\sin(\pi\varepsilon)j!(j+n)!\Gamma(j+1-\varepsilon)\Gamma(j+1+n+\varepsilon)}\right| \leq \frac{(\text{const.})}{j!}. \tag{4.30}$$

Using (4.25) and (4.30) to bound (4.22), we find that

$$|(4.19)| \leq b(x/2)^{\omega} \exp(x^2/4) \tag{4.31}$$

for some constant b.

Finally, we consider the third term (4.20) of $N_\omega(x)$. Again, we calculate the limit as $\varepsilon \to 0$ of (4.20); to do this we apply L'Hôpital's rule to the ratio

$$\begin{aligned}
\frac{R(\omega, j, x)}{\sin(\pi\varepsilon)} &= \frac{1}{\sin(\pi\varepsilon)}\left[(x/2)^{-\omega}(x^2/4)^{j+n} - (x/2)^{\omega}(x^2/4)^{j}\right] \\
&= (x^2/4)^j (x/2)^{-\omega}\left[\frac{(x^2/4)^n - (x^2/4)^{\omega}}{\sin(\pi\varepsilon)}\right] \\
&\equiv (x^2/4)^j (x/2)^{-\omega}\frac{f(\varepsilon)}{\sin(\pi\varepsilon)}.
\end{aligned}$$

On taking the derivative of f we find $f'(\varepsilon) = -(x^2/4)^n(x^2/4)^{\varepsilon}\log(x^2/4)$, which gives $f'(0) = -(x^2/4)^n \log(x^2/4)$. Thus,

$$\frac{R(n+\varepsilon, j, x)}{\sin(\pi\varepsilon)} \to -\frac{2}{\pi}(x/2)^n \log(x/2)(x^2/4)^j \quad \text{as} \quad \varepsilon \to 0,$$

which yields (4.20) tending to

$$\frac{2}{\pi}\log(x/2)(x/2)^n \sum_{j=0}^{\infty} \frac{(-x^2/4)^j}{j!(j+n)!} = \frac{2}{\pi}\log(x/2)J_n(x)$$

as $\varepsilon \to 0$; again, this equals the corresponding term in $N_n(x)$. To bound (4.20), write

$$\begin{aligned}\left|\frac{R(\omega,j,x)}{\sin(\pi\varepsilon)}\right| &= (x^2/4)^j\left|\frac{(x/2)^{-n-\varepsilon}(x/2)^{2n}-(x/2)^{n+\varepsilon}}{\sin(\pi\varepsilon)}\right|\\ &= (x^2/4)^j(x/2)^{n-\varepsilon}\left|\frac{(x/2)^{2\varepsilon}-1}{\sin(\pi\varepsilon)}\right|.\end{aligned}$$

Since $|\exp(p)-1|\le|p|$ for $p\le 0$, we have $|(x/2)^{2\varepsilon}-1|\le|2\varepsilon\log(x/2)|$, where $x\le 1$. Also, as $\varepsilon\in[-1/2,1/2)$ we know that $|\sin(\pi\varepsilon)|\ge|\varepsilon|$. Putting these together gives

$$(x/2)^{n-\varepsilon}\left|\frac{(x/2)^{2\varepsilon}-1}{\sin(\pi\varepsilon)}\right|\le 2(x/2)^{n-\varepsilon}|\log(x/2)|,$$

whence

$$|(4.20)|\le c(x/2)^{n-\varepsilon}|\log(x/2)|\exp(x^2/4) \tag{4.32}$$

for some constant c. Combining the inequalities (4.21), (4.31), and (4.32) results in

$$\begin{aligned}|N_\omega(x)|\le{}& a\Gamma(\omega+1)(x/2)^{-\omega}\exp(x^2/4)+b(x/2)^{\omega}\exp(x^2/4)\\ &+c(x/2)^{n-\varepsilon}|\log(x/2)|\exp(x^2/4).\end{aligned} \tag{4.33}$$

Therefore, for real order we have from (4.11), (4.33), and (4.14) that

$$\begin{aligned}|\mathscr{W}_N\mathscr{K}_N|\le{}& as\exp(s^2/4)+\frac{bs}{\Gamma(\omega+1)}(s/2)^{2\omega}\exp(s^2/4)\\ &+\frac{cs}{\Gamma(\omega+1)}(s/2)^{2n}|\log(s/2)|\exp(s^2/4)\\ &+as(s/r)^{\omega}\exp(r^2/4)+\frac{bs}{\Gamma(\omega+1)}(sr/4)^{\omega}\exp(r^2/4)\\ &+\frac{cs}{\Gamma(\omega+1)}(sr/4)^{n}(s/r)^{\varepsilon}|\log(r/2)|\exp(r^2/4),\end{aligned} \tag{4.34}$$

which is uniformly bounded for $\omega\ge 0$ and $s\le r\le 1$. Regarding the last term in (4.34), ε must belong to $[0,1/2)$ when $n=0$ but for $n\ge 1$, $\varepsilon\in[-1/2,0)$ poses no problem. As with (4.15), the s saves us from the logarithmic divergences at the origin.

4.3.2 The Imaginary Axis

Let $\lambda=i\omega$ with $\omega>0$, and recall that on the imaginary axis we are free to use $J_{-\lambda}(r)$ as the second solution. Taking the lead from the previous section, let us consider each term in equation (4.10) separately. From Abramowitz and Stegun [1965] p. 360 we have

$$J_{i\omega}(s)J_{-i\omega}(s)=\sum_{j=0}^{\infty}\frac{\Gamma(2j+1)}{\Gamma(j+1+i\omega)\Gamma(j+1-i\omega)\Gamma(j+1)}\frac{(-s^2/4)^j}{j!}. \tag{4.35}$$

Also from Abramowitz and Stegun [1965] p. 256 is the formula

$$\Gamma(2z) = \frac{1}{2}\pi^{-1/2}4^z\Gamma(z)\Gamma(z+1/2),$$

which gives

$$\frac{\Gamma(2j+1)}{\Gamma(j+1)} = \frac{2j\Gamma(2j)}{j\Gamma(j)} = \pi^{-1/2}4^j\Gamma(j+1/2). \tag{4.36}$$

Putting (4.36) into equation (4.35) and recognizing that $\Gamma(z^*) = \Gamma(z)^*$ [Abramowitz and Stegun, 1965, p. 256], gives the identity

$$J_{i\omega}(s)J_{-i\omega}(s) = \pi^{-1/2}\sum_{j=0}^{\infty}\frac{\Gamma(j+1/2)}{|\Gamma(j+1+i\omega)|^2}\frac{(-s^2)^j}{j!}. \tag{4.37}$$

To bound this product of Bessel functions, we will use the inequality

$$|\Gamma(\alpha+i\beta)| \geq \sqrt{\operatorname{sech}(\pi\beta)}\Gamma(\alpha), \quad \alpha \geq 1/2 \tag{4.38}$$

found in the book by Carlson [1977] p. 51. This means that

$$\frac{1}{|\Gamma(j+1+i\omega)|} \leq \frac{\sqrt{\cosh(\pi\omega)}}{\Gamma(j+1)},$$

and so from (4.37)

$$|J_{i\omega}(s)J_{-i\omega}(s)| \leq (\text{const.})\cosh(\pi\omega)\exp(s^2). \tag{4.39}$$

Referring to (3.10), equation (4.38) also shows that

$$|J_{i\omega}(s)|^2 \leq \cosh(\pi\omega)\exp(s^2). \tag{4.40}$$

Moreover, $J_{i\omega}(r)$ and $J_{-i\omega}(r)$ are complex conjugates of one another, which means

$$\left|\frac{J_{-i\omega}(r)}{J_{i\omega}(r)}\right| = 1. \tag{4.41}$$

Piecing together (4.39), (4.40), and (4.41) yields

$$\left|\frac{\mathscr{W}_J\mathscr{K}_J}{s}\right| \leq (\text{const.})\cosh(\pi\omega)\exp(s^2). \tag{4.42}$$

This is not a terribly helpful bound for large $|\lambda|$; however, it is not a disaster: $\mathscr{W}_J$ was calculated to be $-(2/\pi)\sin(i\pi\omega) = -i[\exp(\pi\omega) - \exp(-\pi\omega)]/\pi$ (see (4.7)). Hence,

$$\left|\frac{\cosh(\pi\omega)}{\mathscr{W}_J}\right| = \frac{\pi}{2}\left|\frac{e^{2\pi\omega}-1}{e^{2\pi\omega}-1}\right| \leq \frac{\pi}{2}\left(\frac{e^{\pi}+1}{e^{\pi}-1}\right) \tag{4.43}$$

if $\omega \geq 1/2$. That we must stay clear of the origin to get a usable bound was to be expected, it merely reflects the linear dependence of the solutions at $\omega = 0$. Therefore, in coalescing equations (4.42) and (4.43) we acquire the inequality

$$|\mathscr{K}_J| \leq (\text{const.}) s \exp(s^2), \quad \omega \geq 1/2. \tag{4.44}$$

The task now is to patch in the boundedness of the kernel on the imaginary axis for $\omega \in (0, 1/2)$. We will find it useful to revert to using the Neumann function for the second solution: recall the expression for $N_\omega(x)$ given by (4.18) to (4.20), but with the difference that $n = 0$ and $\varepsilon = i\delta$ where $\delta \in (0, 1/2)$, i.e.

$$\begin{aligned} N_{i\delta}(x) = (x/2)^{i\delta} \sum_{j=0}^{\infty} (-x^2/4)^j \left[\frac{\cos(i\pi\delta)/\sin(i\pi\delta)}{j!\Gamma(j+1+i\delta)} - \frac{1/\sin(i\pi\delta)}{j!\Gamma(j+1-i\delta)} \right] \\ - \sum_{j=0}^{\infty} (-1)^j \frac{R(i\delta, j, x)/\sin(i\pi\delta)}{j!\Gamma(j+1-i\delta)} \end{aligned} \tag{4.45}$$

where $R(i\delta, j, x) = (x^2/4)^j \left[(x/2)^{-i\delta} - (x/2)^{i\delta} \right]$. The method by which we bound $N_{i\delta}(x)$ will be quite similar to the one used in the case of real order—in fact, it will be simpler to estimate $N_{i\delta}(x)$. Let us consider the first term in (4.45); in particular, we concentrate on the contents of the square brackets. Rewrite these contents in the form

$$\frac{[\cosh(\pi\delta) - 1]/i\sinh(\pi\delta)}{j!\Gamma(j+1+i\delta)} - \frac{1}{i\sinh(\pi\delta) j!} \left[\frac{1}{\Gamma(j+1-i\delta)} - \frac{1}{\Gamma(j+1+i\delta)} \right], \tag{4.46}$$

and denote the first and second term of equation (4.46) by (I) and (II) respectively. By an application of L'Hôpital's rule, we find that the numerator of (I) is such that

$$\lim_{\delta \to 0} \frac{\cosh(\pi\delta) - 1}{\sinh(\pi\delta)} = 0,$$

and so

$$\begin{aligned} |(\mathrm{I})| &\leq \frac{(\text{const.})\delta}{j!|\Gamma(j+1+i\delta)|} \\ &\leq (\text{const.}) \frac{\sqrt{\cosh(\pi\delta)}}{j!\Gamma(j+1)} \\ &\leq \frac{(\text{const.})}{j!}. \end{aligned} \tag{4.47}$$

This follows from the facts $\sinh(\pi\delta) \geq \delta$ and $\cosh(\pi\delta) - 1 \leq (\text{const.})\delta^2$ for $\delta \in (0, 1/2)$, and the inequality (4.38). Let us rewrite the second term (II) as

$$j!(\mathrm{II}) = \frac{[\Gamma(j+1+i\delta) - \Gamma(j+1-i\delta)]/i\sinh(\pi\delta)}{|\Gamma(j+1+i\delta)|^2};$$

from which, L'Hôpital yields

$$\lim_{\delta\to 0}(\mathrm{II}) = \frac{1}{i\pi\Gamma(j+1)^2 j!}[i\Gamma'(j+1) + i\Gamma'(j+1)] = \frac{2\Gamma'(j+1)}{\pi\Gamma(j+1)^2 j!}.$$

For a bound, we again use the inequality (4.38) to give

$$\begin{aligned}
j!|(\mathrm{II})| &\leq \frac{\cosh(\pi\delta)}{\Gamma(j+1)^2\delta}|\Gamma(j+1+i\delta) - \Gamma(j+1-i\delta)| \\
&\leq \frac{\cosh(\pi\delta)}{\Gamma(j+1)^2}\left|\left(\frac{\Gamma(j+1+i\delta)-\Gamma(j+1)}{\delta}\right) - \left(\frac{\Gamma(j+1+i\delta)-\Gamma(j+1)}{\delta}\right)^*\right| \\
&\leq \frac{(\text{const.})}{\Gamma(j+1)^2}\left|\mathrm{Im}\left\{\frac{\Gamma(j+1+i\delta)-\Gamma(j+1)}{\delta}\right\}\right| \\
&\leq \frac{(\text{const.})}{\Gamma(j+1)^2}\sup_{z\in\Omega}|\mathrm{Im}\{\Gamma'(z)\}| \\
&\leq \frac{(\text{const.})}{\Gamma(j+1)^2}\sup_{z\in\Omega}|\Gamma'(z)|
\end{aligned}$$

where $\Omega = \{j+1+i\zeta/2 : \zeta \in [0,1]\}$; the penultimate line of this calculation is given by the Mean Value Theorem. We require a more general bound from Binet's formula than that of (4.28): let $z = pe^{i\vartheta}$ with $\vartheta \in (-\pi/2, \pi/2)$, then

$$\begin{aligned}
\int_0^\infty \frac{dy}{|y^2+z^2|} &= \int_0^\infty \frac{dy}{|y^2 + p^2\cos(2\vartheta) + ip^2\sin(2\vartheta)|} \\
&= \int_0^\infty \frac{dy}{\sqrt{y^4 + 2y^2p^2\cos(2\vartheta) + p^4}} \\
&\leq \int_0^\infty \frac{dy}{\sqrt{y^4+p^4}}
\end{aligned}$$

only if $\arg(z) \in [0, \pi/4]$. Now, we have the inequality $y^4 + p^4 \geq (y^2+p^2)^2/2$ since it is true that $y^4 + p^4 \geq 2y^2p^2$. Thus, $\sqrt{y^4+p^4} \geq (y^2+p^2)/\sqrt{2}$ and so

$$\int_0^\infty \frac{dy}{\sqrt{y^4+p^4}} \leq \sqrt{2}\int_0^\infty \frac{dy}{y^2+|z|^2} = \frac{\pi\sqrt{2}}{2|z|},$$

whence

$$|\Gamma'(z)| \leq |\Gamma(z)|\left(|\log z| + \frac{1+\sqrt{2}}{|z|}\right), \quad \arg(z) \in [0, \pi/4]. \tag{4.48}$$

Since $\arg(j+1+i\zeta/2) \in [0, \pi/4)$, we may use the bound (4.48) to get

$$j!(\mathrm{II}) \leq \frac{(\text{const.})}{\Gamma(j+1)^2}\sup_{z\in\Omega}|\Gamma(z)|\left(|\log z| + \frac{(\text{const.})}{|z|}\right).$$

With the implementation of yet another inequality $|\Gamma(\alpha+i\beta)| \leq |\Gamma(\alpha)|$, found in, for example, Carlson [1977] p. 51, this bound becomes

$$j!(\mathrm{II}) \leq (\text{const.})\left(\frac{|\log(j+1+i/2)|}{\Gamma(j+1)} + \frac{1}{(j+1)\Gamma(j+1)}\right).$$

Thus,

$$|(\mathrm{II})| \leq \frac{(\text{const.})}{j!} \tag{4.49}$$

and therefore by (4.47) and (4.49),

$$|(4.46)| \leq |(\mathrm{I})| + |(\mathrm{II})| \leq \frac{(\text{const.})}{j!}. \tag{4.50}$$

To estimate the second term in (4.45), we consider $\left[(x/2)^{-i\delta} - (x/2)^{i\delta}\right]/i\sinh(\pi\delta)$. By L'Hôpital's rule, this tends to $-2\log(x/2)/\pi$ in the limit as $\delta \to 0$. Acquiring a bound is very similar to that involving $R(\omega, j, x)$ for $N_\omega(x)$ in §4.3.1, i.e. we have

$$\left|\frac{(x/2)^{-i\delta} - (x/2)^{i\delta}}{\sinh(\pi\delta)}\right| \leq \frac{1}{\delta}|2\delta\log(x/2)|,$$

but we need to check that $|\exp(ip) - 1| \leq |p|$. Well,

$$\exp(ip) - 1 = \int_0^p \frac{d}{dt}[\exp(it)]dt = i\int_0^t \exp(it)dt$$

and this implies the required inequality. Therefore,

$$\begin{aligned}\left|\frac{(x/2)^{-i\delta} - (x/2)^{i\delta}}{\sinh(\pi\delta)\Gamma(j+1-i\delta)}\right| &\leq \frac{2\sqrt{\cosh(\pi\delta)}|\log(x/2)|}{\Gamma(j+1)} \\ &\leq (\text{const.})|\log(x/2)|. \end{aligned} \tag{4.51}$$

Applying the bounds (4.50) and (4.51) to (4.45) yields

$$|N_{i\delta}(x)| \leq \exp(x^2/4)\{d_1 + d_2|\log(x/2)|\} \tag{4.52}$$

where d_1, d_2 are constants.

In view of equation (4.9), we also need estimates on $|J_{i\delta}(s)|$ and $|J_{i\delta}(s)|^2$, as well as on the ratio $|N_{i\delta}(r)/J_{i\delta}(r)|$. Notice that the first two bounds have already been achieved by (4.40) since $\delta \in (0, 1/2)$; however, the latter requires further thought. Let us write out the Neumann function as it is usually defined [Abramowitz and Stegun, 1965, p. 358]:

$$N_{i\delta}(r) = \frac{\cosh(\pi\delta)}{i\sinh(\pi\delta)}J_{i\delta}(r) - \frac{1}{i\sinh(\pi\delta)}J_{-i\delta}(r),$$

from which we get

$$\left|\frac{N_{i\delta}(r)}{J_{i\delta}(r)}\right| = \left|\frac{\cosh(\pi\delta) - J_{-i\delta}(r)/J_{i\delta}(r)}{\sinh(\pi\delta)}\right|.$$

Yet another application of L'Hôpital's rule shows that $N_{i\delta}(r)/J_{i\delta}(r) \to 0$ as $\delta \to 0$; this is a result of cancellation of terms when δ is set to zero in the derivative with respect to δ of $J_{-i\delta}(r)/J_{i\delta}(r)$. Using their conjugate properties, it is possible to write

$$\frac{J_{-i\delta}(r)}{J_{i\delta}(r)} = \exp\{-2i\delta\log(r/2)\}\frac{f(-\delta,r)}{f(\delta,r)}$$

where f is analytic jointly in δ and r in a neighbourhood of the origin, with $f(0,r) = 1$. Hence, define $F(\delta,r) \equiv f(-\delta,r)/f(\delta,r)$ and consider

$$\begin{aligned}\cosh(\pi\delta) - \frac{J_{-i\delta}(r)}{J_{i\delta}(r)} &= \cosh(\pi\delta) - (1 + \exp\{-2i\delta\log(r/2)\} - 1)(1 + [F(\delta,r) - 1]) \\ &= (\cosh(\pi\delta) - 1) - (F(\delta,r) - 1) - (\exp\{-2i\delta\log(r/2)\} - 1) \\ &\quad - (F(\delta,r) - 1)(\exp\{-2i\delta\log(r/2)\} - 1).\end{aligned}$$

Now, we clearly have $|F(\delta,r) - 1| \le e_1|\delta|$ uniformly in a neighbourhood of the origin in the (δ,r)-plane, and $|\cosh(\pi\delta) - 1| \le e_2|\delta|^2$ and $|\exp\{-2i\delta\log(r/2)\} - 1| \le 2|\delta\log(r/2)|$ for e_1, e_2 constants; whence

$$\begin{aligned}\left|\frac{N_{i\delta}(r)}{J_{i\delta}(r)}\right| &\le e_2\delta + e_1 + 2|\log(r/2)| + 2e_1\delta|\log(r/2)| \\ &\le e_3 + e_4|\log(r/2)| \end{aligned} \tag{4.53}$$

for some constants e_3, e_4. The inequalities (4.40), (4.52), and (4.53) yield

$$|\mathscr{W}_N\mathscr{K}_N| \le \alpha\exp(s^2)\{d_1 + d_2|\log(s/2)|\} + \beta\exp(s^2)\{e_3 + e_4|\log(r/2)|\} \tag{4.54}$$

for some constants α and β, with $\lambda = i\omega$, $\omega \in (0, 1/2)$ and $s \le r \le 1$.

We conclude from (4.34), (4.44), and (4.54) that the normalized kernel $\mathscr{K}(r,s,\lambda)$ is bounded by some constant on the boundary comprising the real and imaginary λ-axes. Recall that our 'Phragmén-Lindelöf sector' is given by $\gamma = 1/2$, and since the kernel is analytic inside this sector, we need only show that its growth order is less than $1/\gamma = 2$. In fact, we will demonstrate that the normalized kernel has growth order at most 1.

4.3.3 Growth Order

It is most convenient to calculate the order of the normalized kernel in the form $\mathscr{K}_J$; let us write this version of the kernel in full, i.e. from (4.10) and (4.7) we have

$$\mathscr{K}_J = -\frac{\pi s}{2\sin(\pi\lambda)}\left[J_\lambda(s)J_{-\lambda}(s) - \frac{J_\lambda(r)}{J_\lambda(r)}J_\lambda(s)^2\right] \tag{4.55}$$

In this section, $\lambda \ne 0$ with $\arg(\lambda) \in (0, \pi/2)$ and, as usual, $s \le r \le 1$. Moreover, we will often denote by λ_R and λ_I the real and imaginary parts of λ respectively.

