

Analytic properties of the Jost functions

by Yannick Mvondo-She

Submitted in partial fulfilment of the requirements for the degree Magister Scientiae in the Faculty of Natural and Agricultural Sciences University of Pretoria Pretoria

April 2013



Declaration

I, the undersigned, hereby declare that the dissertation submitted herewith for the degree Magister Scientiae to the University of Pretoria contains my own, independent work and has not been submitted for any degree at this or any other university.

Signature:

Name:

Date:



Acknowledgments

Remember how the Lord your God led you all the way in the desert these forty years, to humble you and to test you in order to know what was in your heart, whether or not you would keep his commands. He humbled you, causing you to hunger and then feeding you with manna, which neither you nor your fathers had known, to teach you that man does not live on bread alone but on every word that comes from the mouth of the Lord. Your clothes did not wear out and your feet did not swell during these forty years. Know then in your heart that as a man disciplines his son, so the Lord your God disciplines you.

Observe the commands of the Lord your God, walking in his way and revering him. For the Lord your God is bringing you into a good land-a land of streams and pools of water, with springs flowing in the valleys and hills.

(Deuteronomy 8:2-7)

Heavenly Father, thank you for, through the good and the bad, you always stood by me, and allowed me to bring this work to completion. Blessed be your name.

I am deeply indebted to my supervisor Professor P. Selyshchev and to my co-supervisor Professor S.A. Rakitiansky, for having involved me in such an interesting project. Thank you for the financial support, for your patience and for the freedom you gave me while working on the project.

My sincere appreciation is expressed to the Pretoria East Church Connect Group for blessing me with the Word of God every Thursday evening and for spiritual growth.

To my family in Cameroon, in France and in the french West Indies, thank you very much for your love and your encouragement.

My last word of thanks goes to my mother, to whom I owe a great debt of gratitude for a life of sacrifice: "Maman, à travers ce petit ouvrage que je te dédie, peut être pouvons nous nous inspirer de Romains 8:18, et nous dire que les souffrances du temps présent (et surtout passé) ne sauraient être comparable à la gloire qui nous sera révélée. Merci beaucoup Maman pour tout ce que tu as fait pour moi."



Title: On some analytic properties of the Jost functions Student: Yannick Mvondo-She Supervisor: Professor Pavel Selyshchev Co-supervisor: Professor Sergei Rakitianski Department: Physics Degree: MSc

Abstract

Recently, was developed a new theory of the Jost function, within which, it was split in two terms involving on one side, singlevalued analytic functions of the energy, and on the other, factors responsible for the existence of the branching-points. For the single-valued part of the Jost function, a procedure for the powerseries expansion around an arbitrary point on the energy plane was suggested. However, this theory lacks a rigorous proof that these parts are entire functions of the energy. It also gives an intuitive (not rigorous) derivation of the domain where they are entire. In the present study, we fill this gap by using a method derived from the method of successive approximations.

Résumé

Récemment, une nouvelle théorie sur les fonctions de Jost a été développée, dans laquelle, les fonctions de Jost sont divisée en deux parties, avec d'une part des fonctions uniformes (univaluées et analytiques) de l'energie, et d'autre part, des facteurs responsables de l'existence de points de ramification. Une procédure permettant le développement en série de la partie contenant les fonctions analytiques de l'énergie autour d'un point quelconque du plan complexe de l'énergie a notamment été suggérée. Cependant, cette théorie souffre d'une preuve rigoureuse de l'analyticité de ces fonctions. La théorie permet également d'obtenir, là encore de facon intuitive, le domaine d'analyticité de ces fonctions. Nous nous proposons donc, à l'aide d'une méthode dérivée de celle des approximations successives de démontrer que ces fonctions sont analytiques dans un domaine particulier que nous déterminerons de facon explicite.



List of Figures

2.1	Function $f(x)$	15
2.2	Path taken by Δz	15
2.3	The energetic Riemann surface	23
2.4	Domain of expansion of the analytic function $f(z)$ in power	
	series	25
2.5	Analytic continuation of $f(z)$ along a path	25
2.6	Rectangular domain R surrounding the point (x_0, y_0)	27
	~ ~ ~	
4.1	Domain of analyticity of the functions $A_l(E,\infty)$ and $B_l(E,\infty)$	53