Applying the inequality (4.38) to the gamma function in the series definition (3.10) of the Bessel function, and using the fact that $|(s/2)^{\lambda}| = (s/2)^{\lambda_R}$, we have

$$\begin{aligned}|J_\lambda(s)| &\leq (s/2)^{\lambda_R} \sum_{j=0}^{\infty} \frac{\sqrt{\cosh(\pi\lambda_I)}}{\Gamma(j+1+\lambda_R)} \frac{(s^2/4)^j}{j!} \\ &\leq \frac{(\text{const.})}{\Gamma(\lambda_R+1)} \exp(\pi\lambda_I/2)(s/2)^{\lambda_R},\end{aligned}$$

from which we get

$$|J_\lambda(s)|^2 \leq \frac{(\text{const.})}{\Gamma(\lambda_R+1)^2} \exp(\pi\lambda_I)(s/2)^{2\lambda_R}. \tag{4.56}$$

Recall the identity (4.37); in this case we have

$$J_\lambda(s)J_{-\lambda}(s) = \pi^{-1/2} \sum_{j=0}^{\infty} \frac{\Gamma(j+1/2)}{\Gamma(j+1+\lambda)\Gamma(j+1-\lambda)} \frac{(-s^2)^j}{j!}.$$

As we have seen, we may decompose gamma functions as follows:

$$\begin{aligned}\Gamma(j+1+\lambda)\Gamma(j+1-\lambda) &= (j+\lambda)(j-1+\lambda)\cdots(1+\lambda)\lambda\Gamma(\lambda) \\ &\quad \times (j-\lambda)(j-1-\lambda)\cdots(1-\lambda)\Gamma(1-\lambda),\end{aligned}$$

which implies that

$$\begin{aligned}|\Gamma(j+1+\lambda)\Gamma(j+1-\lambda)| &\geq \frac{j!}{2}\text{dist}(\lambda,\mathbb{N})|\Gamma(\lambda)\Gamma(1-\lambda)| \\ &= \frac{j!}{2}\text{dist}(\lambda,\mathbb{N})\frac{\pi}{|\sin(\pi\lambda)|}\end{aligned}$$

where $\text{dist}(\lambda,\mathbb{N})$ is the distance from λ to the nearest natural number. Furthermore, we assert the validity of the following inequality:

$$\frac{\text{dist}(\lambda,\mathbb{N})}{|\sin(\pi\lambda)|} \geq (\text{const.})\exp(-\pi\lambda_I). \tag{4.57}$$

To prove this inequality, notice that we have periodicity in λ_R and thus we may restrict our attention to the case $0 < \lambda_R \leq 1$. Let us first consider $1/2 \leq \lambda_R \leq 1$: we are required to show that

$$\frac{|\sin(\pi\lambda)|}{\sqrt{(\lambda_R-1)^2+\lambda_I^2}} \leq (\text{const.})\exp(\pi\lambda_I) \tag{4.58}$$

for $\lambda_I > 0$. Well,

$$|\sin(\pi\lambda)| = |\sin(\pi\lambda_R)\cosh(\pi\lambda_I) + i\cosh(\pi\lambda_R)\sinh(\pi\lambda_I)|;$$

we can immediately bound three of the four terms here: we clearly have $|\sin(y)/y| \leq 1$ and so $|\sin(\pi\lambda_R)| \leq \pi|\lambda_R - 1|$. Also, $|\cos(\pi\lambda_R)| \leq 1$ and $|\cosh(\pi\lambda_I)| \leq \exp(\pi\lambda_I)$. Hence, if we knew the inequality

$$\left|\frac{\sinh(\pi\lambda_I)}{\pi\lambda_I}\right| \le \exp(\pi\lambda_I)$$

to be true, then

$$\begin{aligned}|\sin(\pi\lambda)| &\le (\pi|\lambda_R - 1| + \pi|\lambda_I|)\exp(\pi\lambda_I) \\ &\le 2\pi\sqrt{(\lambda_R - 1)^2 + \lambda_I^2}\exp(\pi\lambda_I) \\ &= 2\pi \mathrm{dist}(\lambda, 1)\exp(\pi\lambda_I).\end{aligned}$$

It remains to prove $|\sinh(y)/y| \le \exp(y)$ or equivalently $\sinh(y) - y\exp(y) \le 0$ for $y \ge 0$. This is an inequality on the real line, it is true for $y \to \infty$ and for $y \to 0$; moreover, the Taylor series shows the validity of this inequality:

$$(y + y^3/3! + y^5/5! + \cdots) - (y + y^2 + y^3/2! + y^4/3! + y^5/4! + \cdots) \le 0.$$

On the other hand, when $0 < \lambda_R \le 1/2$ the denominator in (4.58) is larger, whilst by symmetry, the same bound holds for the numerator. This proves (4.57), and thus we may use it to show

$$|\Gamma(j+1+\lambda)\Gamma(j+1-\lambda)| \ge (\text{const.})j!\exp(-\pi\lambda_I),$$

whence

$$|J_\lambda(s)J_{-\lambda}(s)| \le (\text{const.})\exp(\pi\lambda_I). \tag{4.59}$$

Lastly, we need to consider $J_{-\lambda}(r)/J_\lambda(r)$. Since we do not have any phase method at our disposal, we will need to write the last term in square brackets of (4.55) in a more transparent way. Before doing this, however, let us consider acquiring a lower bound for the denominator: we have on expanding the Bessel series

$$\begin{aligned}J_\lambda(r) &= (r/2)^\lambda \sum_{j=0}^{\infty} \frac{(-r^2/4)^j}{\Gamma(j+1+\lambda)j!} \\ &= (r/2)^\lambda \left[\frac{1}{\Gamma(\lambda+1)} - \frac{r^2/4}{\Gamma(\lambda+2)} + \frac{(r^2/4)^2}{\Gamma(\lambda+3)2!} + \cdots\right] \\ &= \frac{(r/2)^\lambda}{\Gamma(\lambda+1)}\left[1 - \frac{r^2/4}{\lambda+2} + \frac{(r^2/4)^2}{2!(\lambda+2)(\lambda+3)} + \cdots\right]\end{aligned}$$

and so

$$|J_\lambda(r)| \ge \frac{|(r/2)^\lambda|}{2|\Gamma(\lambda+1)|}$$

for all sufficiently large $|\lambda|$. Another application of $|\Gamma(\lambda+1)| \le \Gamma(\lambda_R+1)$ gives

$$|J_\lambda(r)| \ge \frac{(r/2)^{\lambda_R}}{2\Gamma(\lambda_R+1)}. \tag{4.60}$$

Therefore, writing the last term in square brackets of (4.55) as

$$\frac{J_\lambda(s)J_{-\lambda}(r)J_\lambda(s)}{J_\lambda(r)} = \frac{J_\lambda(s)^2}{J_\lambda(r)^2}[J_\lambda(r)J_{-\lambda}(r)],$$

we find from (4.56), (4.59), and (4.60) that

$$\begin{aligned}\left|\frac{J_\lambda(s)J_{-\lambda}(r)J_\lambda(s)}{J_\lambda(r)}\right| &\leq (\text{const.})\exp(\pi\lambda_I)^2\frac{(s/2)^{2\lambda_R}}{(r/2)^{2\lambda_R}} \\ &= (\text{const.})(s/r)^{2\lambda_R}\exp(2\pi\lambda_I) \\ &= (\text{const.})\exp\{2\lambda_R\log(s/r)\}\exp(2\pi\lambda_I) \\ &\leq (\text{const.})\exp(2\pi|\lambda|),\end{aligned}$$

and consequently

$$|\mathscr{W}_J\mathscr{K}_J| \leq (\text{const.})\exp(2\pi|\lambda|).$$

In other words, the product $\mathscr{W}_J\mathscr{K}_J$ is of order 1. Moreover, $\mathscr{W}_J \propto \sin(\pi\lambda)$ and so it is also of order 1 [Markushevich, 1965, p. 252]. We may thus conclude that the normalized kernel $\mathscr{K}_J$ is of order at most 1 from Lemma 1 in Appendix D.2. The Phragmén-Lindelöf Principle then shows that the normalized kernel is bounded by some constant in the first quadrant for $s \leq r \leq 1$; this means that there is a bounded solution $u_{0,w}$ of equation (4.5) for integrable U. This also means that on taking the limit as $|\lambda| \to \infty$ of $u_{0,w}(r,\lambda)$, we can interchange limit and integration. However, it is not terribly straightforward to calculate large $|\lambda|$ asymptotics of the kernel in its current form; in the next section we express the kernel in a different way and compute its asymptotics.

4.4 The D'Alembert Reformulation

For what follows, we consider the second solution $\tilde{u}_0$ to be given by the Neumann function—since it is valid to do so in the whole of the first quadrant. Recall from (4.8) that $\mathscr{W}_N = 2/\pi$; however, we may rescale such that $\mathscr{W}(\mathring{u}_0, \tilde{u}_0) = 1$. Then

$$\frac{\mathring{u}_0\tilde{u}_0' - \mathring{u}_0'\tilde{u}_0}{\mathring{u}_0^2} = \frac{1}{\mathring{u}_0^2}. \tag{4.61}$$

Now,

$$\begin{aligned}\mathscr{K}(r,s,\lambda) &= \frac{\mathring{u}_0(s,\lambda)}{\mathring{u}_0(r,\lambda)}[\mathring{u}_0(r,\lambda)\tilde{u}_0(s,\lambda) - \mathring{u}_0(s,\lambda)\tilde{u}_0(r,\lambda)] \\ &= \frac{\mathring{u}_0(s,\lambda)}{\mathring{u}_0(r,\lambda)}\mathring{u}_0(r,\lambda)\mathring{u}_0(s,\lambda)\left[\frac{\tilde{u}_0(s,\lambda)}{\mathring{u}_0(s,\lambda)} - \frac{\tilde{u}_0(r,\lambda)}{\mathring{u}_0(r,\lambda)}\right] \\ &= -\mathring{u}_0(s,\lambda)^2\int_s^r \frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{\tilde{u}_0(t,\lambda)}{\mathring{u}_0(t,\lambda)}\right\}\mathrm{d}t.\end{aligned}$$

Observe that (4.61) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{\tilde{u}_0(t,\lambda)}{\mathring{u}_0(t,\lambda)}\right\} = \frac{1}{\mathring{u}_0(t,\lambda)^2},$$

whence

$$\mathscr{K}(r,s,\lambda) = -\int_s^r \frac{\mathring{u}_0(s,\lambda)^2}{\mathring{u}_0(t,\lambda)^2}\mathrm{d}t = -\int_s^r \frac{s}{t}\left[\frac{J_\lambda(s)}{J_\lambda(t)}\right]^2 \mathrm{d}t. \tag{4.62}$$

In order to take the limit as $|\lambda| \to \infty$ of (4.62) we require that the integrand be bounded. Firstly, since $s \leq t$ we have $s/t \leq 1$. When $\lambda \geq 0$, the bound (4.14) applies. Furthermore, from the inequalities (4.56) and (4.60) we have

$$\left|\frac{J_\lambda(s)}{J_\lambda(t)}\right|^2 \leq (\text{const.})(s/t)^{2\lambda_R}\exp(\pi\lambda_I) \leq (\text{const.})\exp(\pi|\lambda|),$$

which implies that the integrand is of order 1 in the strict first quadrant. If we could demonstrate boundedness on the imaginary axis, then Phragmën-Lindelöf would give the boundedness of the integrand in the first quadrant. To achieve boundedness on the imaginary axis let us define the quotient

$$Q(s,t,\omega) \equiv \frac{\sum_{j=0}^{\infty} \frac{\Gamma(1+i\omega)}{\Gamma(j+1+i\omega)}\frac{(-s^2/4)^j}{j!}}{\sum_{j=0}^{\infty} \frac{\Gamma(1+i\omega)}{\Gamma(j+1+i\omega)}\frac{(-t^2/4)^j}{j!}}, \quad \omega > 0$$

which corresponds to the ratio $J_{i\omega}(s)/J_{i\omega}(t)$ modulo factors of unit absolute value. Suppose that this is not bounded, then there exists a sequence (s_n, t_n, ω_n) such that $|Q(s_n, t_n, \omega_n)| \to \infty$ as $n \to \infty$. Now, $\omega_n \to \infty$ necessarily on this sequence, whilst (s_n) and (t_n) are bounded sequences—without loss of generality assume $s_n \to s_\infty < \infty$ and $r_n \to r_\infty < \infty$, exctracting convergent subsequences if need be. Letting x stand for either s or t, we claim that

$$\lim_{n\to\infty}\sum_{j=0}^{\infty}\frac{\Gamma(1+i\omega_n)}{\Gamma(j+1+i\omega_n)}\frac{(-x_n^2/4)^j}{j!} = 1. \tag{4.63}$$

We can justify taking the limit inside the sum by noting the following inequalities:

$$\begin{aligned}
|\Gamma(2+i\omega_n)| &= |1+i\omega_n||\Gamma(1+i\omega_n)| \geq |\Gamma(1+i\omega_n)|,\\
|\Gamma(3+i\omega_n)| &= |2+i\omega_n||1+i\omega_n||\Gamma(1+i\omega_n)| \geq 2|\Gamma(1+i\omega_n)|,\\
|\Gamma(4+i\omega_n)| &= |3+i\omega_n||2+i\omega_n||1+i\omega_n||\Gamma(1+i\omega_n)| \geq 3!|\Gamma(1+i\omega_n)|
\end{aligned}$$

and so on; at the general step we have

$$\left|\frac{\Gamma(j+1+i\omega_n)}{\Gamma(1+i\omega_n)}\right| \geq j!$$

and thus the summand is bounded. Swapping limit and summation shows (4.63) to be true, contradicting our assumption that $|Q(s_n, t_n, \omega_n)| \to \infty$. The only logical conclusion is that $J_{i\omega}(s)/J_{i\omega}(t)$ is bounded. Thus, we are justified in taking the limit $|\lambda| \to \infty$ inside the integral defining $\mathscr{K}$ in (4.62). As yet, however, we have no large complex order asymptotics of the Bessel function; these can be found in a seminal paper by Langer [1932].

4.4.1 Langer Asymptotics for the Bessel Function

In his paper, Langer [1932] studied the asymptotic properties of solutions of the second order ordinary differential equation

$$y''(x) + [\nu^2\phi^2(z) - \chi(z)]y(z) = 0 \tag{4.64}$$

for large complex values of the parameter ν^2, with the following hypotheses: $x = \nu\exp(z)$ is real[2] and $\phi^2(x)$ is real, continuous, and non-negative. In the construction of the theory, the complex variable ξ (Langer's variable) was introduced. It is defined as

$$\xi \equiv \nu \int_0^z \phi(z)\mathrm{d}z$$

and is important in the final asymptotic formulae. As an application, Langer considered the special case of $\phi^2(z) = \exp(2z) - 1$ and $\chi(z) = 0$ since this gives rise to the equation satisfied by the general cylinder function. This means that

$$\xi = \nu \int^z \{\exp(2t) - 1\}^{1/2}\mathrm{d}t,$$

$$\xi = \nu \int_0^z \{\exp(2t) - 1\}^{1/2}\mathrm{d}t,$$

where we choose the square root such that $\{\exp(2t) - 1\}^{1/2} = -i\{1 - \exp(2t)\}^{1/2}$. To evaluate this integral let $t = \ln\sqrt{x}$, then

$$\xi = \frac{\nu}{2}\int_1^{e^{2z}} \frac{\sqrt{x-1}}{x}\mathrm{d}x = -\frac{i\nu}{2}\int_1^{e^{2z}} \frac{\sqrt{1-x}}{x}\mathrm{d}x.$$

Next, let $x = \cos^2\vartheta$ so that

$$\begin{aligned}
\xi &= i\nu \int_1^{e^{2z}} \frac{\sin^2\vartheta}{\cos\vartheta}\mathrm{d}\vartheta \\
&= -i\nu \int_1^{e^{2z}} (\cos\vartheta - \sec\vartheta)\,\mathrm{d}\vartheta \\
&= -i\nu\Big[\sin\vartheta - \log(\sec\vartheta + \tan\vartheta)\Big]_{x=1}^{x=e^{2z}} \\
&= -i\nu\left[\sqrt{1-e^{2z}} - \log\left\{\frac{\sqrt{1-e^{2z}}+1}{e^z}\right\}\right],
\end{aligned}$$

[2] The variable x was the independent variable of the differential equation from which the Liouville normal form (4.64) originated; the Louville transformation is discussed in §5.1.1 of Chapter 5.

whence

$$\xi = -i\nu(\Delta - \log(\Delta + 1) + z) \tag{4.65}$$

where $\Delta \equiv \{1 - \exp(2z)\}^{1/2} = (1 - x^2/\nu^2)^{1/2}$. Moreover, we will require the identification

$$g \equiv \left(\frac{2}{\pi\nu\phi(z)}\right)^{1/2},$$

which for our specific function $\phi(z)$ is $g = \sqrt{2/\pi}(x^2 - \nu^2)^{-1/4}$. With the necessary notation introduced, we can now give the asymptotic form of $J_\nu(x)$ for large $|\nu|$ in the first quadrant; however, we must choose the correct region $\Xi^{(h)}$ in Langer [1932] p. 471 table (50). Since $z = \log(x/\nu) = \log x - \log|\nu| - i\arg\nu$, z lies in region $\Xi^{(-2)}$ or $\Xi^{(-1)}$ for ν in the first quadrant [Langer, 1932, p. 472, Fig. 3]. In any case [Langer, 1932, p. 471, table (50)],

$$J_\nu(x) \sim \frac{g}{2}\exp\{i(\xi - \pi/4)\}, \quad |\nu| \to \infty. \tag{4.66}$$

From equation (4.65), $\xi \sim -i\nu\{\alpha + \log x - \log\nu\}$ as $|\nu| \to \infty$, where $\alpha \equiv 1 - \log(2)$. Combining these asymptotics with (4.66) yields

$$\frac{J_\lambda(s)}{J_\lambda(t)} \sim \left(\frac{t^2 - \lambda^2}{s^2 - \lambda^2}\right)^{1/4} \frac{\exp\{\lambda(\alpha + \log s - \log\lambda)\}}{\exp\{\lambda(\alpha + \log t - \log\lambda)\}} \sim \exp\{-\lambda\log(t/s)\},$$

which means that the integrand in (4.62) goes to zero as λ goes to infinity along any ray non-parallel to the imaginary axis, and thus the kernel $\mathscr{K}(r, s, \lambda)$ also tends to zero as λ tends to infinity along non-vertical rays. On a ray that is parallel to the imaginary axis, the integrand becomes more and more oscillatory; thus, the kernel still tends to zero as $\lambda \to \infty$ vertically by the Riemann-Lebesgue Lemma [Bender and Orszag, 1999, p. 277].

Combining these cases, the kernel $\mathscr{K}(r, s, \lambda) \to 0$ as $|\lambda| \to \infty$ in the first quadrant and thus from (4.5), $u_{0,w}(r, \lambda) \sim 1$ or equivalently, $u_0(r, \lambda) \sim \mathring{u}_0(r, \lambda)$ for large $|\lambda|$ locally uniformly in r—the entire analysis has been locally uniform in spatial variable. This shows that the condition (4.1) becomes the free Regge pole condition as $|\lambda| \to \infty$, for which there are no solutions (to be clear, there are no Regge poles for the free problem; in fact, the Wronskian is a constant—see (4.8) and note that the Hankel function is a linear combiniation of the Bessel and Neumann functions), i.e. there are no Regge poles for large $|\lambda|$. Moreover, the Wronskian $\mathscr{W}(u_0, u_\infty)$ is an entire function of λ, which has no zeros for sufficiently large $|\lambda|$ since its λ-zeros are precisely the Regge poles. Therefore, it can only have finitely many zeros by Theorem D.2 in Appendix D.1. These facts have been demonstrated for $k = 1$ and $r \leq 1$; but, as long as $k \leq 1/r_0$ for some finite $r_0 > 0$ then $r \leq r_0$ would suffice. Consequently, we have proved the following result:

Theorem 4. *For a potential which is identically zero for $r > r_0$ and integrable for $r \leq r_0$, there are finitely many associated Regge poles when the energy $k \leq 1/r_0$.*

CHAPTER 5

Boundary Conditions

It is known that there are finitely many Regge poles for an analytic potential with $r^2U(r)$ bounded [Barut and Dilley, 1963], and thus it would be prudent to try and count them. As was described—albeit vaguely—in Chapter 1, the idea for achieving this is as follows: consider (2.74) with boundary condition[1] $u \sim \cos(kr) + i\gamma \sin(kr)$ for large r and $\gamma \in [0, 1]$, where the Regge pole problem corresponds to setting $\gamma = 1$. We do this in order to establish a one-to-one correspondence between the Regge poles and the eigenvalues of the self-adjoint problem associated with $\gamma = 0$; an attempt could then be made to count the Regge poles by counting these eigenvalues, since the technology is already in place to do so. However, as we shall see, there are infinitely many eigenvalues when $\gamma \in [0, 1)$; this is bad news for our proposed approach to counting Regge poles. We do, however, discover a remarkable sensitivity of Regge poles to boundary conditions. In this chapter, we demonstrate that when only the centrifugal term is present, infinitely many 'Regge poles' come from infinity when the value of the coupling constant γ is changed, by any amount, away from unity. Strictly speaking, Regge poles correspond only to $\gamma = 1$; this is the reason for the inverted commas—maybe generalized Regge poles is better.

5.1 The Free Problem

For a localized potential, the boundary condition for distances far from the scattering centre is $u \sim \cos(kr) + i \sin(kr)$. In accordance with our outline above, we introduce a coupling constant γ to acquire the following perturbed boundary condition at infinity:

$$u \sim \cos(kr) + i\gamma \sin(kr), \quad r \to \infty. \tag{5.1}$$

[1]Note that we have the limit circle case at infinity. To emphasize that this is a boundary condition perhaps we should write it as $\lim_{r\to\infty} \mathscr{W}(u, cos(kr) + i\gamma \sin(kr)) = 0$.

In the free case, the solution of (2.74) satisfying (5.1) for $\gamma = 1$ is proportional to $H_\lambda^{(1)}(kr)$, which is a special linear combination of the Bessel and Neumann functions. We require the combination of $J_\lambda(kr)$ and $N_\lambda(kr)$ which satisfies (5.1) for $\gamma \neq 1$. Modulo some constants, we have for large r that

$$\begin{pmatrix} J_\lambda(kr) \\ N_\lambda(kr) \end{pmatrix} \sim r^{-1/2} \begin{pmatrix} \cos(z) & \sin(z) \\ -\sin(z) & \cos(z) \end{pmatrix} \begin{pmatrix} \cos(kr) \\ \sin(kr) \end{pmatrix} \tag{5.2}$$

where $z = (\lambda + 1/2)\pi/2$, since for small argument the Hankel function of the first kind satisfies [Abramowitz and Stegun, 1965, p. 364]

$$H_\nu^{(1)}(x) \sim x^{-1/2} \mathrm{e}^{-i(\nu+1/2)\pi/2} \mathrm{e}^{ix}.$$

The 2×2 matrix in (5.2) is unitary and thus (5.2) can easily be inverted to give

$$\begin{pmatrix} \cos(kr) \\ \sin(kr) \end{pmatrix} \sim r^{1/2} \begin{pmatrix} \cos(z) & -\sin(z) \\ \sin(z) & \cos(z) \end{pmatrix} \begin{pmatrix} J_\lambda(kr) \\ N_\lambda(kr) \end{pmatrix}. \tag{5.3}$$

Therefore, the required combination of the Bessel and Neumann functions is

$$\sqrt{r}[(\cos(z) + i\gamma \sin(z))J_\lambda(kr) + (-\sin(z) + i\gamma\cos(z))N_\lambda(kr)].$$

Thus, we have a 'Regge pole' when $-\sin(z) + i\gamma\cos(z) = 0$ for N_λ entails the singular behaviour of the wavefunction. It is helpful to rewrite this condition as $\tan(z) = i\gamma$ where $z = (\pi/2)(\lambda + 1/2)$ so that, using Euler's formulae, it becomes $\mathrm{e}^{2iz} - 1 = -\gamma(\mathrm{e}^{2iz} + 1)$ or $\mathrm{e}^{2iz} = (1-\gamma)/(1+\gamma)$. Hence, $z = (i/2)\log[(1+\gamma)/(1-\gamma)] + \pi j$ where j is an integer, and thus we finally get

$$\lambda = 2j - \frac{1}{2} + \frac{i}{\pi}\log\left(\frac{1+\gamma}{1-\gamma}\right), \quad j \in \mathbb{Z}, \quad \gamma \in [0, 1). \tag{5.4}$$

5.1.1 Liouville Normal Form

It will be convenient to write the radial Schrödinger equation (2.74) in Liouville normal form, where we think of $1/4 - \lambda^2$ as being the spectral parameter; this suggests that we work in the weighted space $\mathcal{L}^2(\mathbb{R}^+; r^{-2})$. The general classical Sturm-Liouville problem

$$-\frac{\mathrm{d}}{\mathrm{d}r}p(r)\frac{\mathrm{d}f}{\mathrm{d}r} + q(r)f = \mu w(r) f,$$

can be converted to Liouville normal form

$$-\frac{\mathrm{d}^2 g}{\mathrm{d}\rho^2} + Ig = \mu g$$

using Liouville's transformation. This transformation makes $f = mg$ and $\rho = \int (w/p)^{1/2}\mathrm{d}r$ where $m = (pw)^{-1/4}$, provided p, q, and w are sufficiently well-behaved so that I, which can be written as

$$I(\rho) = \frac{q}{w} + m\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}\left(\frac{1}{m}\right),$$

is well-defined [Pryce, 1993]. Consider the independent variable first:

$$\rho = \int (w/p)^{1/2}\mathrm{d}r = \int r^{-1}\mathrm{d}r = \log r + (\text{const.}),$$

i.e. $r = (\text{const.})\mathrm{e}^{\rho}$. Without loss of generality we can take this constant to be 1, and thus we have $r = \mathrm{e}^{\rho}$. The differential $\mathrm{d}r = \mathrm{e}^{\rho}\mathrm{d}\rho$, which means that

$$\frac{\mathrm{d}}{\mathrm{d}r} = \left(\frac{\mathrm{d}r}{\mathrm{d}\rho}\right)^{-1}\frac{\mathrm{d}}{\mathrm{d}\rho} = \mathrm{e}^{-\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}$$

and so (2.74) becomes

$$-\mathrm{e}^{-\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\mathrm{e}^{-\rho}\frac{\mathrm{d}u}{\mathrm{d}\rho}\right) + \left(U(\mathrm{e}^{\rho}) - k^2\right)u = -(\lambda^2 - 1/4)\mathrm{e}^{-2\rho}u. \tag{5.5}$$

Secondly, $u(r) = r^{1/2}\varphi(\rho) = \mathrm{e}^{\rho/2}\varphi(\rho)$. In order to apply this change of variable, it is useful to make some preliminary computations; we have

$$\frac{\mathrm{d}u}{\mathrm{d}\rho} = \frac{1}{2}\mathrm{e}^{\rho/2}\varphi + \mathrm{e}^{\rho/2}\frac{\mathrm{d}\varphi}{\mathrm{d}\rho}, \quad \frac{\mathrm{d}}{\mathrm{d}\rho}\left(\mathrm{e}^{-\rho}\frac{\mathrm{d}u}{\mathrm{d}\rho}\right) = -\frac{1}{4}\mathrm{e}^{-\rho/2}\varphi + \mathrm{e}^{-\rho/2}\frac{\mathrm{d}^2\varphi}{\mathrm{d}\rho^2},$$

which means that (5.5) is now of the form

$$\mathrm{e}^{-3\rho/2}\frac{\mathrm{d}^2\varphi}{\mathrm{d}\rho^2} + \frac{1}{4}\mathrm{e}^{-3\rho/2}\varphi + \left(U(\mathrm{e}^{\rho}) - k^2\right)\mathrm{e}^{\rho/2}\varphi = -(\lambda^2 - 1/4)\mathrm{e}^{-3\rho/2}\varphi. \tag{5.6}$$

Multiplying equation (5.6) by $\mathrm{e}^{3\rho/2}$ yields

$$-\varphi''(\rho) + \left(U(\mathrm{e}^{\rho}) - k^2\right)\mathrm{e}^{2\rho}\varphi(\rho) = \eta\varphi(\rho), \quad \rho \in \mathbb{R} \tag{5.7}$$

where $\eta \equiv -\lambda^2$. In light of Liouville's transformation, we also need to calculate the asymptotics (3.1) and (3.2) for the transformed solutions. These are given by the following few equations: the large negative ρ asymptotics for the regular left-hand solution is

$$\varphi_0(\rho) = \mathrm{e}^{-\rho/2}u_0(\mathrm{e}^{\rho}) \sim \mathrm{e}^{\lambda\rho}, \quad \rho \to -\infty.$$

For the right-hand solution (the 'Hankel-like' solution defined by its behaviour at infinity) we must have

$$\varphi_\infty(\rho) \sim \mathrm{e}^{-\lambda\rho}, \quad \rho \to -\infty.$$

Moreover, the boundary condition at infinity becomes

$$\varphi_\infty(\rho) \sim \mathrm{e}^{-\rho/2}[\cos(k\mathrm{e}^{\rho}) + i\sin(k\mathrm{e}^{\rho})], \quad \rho \to \infty.$$

Consider again the free case. Let $C_\gamma \equiv (1/\pi)\log[(1+\gamma)/(1-\gamma)]$ with $\gamma \in [0,1)$, and note that $C_\gamma > 0$ which is large for γ close to 1. In the η-plane we have from (5.4) that

$$\begin{aligned}\eta &= -[(2j-1/2)^2 - C_\gamma^2 + 2i(2j-1/2)C_\gamma] \\ &= -4j^2 + (2-4iC_\gamma)j + C_\gamma(C_\gamma+i) - 1/4. \end{aligned} \tag{5.8}$$

We note that since $\lambda_R = \mathrm{Re}(\lambda) > 0$ then by equation (5.4) we must have $j \geq 1$. This places the right-most eigenvalue to be at the point $\eta_R \equiv \mathrm{Re}(\eta) = C_\gamma^2 - 9/4$, $\eta_I \equiv \mathrm{Im}(\eta) = -3C_\gamma$. Hence, in terms of η we have the following picture of the spectrum: since we are in the limit circle[2] oscillatory case at infinity there are infintely many eigenvalues (η) tending to negative infinity along some parabola descibed by (5.8) [Pryce, 1993, p. 153]. Moreover, in (5.7) where $U = 0$, all the hypotheses of Proposition B.2 in Appendix B.5 are satisfied. Therefore, the essential spectrum is given by $[0,\infty)$ in the η-plane.

5.1.2 Boundedness of the Resolvent

We wish to show that in the limit as $\gamma \to 1$, infinitely many eigenvalues go to infinity. However, to achieve this we must rule out the possibility of eigenvalues plunging into the essential spectrum. Let us introduce the formal differential operator

$$L = -\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - k^2 \mathrm{e}^{2\rho}, \quad \rho \in \mathbb{R}.$$

Define an operator A_γ by $A_\gamma \varphi = L\varphi$, $\varphi \in \mathscr{D}(A_\gamma)$ where

$$\mathscr{D}(A_\gamma) = \{f \in \mathcal{L}^2(\mathbb{R}) : A_\gamma f \in \mathcal{L}^2(\mathbb{R}) \text{ and } f \sim \mathrm{e}^{-\rho/2}[\cos(k\mathrm{e}^\rho) + i\gamma\sin(k\mathrm{e}^\rho)], \rho \to \infty\}$$

and $\gamma \in [0,1]$. In light of what we want to accomplish, we need to show that the norm of the resolvent $\|(A_\gamma - \eta)^{-1}\|$ is bounded with respect to η in some region which separates the eigenvalues from the essential spectrum. Firstly, in order to acquire an explicit expression for this resolvent, we must apply Liouville's transformation to the inhomogeneous free problem associated with equation (2.74), i.e.

$$-u'' + \left(\frac{\lambda^2 - 1/4}{r^2} - k^2\right)u = \frac{1}{r^2}g, \quad g \in \mathcal{L}^2(\mathbb{R}^+; r^{-2}). \tag{5.9}$$

Recalling the transformation calculations in §5.1.1, we need only consider the final step of multiplication by $\mathrm{e}^{3\rho/2}$ to get

$$-\varphi''(\rho) - \left(k^2\mathrm{e}^{2\rho} + \eta\right)\varphi(\rho) = \tilde{g}(\rho) \tag{5.10}$$

where $\tilde{g}$ is defined by $\tilde{g}(\rho) \equiv \mathrm{e}^{-\rho/2}g(\mathrm{e}^\rho)$. Observe that $\tilde{g} \in \mathcal{L}^2(\mathbb{R})$ since we clearly have $\int_\mathbb{R} |\tilde{g}|^2 \mathrm{d}\rho = \int_0^\infty |g|^2/r^2 \mathrm{d}r < \infty$. Hence, $\tilde{g}$ is an isometry and we may continue to work with

[2] This is given by Weyl's alternative—Theorem A.10—which is described briefly in Appendix A.3.

the new differential equation for ρ, namely, (5.10).

We use the method of variation of parameters on the inhomogeneous equation (5.10); this is the standard method for acquiring an explicit expression for the resolvent. Suppose that φ_0 and φ_∞ constitute a fundamental system for the associated homogeneous $U = 0$ equation (5.7), or equivalently for the following first order system:

$$\begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -(k^2 e^{2\rho} + \eta) & 0 \end{pmatrix} \begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}.$$

To solve the inhomogeneous first order system

$$\begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -(k^2 e^{2\rho} + \eta) & 0 \end{pmatrix} \begin{pmatrix} \varphi \\ \varphi' \end{pmatrix} + \begin{pmatrix} 0 \\ -\tilde{g} \end{pmatrix}$$

we write

$$\begin{pmatrix} \varphi \\ \varphi' \end{pmatrix} = \Phi F, \quad \Phi = \begin{pmatrix} \varphi_0 & \varphi_\infty \\ \varphi_0' & \varphi_\infty' \end{pmatrix}$$

where F is as yet undetermined. Then

$$\begin{aligned} \begin{pmatrix} 0 & 1 \\ -(k^2 e^{2\rho} + \eta) & 0 \end{pmatrix} \Phi F + \begin{pmatrix} 0 \\ -\tilde{g} \end{pmatrix} = \begin{pmatrix} \varphi \\ \varphi' \end{pmatrix}' &= \Phi' F + \Phi F' \\ &= \begin{pmatrix} 0 & 1 \\ -(k^2 e^{2\rho} + \eta) & 0 \end{pmatrix} \Phi F + \Phi F', \end{aligned}$$

which implies that $F' = \Phi^{-1} \left(\begin{smallmatrix} 0 \\ -\tilde{g} \end{smallmatrix} \right)$. Now,

$$\Phi^{-1} = \mathscr{W}^{-1} \begin{pmatrix} \varphi_\infty' & -\varphi_\infty \\ -\varphi_0' & \varphi_0 \end{pmatrix}$$

where $\mathscr{W} \equiv \mathscr{W}(\varphi_0, \varphi_\infty)$ is the Wronskian of φ_0 and φ_∞. Hence

$$F' = \frac{1}{\mathscr{W}} \begin{pmatrix} \varphi_\infty \tilde{g} \\ -\varphi_0 \tilde{g} \end{pmatrix},$$

which gives

$$F = \begin{pmatrix} \int_\rho^\infty \frac{\varphi_\infty \tilde{g}}{\mathscr{W}} + c_1 \\ -\int_0^\rho \frac{\varphi_0 \tilde{g}}{\mathscr{W}} + c_2 \end{pmatrix}.$$

Since $\left(\begin{smallmatrix} \varphi \\ \varphi' \end{smallmatrix} \right) = \Phi F$, it follows that

$$\varphi(\rho) = c_1 \varphi_0(\rho) + c_2 \varphi_\infty(\rho) - \varphi_\infty(\rho) \int_0^\rho \frac{\varphi_0(s) \tilde{g}(s)}{\mathscr{W}} ds + \varphi_0(\rho) \int_\rho^\infty \frac{\varphi_\infty(s) \tilde{g}(s)}{\mathscr{W}} ds. \quad (5.11)$$

Using the fact that $c_1 \varphi_0(\rho) + c_2 \varphi_\infty(\rho)$ is the general solution to equation (5.7) with zero potential, we are free to choose $c_1 = c_2 = 0$. Let $\varphi_{\infty,\gamma} \in \mathscr{D}(A_\gamma)$, then on absorbing the non-zero constant $\mathscr{W}$ into $\varphi_{\infty,\gamma}$ we have

$$((A_\gamma - \eta)^{-1}\tilde{g})(\rho) = -\varphi_{\infty,\gamma}(\rho)\int_{-\infty}^{\rho}\varphi_0(s)\tilde{g}(s)\mathrm{d}s + \varphi_0(\rho)\int_{\rho}^{\infty}\varphi_{\infty,\gamma}(s)\tilde{g}(s)\mathrm{d}s. \tag{5.12}$$

By the same reasoning that led to the utilization of the norm (3.36) in Chapter 3, we may use the norm given by

$$\|\cdot\|_{\mathcal{L}^2(\mathbb{R})} = \sup_{h\in\mathcal{L}^2(\mathbb{R})}\frac{|\langle h|\cdot\rangle|}{\|h\|_{\mathcal{L}^2(\mathbb{R})}} \tag{5.13}$$

in order to estimate $\|(A_\gamma - \eta)^{-1}\tilde{g}\|$. Suppose $h \in \mathcal{L}^2(\mathbb{R})$. Therefore, for the first term in equation (5.12) we consider the quantity

$$\begin{aligned}\left|\int_{\mathbb{R}} h(\rho)\varphi_{\infty,\gamma}(\rho)\int_{-\infty}^{\rho}\varphi_0(s)\tilde{g}(s)\mathrm{d}s\mathrm{d}\rho\right| &\leq \int_{\mathbb{R}}|h(\rho)||\varphi_{\infty,\gamma}(\rho)|\int_{-\infty}^{\rho}|\varphi_0(s)||\tilde{g}(s)|\mathrm{d}s\mathrm{d}\rho\\ &= \int_{\mathbb{R}}|h(\rho)||\varphi_{\infty,\gamma}(\rho)|\int_{-\infty}^{0}|\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}t\mathrm{d}\rho\\ &= \int_{-\infty}^{0}\mathrm{d}t\int_{\mathbb{R}}|h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho,\end{aligned} \tag{5.14}$$

where on the second line of equation (5.14) we have made the substituation $s = \rho + t$. To bound $|\varphi_0(\rho)|$, the solution defined by its good behaviour at negative infinity, for $\rho \in (0,\infty)$, we need a second solution. Let $\tilde{\varphi}_\infty(\rho) \sim \mathrm{e}^{-\rho/2}\cos(k\mathrm{e}^{\rho})$ as $\rho \to \infty$ be this second solution. Since $\tilde{\varphi}_\infty$ and φ_∞ are linearly independent[3], we must have a relation of the kind $\varphi_0(\rho) = c_1\tilde{\varphi}_\infty(\rho) + c_2\varphi_\infty(\rho)$ where φ_∞ is the solution that blows up at negative infinity. Moreover, it follows from the behaviour of φ_0 that c_2 must be zero and so $\varphi_0(\rho) \sim \mathrm{e}^{-\rho/2}\cos(k\mathrm{e}^{\rho})$ as $\rho \to \infty$. From the asymptotic behaviour of the solutions we may summarize their bounds as follows:

$$|\varphi_0(x)| \leq (\text{const.})\begin{cases}\mathrm{e}^{-x/2} & \text{if } x > 0,\\ \mathrm{e}^{\lambda_R x} & \text{if } x < 0,\end{cases} \tag{5.15}$$

and

$$|\varphi_{\infty,\gamma}(x)| \leq (\text{const.})\begin{cases}(1+\gamma)\mathrm{e}^{-x/2} & \text{if } x > 0,\\ \mathrm{e}^{-\lambda_R x} & \text{if } x < 0.\end{cases} \tag{5.16}$$

On splitting up the integral over the whole real line in equation (5.14), we must concentrate on bounding the first integral for which $\rho \in (-\infty, 0)$. If $\rho \in (-\infty, 0)$ then necessarily $\rho + t < 0$, and so by (5.15) and (5.16) we have

$$|\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)| \leq (\text{const.})\mathrm{e}^{\lambda_R t}.$$

[3]To see this, suppose they are linearly dependent. In this case they must have the same asymptotic behaviour, and so we have an eigenfunction. Thus, η is an eigenvalue, which cannot be.