Contents

1	Intr	oduction	2
	1.1	Historical background	2
	1.2	The Jost function	4
		1.2.1 Basic concepts	4
		1.2.2 Boundary conditions	6
	1.3	Transformation of the Schrödinger equation	7
		1.3.1 Factorization	11
		1.3.2 Analytic properties of the Jost function	13
2	Mat	thematical background	14
	2.1	Functions of a complex variable	14
		2.1.1 Analytic function	14
		2.1.2 Single-valued and many-valued functions	17
		2.1.3 Riemann surfaces	20
		2.1.4 Factorization revisited	21
		2.1.5 Properties of analytic functions	24
	2.2	Existence and nature of solutions of ordinary differential equa-	
		tions	26
		2.2.1 Background	26
		2.2.2 The existence theorem	27
	2.3	The method of successive approximations	28
	2.4	Gronwall inequality	33
		2.4.1 Gronwall Lemma $[34]$	33
	2.5	On certain methods of successive approximations	34
	2.6	A general theorem on linear differential equations that depend	
		on a parameter	34
	2.7	Extension of the method of successive approximation to a sys-	
		tem of differential equations of the first-order; vector-matrix	
		notation \ldots	36
		2.7.1 A glance at existence and uniqueness	36
		2.7.2 Application to linear equations	37
		2.7.3 Vector-matrix notation	37
	2.8	Norms of matrices	38



1

CONTENTS

	2.8.1 An inequality involving norms and integrals	39
3	Analyticity of the functions $\tilde{A}_l(E,r)$ and $\tilde{B}_l(E,r)$ 3.1 Existence and uniqueness	41 42 44
4	Analyticity of the functions $\tilde{A}_l(E,\infty)$ and $\tilde{B}_l(E,\infty)$ 4.1 Asymptotics of the Ricatti-Bessel and of the Ricatti-Neumann	47
	functions	48
5	Conclusion	54



Chapter 1

Introduction

1.1 Historical background

By the past, as a conventional way to treat quantum collision processes, common practice was to focus on the scattering amplitude of the physical wave function [1] [2]. Yet, the analysis of non relativistic quantum mechanical problems can be done adequately in terms of the Jost functions, and the Jost solutions of the Schrödinger equation. The Jost function was introduced in 1947 by Res Jost [3]. It can be described in substance as a complex function of the total energy of a quantum state, where the energy is allowed to have not only real but also complex values [4]. The Jost functions, when defined for all complex values of the momentum possess all information about a given physical system. An interesting feature in the Jost function approach is that it allows a simultaneous treatment of bound, virtual, scattering and resonance states.

Abundant litterature on Scattering Theory has chapters devoted to the Jost function, where usually it is expressed either via an integral containing the regular solution [1] [2], or via a Wronskian of the Jost solutions [5]. In all cases, they are expressed in terms of the wave function. But to make use of the Jost functions in such a form, one must find the wave function first. This means that the problem is practically solved and nothing more is needed [6]. Hence in spite of the usefulness of the Jost functions in studying spectral properties of hamiltonians, for quite some time they were regarded rather as purely mathematical entities, elegant and useful in formal scattering theory [7], but with no computational use.

In the early nineteen nineties, linear first-order differential equations for functions closely related to the Jost solutions were proposed [8]. Based on the variable-phase approach [9], the equations and their solutions provide the Jost function at any fixed value of the radial variable r, and its complex



conjugate counterpart, which corresponds to the potential truncated at the point r. An inconvenience though, was that the method was suitable only for bound and scattering state calculations, meaning, for calculations in the upper-half of the complex plane and on the real axis. An extension of the method to the unphysical sheet was proposed in [10], in order to include the resonant state region. Such development was made by combining the variable constant method [11], and the complex coordinate rotation method [12].

As a result, the combination used to recast the Schrödinger equation into a set of linear first ordered coupled equations for Jost type solutions allowed for a treatment of all possible states in a unified way. Conclusive tests confirmed the effectiveness of the approach, in particular, in locating bound states and resonances, through numerical integrations of the derived equations in order to obtain the Jost functions (Jost matrices in the case of multichannels) for all momenta of physical interest.

Although the method enjoyed success, it also had drawbacks. One of them concerned the point k = 0 at which the proposed equations are singular. The method was thereafter refined by using a procedure taken from [13]. The prescription lies in the fact that within a small region around k = 0, the Ricatti-Hankel functions $h_l^{(\pm)}(kr)$ can be expanded in power series [14], and each term therein can be factorized in k and r. Similarly, the Jost functions can be expanded in powers of k with unknown r-dependent coefficients in this region, the coefficients being specified by the resulting system of k-independent differential equations. This is of a crucial importance in fields such a Quantum few-Body Theory, especially when it comes to locating quantum resonances...

Historically, after the advent of Quantum Mechanics, attention to resonance states was first drawn by nuclear physicists. In particular, we can think of George Gamow's seminal work on the α -decay. The role of quantum resonances in Solid State and Chemical Physics for instance was understood much later [15] [16]. More recently, efforts in a Condensed Matter and Molecular Physics oriented research have converged to construct the solutions of the set of first order differential equations in the form of Taylor-type power series near an arbitrary point on the Riemann surface of the energy [17], in a way that is similar to the effective expansion range, but more generalized.

A fundamental point in the expansion of a function, is the analycity of the given function. For all the aforementionned work, it was given that the Jost function is analytic at all complex energies and that for the so called spectral points, it has simple zeros. The spectral points being the energies



at which the system forms bound and resonant states, the location of the bound states and the resonances is done by calculating the Jost function and the points of its zeros. Yet, the analytic properties of the Jost functions suffers a lack of rigorous treatment. A special attention to the problem will be given here.

1.2 The Jost function

1.2.1 Basic concepts

A range of macroscopic phenomena can be described on the basis of nonrelativistic Quantum Mechanics. Molecular, Atomic, Nuclear and Solid State phenomena span this range.

At a given time t, the state of a physical system can be described within the framework of non-relativistic Quantum Mechanics, by a complex-valued wave function $\Psi(\vec{r}, t)$, where the wave function Ψ depends on the timeparameter t, and on a complete set of variables summarized as \vec{r} . The physical system can usually be found in a quantum state, which is characterized by a full set of quantum numbers, such as total energy, angular momentum, etc,... The hermitian operator \hat{H} that describes the energy of a system is the Hamiltonian. It consists of the kinetic energy operator

$$\widehat{T} = \sum_{i=1}^{N} \frac{\widehat{p}_i^2}{2m_i},$$
(1.1)

of a system of N spinless particles of mass m_i and momentum p_i , of a potential energy operator \hat{V} , which is in general the function of the N interparticles displacement vectors (plus a potential generated by an external field, if any)

$$\widehat{H} = \widehat{T} + \widehat{V}.\tag{1.2}$$

The hamiltonian of a physical system determines its evolution in time. In coordinate representation, the evolution of a state is described by a partial differential equation, the *Schrödinger equation*

$$\widehat{H}\Psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t}\Psi(\vec{r},t).$$
(1.3)

For a time-independent Hamiltonian \hat{H} , the wave function

$$\Psi(\vec{r},t) = \exp\left(-\frac{i}{\hbar}Et\right)\psi\left(\vec{r}\right)$$
(1.4)



is said to be a solution of the Schrödinger equation (1.3), if and only if $\psi(\vec{r})$ is an eigenfunction of \hat{H} , with eigenvalue E, such that

$$\widehat{H}\psi(\vec{r}) = E\psi\left(\vec{r}\right). \tag{1.5}$$

Equation (1.5) is called the *time-independent*, or *stationary Schrödinger* equation. For a point particle in a radially symmetric potential $V(\vec{r})$, in coordinate representation, the time-independent Schrödinger equation is

$$\left(-\frac{\hbar^2}{2\mu}\Delta_r + V(r)\right)\psi(\vec{r}) = E\psi(\vec{r}).$$
(1.6)

It is possible with the help of the orbital angular momentum \hat{L} , to express the Laplacian operator $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{-\hat{p}^2}{\hbar^2}$ in spherical coordinate

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{-\vec{L}^2}{r^2\hbar^2}.$$
(1.7)

The square and the z-component of the angular momentum, respectively $\hat{\vec{L}}^2$ and \hat{L}_z being constants of motion, the solutions of the Schödinger equation (1.5) can be labelled by the good quantum numbers l and m, and the energy E, to give [1] [2] [5]

$$\psi(\vec{r}) = \phi_l(E, r) Y_{l,m}(\theta, \varphi). \tag{1.8}$$

In equation (1.8), the so-called *spherical harmonic* function $Y_{l,m}(\theta, \varphi)$ is an eigenfunction of both operators $\hat{\vec{L}}^2$ and \hat{L}_z , while l and m are eigenvalues of $\hat{\vec{L}}^2$ and \hat{L}_z respectively. The solutions of the stationary Schrödinger hence have a radial part in $\phi_l(E, r)$ and an angular part from the spherical harmonic function expressed in terms of θ and φ , the polar angles of \vec{r} . Inserting (1.8) into (1.6) leads to an equation for the *radial wave function*

inserting (1.3) into (1.5) leads to an equation for the value function
$$\phi_l(E,r)$$

$$\left[-\frac{\hbar}{2\mu}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right]\phi_l(E,r) = E\phi_l(E,r), \quad (1.9)$$

that is independent of the azimutal quantum number m.