Thus, for $\rho \in (-\infty, 0)$ we have

$$\int_{-\infty}^{0} \mathrm{d}t \int_{-\infty}^{0} |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho \le \int_{-\infty}^{0} \mathrm{e}^{\lambda_R t}\mathrm{d}t \int_{-\infty}^{0} |h(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho$$
$$\le (\text{const.}) \frac{\|h\|\|\tilde{g}\|}{\lambda_R}. \tag{5.17}$$

For $\rho \in (0, \infty)$ there is an ambiguity in the sign of $\rho + t$ and thus we need to split up the second integral in (5.14) once more, i.e.

$$\int_{-\infty}^{0} \mathrm{d}t \int_{0}^{\infty} |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho$$
$$= \int_{-\infty}^{0} \mathrm{d}t \left[\int_{0}^{-t} |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho \right.$$
$$\left. + \int_{-t}^{\infty} |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho \right].$$

Now, from equations (5.15) and (5.16) we have the bounds

$$|\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)| \le (\text{const.}) \begin{cases} (1+\gamma)\mathrm{e}^{-\rho/2}\mathrm{e}^{-(\rho+t)/2} & \text{if} \quad \rho+t>0, \\ (1+\gamma)\mathrm{e}^{-\rho/2}\mathrm{e}^{\lambda_R(\rho+t)} & \text{if} \quad \rho+t<0. \end{cases} \tag{5.18}$$

Thus, from (5.18) we have

$$\int_{-\infty}^{0} \mathrm{d}t \int_{0}^{-t} |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho$$
$$\le (\text{const.})(1+\gamma) \int_{-\infty}^{0} \mathrm{d}t \int_{0}^{-t} |h(\rho)||\tilde{g}(\rho+t)|\mathrm{e}^{-\rho/2}\mathrm{e}^{\lambda_R(\rho+t)}\mathrm{d}\rho$$
$$= (\text{const.})(1+\gamma) \int_{0}^{\infty} \mathrm{d}\rho \int_{-\infty}^{-\rho} |h(\rho)||\tilde{g}(\rho+t)|\mathrm{e}^{-\rho/2}\mathrm{e}^{\lambda_R(\rho+t)}\mathrm{d}t$$
$$\le (\text{const.})(1+\gamma) \int_{0}^{\infty} \mathrm{e}^{-\rho/2}|h(\rho)|\mathrm{d}\rho \left[\int_{-\infty}^{-\rho} |\tilde{g}(\rho+t)|^2\mathrm{d}t \right]^{1/2} \left[\int_{-\infty}^{-\rho} \mathrm{e}^{2\lambda_R(\rho+t)}\mathrm{d}t \right]^{1/2}$$
$$\le (\text{const.})(1+\gamma)(2\lambda_R)^{-1/2}\|\tilde{g}\| \left[\int_{0}^{\infty} \mathrm{e}^{-\rho}\mathrm{d}\rho \right]^{1/2} \left[\int_{0}^{\infty} |h(\rho)|^2\mathrm{d}\rho \right]^{1/2}$$
$$\le (\text{const.})(1+\gamma)(2\lambda_R)^{-1/2}\|h\|\|\tilde{g}\|. \tag{5.19}$$

Again from equation (5.18) we have

$$\int_{-\infty}^{0} \mathrm{d}t \int_{-t}^{\infty} |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho$$
$$\le (\text{const.})(1+\gamma) \int_{-\infty}^{0} \mathrm{d}t \int_{-t}^{\infty} |h(\rho)||\tilde{g}(\rho+t)|\mathrm{e}^{-\rho/2}\mathrm{e}^{-(\rho+t)/2}\mathrm{d}\rho$$
$$= (\text{const.})(1+\gamma) \int_{0}^{\infty} \mathrm{e}^{-\rho}|h(\rho)|\mathrm{d}\rho \int_{-\rho}^{0} |\tilde{g}(\rho+t)|\mathrm{e}^{-t/2}\mathrm{d}t$$

$$
\begin{aligned}
&\leq (\text{const.})(1+\gamma)\|\tilde{g}\| \int_0^\infty \mathrm{e}^{-\rho}|h(\rho)|\mathrm{d}\rho \left[\int_{-\rho}^0 \mathrm{e}^{-t}\mathrm{d}t\right]^{1/2} \\
&= (\text{const.})(1+\gamma)\|\tilde{g}\| \int_0^\infty \mathrm{e}^{-\rho}\sqrt{\mathrm{e}^{\rho}-1}|h(\rho)|\mathrm{d}\rho \\
&\leq (\text{const.})(1+\gamma)\|h\|\|\tilde{g}\| \left[\int_0^\infty \left(\mathrm{e}^{-\rho}-\mathrm{e}^{-2\rho}\right)\mathrm{d}\rho\right]^{1/2} \\
&= 2^{-1/2}(\text{const.})(1+\gamma)\|h\|\|\tilde{g}\|. \qquad (5.20)
\end{aligned}
$$

Combining equations (5.19) and (5.20) yields

$$
\begin{aligned}
&\int_{-\infty}^0 \mathrm{d}t \int_0^\infty |h(\rho)||\varphi_{\infty,\gamma}(\rho)||\varphi_0(\rho+t)||\tilde{g}(\rho+t)|\mathrm{d}\rho \\
&\qquad\qquad \leq (\text{const.})(1+\gamma)\|h\|\|\tilde{g}\|\left[(2\lambda_R)^{-1/2}+2^{-1/2}\right], \qquad (5.21)
\end{aligned}
$$

whence from (5.17), (5.21), and (5.14)

$$
\left|\int_{\mathbb{R}} h(\rho)\varphi_{\infty,\gamma}(\rho)\int_{-\infty}^{\rho}\varphi_0(s)\tilde{g}(s)\mathrm{d}s\mathrm{d}\rho\right| \leq (\text{const.})\|h\|\|\tilde{g}\|\left[\frac{1}{\lambda_R}+\frac{1+\gamma}{\sqrt{2}}\left(1+\frac{1}{\sqrt{\lambda_R}}\right)\right]. \qquad (5.22)
$$

Finding a bound for the second term in equation (5.12) is very similar, but we shall derive the result anyway. Suppose $h \in \mathcal{L}^2(\mathbb{R})$. For the second term consider

$$
\left|\int_{\mathbb{R}} h(\rho)\varphi_0(\rho)\int_{\rho}^{\infty}\varphi_{\infty,\gamma}(s)\tilde{g}(s)\mathrm{d}s\mathrm{d}\rho\right| \leq \int_0^\infty \mathrm{d}t\int_{\mathbb{R}}|h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho. \qquad (5.23)
$$

Writing the integral over the whole real line in equation (5.23) as two integrals, we need to consider bounding the second integral for which $\rho \in (0,\infty)$. If $\rho \in (0,\infty)$ then $\rho+t>0$ always and so by (5.15) and (5.16)

$$
|\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)| \leq (\text{const.})(1+\gamma)\mathrm{e}^{-\rho}\mathrm{e}^{-t/2}.
$$

Thus, for $\rho \in (0,\infty)$ we have

$$
\begin{aligned}
&\int_0^\infty \mathrm{d}t\int_0^\infty |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho \\
&\quad \leq (\text{const.})(1+\gamma)\int_0^\infty \mathrm{d}t\int_0^\infty |h(\rho)||\tilde{g}(\rho+t)|\mathrm{e}^{-\rho}\mathrm{e}^{-t/2}\mathrm{d}\rho \\
&\quad \leq (\text{const.})(1+\gamma)\int_0^\infty |h(\rho)|\mathrm{e}^{-\rho}\mathrm{d}\rho\int_0^\infty |\tilde{g}(\rho+t)|\mathrm{e}^{-t/2}\mathrm{d}t \\
&\quad \leq (\text{const.})(1+\gamma)\|h\|\|\tilde{g}\|\left[\int_0^\infty \mathrm{e}^{-2\rho}\mathrm{d}\rho\right]^{1/2} \\
&\quad = 2^{-1/2}(\text{const.})(1+\gamma)\|h\|\|\tilde{g}\|. \qquad (5.24)
\end{aligned}
$$

For $\rho \in (-\infty, 0)$ we must split up the first integral in (5.23) as follows

$$\int_0^\infty \mathrm{d}t \int_{-\infty}^0 |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho$$
$$= \int_0^\infty \mathrm{d}t \left[\int_{-\infty}^{-t} |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho + \int_{-t}^0 |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho \right]$$

and consider the sign of $\rho + t$. We observe from equations (5.15) and (5.16) that we have the following bounds:

$$|\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)| \le (\text{const.}) \begin{cases} (1+\gamma)\mathrm{e}^{-(\rho+t)/2}\mathrm{e}^{\lambda_R \rho} & \text{if} \quad \rho+t>0, \\ \mathrm{e}^{-\lambda_R t} & \text{if} \quad \rho+t<0. \end{cases} \tag{5.25}$$

Hence, from (5.25) we have

$$\begin{aligned} &\int_0^\infty \mathrm{d}t \int_{-\infty}^{-t} |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho \\ &\le (\text{const.}) \int_0^\infty \mathrm{d}t \int_{-\infty}^{-t} |h(\rho)||\tilde{g}(\rho+t)|\mathrm{e}^{-\lambda_R t}\mathrm{d}\rho \\ &\le (\text{const.})\|h\|\|\tilde{g}\| \int_0^\infty \mathrm{e}^{-\lambda_R t}\mathrm{d}t \\ &= (\text{const.})\frac{\|h\|\|\tilde{g}\|}{\lambda_R} \end{aligned} \tag{5.26}$$

and

$$\begin{aligned} &\int_0^\infty \mathrm{d}t \int_{-t}^0 |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho \\ &\le (\text{const.})(1+\gamma) \int_0^\infty \mathrm{d}t \int_{-t}^0 |h(\rho)||\tilde{g}(\rho+t)|\mathrm{e}^{-(\rho+t)/2}\mathrm{e}^{\lambda_R\rho}\mathrm{d}\rho \\ &= (\text{const.})(1+\gamma) \int_{-\infty}^0 |h(\rho)|\mathrm{e}^{\lambda_R\rho}\mathrm{d}\rho \int_{-\rho}^\infty |\tilde{g}(\rho+t)|\mathrm{e}^{-(\rho+t)/2}\mathrm{d}t \\ &\le (\text{const.})(1+\gamma)\|g\| \int_{-\infty}^0 |h(\rho)|\mathrm{e}^{\lambda_R\rho}\mathrm{d}\rho \left[\mathrm{e}^{-\rho}\int_{-\rho}^\infty \mathrm{e}^{-t}\mathrm{d}t\right]^{1/2} \\ &\le (\text{const.})(1+\gamma)\|h\|\|\tilde{g}\| \left[\int_{-\infty}^0 \mathrm{e}^{2\lambda_R\rho}\mathrm{d}\rho\right]^{1/2} \\ &= (\text{const.})(1+\gamma)(2\lambda_R)^{-1/2}\|h\|\|\tilde{g}\|. \end{aligned} \tag{5.27}$$

Combining equations (5.26) and (5.27) gives

$$\int_0^\infty \mathrm{d}t \int_{-\infty}^0 |h(\rho)||\varphi_{\infty,\gamma}(\rho+t)||\varphi_0(\rho)||\tilde{g}(\rho+t)|\mathrm{d}\rho \le (\text{const.})\|h\|\|\tilde{g}\| \left[\frac{1}{\lambda_R} + \frac{1+\gamma}{\sqrt{2\lambda_R}}\right], \tag{5.28}$$

and so from (5.24), (5.28), and (5.23)

$$\left| \int_{\mathbb{R}} h(\rho)\varphi_0(\rho) \int_\rho^\infty \varphi_{\infty,\gamma}(s)\tilde{g}(s)\mathrm{d}s\mathrm{d}\rho \right| \leq (\text{const.})\|h\|\|\tilde{g}\| \left[\frac{1}{\lambda_R} + \frac{1+\gamma}{\sqrt{2}} \left(1 + \frac{1}{\sqrt{\lambda_R}} \right) \right]. \tag{5.29}$$

Therefore, we finally have from equations (5.12), (5.22), and (5.29) that

$$\|(A_\gamma - \eta)^{-1}\tilde{g}\| \leq (\text{const.})\|\tilde{g}\| \left[\frac{2}{\lambda_R} + \sqrt{2}(1+\gamma) \left(1 + \frac{1}{\sqrt{\lambda_R}} \right) \right]. \tag{5.30}$$

5.1.3 Finding an Eigenvalue Free Region

In terms of the generalized CAM we have $\lambda_R = \mathrm{Re}\sqrt{-\eta}$; we choose the branch of square root such that its real part is greater than zero, since $\lambda_R > 0$ is the regularity condition on the solutions at the origin—this is discussed on p. 20 in Chapter 2.

Recall that we need to find a region in the η-plane in which there are no eigenvalues, or better, a region for which the resolvent $(A_\gamma - \eta)^{-1}$ is bounded with respect to η. Let us first consider the right-half plane, this is where $-\eta = -\alpha^2 + i\beta$ with $\alpha, \beta > 0$. On choosing $+i$ for the square root in order to gain the correct sign for the real part of λ, we have

$$\begin{aligned} \sqrt{-\eta} &= i\alpha\sqrt{1 - i\beta/\alpha^2} \\ &\approx i\alpha(1 - i\beta/2\alpha^2) \\ &= \beta/2\alpha + i\alpha. \end{aligned}$$

For $1/\lambda_R$ to be bounded we must have $\alpha = \mathcal{O}(\beta)$ or $\sqrt{\eta_R} = \mathcal{O}(\eta_I)$. Therefore, we require $\eta_R \leq \eta_I^2$. A parabola could give the desired region in the right-half plane. To check this, consider the problem of never allowing the point (g_a, h_a) inside some parabola $y = f_a(x-b)^2$ where $x > b$: to solve this we require $x - b < g_a$ where $y > h_a$. As a consequence, $f_a(x-b)^2 > h_a$ or $f_a > h_a/(x-b)^2$. However, $x - b < g_a$ and so we need

$$f_a > \frac{h_a}{g_a^2}. \tag{5.31}$$

In our case we require the right-most eigenvalue $(\eta_I, \eta_R) = (-3C_\gamma, C_\gamma^2 - 9/4)$ to always lie outside the parabola $\eta_R = f_\gamma(\eta_I - \beta)^2$, $\eta_I > \beta$ (see p. 78 for the definitions of η and C_γ). The solution is provided by (5.31), i.e.

$$f_\gamma > 1/9 - 1/4C_\gamma^2.$$

Thus, the region enclosed by the two parabolas $\eta_R = f_\gamma(\eta_I - \beta/2)^2$ and $\eta_R = f_\gamma(\eta_I - \beta)^2$ deals with the case $C_\gamma > 3/2$. On the other hand, for C_γ such that $0 < C_\gamma \leq 3/2$ we are to consider computing the desired 'eigenvalue-less' region in the left-half plane. For this purpose, let us now write $-\eta = \alpha^2 + i\beta$ with $\alpha, \beta > 0$, and in a similar fashion to above we can show that $\sqrt{-\eta} \approx \alpha + i\beta/2\alpha$. Since $\eta_R = -\alpha^2$ and $-\eta_I = \beta$, it follows that

$$\begin{aligned}\frac{1}{\lambda_R} &\approx \frac{\sqrt{-\eta_R}}{-\eta_R - \eta_I^2/4\eta_R} \\ &= \frac{1}{\sqrt{-\eta_R} - \eta_I^2/4\eta_R\sqrt{-\eta_R}}.\end{aligned} \tag{5.32}$$

For λ_R^{-1} in equation (5.32) to be bounded, we require $\eta_R \to -\infty$ and $\eta_I \neq 0$. An infinite strip in the fourth quadrant formed by the lines $\eta_I = -\beta/2$ and $\eta_I = -\beta$ with β satisfying $0 < \beta < 3C_\gamma$ would certainly suffice.

These calculations culminate in a region of boundedness for the resolvent $(A_\gamma - \eta)^{-1}$; this region is depicted in Figure 5.1, and it separates the eigenvalues from the essential spectrum as desired. Note that the boundedness of $1/\sqrt{\lambda_R}$ in this region is a direct consequence of the boundedness of $1/\lambda_R$.

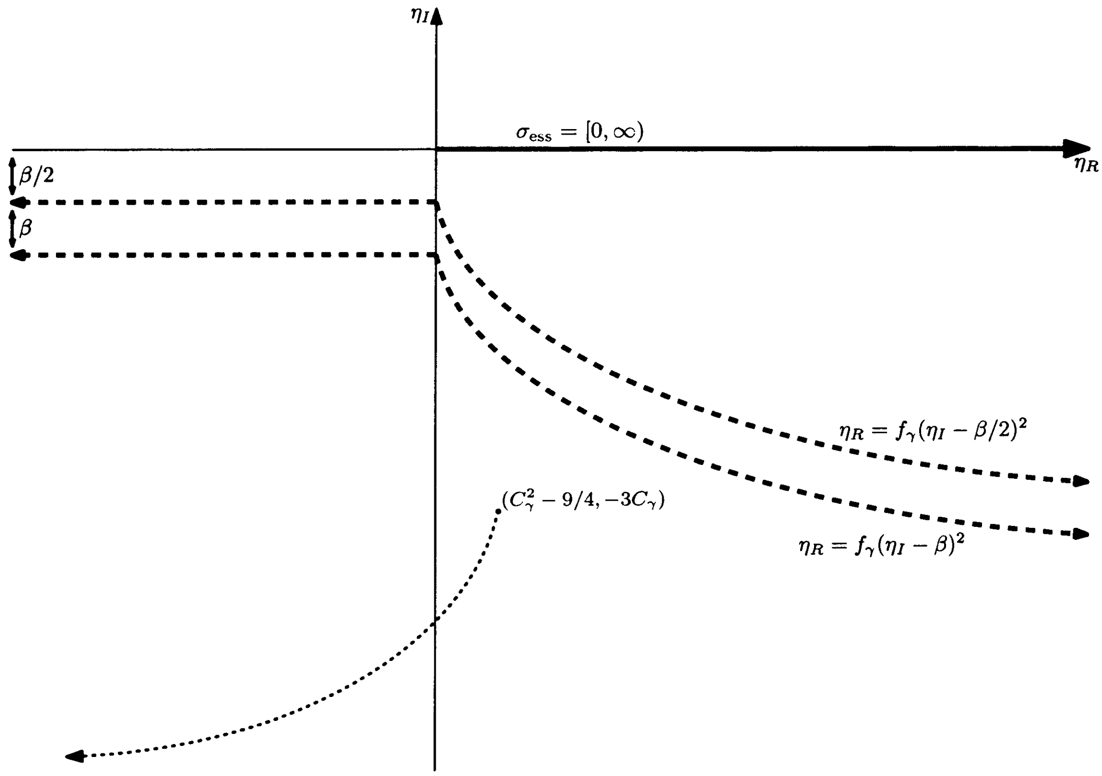

Figure 5.1: The eigenvalues lie on the dotted parabola, whilst the region bounded between the thick dashed lines forms the eigenvalue-free region.

By construction, the Regge pole problem (2.74) corresponds to setting the coupling constant γ to unity. However, if the potential is identically zero then as we know there are no associated Regge poles; this observation, together with Figure 5.1, yields the result

Theorem 5. *For the free particle Regge pole problem, every generalized Regge pole $\eta_j(\gamma)$ is such that* $\lim_{\gamma\to 1} |\eta_j(\gamma)| = +\infty$.

CHAPTER 6

Conclusion and Future Work

For many decades it has been believed on physical grounds that the Regge trajectory describing resonances (positive energy) should connect continuously at threshold to the Regge trajectory describing bound states (negative energy). We have seen in §2.5.1 that for the Coulomb attraction, this is certainly not the case; however, it is expected to be true for shorter range potentials—such as the screened Coulomb potentials. In Chapter 3 we were able to resolve this long-standing conjecture: for potentials with $r|V(r)|$ bounded at the origin, which satisfy the moment-type condition

$$\int_0^{\infty} |(1+r)V(r)| \mathrm{d}r < +\infty, \tag{6.1}$$

each Regge trajectory is either continuous at $E = 0$ or else goes to infinity as E approaches zero from above; moreover, every bound state trajectory ($E < 0$) has a corresponding Regge trajectory ($E > 0$) to which it connects continuously at zero energy. Apart from the Coulomb interaction, are Regge trajectories which go to infinity really possible? This remains an open question. There are some (unreliable) numerical experiments to indicate that singular behaviour of the trajectories may be possible for rational approximations to Thomas-Fermi potentials; as yet, however, there are no proofs or counter-examples. On the other hand, it has been known for half a century that Regge trajectories extend to infinity in the CAM plane as the energy $k \to \infty$ [Barut and Calogero, 1962].

In the sequel chapter we proved that for a compactly supported integrable potential, the associated scattering problem has only finitely many Regge poles in the right-half generalized CAM plane. In terms of analyticity, this significantly weakens the assumptions made in Barut and Dilley [1963]; for example, the result (Theorem 4) of Chapter 4 enables us to deal with the finite spherical well. However, it is desirable to extend these results to non-analytic potentials without compact support. We have made several unsuccessful attempts to achieve this generalization, their failure was essentially due to the lack of suitable normalization of the integral equation definining the right-hand solution when λ is not fixed—a consequence of the Hankel function of the first kind possessing infintely many λ-zeros in the first quadrant. The next best candidate for a normalizer would be the Hankel function of the second kind. This was a promising idea, largely because it has its infinitely many λ-zeros in the second quadrant [Cochran, 1965]; but, the large CAM asymptotics could not be handled. There were similar issues with using any normalizer concocted from Hankel functions. However, there was encouraging numerical evidence that using $\mathrm{e}^{-i\pi\lambda}H_{\lambda}^{(2)}(r)$ as a normalizer could work, the problem was in seeing this from an analytic perspective; there seemed to be some conflict between the numerical outputs and what could be calculated explicitly.

We conjecture that there are finitely many Regge poles associated with a potential satisfying the moment-type condition (6.1). This result would allow treatment of a much larger class of potential functions; for example, potentials such as

$$V(r) = \frac{c}{(1+ar)^2(1+b(r-1)^2)},$$

which is rather similar to a rational Thomas-Fermi potential (see (1.1)) but has singularities at $r = 1 \pm i/\sqrt{b}$. Furthermore, what we believe would be of considerable interest, is an estimate of the number of Regge poles in terms of the potential, in the spirit of the Cwikel-Lieb-Rosenblum estimates for the number of bound states. This would be the focal point for future work, the reason being the following. Knowledge that there are only finitely many pole contributions to the sum in the Regge representation of the scattering amplitude (2.73) is not terribly helpful, since in principle there could still be 'too many'; i.e. the number of Regge poles could still be very large and so for practical purposes, infinite. We therefore justify the need for knowledge of the explicit numbers of Regge poles. However, compared with counting bound states, the counting of Regge poles is an order of magnitude more difficult. Moreover, it is at least as difficult as counting resonances. The attempt made in this thesis to achieve Regge pole estimates was unsuccessful; but, it did reveal an almost pathological sensitivity of Regge poles toward boundary conditions, and this illustrates well the richness of the theory.

APPENDIX A

Self-Adjointness

A.1 Closed Operators

Definition A.1. *If X is a subset of a metric space $\mathscr{X}$, then the closure of X in $\mathscr{X}$ is the set of all $x \in \mathscr{X}$ such that x is adherent to X; it is denoted by $\overline{X}$. In other words, $x \in \overline{X}$ if and only if there is a sequence (x_n) in X such that $x_n \to x$.*

We make the following remarks: if $\overline{X} = \mathscr{X}$ then X is called dense in $\mathscr{X}$. X is a closed if and only if $X = \overline{X}$. If $X \subset Y$ then $\overline{X} \subset \overline{Y}$ for suppose $x \in \overline{X}$ and $x_n \to x$ where $x_n \in X$, then since $x_n \in Y$, x is adherent to Y. $\overline{X}$ is the smallest closed subset of $\mathscr{X}$ which contains X for if $X \subset Y$ and Y is closed, then $\overline{X} \subset \overline{Y} = Y$.