The ordinary differential equation of second order for the radial wave function $\phi_l(E, r)$ (1.9) is called the *radial Schrödinger equation*. It provides a

5



significant simplification of the partial differential equation (1.6). Yet, with a little bit more algebra a greater simplification can be obtained by formulating an equation not for $\phi_l(E, r)$, but for $u_l = r\phi_l$, i.e for the radial wave function of $u_l(r)$ defined by

$$\psi(\vec{r}) = \frac{u_l(E,r)}{r} Y_{l,m}(\theta,\varphi). \tag{1.10}$$

We end up with the following expression of the radial Schrödinger equation

$$\left(-\frac{\hbar}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right)u_l(E,r) = Eu_l(E,r).$$
 (1.11)

Equation (1.11) is actually the Schrödinger equation for a single particle of mass μ moving in a one spatial dimension, in an effective potential consisting of V(r) plus the *centrifugal potential* $l(l+1)\hbar^2 \langle 2\mu r^2 \rangle$

$$V_{eff}(l,r) = V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}.$$
(1.12)

1.2.2 Boundary conditions

The radial Schrödinger equations (1.9) and (1.11) are defined only for nonnegative values of the radial coordinate r, *i.e* on the interval $r \in [0, \infty)$. The boundary condition imposed on the radial wave function $u_l(E, r)$ at r = 0, can be derived by inserting an ansatz $u_l(E, r) \propto r^{\alpha}$ into equation (1.11). As long as the potential V(r) is less singular than r^{-2} , the leading term on the left-hand side of the ansatz is proportional to $r^{\alpha-2}$, and vanishes only if $\alpha = l+1$ or $\alpha = -l$ [18]. The latter option must be discarded, for an infinite value of $u_l(E, r \to 0)$ would lead to an infinite contribution to the norm of the wave function near the origin; a finite value would lead to a delta function singularity coming from $\Delta\left(\frac{1}{r}\right)$ in equation (1.6), which cannot be compensated by any other term in the equation. The boundary condition imposed at r = 0 on the radial wave function is thus

$$u_l(E,0) = 0,$$
 for all *l*. (1.13)

The behaviour of the radial wave function near the origin is given by

$$u_l(E,r) \propto r^{l+1}, \qquad \text{for } r \to 0$$
 (1.14)

(for potentials that are less singular than r^{-2}). These conditions remain the same for all types of solutions. However, when



the radial coordinate tends to an infinite value, the boundary condition is different for the bound, scattering and resonant states. In particular, when the potential V(r) at large distances is less singular than r^{-2} , and therefore vanishes fast enough, the radial Schrödinger equation (1.11) becomes

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right) u_l(E,r) = 0, \qquad \text{for } r \to \infty , \qquad (1.15)$$

where k is called the *wave number* and is related to the energy by $2mE = \hbar^2 k^2$ (and therefore $\hbar \vec{k} = \vec{p}, \vec{p}$ being the momentum). Equation (1.15) is also called the *free* radial Schrödinger equation. Its general solution can be constructed as the linear combination of two linearly independent solutions $h_l^{(\pm)}(kr)$. These solutions are the Ricatti-Hankel functions, which behave exponentially

$$h_l^{(\pm)}(kr) \xrightarrow{r \to \infty} \mp i e^{\left[\pm i\left(kr - l\frac{\pi}{2}\right)\right]},$$
 (1.16)

and the general asymptotic form of $u_l(E, r)$ reads

$$u_l(E,r) \xrightarrow{r \to \infty} ah_l^{(-)}(kr) + bh_l^{(+)}(kr), \qquad (1.17)$$

where a and b are arbitrary complex numbers that by an appropriate combination determine the solution type (bound, scattering or resonant). In fact, these coefficients are complex functions of the total energy of the system and differ with the angular momenta. Equation (1.17) can then be rewritten as

$$u_l(E,r) \xrightarrow{r \to \infty} h_l^{(-)}(kr) f_l^{(in)}(E) + h_l^{(+)}(kr) f_l^{(out)}(E), \qquad (1.18)$$

with $a = f_l^{(in)}(E)$ and $b = f_l^{(out)}(E)$. These two functions are called the Jost functions. Since $h_l^{(-)}(kr)$ represents the incoming spherical wave, and $h_l^{(+)}(kr)$ the outgoing spherical wave, these two functions are just the amplitudes of the corresponding waves.

1.3 Transformation of the Schrödinger equation

At stake here is to show the analytic properties of the Jost function. This is equivalent to expressing it in such a way that all possible terms that are not analytically dependent on the energy are given explicitly. This can be done by transforming the radial Schrödinger equation (1.9) into simple differential equations of the first order. The radial Schrödinger equation reads



$$\left(\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right) u_l(E,r) = V(r)u_l(E,r).$$
(1.19)

Using a systematic method taken from the theory of Ordinary Differential Equations, and known as the method of Variation of Parameters [11] [19], we look for the unknown function $u_l(E, r)$ in special form

$$u_l(E,r) = h_l^{(-)}(kr)F_l^{(in)}(E,r) + h_l^{(+)}(kr)F_l^{(out)}(E,r), \qquad (1.20)$$

where $F_l^{(in)}(E,r)$ and $F_l^{(out)}(E,r)$ are new unknown functions. This implies that, with the Jost functions as a case of interest, we will look for an asymptotic-like solution, for it is known that at large distances, where the potential vanishes, the wave function behaves as a linear combination of the Ricatti-Hankel functions obeying the equation

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right) u_l(E,r) = 0.$$
(1.21)

So at large distances, these functions are constant.

As indicated in [10], the introduction of two unknown functions $F_l^{(in/out)}$ instead of the original unknown function u_l implies they cannot be independent. Therefore, an arbitrary condition relating them to each other can be imposed. Conveniently, using ∂_r as $\frac{d}{dr}$, the following equation can be chosen

$$h_l^{(-)}(kr)\partial_r F_l^{(in)}(E,r) + h_l^{(+)}(kr)\partial_r F_l^{(out)}(E,r) = 0.$$
(1.22)

This condition is known as the Lagrange condition in the method of Variation of Parameters. Substituting equation (1.20) into equation (1.19), and using the Lagrange condition and the Wronskian of the Ricatti-hankel function

$$h_l^{(-)}(kr)\partial_r h_l^{(+)}(kr) + h_l^{(+)}(kr)\partial_r h_l^{(-)}(kr) = 2ik, \qquad (1.23)$$

yields a coupled system of first order differential equations for the unknown functions, that are nothing else but an equivalent form of the original Schrödinger equation [10]

$$\begin{cases} \partial_r F_l^{(in)}(E,r) &= -\frac{h_l^{(+)}(kr)}{2ik} V(r) \left[h_l^{(-)}(kr) F_l^{(in)}(E,r) + h_l^{(+)}(kr) F_l^{(out)}(E,r) \right] \\ \partial_r F_l^{(out)}(E,r) &= -\frac{h_l^{(-)}(kr)}{2ik} V(r) \left[h_l^{(-)}(kr) F_l^{(in)}(E,r) + h_l^{(+)}(kr) F_l^{(out)}(E,r) \right] \end{cases}$$



While trying to find the boundary conditions that should be imposed on the functions $F_l^{(in/out)}(E,r)$, it must be remembered with the restrictions on the potential, that the physical solution $u_l(E,r)$ must be regular everywhere. This implies [17] that the wave function $u_l(E,r)$ must be zero when r is zero

$$u_l(E,r) \xrightarrow{r \to 0} 0, \tag{1.24}$$

and is proportional to the Ricatti-Bessel function at short distances

$$u_l(E,r) \propto j_l(E,r). \tag{1.25}$$

It could be argued that it is not the case because $h_l^{(+)}(kr)$ and $h_l^{(-)}(kr)$ in equation (1.20) are singular at r = 0. But their singularities can cancel each other if they are superimposed with a same coefficient [20]

$$h_l^{(+)} + h_l^{(-)} = 2j_l(kr).$$
 (1.26)

The condition

$$u_l(E,0) = 0, (1.27)$$

can only be achieved if both $F_l^{(in/out)}(E,r)$ are equal to the same constant at r=0

$$F_l^{(in)}(E,0) = F_l^{(out)}(E,0).$$
(1.28)

Since we are not concerned about their normalization, we chose any arbitrary value for the constant. We chose the constant to be $\frac{1}{2}$ for $u_l(E, r)$ to behave near the origin as the Ricatti-Bessel function, as prescribed by equation (1.26)

$$F_l^{(in)}(E,0) = F_l^{(out)}(E,0) = \frac{1}{2}.$$
(1.29)

In order to express the non-analytic dependencies of the Jost functions in an explicit form, the ansatz (1.20) can be recast by using either the Ricatti-Bessel and Ricatti-Newmann functions, $j_l(kr)$ and $y_l(kr)$, or the Ricatti-Hankel functions, that are related by

$$h_l^{(\pm)}(kr) = j_l(kr) \pm iy_l(kr).$$
(1.30)