Definition A.2 (Kato [1966] p. 164)**.** *Let $T : \mathscr{X}_1 \to \mathscr{X}_2$ be an operator. A sequence (x_n) in the domain $\mathscr{D}(T)$ is called T-convergent to $x \in \mathscr{X}_1$ if both (x_n) and (Tx_n) are Cauchy sequences and $x_n \to x$. In this case, we write $x_n \xrightarrow{T} u$. Moreover, T is called closed if $x_n \xrightarrow{T} x$ implies $x \in \mathscr{D}(T)$ and $Tx = \lim Tx_n$.*

It is useful in the study of closed operators to introduce the notion of the graph of an operator [Kato, 1966, pp. 164-165]: the cartesian product space $\mathscr{X}_1 \times \mathscr{X}_2$ is a vector space with linear operation defined by $\alpha(x_1, x_2) + \beta(x_1', x_2') = (\alpha x_1 + \beta x_1', \alpha x_2 + \beta x_2')$ and becomes a normed space when equipped with the norm $\|(x_1, x_2)\| = (\|x_1\|^2 + \|x_2\|^2)^{1/2}$, which is complete making $\mathscr{X}_1 \times \mathscr{X}_2$ a Banach space. The graph $G(T)$ is the subset of $\mathscr{X}_1 \times \mathscr{X}_2$ consisting of all elements (x, Tx) with $x \in \mathscr{D}(T)$, and is a linear subspace of $\mathscr{X}_1 \times \mathscr{X}_2$. Moreover, $G'(\tilde{T})$ is a linear subspace of $\mathscr{X}_1 \times \mathscr{X}_2$ consisting of all pairs $(\tilde{T}x, x)$ with $x \in \mathscr{D}(\tilde{T})$, and is the inverse graph of the operator $\tilde{T} : \mathscr{X}_2 \to \mathscr{X}_1$.

A sequence (x_n) in $\mathscr{X}_1$ is T-convergent if and only if (x_n, Tx_n) is a Cauchy sequence in $\mathscr{X}_1 \times \mathscr{X}_2$. Therefore, T is closed if and only if $G(T)$ is a closed subspace of $\mathscr{X}_1 \times \mathscr{X}_2$.

Definition A.3 (Kato [1966] p. 165). *An operator* $T : \mathscr{X}_1 \to \mathscr{X}_2$ *is called closable if* T *has a closed extension. Equivalently,* T *is closable if and only if the closure* $\overline{G(T)}$ *of* $G(T)$ *is a graph. In this case, there is a closed operator* $\overline{T}$ *with graph* $G(\overline{T}) = \overline{G(T)}$ *and* $\overline{T}$ *is called the closure of* T. *Moreover,* $\overline{T}$ *is the smallest closed extension of* T.

In view of this, if T is closable then $\mathscr{D}(\overline{T})$ is the set of all $x \in \mathscr{X}_1$ such that there exists a sequence (x_n) in $\mathscr{D}(T)$ with $x_n \to x$, where (Tx_n) also converges. Furthermore, we also have $\overline{T}x = \lim Tx_n$ for $x \in \mathscr{D}(\overline{T})$. With this information, we have

Theorem A.1 (Weidmann [1980] p. 58). *Suppose we have a bounded linear operator* $T \in \mathscr{L}(\mathscr{E}, \mathscr{B})$ *where* $\mathscr{E}$ *is any normed space and* $\mathscr{B}$ *is a Banach space. Then there exists a unique bounded extension* $\tilde{T}$ *of* T *satisfying* $\mathscr{D}(\tilde{T}) = \overline{\mathscr{D}(T)}$.

Proof. Assume $\tilde{T}$ is a bounded extension of T such that $\mathscr{D}(\tilde{T}) = \overline{\mathscr{D}(T)}$. If $x \in \mathscr{D}(\tilde{T})$ then there is a sequence (x_n) from $\mathscr{D}(T)$ such that $x_n \to x$. Since $\tilde{T}$ is continuous, $\tilde{T}x = \lim \tilde{T}x_n = \lim Tx_n$ and so $\tilde{T}$ is determined uniquely by T, if it exists.

To show existence, let $x \in \overline{\mathscr{D}(T)}$ and (x_n) be a sequence in $\mathscr{D}(T)$ such that $x_n \to x$, which means (x_n) is a Cauchy sequence. Since T is bounded, (Tx_n) is also Cauchy as $\|Tx_n - Tx_m\| \leq \|T\|\|x_n - x_m\|$. Hence, there exists a $y \in \mathscr{B}$ such that $Tx_n \to y$ and y is independent of the choice of (x_n). So, we can define $\tilde{T}x = y$.

To demonstrate the linearity of $\tilde{T}$ suppose $x, x' \in \overline{\mathscr{D}(T)}$ and $(x_n), (x'_n)$ are sequences in $\mathscr{D}(T)$ with $x_n \to x$ and $x'_n \to x'$. Then for all $\alpha, \beta \in \mathbb{C}$, we have

$$\begin{aligned}\tilde{T}(\alpha x + \beta x') &= \lim T(\alpha x_n + \beta x'_n)\\ &= \lim(\alpha T x_n + \beta T x'_n)\\ &= \alpha\tilde{T}x + \beta\tilde{T}x'.\end{aligned}$$

In addition, if $x \in \overline{\mathscr{D}(T)}$ and (x_n) in $\mathscr{D}(T)$ such that $x_n \to x$, then their norms also converge, i.e. $\|x_n\| \to \|x\|$.[1] Hence, we have

$$\|\tilde{T}x\| = \lim \|Tx_n\| \leq \lim \|T\|\|x_n\| = \|T\|\|x\|,$$

which shows that $\tilde{T}$ is bounded. □

A.2 The Adjoint Operator

Definition A.4. *An operator* $T : \mathscr{H} \to \mathscr{H}$ *on Hilbert space* $\mathscr{H}$ *is called Hermitian if it is a formal adjoint of itself, i.e.* $\langle Tf|g\rangle = \langle f|Tg\rangle$ *for all* $f, g \in \mathscr{D}(T)$. *Moreover, an operator* T *on* $\mathscr{H}$ *is called symmetric if it is Hermitian and densely defined, where by densely defined we mean* $\overline{\mathscr{D}(T)} = \mathscr{H}$.

[1] This is a consequence of the standard inequality $|\|x\| - \|y\|| \leq \|x - y\|$. To derive this inequality, we use $|d(x,z) - d(y,z)| \leq d(x,y)$, which in turn is the result of interchanging x and y in the triangle inequality $d(x,z) \leq d(x,y) + d(y,z)$.

We now discuss the notion of self-adjointness and to do so we cite the description given in Weidmann [1980] pp. 67–68. If S is a formal adjoint of an operator $T : \mathscr{H}_1 \to \mathscr{H}_2$, then for each $g \in \mathscr{D}(S)$ the linear functional L_g defined by $L_g f = \langle g|Tf\rangle$ with $\mathscr{D}(L_g) = \mathscr{D}(T)$ is continuous. This is because for all $f \in \mathscr{D}(L_g)$, we have $L_g f = \langle g|Tf\rangle = \langle Sg|f\rangle$, which means that L_g is the restriction to $\mathscr{D}(T)$ of the continuous linear functional T_{Sg}. If $\mathscr{D}(T)$ is dense, then by Theorem A.1, L_g can be uniquely extended to $\mathscr{H}_1 = \overline{\mathscr{D}(T)}$. Hence, there exists a $h_g \in \mathscr{H}_1$, uniquely determined by g and T via $\langle g|Tf\rangle = L_g f = \langle h_g|f\rangle$ for all $f \in \mathscr{D}(T)$. Moreover, if S is a formal adjoint of T and $g \in \mathscr{D}(S)$ then we have $h_g = Sg$. Therefore, every formally adjoint operator of T is a restriction of the adjoint operator $T^\dagger$, which we now describe: suppose $T : \mathscr{H}_1 \to \mathscr{H}_2$ is densely defined and

$$\mathscr{D}^\dagger \equiv \{g \in \mathscr{H}_2 : \text{there exists a } h_g \in \mathscr{H}_1 \text{ such that } \langle h_g|f\rangle = \langle g|Tf\rangle \text{ for all } f \in \mathscr{D}(T)\}.$$

The element h_g is unique for if $\langle h_1|f\rangle = \langle h_2|f\rangle = \langle g|Tf\rangle$ for all $f \in \mathscr{D}(T)$, then clearly $\langle h_1 - h_2|f\rangle = 0$ for all $f \in \mathscr{D}(T)$, which means that $h_1 - h_2 \in \mathscr{D}(T)^\perp$. Now, $\overline{\mathscr{D}(T)} = \mathscr{H}_1$ since $\mathscr{D}(T)$ is dense and $\mathscr{H}_1 = \overline{\mathscr{D}(T)} \oplus \overline{\mathscr{D}(T)}^\perp$ since $\overline{\mathscr{D}(T)}$ is closed. Hence, $\overline{\mathscr{D}(T)}^\perp = \{0\}$. Furthermore, $\overline{\mathscr{D}(T)}^\perp = (\mathscr{D}(T)^{\perp\perp})^\perp$ since both $\overline{\mathscr{D}(T)}$ and $\mathscr{D}(T)^{\perp\perp}$ are the smallest closed linear subspaces of $\mathscr{H}_1$ containing $\mathscr{D}(T)$. Finally, as $(\mathscr{D}(T)^{\perp\perp})^\perp = \mathscr{D}(T)^\perp$, we have that $\mathscr{D}(T)^\perp = \{0\}$ and thus $h_1 = h_2$. Also, $\mathscr{D}^\dagger$ is a subspace of $\mathscr{H}_2$ and $\mathscr{D}^\dagger \to \mathscr{H}_1$, $g \mapsto h_g$ is linear since for $g_1, g_2 \in \mathscr{D}^\dagger$ and $\alpha, \beta \in \mathbb{C}$, $h_{\alpha g_1 + \beta g_2} = \alpha h_{g_1} + \beta h_{g_2}$.

Hence, by $\mathscr{D}(T^\dagger) = \mathscr{D}^\dagger$, $T^\dagger g = h_g$ for $g \in \mathscr{D}(T^\dagger)$ a linear operator $T^\dagger : \mathscr{H}_2 \to \mathscr{H}_1$ is defined. $T^\dagger$ is a formal adjoint of T and is the extension of all formal adjoints of T. Since a densely defined operator T is Hermitian if and only if it is a restriction of $T^\dagger$, we have that an operator T is symmetric if and only if T is densely defined and $T \subset T^\dagger$. An operator T on $\mathscr{H}$ is self-adjoint if T is densely defined and $T = T^\dagger$.

Theorem A.2. *If $\mathscr{J}$ is any subspace of $\mathscr{H}$, then $\mathscr{J}^\perp$ is a closed linear subspace of $\mathscr{H}$.*

Proof. Firstly, we clearly have $0 \in \mathscr{J}^\perp$. If $f \perp g_j$ for all j and $g = \sum_{j=1}^n \lambda_j g_j$, then $\langle f|g\rangle = \sum_{j=1}^n \lambda_j \langle f|g_j\rangle = 0$ and so $\mathscr{J}^\perp$ is a linear subspace of $\mathscr{H}$. Suppose $(f_n) \in \mathscr{J}^\perp$ and $f_n \to f \in \mathscr{H}$, then for any $g \in \mathscr{J}$ we have $\langle f|g\rangle = \lim\langle f_n|g\rangle = 0$. Hence $f \in \mathscr{J}^\perp$. □

Theorem A.3 (Hutson and Pym [1980] pp. 171–172). *The adjoint operator is closed.*

Proof. We first demonstrate that $G'(-T^\dagger) = G(T)^\perp$. By definition of the inner product in $\mathscr{H} \times \mathscr{H}$, $\langle (f, Tf)|(-T^\dagger g, g)\rangle = \langle f| - T^\dagger g\rangle + \langle Tf|g\rangle = 0$, $f \in \mathscr{D}(T)$, $g \in \mathscr{D}(T^\dagger)$. Thus, $G'(-T^\dagger) \subset G(T)^\perp$. On the other hand, take an element $(h, g) \in G(T)^\perp$. Then we have the equation $\langle f|h\rangle + \langle Tf|g\rangle = \langle (f, Tf)|(h, g)\rangle = 0$, which means that $g \in \mathscr{D}(T^\dagger)$ and $h = -T^\dagger g$, i.e. $G(T)^\perp \subset G'(-T^\dagger)$.

Now, $G(T)^\perp$ is closed by Theorem A.2 and therefore $G'(-T^\dagger)$ is also closed, which means that $T^\dagger$ is a closed operator. □

Theorem A.4 (Weidmann [1980] p. 91). *Every symmetric operator T on $\mathscr{H}$ is closable and $\overline{T}$ is also symmetric.*

Proof. It follows immediately from Theorem A.3 that T is closable since we have $T \subset T^\dagger$ where $T^\dagger$ is closed.

Since T is closable we can take any $f, g \in \mathscr{D}(\overline{T})$ such that there are sequences (f_n), (g_n) in $\mathscr{D}(T)$ with $f_n \to f$, $g_n \to g$, $Tf_n \to \overline{T}f$, and $Tg_n \to \overline{T}g$. Therefore, since we assume that T is symmetric, $\langle \overline{T}f|g\rangle = \lim\langle Tf_n|g_n\rangle = \lim\langle f_n|Tg_n\rangle = \langle f|\overline{T}g\rangle$. It only remains to demonstrate the density of $\mathscr{D}(\overline{T})$. We note that if $\mathscr{J}_1 \subset \mathscr{J}_2$, then $\overline{\mathscr{J}_1} \subset \overline{\mathscr{J}_2}$ for suppose $f \in \overline{\mathscr{J}_1}$ and $(f_n) \in \mathscr{J}_1$ with $f_n \to f$, then also $(f_n) \in \mathscr{J}_2$ and so f is adherent to $\mathscr{J}_2$. Now, the inclusion $T \subset \overline{T}$ means that $\mathscr{D}(T) \subset \mathscr{D}(\overline{T}) \subset \mathscr{H}$. Furthermore, $\overline{\mathscr{D}(T)} = \mathscr{H}$ by hypothesis and so $\overline{\mathscr{D}(\overline{T})} = \mathscr{H}$. □

Theorem A.5. *If T is a symmetric operator on $\mathscr{H}$, then $\overline{T} = T^{\dagger\dagger}$ and $\overline{T}^\dagger = T^\dagger$.*

Proof. It is clear that T is closable by Theorem A.4. Thus, from the proof of Theorem A.3 we have $G(\overline{T}) = \overline{G(T)} = G(T)^{\perp\perp} = G'(-T^\dagger)^\perp$. We also have that $G(T^{\dagger\dagger}) = G'(-T^\dagger)^\perp$ since $\langle (f, T^{\dagger\dagger}f)|(-T^\dagger g, g)\rangle = \langle f|-T^\dagger g\rangle + \langle T^{\dagger\dagger}f|g\rangle = 0$ for $f \in \mathscr{D}(T^{\dagger\dagger})$, $g \in \mathscr{D}(T^\dagger)$. Hence, $G(T^{\dagger\dagger}) \subset G'(-T^\dagger)^\perp$. Conversely, suppose we have an element $(h, g) \in G'(-T^\dagger)^\perp$. Then, $\langle -T^\dagger f|h\rangle + \langle f|g\rangle = \langle (-T^\dagger f, f)|(h, g)\rangle = 0$, which means that $h \in \mathscr{D}(T^{\dagger\dagger})$ and $g = T^{\dagger\dagger}h$, i.e. $G'(-T^\dagger)^\perp \subset G(T^{\dagger\dagger})$. This justifies the claim that $G(T^{\dagger\dagger}) = G'(-T^\dagger)^\perp$ and hence $T^{\dagger\dagger} = \overline{T}$. Moreover, $T^\dagger = \overline{T^\dagger} = (T^\dagger)^{\dagger\dagger} = (T^{\dagger\dagger})^\dagger = \overline{T}^\dagger$. □

Definition A.5. *A symmetric operator T on $\mathscr{H}$ is called essentially self-adjoint if $\overline{T}$ is self-adjoint.*

Theorem A.6. *Let T be a symmetric operator on $\mathscr{H}$, then T is essentially self-adjoint if and only if $T^\dagger$ is symmetric. In this case, we have $\overline{T} = T^\dagger$.*

Proof. If T is essentially self-adjoint then $T^\dagger = \overline{T}^\dagger = \overline{T} = T^{\dagger\dagger}$ by Theorem A.5, the hypothesis and Theorem A.5 respectively. Thus, $T^\dagger$ is self-adjoint and so is also symmetric.

If, on the other hand, $T^\dagger$ is symmetric then as $\overline{T}$ is symmetric by Theorem A.4 and $\overline{T}^\dagger = T^\dagger$, we have $\overline{T} \subset \overline{T}^\dagger = T^\dagger$. Also, $T^\dagger \subset T^{\dagger\dagger} = \overline{T}$ by Theorem A.5 and so $\overline{T} = T^\dagger = \overline{T}^\dagger$, which means that T is essentially self-adjoint. □

A.3 The Sturm-Liouville Operator

Our task for this section is to study the self-adjointness of the Sturm-Liouville operator; we give the account due to Weidmann [1980] pp. 248–250. Before embarking on this, let us first present a result which will be of great use in the study of the Sturm-Liouville operator. This result concerning finite linear combinations of (complex) linear functionals can be found, for example, in the book of Weidmann [1980] p. 53; for our purpose we will only make the statement, but it may be proved by mathematical induction. Setting our notation for the null space, $\mathscr{N}(T) \equiv \{f \in \mathscr{D}(T) : Tf = 0\}$, we have

Theorem A.7. *Suppose $F_1, F_2, \ldots F_n$ are linear functionals on a complex Hilbert space $\mathscr{H}$ with $\mathscr{D}(F_j) = \mathscr{D}(F) = \mathscr{H}$ for $j \in \{1, 2, \ldots n\}$. If $\bigcap_{j=1}^n \mathscr{N}(F_j) \subset \mathscr{N}(F)$, then there exists $\alpha_j \in \mathbb{C}$ such that $F = \sum_{j=1}^n \alpha_j F_j$.*

We now describe the Sturm-Liouville operator, and also introduce some concepts and notation to be used throughout. Consider the formal differential operator

$$Lf = \frac{1}{w}(-(pf')' + qf)$$

on (a, b), with $p, w > 0$ and p, q, w real-valued and continuous functions defined on (a, b). The maximal operator T corresponding to L is defined by $Tf = Lf$, with $\mathscr{D}(T)$ consisting of all $f \in \mathcal{L}^2(a, b; w)$ such that f is continuously differentiable in (a, b), f' is absolutely continuous in (a, b), and $Lf \in \mathcal{L}^2(a, b; w)$. The minimal operator T_0 corresponding to L is defined by $T_0 f = Lf$ with $\mathscr{D}(T_0) = C_0^\infty(a, b)$. Both T and T_0 are densely defined.

If $z \in \mathbb{C}$ and g is locally integrable, then f is a solution of the equation $(L-z)f = g$ if f is continuously differentiable, f' is absolutely continuous, and $(L-z)f(x) = g(x)$ for almost all $x \in (a, b)$. Two solutions f_1 and f_2 of the homogeneous equation $(L-z)f = 0$ constitute a fundamental system if their weighted Wronskian $\mathscr{W} \equiv \mathscr{W}(f_1, f_2) = p(f_1 f_2' - f_2 f_1') \neq 0$ for some (and hence for all) $x \in (a, b)$. In this instance, solutions f of the equation $(L - z)f = g$ are given by the variation of parameters formula

$$\begin{aligned} f(x) = c_1 f_1(x) + c_2 f_2(x) + f_1(x) \int_c^x \mathscr{W}^{-1} f_2(s) g(s) w(s) \mathrm{d}s \\ - f_2(x) \int_c^x \mathscr{W}^{-1} f_1(s) g(s) w(s) \mathrm{d}s \end{aligned}$$

where $c \in (a, b)$ and $c_1, c_2 \in \mathbb{C}$. Suppose f and g are continuously differentiable, then we define the Liouville bracket to be

$$[f, g]_x \equiv p(x)(f'(x)^* g(x) - f(x)^* g'(x)).$$

Furthermore, for f' and g' absolutely continuous we have by integration by parts that

$$\int_\alpha^\beta (f^* Lg - (Lf)^* g) w \mathrm{d}x = [f, g]_\beta - [f, g]_\alpha$$

for $[\alpha, \beta] \subset (a, b)$. Therefore, for $f, g \in \mathscr{D}(T)$ we have

$$\langle f | Tg \rangle - \langle Tf | g \rangle = [f, g]_b - [f, g]_a.$$

Theorem A.8. *Let $\mathcal{L}_0^2(a, b; w)$ be the subspace of those functions in $\mathcal{L}^2(a, b; w)$ that vanish for almost all x near a and b. Then, the range $\mathscr{R}(T_0) \equiv \mathscr{R}$ consists of those functions $v \in \mathcal{L}_0^2(a, b; w)$ such that $\int_a^b \phi^* v w \mathrm{d}x = 0$ for every solution ϕ of $L\phi = 0$.*

Proof. For $f \in \mathscr{D}(T_0)$ (so $T_0 f \in \mathscr{R}(T_0)$) and for every ϕ such that $L\phi = 0$, we have by integration by parts that $\int_a^b \phi^* (T_0 f) w \mathrm{d}x = \int_a^b (L\phi)^* f w \mathrm{d}x = 0$, which means that $T_0 f \in \mathscr{R}$ or $\mathscr{R}(T_0) \subset \mathscr{R}$. Now, take $v \in \mathscr{R}$ and $[\alpha, \beta] \subset (a, b)$ with v vanishing outside $[\alpha, \beta]$. For $c \in (a, b)$ and $c_1 = c_2 = 0$, let h be such that $Lh = v$ given by the variation of parameters formula met earlier for $z = 0$. Then, h' is absolutely continuous and $h(x) = 0$ for $x \in (a, \alpha)$.