This leads to another representation of the physical solution of equation (1.19) in the form

$$u_l(E,r) = j_l(E,r)A_l(E,r) - y_l(E,r)B_l(E,r),$$
(1.31)

equivalent to the ansatz (1.20), not only at large distances, but everywhere on the interval $r \in [0, \infty)$. When $r \to \infty$, the functions $A_l(E, r)$ and $B_l(E, r)$, and similarly $F^{(in/out)}(E, r)$ tend to r-independent constants. In particular, the asymptotic behaviour of the wave function leads to

$$u_l(E,r) \xrightarrow{r \to \infty} h_l^{(-)}(kr) f_l^{(in)}(E) + h_l^{(+)}(kr) f_l^{(out)}(E), \qquad (1.32)$$

where, when comparing equation (1.32) and equation (1.20), we see that $F^{(in/out)}(E, r)$ converge to the Jost functions when $r \to \infty$

$$\lim_{r \to \infty} F_l^{(in)}(E, r) = f_l^{(in)}(E),$$
(1.33)

and

$$\lim_{r \to \infty} F_l^{(out)}(E, r) = f_l^{(out)}(E).$$
(1.34)

The unknown functions $A_l(E, r)$ and $B_l(E, r)$ can be expressed in terms of $F^{(in/out)}(E, r)$, by using equation (1.30), and making a linear combination of the system between equation (1.23) and equation (1.24), leading to

$$\begin{cases}
A_{l}(E,r) = F_{l}^{(in)}(E,r) + F_{l}^{(out)}(E,r) \\
B_{l}(E,r) = i \left[F_{l}^{(in)}(E,r) - F_{l}^{(out)}(E,r) \right].
\end{cases}$$
(1.35)

and asymptotically to

$$\begin{cases}
A_{l}(E) = f_{l}^{(in)}(E) + f_{l}^{(out)}(E) \\
B_{l}(E) = i \left[f_{l}^{(in)}(E) - f_{l}^{(out)}(E) \right].
\end{cases}$$
(1.36)

From (1.36), a new expression of $F^{(in/out)}(E,r)$ is found as



and from which the Jost functions can be obtained, considering the asymptotic behaviour of (1.37), by writing

$$\begin{cases} f_l^{(in)}(E) = \frac{1}{2} [A_l(E) + iB_l(E)] \\ f_l^{(out)}(E) = \frac{1}{2} [A_l(E) - iB_l(E)]. \end{cases}$$
(1.38)

A new system of firt order differential equations equivalent to the system between equations (1.23) and (1.24), and to equation (1.19) is obtained for the new unknown functions $A_l(E, r)$ and $B_l(E, r)$, and reads [20]

$$\begin{cases} \partial_r A_l(E,r) = -\frac{y_l(kr)}{k} V(r) \left[j_l(kr) A_l(E,r) - y_l(kr) B_l(E,r) \right] \\ \partial_r B_l(E,r) = -\frac{j_l(kr)}{k} V(r) \left[j_l(kr) A_l(E,r) - y_l(kr) B_l^{(}E,r) \right]. \end{cases}$$
(1.39)

Following from equation (1.29), the system has the physical boundary conditions

$$A_l(E,0) = 1,$$
 $B_l(E,0) = 0.$ (1.40)

What was showed here is a simple procedure to express the Jost functions for finite range potentials. For such potentials, when large enough values of r are reached, or if the potential is cut off at a certain (large) value of r, the functions do not change anymore, and eventually give us the Jost functions.

1.3.1 Factorization

The main goal being to show that the Jost function can be split into two parts, one of which is analytic and can therefore be expressed in power-series expansion, a further transformation of equation (1.39) is required to explicitly separate the non-analytic factors. Using the fact that the Ricatti-Bessel and Ricatti-Neumann functions can be represented by absolutely convergent series [20]

$$\begin{cases} j_{l}(kr) = \left(\frac{kr}{2}\right)^{l+1} \sum_{n=0}^{\infty} \frac{(-1)^{n} \sqrt{\pi}}{\Gamma\left(l+\frac{3}{2}+n\right) n!} \left(\frac{kr}{2}\right)^{2n} = k^{l+1} \tilde{j}_{l}(E,r) \\ y_{l}(kr) = \left(\frac{2}{kr}\right)^{l} \sum_{n=0}^{\infty} \frac{(-1)^{n+l+1}}{\Gamma\left(-l+\frac{1}{2}+n\right) n!} \left(\frac{kr}{2}\right)^{2n} = k^{-l} \tilde{y}_{l}(E,r). \end{cases}$$
(1.41)



The factorized functions $\tilde{j}_l(E,r)$ and $\tilde{y}_l(E,r)$ are obtained. These functions have the advantage that they do not depend on odd powers of k, and thus are single-valued functions of the energy E. Using equation (1.41) [20], it is possible to express $A_l(E,r)$ and $B_l(E,r)$ as a linear combination of products momenta factors and new functions $\tilde{A}_l(E,r)$ and $\tilde{B}_l(E,r)$, such that equation (1.39) can be transformed. If we write

$$\begin{cases} j_l(kr) &= k^{l+1} \tilde{j}_l(E,r) \\ \\ y_l(kr) &= k^{-l} \tilde{y}_l(E,r), \end{cases}$$

equation (1.39) becomes

$$\begin{cases} \partial_r A_l(E,r) &= -\frac{k^{-l} \tilde{y}_l(kr)}{k} V(r) \left[k^{l+1} \tilde{j}_l(kr) A_l(E,r) - k^{-l} \tilde{y}_l(kr) B_l(E,r) \right] \\ \\ \partial_r B_l(E,r) &= -\frac{k^{l+1} \tilde{j}_l(kr)}{k} V(r) \left[k^{l+1} \tilde{j}_l(kr) A_l(E,r) - k^{-l} \tilde{y}_l(kr) B_l^{\dagger}(E,r) \right], \end{cases}$$

or again

$$\begin{cases} \partial_r A_l(E,r) &= -\frac{\tilde{y}_l(kr)}{k^{l+1}} V(r) \left[\tilde{j}_l(kr) k^{l+1} A_l(E,r) - \tilde{y}_l(kr) k^{-l} B_l(E,r) \right] \\ \partial_r B_l(E,r) &= -k^l \tilde{j}_l(kr) V(r) \left[\tilde{j}_l(kr) k^{l+1} A_l(E,r) - \tilde{y}_l(kr) k^{-l} B_l(E,r) \right], \end{cases}$$

which in turn gives

$$\begin{cases} k^{l+1}\partial_{r}A_{l}(E,r) &= -\tilde{y}_{l}(kr)V(r)\left[\tilde{j}_{l}(kr)k^{l+1}A_{l}(E,r) - \tilde{y}_{l}(kr)k^{-l}B_{l}(E,r)\right] \\ k^{-l}\partial_{r}B_{l}(E,r) &= -\tilde{j}_{l}(kr)V(r)\left[\tilde{j}_{l}(kr)k^{l+1}A_{l}(E,r) - \tilde{y}_{l}(kr)k^{-l}B_{l}(E,r)\right], \end{cases}$$

or

$$\begin{cases} \partial_r \left[k^{l+1} A_l(E,r) \right] &= -\tilde{y}_l(kr) V(r) \left[\tilde{j}_l(kr) k^{l+1} A_l(E,r) - \tilde{y}_l(kr) k^{-l} B_l(E,r) \right] \\ \partial_r \left[k^{-l} B_l(E,r) \right] &= -\tilde{j}_l(kr) V(r) \left[\tilde{j}_l(kr) k^{l+1} A_l(E,r) - \tilde{y}_l(kr) k^{-l} B_l(E,r) \right], \\ \text{and if we write} \end{cases}$$

 $\tilde{A}_l(E,r) = k^{l+1} A_l(E,r)$ and $\tilde{B}_l(E,r) = k^{-l} B_l(E,r),$ (1.42)

we finally have an expression



$$\begin{cases} \partial_r \tilde{A}_l(E,r) = -\tilde{y}_l(E,r)V(r) \left[\tilde{j}_l(E,r)\tilde{A}_l(E,r) - \tilde{y}_l(E,r)\tilde{B}_l(E,r) \right] \\ \partial_r \tilde{B}_l(E,r) = -\tilde{j}_l(E,r)V(r) \left[\tilde{j}_l(E,r)\tilde{A}_l(E,r) - \tilde{y}_l(E,r)\tilde{B}_l^{\dagger}(E,r) \right], \end{cases}$$
(1.43)

devoid of all momenta factors, where remains a system of first order differential equations, whose coefficients and solutions are single-valued functions of the energy E.

1.3.2 Analytic properties of the Jost function

Up to this point we have expressed the system of first-order differential equations between equations (1.23) and (1.24) by a new set of first-order differential equation (1.43). The analytic properties of the Jost functions that we are trying to establish, are subject to the proof that for any r on the interval $[0,\infty)$, the solutions of equation (1.43), namely $\tilde{A}_l(E,r)$ and $\tilde{B}_l(E,r)$, are entire (analytic single-valued) functions of the complex variable E.