For each solution ϕ of the equation $L\phi = 0$ and for each $x_0 \in (a, \alpha)$, $x \in (\beta, b)$, we have

$$\begin{aligned}[\phi, h]_x &= [\phi, h]_x - [\phi, h]_{x_0} \\ &= \int_{x_0}^{x} (\phi^* v - (L\phi)^* h) w \mathrm{d}x \\ &= 0.\end{aligned}$$

This holds for every ϕ with the property that $L\phi = 0$ and so it must be that $h(x) = 0$ for all $x \in (\beta, b)$. Therefore, $h \in \mathscr{D}(T_0)$ and $T_0 h = v \in \mathscr{R}(T_0)$ or equivalently, $\mathscr{R} \subset \mathscr{R}(T_0)$. □

Theorem A.9. $T_0{}^\dagger = T$.

Proof. Integration by parts shows that $\langle T_0 f | g \rangle = \langle f | T g \rangle$ for all $f \in \mathscr{D}(T_0)$, $g \in \mathscr{D}(T)$, i.e. that they are formal adjoints of each other. This means that $T \subset T_0{}^\dagger$ since every formally adjoint operator of T_0 is a restriction of $T_0{}^\dagger$.

To show that $T_0{}^\dagger \subset T$, take $f \in \mathscr{D}(T_0{}^\dagger)$. Then, $g = T_0{}^\dagger f$ is locally integrable. Suppose h is such that $Lh = g$, then

$$\int_a^b (f - h)^* (T_0 v) w \mathrm{d}x = \int_a^b [(T_0{}^\dagger f) - (Lh)]^* v w \mathrm{d}x = 0$$

for all $v \in \mathscr{D}(T_0)$. Defining the functional

$$F : \mathcal{L}_0^2(a, b; w) \to \mathbb{C}, \quad l \mapsto \int_a^b (f - h)^* l w \mathrm{d}x,$$

we see that $\mathscr{R}(T_0) \subset \mathscr{N}(F)$. By Theorem A.8, $\mathscr{R}(T_0)$ consists of all $l \in \mathcal{L}_0^2(a, b; w)$ such that $\int_a^b \phi^* l w \mathrm{d}x = 0$ for every solution ϕ of $L\phi = 0$. Moreover, $\mathscr{R}(T_0) = \mathscr{N}(F_j)$ where $F_j : \mathcal{L}_0^2(a, b; w) \to \mathbb{C}$, $l \mapsto \int_a^b \phi_j{}^* l w \mathrm{d}x$, $j = 1, 2$ and ϕ_1, ϕ_2 constitute a fundamental system for $L\phi = 0$. Therefore, by Theorem A.7 we can write $F = \alpha_1 F_1 + \alpha_2 F_2$ for some $\alpha_1, \alpha_2 \in \mathbb{C}$. Defining $\mu(x) \equiv \alpha_1 \phi_1(x) + \alpha_2 \phi_2(x)$, we have $\int_a^b (f - h - \mu)^* l w \mathrm{d}x = 0$, which means $f - h = \alpha_1 \phi_1 + \alpha_2 \phi_2$ for almost all $x \in (a, b)$. Hence, f is a solution of $Lf = g$ and since $f \in \mathcal{L}^2(a, b; w)$ it follows that $f \in \mathscr{D}(T)$, i.e. $T_0{}^\dagger \subset T$. □

Theorem A.10 (Weidmann [1980] p. 254). *Let L be a Sturm-Liouville formal differential operator on (a, b) and let $c \in (a, b)$. Either every solution u of the equation $(L - z)u = 0$ lies in $\mathcal{L}^2(c, b; w)$ for every $z \in \mathbb{C}$, or for each $z \in \mathbb{C} \setminus \mathbb{R}$ there exists (up to multiplication by a constant) exactly one solution u of the equation $(L - z)u = 0$ with $u \in \mathcal{L}^2(c, b; w)$. The exact analogue holds for the boundary point a. This is known as Weyl's alternative.*

The original analysis of Hermann Weyl refers to the first case in Theorem A.10 as the limit circle case at b (or at a), whilst the second is referred to as the limit point case at b (or at a). These are not merely semantics, but are accurate descriptions of the possible cases that can arise in solving the Sturm-Liouville equation with a singular boundary point, by letting $b \to \infty$ and approximating the singular problem by a sequence of regular ones.

Theorem A.11 (Weidmann [1980] p. 255).

(a) $[f,g]_a = 0$ *for* $f \in \mathscr{D}(\overline{T_0})$ *and* $g \in \mathscr{D}(T)$,

(b) In the limit circle case at a; if ϕ *is a solution of* $(L-z)\phi = 0$ *for some* $z \in \mathbb{C}$, ϕ_0 *is twice continuously differentiable on* (a,b), $\phi_0(x) = \phi(x)$ *near a, and* $\phi_0(x) = 0$ *near b, then we have* $\phi_0 \in \mathscr{D}(T) \setminus \mathscr{D}(\overline{T_0})$,

(c) In the limit point case at a, $[f,g]_a = 0$ *for all* $f, g \in \mathscr{D}(T)$. *Similarly for b.*

Proof.

(a) Let $f \in \mathscr{D}(\overline{T_0})$ and $g \in \mathscr{D}(T)$, then there is a $g_0 \in \mathscr{D}(T)$ with the property that $g_0(x) = g(x)$ near a and $g_0(x) = 0$ near b. This can be seen by multiplying g by a mollifier χ with the property that $\chi(x) = 1$ near a and $\chi(x) = 0$ near b, i.e. let $g_0 = \chi g$ then $g_0' = \chi g' + \chi' g$ exists and is absolutely continuous. So,

$$[f,g]_a = [f,g_0]_a - [f,g_0]_b = -(\langle f|Tg_0\rangle - \langle \overline{T_0} f|g_0\rangle) = \langle f|\overline{T_0}^{\dagger} g_0\rangle - \langle f|Tg_0\rangle = 0$$

since T is closed by Theorems A.9 and A.3, and so $\overline{T_0}^{\dagger} = T^{\dagger}$ by Theorem A.5.

(b) Now, $\phi_0 \in \mathscr{D}(T)$. If v is such that $(L-z)v = 0$ with $\mathscr{W}(\phi, v) \neq 0$ and v_0 is defined analogously to ϕ_0, then $v_0{}^* \in \mathscr{D}(T)$ and $[\phi_0, v_0{}^*]_a = [\phi, v^*]_a = -\mathscr{W}(u,v)^* \neq 0$. Thus, it follows from (a) that $\phi_0 \notin \mathscr{D}(\overline{T_0})$.

(c) We are free to suppose that L is regular at b, then the defect indicies of T_0 are $(1,1)$ by Weyl's alternative—for our purposes we take as our definition of the defect indicies (γ_+, γ_-) of T_0 to be as follows: γ_+ (γ_-) is equal to the number of linearly independent solutions of the equation $(L+i)u = 0$ $((L-i)u = 0)$ that belong to $\mathcal{L}^2(a,b;w)$. Let ϕ_1, ϕ_2 be linearly independent solutions of $L\phi = 0$, and let v_1, v_2 be twice continuously differentiable functions such that $v_j(x) = \phi_j(x)$ near b and $v_j(x) = 0$ near a. By part (b), $v_1, v_2 \in \mathscr{D}(T)$ and are linearly independent modulo $\mathscr{D}(\overline{T_0})$. Thus, $\mathscr{D}(T) = \mathscr{D}(\overline{T_0}) + \operatorname{span}(v_1, v_2)$. Hence, any $f, g \in \mathscr{D}(T)$ have elements $f_0, g_0 \in \mathscr{D}(\overline{T_0})$ that agree with f and g in a neighbourhood of a respectively. It follows from part (a) that $[f,g]_a = [f_0, g_0]_a = 0$.

□

Theorem A.12. *If we have the limit point case at both singular endpoints, then it follows that T is self-adjoint.*

Proof. In this case we have for $f, g \in \mathscr{D}(T)$ that $\langle f|Tg\rangle - \langle Tf|g\rangle = [f,g]_b - [f,g]_a = 0$ by Theorem A.11 (c). Thus T is symmetric. We also know that T_0 is symmetric since we have that $T_0 \subset T = T_0{}^{\dagger}$ by Theorem A.9. Consequently, as both T_0 and $T_0{}^{\dagger}$ are symmetric, T_0 is essentially self-adjoint by Theorem A.6. Another application of Theorem A.6 yields that $\overline{T_0} = T_0{}^{\dagger} = T$ and so by definition of essential self-adjointness, T is self-adjoint. □

APPENDIX B

The Spectrum

B.1 Spectral Theory in Finite Dimensions

Let $\mathscr{E}$ denote the space $\mathbb{C}^n$ with any appropriate norm, and suppose that A is a linear operator on $\mathscr{E}$ corresponding to a matrix $\tilde{A} = (a_{ij})_{i,j}^n$. A non-zero vector $v \in \mathscr{E}$ is called an eigenvector of the operator A, belonging to eigenvalue λ, if we have

$$Av = \lambda v. \tag{B.1}$$

The collection of all eigenvalues of A is called the spectrum of A. Clearly, the spectrum of A coincides with the set of all roots $\{\lambda_1, \ldots, \lambda_m\}$, $m \leq n$, of the characteristic equation

$$\det \begin{pmatrix} a_{11} - \lambda & a_2 & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{2n} & \cdots & a_{nn} - \lambda \end{pmatrix} = 0.$$

This is justified by the fact that all matrices representing a given operator on a finite dimensional normed space $\mathscr{E}$—relative to various bases for $\mathscr{E}$—have the same eigenvalues. Therefore, if $\lambda \in \{\lambda_1, \ldots, \lambda_n\}$ then the corresponding operator $A - \lambda\mathbf{1}$ is not invertible, where $\mathbf{1}$ denotes the identity operator.

Before we continue our brief introduction to spectral theory let us, in anticipation of what is to come in the next section, note the following fundamental result concerning linear operators and their inverses on general vector spaces [Kreyszig, 1978, p. 88]:

Theorem B.1. *Let $\mathscr{V}_1$ and $\mathscr{V}_2$ be complex vector spaces, and let $T : \mathscr{D}(T) \to \mathscr{R}(T)$ be a linear operator with domain $\mathscr{D}(T) \subset \mathscr{V}_1$ and range $\mathscr{R}(T) \subset \mathscr{V}_2$. Then, the inverse $T^{-1} : \mathscr{R}(T) \to \mathscr{D}(T)$ exists if and only if $Tv = 0$ implies $v = 0$, and is a linear operator.*

Proof. Suppose $Tv = 0$ implies $v = 0$. If $Tv_1 = Tv_2$, then $T(v_1 - v_2) = 0$ which implies $v_1 = v_2$ by assumption. Conversely, if the inverse of T exists then $Tv_1 = Tv_2$ implies $v_1 = v_2$; setting $v_2 = 0$ shows that $Tv_1 = 0$ implies $v_1 = 0$. We now show that if it exists, T^{-1} is a linear operator: let $v_1, v_2 \in \mathscr{D}(T)$, $w_1 = Tv_1$, and $w_2 = Tv_2$. Then, $v_1 = T^{-1}w_1$ and $v_2 = T^{-1}w_2$. Since T is linear we have for any $a, b \in \mathbb{C}$ that $aw_1 + bw_2 = T(av_1 + bv_2)$, which means that $T^{-1}(aw_1 + bw_2) = av_1 + bv_2 = aT^{-1}w_1 + bT^{-1}w_2$. □

B.2 The Resolvent

Thus motivated, we now consider spaces of arbitrary dimension; in particular, we are no longer restricted (as we were in the previous section) to finite dimensional spaces. Spectral theory is a much richer subject in infinite dimensions since in general, the spectrum will no longer comprise of isolated points only. Let $\mathscr{E}$ denote some complex normed space and let $T : \mathscr{D}(T) \to \mathscr{E}$ be a linear operator. We may associate with T the linear operator

$$(T - \lambda \mathbf{1})^{-1} = (T - \lambda)^{-1} \tag{B.2}$$

called the resolvent of T—we know that it is linear because of Theorem B.1. The resolvent provides the solution to equations such as $(T - \lambda)v = w$, i.e. $v = (T - \lambda)^{-1}w$ provided, of course, that $(T - \lambda)^{-1}$ exists. The resolvent clearly depends upon λ and, in fact, spectral theory revolves around this dependence. The existence, boundedness, and density of the domain of $(T - \lambda)^{-1}$ are of particular interest, since these properties of the resolvent give rise to the different types of spectrum associated with infinite dimensional spaces. We now give the standard classification of the spectrum of an operator: the definition to follow can be found in, for example, Kreyszig [1978] p. 371.

Definition B.1. *A regular value λ of the operator T is a complex number such that*

1. $(T - \lambda)^{-1}$ *exists,*
2. $(T - \lambda)^{-1}$ *is bounded,*
3. $\mathscr{D}((T - \lambda)^{-1})$ *is dense in $\mathscr{E}$.*

The resolvent set $\rho(T)$ is the set of all regular values of T. The complement of $\rho(T)$ in the complex plane is called the spectrum of T, denoted by $\sigma(T)$. The spectrum is partitioned into three disjoint sets, corresponding to the properties of $(T - \lambda)^{-1}$ listed above:

- *The point spectrum, denoted by $\sigma_p(T)$, is the set of λ such that the resolvent does not exist; members of the point spectrum are called eigenvalues,*
- *The continuous spectrum, denoted by $\sigma_c(T)$, is the set of λ such that the resolvent exists and has dense domain, but is not bounded,*
- *The residual spectrum, denoted by $\sigma_r(T)$, is the set of λ such that the resolvent exists but is not densely defined—it may or may not be bounded.*

Theorem B.1 shows that the resolvent $(T-\lambda)^{-1} : \mathscr{R}(T-\lambda) \to \mathscr{D}(T-\lambda)$ exists if and only if $(T-\lambda)v = 0$ implies $v = 0$. Thus, if $(T-\lambda)v = 0$ but $v \neq 0$ then $\lambda \in \sigma_{\mathrm{p}}(T)$ by Definition B.1. The element v is called an eigenvector of T—or an eigenfunction if we are working in a function space—belonging to eigenvalue λ. This demonstrates that the current definition of an eigenvalue is consistent with our previous one involving (B.1).

B.3 The Essential Spectrum

We have seen in section B.1 that the spectum of a linear operator T can be decomposed as follows: $\sigma(T) = \sigma_{\mathrm{p}}(T) \cup \sigma_{\mathrm{c}}(T) \cup \sigma_{\mathrm{r}}(T)$. However, we may define yet another subset of the spectrum called the essential spectrum, which is denoted by $\sigma_{\mathrm{e}}(T)$. The reason for introducing the essential spectrum is that it is a more general concept with many useful properties. There are various definitions of the essential spectrum in the literature, and they are not generally equivalent, except when T is a self-adjoint operator—on a Hilbert space of course [Edmunds and Evans, 1987, p. 417]. Furthermore, in the case where T is a bounded self-adjoint operator, we have a simple decomposition of the spectrum into two disjoint subsets given by $\sigma(T) = \sigma_{\mathrm{p}}(T) \cup \sigma_{\mathrm{e}}(T)$ [Reed and Simon, 1980, p. 236]. In order to introduce the notion of essential spectrum, we must first make some preliminary definitions; we take these from Edmunds and Evans [1987] pp. 7 and 39.

Definition B.2. *Let $\mathscr{W}$ be a subspace of the vector space $\mathscr{V}$. The coset of $v \in \mathscr{V}$ with respect to $\mathscr{W}$ is denoted by $v + \mathscr{W}$, and is defined as*

$$v + \mathscr{W} \equiv \{v + w, w \in \mathscr{W}\}.$$

The cosets constitute the elements of a vector space; this space is called the quotient space, which is denoted by $\mathscr{V}/\mathscr{W}$.

Definition B.3. *Suppose that $\mathscr{B}_1$ and $\mathscr{B}_2$ are two Banach spaces, then a closed linear operator $T \in \mathscr{C}(\mathscr{B}_1, \mathscr{B}_2)$ is said to be semi-Fredholm if $\mathscr{R}(T)$ is closed and at least one of the nullity,* $\mathrm{nul}(T) \equiv \dim(\mathscr{N}(T))$ *and deficiency,* $\mathrm{def}(T) \equiv \dim(\mathscr{B}_2/\mathscr{R}(T))$ *is finite.*

Now that we have introduced the notion of a semi-Fredholm operator, we are in a position to define the essential spectrum of a closed linear operator $\sigma_{\mathrm{e}}(T)$; this is given, for example, by the following [Edmunds and Evans, 1987, p. 40]:

Definition B.4. *Let $\mathscr{B}$ be a complex Banach space and let $T \in \mathscr{C}(\mathscr{B})$. Then the essential spectrum of T is given by the set*

$$\sigma_{\mathrm{e}}(T) \equiv \mathbb{C} \setminus \{\lambda \in \mathbb{C} : T - \lambda \ \textit{is semi-Fredholm} \ (\mathscr{N}(T) < \infty)\}.$$

As we have already mentioned there are several different definitions of $\sigma_{\mathrm{e}}(T)$; we favour this particular definition because it yields an equivalent definition which is usually more convenient to work with in practice. In fact, this equivalent characterization will be useful imminently. To be able to recharacterize the essential spectrum, we must first introduce singular sequences; these are defined as follows [Edmunds and Evans, 1987, p. 415]:

Definition B.5. *A sequence (x_n) in $\mathscr{D}(T)$ is called a singular sequence of T corresponding to $\lambda \in \mathbb{C}$ if it contains no convergent subsequence in a complex Banach space $\mathscr{B}$, and is such that $\|x_n\|_{\mathscr{B}} = 1$ and $(T - \lambda)x_n \to 0$ as $n \to \infty$.*

With this in mind, we have [Edmunds and Evans, 1987, p. 415]

Theorem B.2. *For $T \in \mathscr{C}(\mathscr{B})$ densely defined, $\lambda \in \sigma_e(T)$ if and only if there is a singular sequence of T corresponding to λ.*

In spectral theory, the numerical range of an operator in Hilbert space is a most important tool; in our case, we will require it for the purpose of calculating the essential spectrum, by means of a well-used argument. The importance of the numerical range is due to the fact that it contains the essential spectrum (and also the point spectrum). The proof of this is given after the following definition [Edmunds and Evans, 1987, p. 99]:

Definition B.6. *The numerical range $\Phi(T)$ of a linear operator T in Hilbert space $\mathscr{H}$, is the set of complex numbers*

$$\Phi(T) \equiv \overline{\{\langle Tx|x\rangle : x \in \mathscr{D}(T), \|x\| = 1\}}.$$

Theorem B.3. *$\sigma_e(T) \subset \Phi(T)$.*

Proof. Let $\lambda \in \sigma_e(T)$. Then, by Theorem B.2 there exists a sequence (x_n) in $\mathscr{D}(T)$, with $\|x_n\| = 1$ such that $\|Tx_n - \lambda x_n\| \to 0$ or $\langle Tx_n|x_n\rangle - \lambda\langle x_n|x_n\rangle \to 0$. This means that $\langle Tx_n|x_n\rangle - \lambda \to 0$ and so $\lambda \in \Phi(T)$. Hence, $\sigma_e(T) \subset \Phi(T)$. □

Aided by the following definition from Kato [1966] p. 194 concerning the relative compactness of operators, we give a generalization of the seminal result due to Weyl [1909] on self-adjoint operators in a Hilbert space; it describes the invariance of the essential spectrum under a relatively compact perturbation [Kato, 1966, p. 244].

Definition B.7. *Let S and T be linear operators satisfying $\mathscr{D}(S) \subset \mathscr{D}(T)$. Assume that for any sequence $(v_n) \in \mathscr{D}(S)$ with both (v_n) and (Sv_n) bounded, (Tv_n) contains a convergent subsequence. Then T is said to be relatively compact with respect to S, or simply, S-compact.*

Theorem B.4. *Let $\mathscr{B}$ be a complex Banach space. Suppose $S \in \mathscr{C}(\mathscr{B})$ and let the linear operator T be S-compact. Then, $\sigma_e(S) = \sigma_e(S + T)$.*

The next theorem is the core of this section; it is indispensable in the development of the proposition which we are to use in the main body of the thesis—in Chapter 5. In essence, the following is an application of Theorem B.4, but we will require the machinery of an intermediate result in order to present its proof satisfactorily.

Theorem B.5. *Consider the following operator:*

$$T = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \quad \text{on} \quad \mathcal{L}^2(\mathbb{R}).$$

If V is bounded and decays at $\pm\infty$, then $\sigma_e(T) = [0, \infty)$.

Proof. To prove this we trace Kato [1966] p. 304. For the operator $T_0 = -\mathrm{d}/\mathrm{d}x^2$ on $\mathcal{L}^2(\mathbb{R})$, $\sigma(T_0) = \sigma_e(T_0) = [0, \infty)$. Thus, in view of Theorem B.3 it suffices to prove that $T - T_0$ is relatively compact with respect to T_0. Let (f_n) be a bounded sequence in $\mathcal{L}^2(\mathbb{R})$ such that $(T_0 f_n)$ is also bounded. We have to show that $((T - T_0)f_n)$ contains a convergent subsequence. To continue we require the following proposition [Kato, 1966, p. 301]:

Proposition B.1. *Let $f(x) \in \mathcal{L}^2(\mathbb{R})$ be such that $|k|^2\hat{f}(k) \in \mathcal{L}^2(\mathbb{R})$, $k \in \mathbb{R}$, where we define $\hat{f}(k) = Ff(x)$ to be the Fourier transform of $f(x)$. Then f is a bounded function which is Hölder continuous with exponent smaller than $1/2$.*

Proof. Firstly, observe that by an application of the Hölder inequality the Fourier transform of f is integrable:

$$\left(\int_{\mathbb{R}} |\hat{f}(k)|\mathrm{d}k\right)^2 \le \int_{\mathbb{R}} \frac{\mathrm{d}k}{(|k|^2 + \alpha^2)^2} \int_{\mathbb{R}} |\hat{f}(k)|^2(|k|^2 + \alpha^2)^2\mathrm{d}k < \infty$$

for some arbitrary $\alpha > 0$. Now, the Riemann-Lebesgue Theorem states that a function f whose Fourier transform $\hat{f}(k) \in \mathcal{L}^1(\mathbb{R})$ is bounded and continuous. To see this, we have

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{ikx}\hat{f}(k)\mathrm{d}k \tag{B.3}$$

and so

$$|f(x)| \le \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} |\hat{f}(k)|\mathrm{d}k < \infty$$

for almost all $x \in \mathbb{R}$, i.e. f is essentially bounded. The continuity of f follows directly from the continuity of the integral in (B.3). Hence, f is bounded and continuous.

Next, we need to show that for all $\gamma \in (0, 1/2)$ there exists a non-negative constant C such that for all $x, y \in \mathbb{R}$,

$$|f(x) - f(y)| \le C|x - y|^\gamma.$$

To this end, we have

$$|f(x) - f(y)| = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} |\mathrm{e}^{ikx} - \mathrm{e}^{iky}||\hat{f}(k)|\mathrm{d}k.$$

Now,

$$\mathrm{e}^{ikx} - \mathrm{e}^{iky} = ik\int_y^x \mathrm{e}^{ikt}\mathrm{d}t,$$

which implies that

$$|\mathrm{e}^{ikx} - \mathrm{e}^{iky}| \le |k||x - y|.$$

We note that $|e^{ikx} - e^{iky}|$ does not exceed 2, and thus

$$\begin{aligned}|e^{ikx} - e^{iky}| &= |e^{ikx} - e^{iky}|^{\gamma}|e^{ikx} - e^{iky}|^{1-\gamma} \\ &\leq 2^{1-\gamma}|k|^{\gamma}|x-y|^{\gamma}.\end{aligned}$$

Hence,

$$\frac{|f(x)-f(y)|}{|x-y|^{\gamma}} \leq \frac{2^{1-\gamma}}{\sqrt{2\pi}}\int_{\mathbb{R}}|k|^{\gamma}|\hat{f}(k)|\mathrm{d}k.$$

By the Hölder inequality

$$\left(\int_{\mathbb{R}}|k|^{\gamma}|\hat{f}(k)|\mathrm{d}k\right)^2 \leq \left(\int_{\mathbb{R}}|k|^{2\gamma}\mathrm{d}k\right)\left(\int_{\mathbb{R}}|\hat{f}(k)|^2\mathrm{d}k\right),$$

which implies

$$\left(\int_{\mathbb{R}}|k|^{\gamma}|\hat{f}(k)|\mathrm{d}k\right)^2 \leq \left(\int_{\mathbb{R}}\frac{|k|^{2\gamma}}{(|k|^2+\alpha^2)^2}\mathrm{d}k\right)\left(\int_{\mathbb{R}}|\hat{f}(k)|^2(|k|^2+\alpha^2)^2\mathrm{d}k\right) \tag{B.4}$$

for some arbitrary $\alpha > 0$. Looking at (B.4), the second integral is finite by hypothesis. Denote the integrand in the first integral by I_{γ}, then if $\gamma \in (0, 1/2)$ we have

$$I_{\gamma} \sim \begin{cases} |k|^{2\gamma}\alpha^{-4} & \text{as} \quad k \to 0, \\ |k|^{2\gamma-4} & \text{as} \quad k \to \pm\infty \end{cases}$$

and so in both cases I_{γ} is integrable. Therefore,

$$\frac{|f(x)-f(y)|}{|x-y|^{\gamma}} \leq C$$

□

In order to make use of Proposition B.1, we need to show that $|k|^2\hat{f}(k) \in \mathcal{L}^2(\mathbb{R})$ since we already have by hypothesis that our sequence of bounded functions lives in the Lebesgue space $\mathcal{L}^2(\mathbb{R})$. To do this we first note that $-\mathrm{d}^2f/\mathrm{d}x^2$ is the inverse Fourier transform of $|k|^2\hat{f}(k)$, as the following straight-forward calculation demonstrates:

$$\begin{aligned}F^{-1}|k|^2\hat{f}(k) &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}|k|^2 e^{ikx}\hat{f}(k)\mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\frac{\mathrm{d}^2(-e^{ikx})}{\mathrm{d}x^2}\hat{f}(k)\mathrm{d}k \\ &= -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left[\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}e^{ikx}\hat{f}(k)\mathrm{d}k\right] \\ &= -\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(x).\end{aligned}$$

But, by assumption we know that $F^{-1}|k|^2\hat{f} = T_0 f \in \mathcal{L}^2(\mathbb{R})$, and thus by Parseval's Theorem [Boas, 2006, p. 383] we get $|k|^2\hat{f}(k) \in \mathcal{L}^2(\mathbb{R})$. Therefore, applying Proposition B.1 to our sequence (f_n), we find that the $f_n(x)$ are uniformly bounded in x and n, and equicontinuous. By the famous Arzelá-Ascoli Theorem [Kato, 1966, p. 157], (f_n) contains a subsequence, (f_{n_j}) say, that converges uniformly on any bounded interval of $\mathbb{R}$. Let f be the limit of this subsequence, then f is bounded, continuous, and resides in $\mathcal{L}^2(\mathbb{R})$. All that remains is to show that $Vf_{n_j} \to Vf$ in $\mathcal{L}^2(\mathbb{R})$.

Let $\varepsilon > 0$ and suppose R is sufficiently large as to ensure that $|V(x)| \leq \varepsilon$ for $|x| \geq R$, which can be done since V decays for large $|x|$ by assumption. Then,

$$\begin{aligned}\int_{|x|\geq R} |Vf_{n_j} - Vf|^2 \mathrm{d}x &\leq 2\varepsilon^2(\|f_{n_j}\|^2 + \|f\|^2) \\ &\leq 4(\sup \|f_{n_j}\|)^2\varepsilon^2\end{aligned}$$

for all n, and

$$\int_{|x|\leq R} |Vf_{n_j} - Vf|^2 \mathrm{d}x \to 0 \quad \text{as} \quad n \to \infty$$

by the assumed boundedness of V and the uniform convergence $f_{n_j} \to f$ on $|x| \leq R$. It follows that $Vf_{n_j} \to Vf$ in $\mathcal{L}^2(\mathbb{R})$. □

What we actually want to prove is slightly different from Theorem B.5, namely, the hypotheses on the function V are more complicated. To cope with such modifications, we must consider the Glazman decomposition; this is the topic of the next section.

B.4 The Glazman Decomposition

The Glazman decomposition is a strategy for calculating the essential spectrum under the special circumstances in which the operator can be split up in some helpful way. The method is described in the book of Akhiezer and Glazman [1993]. We study the operator

$$T = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \quad \text{on} \quad \mathcal{L}^2(\mathbb{R})$$

and consider the equation

$$(T - z)u = f, \quad f \in \mathcal{L}^2(\mathbb{R}).$$

Let L be the differential expression associated with the operator T and define

$$f_1 \equiv f\big|_{(-\infty,0]}, \quad f_2 \equiv f\big|_{[0,\infty)}.$$

Thus, we need

$$(L - z)u_1 = f_1, \quad (L - z)u_2 = f_2$$

with $u_1(0) = u_2(0) := h$, $h \in \mathbb{C}$ and $u_1'(0) = u_2'(0)$. We attempt to solve

$$(L - z)u_1 = f_1, \quad u_1(0) = h,$$

in $\mathcal{L}^2((-\infty, 0])$. This is only possible provided $z \notin \sigma(T_1)$, where

$$\mathscr{D}(T_1) = \{\omega \in \mathcal{L}^2((-\infty, 0]) : L\omega \in \mathcal{L}^2((-\infty, 0]), \omega(0) = 0\}.$$

Let $K_1 h \in \mathcal{L}^2((-\infty, 0])$, which depends on z, be such that

$$(L - z)(K_1 h) = 0, \quad (K_1 h)(0) = h$$

and note that $K_1 : \mathbb{C} \to \mathcal{L}^2((-\infty, 0])$ is rank 1 since $\mathscr{D}(K_1)$ has dimension one. Let $v_1 \equiv u_1 - K_1 h$ and apply the operator $(L - z)$ to both sides to get

$$\begin{aligned}(L - z)v_1 &= f_1 - (L - z)(K_1 h)\\ &= f_1.\end{aligned}$$

Also, $v_1(0) = h - h = 0$, which implies $v_1 \in \mathscr{D}(T_1)$ and hence $v_1 = (T_1 - z)^{-1} f_1$. Therefore,

$$\begin{aligned}u_1 &= v_1 + K_1 h\\ &= (T_1 - z)^{-1} f_1 + K_1 h.\end{aligned} \tag{B.5}$$

Similarly, we solve in $\mathcal{L}^2([0, \infty))$, the problem $(L - z)u_2 = f_2$, $u_2(0) = h$. Again, this is possible only when z is not in $\sigma(T_2)$, where

$$\mathscr{D}(T_2) = \{\omega \in \mathcal{L}^2([0, \infty)) : L\omega \in \mathcal{L}^2([0, \infty)), \omega(0) = 0\}.$$

Suppose $K_2 h \in \mathcal{L}^2([0, \infty))$ is such that

$$(L - z)(K_2 h) = 0, \quad (K_2 h)(0) = h$$

and note once again that $K_2 : \mathbb{C} \to \mathcal{L}^2([0, \infty))$ is rank 1. Let $v_2 \equiv u_2 - K_2 h$, then applying the operator $(L - z)$ to both sides yields

$$u_2 = (T_2 - z)^{-1} f_2 + K_2 h. \tag{B.6}$$

We need to eliminate h. To achieve this we take derivatives at the origin. Let ∂_j for $j \in \{1, 2\}$ be defined by

$$\partial_1 u = \lim_{x \uparrow 0} u'(x) \quad \text{and} \quad \partial_2 u = \lim_{x \downarrow 0} u'(x).$$

From our initial data, we want $\partial_1 u_1 = \partial_2 u_2$, i.e.

$$\partial_1(T_1 - z)^{-1} f_1 + \partial_1 K_1 h = \partial_2(T_2 - z)^{-1} f_2 + \partial_2 K_2 h. \tag{B.7}$$

It is important to notice that the operators $\partial_1 K_1 \equiv M_1$ and $\partial_2 K_2 \equiv M_2$ are so-called Titchmarsh-Weyl M-functions. To see this, consider the following for K_2 (the same argument applies to K_1). By definition the function

$$\xi_h \equiv K_2 h$$

solves the problem

$$(L - z)\xi_h = 0 \quad \text{on} \quad [0, \infty), \quad \xi_h \in \mathcal{L}^2([0, \infty)), \quad \xi_h(0) = h.$$

Therefore,

$$\begin{aligned} \partial_2 K_2 &= \frac{1}{h}\partial_2 K_2 h \\ &= \frac{\xi_h'(0+)}{\xi_h(0)} \\ &= \frac{\xi'(0+)}{\xi(0)} \end{aligned} \tag{B.8}$$

where ξ is such that

$$(L - z)\xi = 0 \quad \text{on} \quad [0, \infty), \quad \xi \in \mathcal{L}^2([0, \infty)), \quad \xi(0) = 1.$$

Equation (B.8) is the definition of the Titchmarsh-Weyl M-function. Therefore, assuming the same has been done for K_1, we have

$$M_1(z) = \frac{\xi'(0+)}{\xi(0)} \quad \text{and} \quad M_2(z) = \frac{\xi'(0-)}{\xi(0)}.$$

It is well-known that the functions $M_1(z)$ and $M_2(z)$ have poles at the eigenvalues of T_1 and T_2 respectively [Coddington and Levinson, 1955, Ch. 9]. Hence, equation (B.7) gives

$$\partial_1(T_1 - z)^{-1} f_1 + M_1 h = \partial_2(T_2 - z)^{-1} f_2 + M_2 h,$$

which implies

$$h = \frac{1}{M_1 - M_2}[-\partial_1(T_1 - z)^{-1} f_1 + \partial_2(T_2 - z)^{-1} f_2].$$

Therefore, from equations (B.5) and (B.6) we have

$$\begin{aligned} u_1 &= (T_1 - z)^{-1} f_1 + \frac{1}{M_1 - M_2}[-K_1\partial_1(T_1 - z)^{-1} f_1 + K_1\partial_2(T_2 - z)^{-1} f_2], \\ u_2 &= (T_2 - z)^{-1} f_2 + \frac{1}{M_1 - M_2}[-K_2\partial_1(T_1 - z)^{-1} f_1 + K_2\partial_2(T_2 - z)^{-1} f_2]. \end{aligned}$$

We may write these equations in the more succinct form

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = R(z) \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

where

$$R(z) = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix}, \tag{B.9}$$

and

$$\begin{aligned}
R_{11}(z) &= (T_1 - z)^{-1} - \frac{1}{M_1 - M_2} K_1 \partial_1 (T_1 - z)^{-1}, \\
R_{12}(z) &= \frac{1}{M_1 - M_2} K_1 \partial_2 (T_2 - z)^{-1}, \\
R_{21}(z) &= -\frac{1}{M_1 - M_2} K_2 \partial_2 (T_1 - z)^{-1}, \\
R_{22}(z) &= (T_2 - z)^{-1} + \frac{1}{M_1 - M_2} K_2 \partial_2 (T_2 - z)^{-1}.
\end{aligned}$$

In a finite dimensional normed space $\mathscr{E}$, the Bolzano-Weierstrass Theorem holds true, namely, we can extract from each bounded sequence (x_n) in $\mathscr{E}$ a subsequence (x_{n_j}) that converges to some element $x \in \mathscr{E}$. In this case, the normed space $\mathscr{E}$ is said to be locally compact [Kato, 1966, p. 7]. This means that a bounded operator with finite rank is compact. The justification for this is as follows: an operator having finite rank means that the range of that operator is finite dimensional. Moreover, by definition an operator T is compact if the sequence (Tx_n) contains a Cauchy subsequence for any bounded sequence (x_n) [Kato, 1966, p. 157]; but, since the range is finite dimensional it is locally compact, and so the result follows. As a corollary, the rank 1 operators

$$\begin{aligned}
&\frac{1}{M_1 - M_2} K_1 \partial_1 (T_1 - z)^{-1}, \\
&\frac{1}{M_1 - M_2} K_1 \partial_2 (T_2 - z)^{-1}, \\
&\frac{1}{M_1 - M_2} K_2 \partial_2 (T_1 - z)^{-1}, \\
&\frac{1}{M_1 - M_2} K_2 \partial_2 (T_2 - z)^{-1}
\end{aligned}$$

are all compact. By Theorem B.4, the essential spectrum does not 'see' these compact operators and so from equation (B.9) we have

$$\begin{aligned}
\sigma_e(R) &= \sigma_e \begin{pmatrix} (T_1 - z)^{-1} & 0 \\ 0 & (T_2 - z)^{-1} \end{pmatrix} \\
&= \sigma_e \left((T_1 - z)^{-1} \right) \cup \sigma_e \left((T_2 - z)^{-1} \right) \\
&= \frac{1}{\sigma_e(T_1) - z} \cup \frac{1}{\sigma_e(T_2) - z}
\end{aligned} \tag{B.10}$$

by the Spectral Mapping Theorem [Edmunds and Evans, 1987, p. 419]. Applying the Spectral Mapping Theorem once again to $\sigma_e(R)$ on the left side of equation (B.10) yields the well-known result $\sigma_e(T) = \sigma_e(T_1) \cup \sigma_e(T_2)$.

B.5 Chasing Away the Essential Spectrum

We now have the necessary information to present the result that we require. The proof of the following proposition involves chasing away the essential spectrum to infinity; this is quite standard and is often used in circumstances in which the function V is unbounded.

Proposition B.2. *Consider the following operator:*

$$T = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \quad \textit{on} \quad \mathcal{L}^2(\mathbb{R}),$$

where the function V is such that it is bounded on $(-\infty, 0]$ and tends to zero as $x \to -\infty$, but $V \to +\infty$ as $x \to +\infty$. Then, $\sigma_e(T) = [0, \infty)$.

Proof. Allow us to decouple T into the two operators

$$T_1 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \quad \text{on} \quad \mathcal{L}^2((-\infty, 0])$$

and

$$T_2 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \quad \text{on} \quad \mathcal{L}^2([0, +\infty)),$$

with some (Dirichlet) boundary condition at zero. By Theorem B.5, $\sigma_e(T_1) = [0, \infty)$. For the essential spectrum of T_2 we have the following lemma:

Lemma B.1. *Given some $Y > 0$, and assuming $X > 0$ is large enough as to ensure that $V(x) > Y$ for all $x \geq X$, then $\sigma_e(T_2) = \emptyset$.*

Proof. Decouple T_2 into a further two operators, say

$$T_3 f = -\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + V(x)f, \quad f \in \mathcal{L}^2([0, X])$$

and

$$T_4 f = -\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + V(x)f, \quad f \in \mathcal{L}^2([X, +\infty))$$

with, for example, $f(X) = 0$. The operator T_3 has only eigenvalues, being a regular problem. Hence, in terms of finding the essential spectrum of T_2, we need only consider $\sigma_e(T_4)$; we will find that the essential spectrum of T_4 is also empty. The idea for showing this is simple: take an element of the numerical range $\Phi(T_4)$ and show that the real part of this complex number exceeds Y. Since $Y > 0$ was arbitrary and $\sigma_e(T_4) \subset \Phi(T_4)$ by Theorem B.3, we chase away $\sigma_e(T_4)$. Suppose $\phi \in \mathscr{D}(T_4)$ such that $\|\phi\| = 1$, where

$$\mathscr{D}(T_4) = \{f \in \mathcal{L}^2([X, +\infty)) : T_4 f \in \mathcal{L}^2([X, +\infty)), f(X) = 0\}.$$

It follows from integration by parts that

$$\begin{aligned}\langle T_4\phi|\phi\rangle &= -\int_X^\infty \phi''\phi + \int_X^\infty V\phi^2 \\ &= \int_X^\infty (\phi')^2 + \int_X^\infty V\phi^2,\end{aligned}$$

and thus taking real parts we obtain

$$\mathrm{Re}\langle T_4\phi|\phi\rangle = \int_X^\infty (\phi')^2 + \int_X^\infty \mathrm{Re}(V)\phi^2 > Y.$$

This implies that $\sigma_{\mathrm{e}}(T_4) = \emptyset$. Hence, by the Glazman decomposition, $\sigma_{\mathrm{e}}(T_2) = \emptyset$. □

Therefore, we conclude by another application of the Glazman decomposition that the essential spectrum of T is indeed $[0, \infty)$, as required. □

APPENDIX C

Montel's Theorem

We begin with some fundamental results in complex analysis and in particular, the Analytic Convergence Theorem due to Weierstrass. We then give a proof of Montel's Theorem, in which the Analytic Convergence Theorem plays a central role.

Theorem C.1 (Morera's Theorem). *Suppose f is continuous in a region $G \subset \mathbb{C}$ and $\int_\Gamma f = 0$ for every closed curve Γ in G. Then f is analytic on G.*

Proof. Let $z_0 \in G$ and define for each z_0 the function $F(z) \equiv \int_{z_0}^{z} f(w)\mathrm{d}w$. Since we know that $\int_\Gamma f = 0$ for all closed curves Γ, the function F is well-defined because the integral is path independent. To see this, let Γ_0 and Γ_1 be paths joining z_0 and z, and $\int_\Gamma f = 0$ for all closed curves Γ. Then we have that $\int_{\Gamma_0} f = \int_{\Gamma_1} f$ by Γ_0 and $-\Gamma_1$ to form a closed curve in G (the path $-\Gamma_1$ is just the reversal of Γ_1).

We show that F is differentiable on G with $F' = f$; in this case, we would conclude that F is analytic along with all its derivatives on G, which would mean that f is analytic on G. So, suppose $h \in \mathbb{C}$ such that $z+h \in G$, then $(F(z+h)-F(z))/h = (1/h)\int_z^{z+h} f(w)\mathrm{d}w$. By writing $f(z) = (1/h)\int_z^{z+h} f(z)\mathrm{d}w$, we find that

$$\left|\frac{F(z+h)-F(z)}{h} - f(z)\right| = \left|\frac{1}{h}\int_z^{z+h}(f(w)-f(z))\mathrm{d}w\right|.$$

Since f is continuous at z, $f(w) \to f(z)$ as $w \to z$, i.e. $f(w) \to f(z)$ as $h \to 0$. More precisely, given any $\varepsilon > 0$ there exists a $\delta > 0$ such that $|f(w) - f(z)| < \varepsilon$ whenever $|h| < \delta$. Hence, for any $\varepsilon > 0$ there exists a $\delta > 0$ such that

$$\left|\frac{F(z+h)-F(z)}{h} - f(z)\right| < \frac{\varepsilon}{|h|}\left|\int_z^{z+h}\mathrm{d}w\right| = \varepsilon$$

whenever $|h| < \delta$. Therefore, $F'(z) = f(z)$. □

Proposition C.1 (Marsden and Hoffman [2003] p. 188). *Suppose (f_n) is a sequence of continuous functions defined on G and $f_n \to f$ uniformly, then f is continuous on G.*

Proof. Suppose we choose N such that $|f_N(z) - f(z)| < \varepsilon/3$ for all $z \in G$, which poses no problem since $f_n \to f$ uniformly. Since f_N is continuous, there exists a $\delta > 0$ such that $|f_N(z) - f_N(z_0)| < \varepsilon/3$ whenever $|z - z_0| < \delta$. Hence,

$$\begin{aligned}|f(z) - f(z_0)| &\leq |f(z) - f_N(z)| + |f_N(z) - f_N(z_0)| + |f_N(z_0) - f(z_0)| \\ &< \varepsilon/3 + \varepsilon/3 + \varepsilon/3 = \varepsilon\end{aligned}$$

and f is continuous on G. □

Proposition C.2 (Marsden and Hoffman [2003] p. 191). *Let $\Gamma : [a, b] \to G$ be a curve and suppose (f_n) is a sequence of continuous functions defined on $\Gamma([a, b])$, which converges uniformly to f on $\Gamma([a, b])$. Then, $\int_\Gamma f_n \to \int_\Gamma f$.*

Proof. We know f is continuous and thus it is integrable. For each $\varepsilon > 0$ we may choose $n \geq N$ such that $|f_n(z) - f(z)| < \varepsilon$ for all z on Γ. By the aptly named ML Theorem, we have $|\int_\Gamma f_n - \int_\Gamma f| \leq \int_\Gamma |f_n - f| < \varepsilon L$ where L is the length of Γ. The result follows. □

Theorem C.2 (Marsden and Hoffman [2003] p. 191). *Let $G \subset \mathbb{C}$ be an open set and suppose that (f_n) is a sequence of analytic functions defined on G. If $f_n \to f$ uniformly on every closed disk in G, then f is analytic. This is the Analytic Convergence Theorem.*

Proof. Let $z_0 \in G$ and let $\overline{\mathrm{D}}(z_0; r) = \{z \in G : |z - z_0| \leq r\}$ be a closed disk around z_0 contained in G—as G is open. Since $f_n \to f$ uniformly in $\overline{\mathrm{D}}(z_0; r)$, $f_n \to f$ uniformly in the open disk $\mathrm{D}(z_0; r) = \{z \in G : |z - z_0| < r\}$. By Propostion C.1, f is continuous on $\mathrm{D}(z_0; r)$. If Γ is any closed curve in $\mathrm{D}(z_0; r)$, then since f_n is analytic, $\int_\Gamma f_n = 0$ by Cauchy's Theorem. By Proposition C.2, $\int_\Gamma f_n \to \int_\Gamma f$ and hence $\int_\Gamma f = 0$. Therefore, by Morera's Theorem (Theorem C.1), f is analytic on $\mathrm{D}(z_0; r)$. □

Definition C.1. *A family $\mathscr{F}$ of analytic functions defined on an open set in $\mathbb{C}$ is called normal if each sequence of functions in $\mathscr{F}$ has a subsequence which converges uniformly on compacta to an analytic function.*

Theorem C.3 (Conway [1978] p. 153). *If $\mathscr{F}$ is a locally bounded family of analytic functions on G, then $\mathscr{F}$ is a normal family in G. This is known as Montel's Theorem.*

Proof. Take any sequence (f_n) from $\mathscr{F}$ and consider the sequence $(f_n(z_1))$. We know $|f_n(z_1)| < M$ for some M and $n \in \mathbb{N}$. This bounded sequence has a convergent subsequence by the Bolzano-Weierstrass Theorem, say $(f_{n_j}^{(1)})$ converging at z_1. Similarly, at z_2 the sequence $(f_{n_j}^{(1)}(z_2))$ is bounded and so we can extract a convergent subsequence $(f_{n_j}^{(2)})$ which converges at z_2 and z_1. Thus, we have subsequences which converge at $z_1, z_2, \ldots z_p$ for each $p \in \mathbb{N}$. On extracting the diagonal sequence $(f_{n_j}^{(j)})$ we find that this sequence converges at every z_n. Let us define $(g_j) \equiv (f_{n_j}^{(j)})$; we now show that the sequence (g_j) converges uniformly on compact sets.

Let $K \subset G$ be compact. We prove that $\mathscr{F}$ is equicontinuous on K. Let Γ be the boundary of a closed disk of radius r contained in G. If $z, z_0 \in \Gamma$, then by Cauchy's integral formula we have

$$\begin{aligned} f(z) - f(z_0) &= \frac{1}{2\pi i} \int_\Gamma \left(\frac{1}{\zeta - z} - \frac{1}{\zeta - z_0} \right) f(\zeta) \mathrm{d}\zeta \\ &= \frac{z - z_0}{2\pi i} \int_\Gamma \frac{f(\zeta)\mathrm{d}\zeta}{(\zeta - z)(\zeta - z_0)}. \end{aligned}$$

If we restrict z and z_0 to the smaller concentric disk of radius $r/2$, then since $|f| \leq M$ on Γ we have the following inequality:

$$|f(z) - f(z_0)| \leq 4M|z - z_0|/r. \tag{C.1}$$

Equation (C.1) shows equicontinuity on the smaller disk. Now, each point in K is the centre of a disk with radius r as described. The open disks of radius $r/4$ form an open covering of K. We may choose a finite subcovering and denote the centres, radii, and bounds by ζ_j, r_j, and M_j respectively. Let r be the smallest of the r_j and M the largest of the M_j. For each $\varepsilon > 0$ let δ be the smaller of $r/4$ and $\varepsilon r/4M$. If $|z - z_0| < \delta$ and $|z_0 - \zeta_j| < r_j/4$, then $|z - \zeta_j| = |z - z_0 + z_0 - \zeta_j| < \delta + r_j/4 \leq r_j/2$. Hence, (C.1) applies and we find that $|f(z) - f(z_0)| < 4M_j\delta/r_j \leq 4M\delta/r \leq \varepsilon$ as required.

Since $\mathscr{F}$ is equicontinuous on K, there exists a $\delta > 0$ such that $|g_n(z) - g_n(z')| < \varepsilon/3$, $n \in \mathbb{N}$, whenever $z, z' \in K$ with $|z - z'| < \delta$. Additionally, we know that $K \subset \bigcup_{j=1}^{j_0} \mathrm{D}(z_j; \delta)$. Therefore, there is an $N \in \mathbb{N}$ such that $n, m \geq N$ implies $|g_n(z_j) - g_m(z_j)| < \varepsilon/3$ for $j = 1, 2, \ldots j_0$. Finally, for any $z \in K$, $z \in \mathrm{D}(z_i; \delta)$ for some $i \in [1, j_0]$ and so

$$\begin{aligned} |g_n(z) - g_m(z)| &\leq |g_n(z) - g_n(z_i)| + |g_n(z_i) - g_m(z_i)| + |g_m(z_i) - g_m(z)| \\ &< \varepsilon/3 + \varepsilon/3 + \varepsilon/3 = \varepsilon. \end{aligned}$$

We conclude that (g_n) converges uniformly on K to a function which is analytic by the Analytic Convergence Theorem (Theorem C.2). □

APPENDIX D

Some Results on Entire Functions

D.1 The Zeros of an Entire Function

The fact that an entire function has finitely many zeros in any compact set may be demonstrated with the aid of the following preliminary result [Holland, 1973, p. 16]:

Theorem D.1. *Suppose $f(z)$ is a non-zero entire function, then for all $z = z_0 \in \mathbb{C}$ there exists a disk centred at z_0 in which $f(z)$ has no zeros, except possibly at $z = z_0$ itself.*

Proof. Suppose $f(z_0) \neq 0$, then $|f(z_0)| > 0$. Since f is continuous, there exists a disk centred at z_0 such that $|f(z) - f(z_0)| < \varepsilon$ for all $\varepsilon > 0$. Thus,

$$\begin{aligned} |f(z)| &= |f(z_0) + [f(z) - f(z_0)]| \\ &\geq |f(z_0)| - |f(z) - f(z_0)| \\ &> |f(z_0)| - \varepsilon. \end{aligned}$$

Taking $\varepsilon = |f(z_0)|$, we get $|f(z)| > 0$, which means that $|f(z)| \neq 0$. Therefore, for $f(z_0) \neq 0$ there exists a disk centred at z_0 containing no zeros of f. Furthermore, suppose $f(z_0) = 0$ and m is the order of the zero at $z = z_0$. Then $f(z) = (z - z_0)^m g(z)$ where g is entire and $g(z_0) \neq 0$. Thus, there exists a disk centred at z_0 such that $g(z) \neq 0$. Therefore, f has no zeros other than z_0 inside this disk. □

Theorem D.2 (Holland [1973] p. 17). *An entire function f cannot have infinitely many zeros in any closed disk of finite radius.*

Proof. Assume to the contrary, namely, that f has infinitely many zeros in the closed disk $\overline{\mathrm{D}}(0; r)$. By the Bolzano-Weierstrass Theorem, there exists a z_0 in this disk which is a point of accumulation of the set of zeros of f. Thus, in an any disk centred at z_0 there are infinitely many zeros of f; this is at odds with Theorem D.1. □

D.2 A Lemma on the Growth Order

This section provides a brief study of the growth order of an entire function with the aim of proving a lemma required in Chapter 4; since the majority of the results leading up to this lemma are well-known, they are presented without proof.

Our discussion begins with the basic notion of the upper limit (limit superior) of a real sequence (x_n), denoted by $\limsup_{n\to\infty} x_n$. It is defined as follows: if (x_n) is unbounded above, then we set $\limsup_{n\to\infty} x_n = +\infty$; otherwise, define $x_N^+ \equiv \sup_{n\geq N} x_n$, which means (x_N^+) is a non-increasing sequence so that the limit $\lim_{N\to\infty} x_N^+$ exists. We then set $\limsup_{n\to\infty} x_n = \lim_{N\to\infty} x_N^+$. An alternative and perhaps more practical definition is as follows: $\limsup_{n\to\infty} x_n = +\infty$ if (x_n) is unbounded above; $\limsup_{n\to\infty} x_n = -\infty$ if $x_n \to -\infty$ as $n \to \infty$; or $\limsup_{n\to\infty} = x$ (x finite) if, given any $\varepsilon > 0$, we have $x_n < x+\varepsilon$ for all sufficiently large n and $x_n < x - \varepsilon$ for some arbitrarily large n.

In anticipation of the language used in the theory of entire functions, we introduce the concepts of genus and canonical products. The following definition is quite standard in complex analysis and can be found in, for example, Holland [1973].

Definition D.1. *Given an infinite sequence of complex numbers (z_n) with $z_n \neq 0$ for all n, $|z_n| \to \infty$ as $n \to \infty$ and $\sum_{n=1}^{\infty} 1/|z_n|^{h+1}$ converges for some integer h, its genus is defined as the smallest non-negative integer k such that $\sum_{n=1}^{\infty} 1/|z_n|^{k+1}$ converges. If the z_n arise as the zeros of an entire function, then k is referred to as the genus of the entire function. Given such a sequence (z_n) of genus k, the corresponding product*

$$\prod_{n=1}^{\infty}\left(1-\frac{z}{z_n}\right)\exp\left(\frac{z}{z_n}+\frac{z^2}{2z_n^2}+\cdots+\frac{z^k}{kz_n^k}\right)$$

is called the canonical product corresponding to the sequence.

An important theorem linking genus, canonical products, and entire functions is the following, which is a stronger version of Weierstrass's Factorization Theorem.

Theorem D.3 (Markushevich [1965] p. 287). *If f is an entire function of genus k with the sequence (z_n) as its non-zero zeros, and a zero of order m at the origin (set $m = 0$ if $z = 0$ is not a zero), then*

$$f(z) = z^m\prod_{n=1}^{\infty}\left(1-\frac{z}{z_n}\right)\exp\left(\frac{z}{z_n}+\frac{z^2}{2z_n^2}+\cdots+\frac{z^k}{kz_n^k}\right)$$

where the right side is called the canonical product corresponding to f.

Probably the most fundamental property associated with a transcendental entire function $f(z)$—we refer to an entire function as being transcendental in order to emphasize that we are considering entire functions that are not polynomials—is the maximum modulus function. It is defined for $r \geq 0$ by

$$M(r) \equiv \max_{|z|=r} |f(z)|.$$

Unless $f(z)$ is a constant function, $M(r)$ is a strictly increasing function of r which, by Liouville's Theorem on bounded entire functions, is such that $M(r) \to \infty$ as $r \to \infty$. Moreover, the maximum modulus function satisfies [Markushevich, 1965, p. 250]

$$\frac{M(r)}{r^{\mu}} \to \infty, \quad r \to \infty$$

for every $\mu \geq 0$. Thus, whilst it is natural to compare $M(r)$ with r^n for polynomials, we clearly require more rapid growth for use with transcendental entire functions. Since $\exp(z), \exp(z^2), \exp(z^3), \ldots$ are relatively simple entire functions with maximum modulus functions $\exp(r), \exp(r^2), \exp(r^3), \ldots$, it is natural to use $\exp(r^{\rho})$ for comparison with transcendental entire functions. Loosely speaking, a function will be called of order ρ if its maximum modulus function grows like $\exp(r^{\rho})$. To make this more precise we have the following definition [Markushevich, 1965, pp. 250–251]:

Definition D.2. *If $f(z)$ is entire with maximum modulus $M(r)$ and there exists a number $\rho \geq 0$ such that, given any $\varepsilon > 0$, we have $M(r) < \exp\{r^{\rho+\varepsilon}\}$ for all sufficiently large r and $M(r) > \exp\{r^{\rho-\varepsilon}\}$ for some arbitrarily large r. Then we say that f is of finite order, namely, ρ; if no such ρ exists then f is said to be of infinite order.*

If the maximum modulus function is given by $M(r) = \exp(r^{\rho})$, then $\log M(r) = r^{\rho}$ and so $\log \log M(r) = \rho \log r$, which implies that

$$\rho = \frac{\log \log M(r)}{\log r}, \quad r > 0$$

provided $M(r) > 1$. An equivalent definition is thus

$$\rho = \limsup_{r \to \infty} \frac{\log \log M(r)}{\log r}. \tag{D.1}$$

Equation (D.1) is not quite equivalent to Definition D.2; this is because of the restriction on $M(r)$ to be greater than 1. However, since $M(r) \to \infty$ as $r \to \infty$ unless we have a constant function, the only exceptions are the constant functions $f(z) = C$ with $|C| \leq 1$. We assume that we are dealing with entire functions a little more complicated than these. A result which will be most useful in the development of the lemma we require is the following, which can be found in Boas [1954] p. 9.

Theorem D.4. *Suppose f_1 and f_2 are entire functions of orders ρ_1 and ρ_2 respectively, and ρ is the order of their product $f_1 f_2$. Then $\rho \leq \max\{\rho_1, \rho_2\}$.*

We require the introduction of one more quantity: the exponent of convergence. This is also a standard concept and we take its definition from [Markushevich, 1965, p. 285].

Definition D.3. *Let (z_n) be an infinite sequence with $z_n \neq 0$ for all n and $|z_n| \to \infty$ as $n \to \infty$. Suppose there exists a number $\rho_c \geq 0$ such that $\sum_{n=1}^{\infty} 1/|z_n|^{\rho_c+\varepsilon}$ converges for all $\varepsilon > 0$, but $\sum_{n=1}^{\infty} 1/|z_n|^{\rho_c-\varepsilon}$ diverges for all $\varepsilon > 0$. Then we call ρ_c the exponent of convergence of the sequence (z_n). If (z_n) is the sequence of non-zero zeros of an entire function f, then ρ_c is called the exponent of convergence of the zeros of f. For a finite sequence, convention dictates that $\rho_c = 0$.*

Every sequence of finite genus has an exponent of convergence and conversely, every infinite sequence for which an exponent of convergence exists is of finite genus. In one sense, the exponent of convergence is a more precise measure of the growth of $|z_n|$ than its genus, for it need not be an integer. For example, the sequence $1^2, 2^2, 3^2, \ldots$ has exponent of convergence 1/2, this is because $\sum 1/(n^2)^{1/2+\varepsilon}$ converges but $\sum 1/(n^2)^{1/2-\varepsilon}$ diverges for all $\varepsilon > 0$; however, this sequence has genus zero since $\sum 1/n^2$ converges. On the other hand, we have no information about the convergence of $\sum 1/|z_n|^{\rho_c}$, whilst we do know that $\sum 1/|z_n|^{k+1}$ converges. A useful characterization of the exponent of convergence is given by the following result [Markushevich, 1965, p. 285]:

Theorem D.5. *Let (z_n) be an infinite sequence with $z_n \neq 0$, $|z_n| \leq |z_{n+1}|$ for all n, and $|z_n| \to \infty$ as $n \to \infty$. Then, if (z_n) has exponent of convergence ρ_c, we have*

$$\rho_c = \limsup_{n\to\infty} \frac{\log n}{\log |z_n|}$$

and conversely.

A direct consequence of Theorem D.5 is

Theorem D.6. *Defining $n(r)$ to be the zero counting function, i.e. $n(r)$ gives the number of zeros of an entire function f in $|z| \leq r$, we have*

$$\rho_c = \limsup_{r\to\infty} \frac{\log n(r)}{\log r}.$$

Let us now exhibit two famous theorems due to J S Hadamard [Markushevich, 1965, pp. 288–289]; they will be of utmost importance in the proof of our lemma.

Theorem D.7 (Hadamard's First Theorem). *If an entire function is of order ρ and ρ_c is the exponent of convergence of its zeros, then $\rho_c \leq \rho$.*

Theorem D.8 (Hadamard's Factorization Theorem). *Let f be an entire function of order ρ with an infinite number of zeros. Then we have*

$$f(z) = z^m \exp\{Q(z)\} P(z)$$

where $P(z)$ is the canonical product formed using the non-zero zeros of f, and $Q(z)$ is a polynomial of degree at most ρ.

In the Hadamard factorization $f(z) = z^m \exp\{Q(z)\}P(z)$, suppose f is of order ρ with exponent of convergence of its zeros ρ_c, and Q to be of degree q. By Borel's Theorem on the order of canonical products [Holland, 1973, p. 71] we find that P is of order ρ_c; we also know that the order of $\exp\{Q\}$ is q [Markushevich, 1965, pp. 253–254]. As a consequence, $\rho \leq \max\{q, \rho_c\}$ by Theorem D.4. However, Hadamard's First Theorem says that $\rho_c \leq \rho$, whilst Hadamard's Factorization Theorem says that $q \leq \rho$, whence $\rho \geq \max\{q, \rho_c\}$. We must conclude that $\rho = \max\{q, \rho_c\}$. These observations will be indispensable when proving the next theorem[1], which in turn is used to prove the subsequent desired lemma.

Theorem D.9. *If f_1 and f_2 are entire functions of orders ρ_1 and ρ_2 respectively with $\rho_1 > \rho_2$, then the order of their product $f_1 f_2$ is ρ_1.*

Proof. Suppose the Hadamard's factorizations to be $f_1(z) = z^{m_1} \exp\{Q_1(z)\}P_1(z)$ and $f_2(z) = z^{m_2} \exp\{Q_2(z)\}P_2(z)$, where the $P_i(z)$ are canonical products. Then,

$$f_1(z)f_2(z) = z^{m_1+m_2} \exp\{Q_1(z) + Q_2(z)\}P_1(z)P_2(z). \tag{D.2}$$

Let ρ be the order of $f_1 f_2$, then there are two cases to consider: either the order of $P_1(z)$ is ρ_1 or else it is less than ρ_1. Suppose $P_1(z)$ is of order ρ_1 so that ρ_1 is the exponent of convergence of its zeros. Adding in the zeros of $P_2(z)$ cannot decrease the exponent of convergence of the zeros—as can be seen from Theorem D.6. Thus, the exponent of convergence of the zeros of $f_1 f_2$, say $\hat{\rho}$, is at least ρ_1. Hadamard's First Theorem tells us that $\rho_1 \leq \hat{\rho} \leq \rho$, but we already know that $\rho \leq \rho_1$ and so $\rho = \rho_1$.

Alternatively, suppose $P_1(z)$ is of order less than ρ_1. Now, ρ_1 is equal to the maximum of the degree of $Q_1(z)$ and the order of $P_1(z)$, which implies that ρ_1 is the degree of $Q_1(z)$ and is an integer. Since the degree of $Q_2(z)$ is smaller than ρ_1, the degree of $Q_1(z) + Q_2(z)$ is ρ_1. Note that $P_1(z)P_2(z)$ is of order less than ρ_1 and again use Hadamard to write $P_1(z)P_2(z) = \exp\{Q_3(z)\}P_3(z)$, where $P_3(z)$ is the canonical product associated with the zeros of both $P_1(z)$ and $P_2(z)$ and is of order less than ρ_1, and $Q_3(z)$ is a polynomial of degree less than ρ_1. The product factorization (D.2) therefore becomes

$$f_1(z)f_2(z) = z^{m_1+m_2} \exp\{Q_1(z) + Q_2(z) + Q_3(z)\}P_3(z) \tag{D.3}$$

where $Q_1(z) + Q_2(z) + Q_3(z)$ is of degree ρ_1, whilst $P_3(z)$ is a canonical product of order less than ρ_1. Now, equation (D.3) is the Hadamard factorization of $f_1 f_2$, which implies that $\rho_1 \leq \rho$ but also $\rho \leq \rho_1$ by Theorem D.4, whence $\rho = \rho_1$. □

Lemma 1. *Suppose that f_1 is entire, f_2 is entire with order 1 and $f_1 f_2$ is of order 1, then f_1 is of order at most 1.*

Proof. Assume to the contrary, namely that f_1 is of order $\rho > 1$. Then by Theorem D.9, $f_1 f_2$ would be of order ρ, which is impossible. □

[1]This result was found in Edinburgh lecture notes from 1986, the lecturer was Stanley Richardson. Attempts to find an official citation for this theorem and its proof were in vain.

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