The approach for this is to use a theorem taken from a treatise published in 1896 by french mathematician Emile Picard (1856-1941), based on a theory called the *Method of Approximations*. This method, although probably known to Cauchy, originates in 1838 when Joseph Liouville applied it to the case of the homogeneous linear equation of the second order [21]. The theory was extended to linear equations of order n by J. Caqué in 1864 [22], L. Fuchs in 1870 [23] and G. Peano in 1888 [24], but in its most general form (including non linear differential equations), it was developed by Picard in 1893 [25].

In particular, is found in the treatise a theorem that states [26] the following: Let a linear differential equation of the form:

$$\frac{d^n y}{dx^n} + P_1(x,k)\frac{d^{n-1}y}{dx^{n-1}} + \dots + P_n(x,k)y = Q(x,k),$$
(1.44)

where $P_i(x,k)$ (with i = 1, 2, ..., n) and Q(x,k) are continuous functions of the real variable x and single-valued analytic functions of the complex parameter k. The method of successive approximations shows that there exists a unique solution (real or not), with given initial conditions (real or not), and that if these initial conditions are independent of k, the solution is also an analytic function of k. This result was also proved by Poincaré using a different method [27].

The theorem also mentions that for a system where Q(x, k) = 0, the system of solutions formed must be independent of k-and in fact must assume numerical values- at the initial conditions.

The application of this theorem is the object of the next chapters.



Chapter 2

Mathematical background

We will discuss here, some topics that are of specific interest to us. In this view, this chapter should merely be regarded as a tool-box.

2.1 Functions of a complex variable

In trying to investigate differential equations with the help of power series, one realises quickly that a knowledge of the theory of functions of a complex variable is needed. Here, we will confine our development to the part of Complex Analysis that will be useful to our present study of the analytic properties of the solutions of the system of linear differential equations under consideration. The basic properties of Complex Functions can be found in [11].

2.1.1 Analytic function

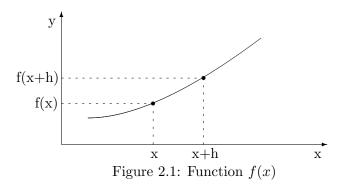
Consider a complex variable z = x + iy, where x and y are independent real variables. z usually represents a point in a complex z-plane. Let f(z) = u + iv, a function of the complex variable z be defined by associating to each point z a given complex number f(z). The function f(z) is called a *single-valued analytic function* of z, if u and v are real single-valued functions of x and y.

In Real Analysis, f(x) is usually defined as a function of a real variable x. When f(x) has a derivative, then the quotient

$$\frac{f(x+h) - f(x)}{h} \tag{2.1}$$

approaches f'(x) when h approaches zero.





In the same way, in Complex Analysis, if we write $\Delta z = z - z_0$ and $\Delta f(z) = f(z) - f(z_0) = f(z_0 + \Delta z) - f(z_0)$, it is possible to determine under which conditions the quotient $\frac{\Delta f(z)}{\Delta z}$ will approach a definite limit when the absolute value of Δz approaches zero.

By letting x and y have independent increments Δx and Δy , z will be incremented by $\Delta z = \Delta x + i\Delta y$. If $\Delta f(z)$ is a single-valued function of z, f(z) will receive an increment $\Delta f(z) = \Delta u + i\Delta v$. The derivative of f(z) with respect to z can then be expressed as

$$\frac{df(z)}{dz} = \lim_{\Delta z \to 0} \frac{\Delta f(z)}{\Delta z} = \lim_{(\Delta x, \Delta y) \to (0,0)} \frac{\Delta u + i\Delta v}{\Delta x + i\Delta y},$$
(2.2)

where the limit, if it exists, must have a single value, which is independent of the path taken by Δz (or Δx and Δy) to approach zero. This means that the limit in equation (2.2) is a double limit with respect to the increments Δx and Δy .

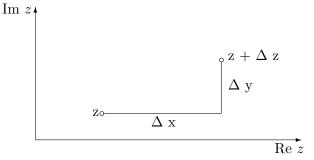


Figure 2.2: Path taken by Δz

The existence of a double limit implies that the corresponding iterated limits also exist and are equal. Let Δx and Δy in figure (2.2) approach zero in the following way: first $\Delta y \to 0$, then $\Delta x \to 0$. Letting Δz in that way allows to write



$$\frac{dw}{dz} = \lim_{\Delta x \to 0} \lim_{\Delta y \to 0} \frac{\Delta u + i\Delta v}{\Delta x + i\Delta y}$$
$$= \lim_{\Delta x \to 0} \frac{\Delta u + i\Delta v}{\Delta x}$$
$$= \lim_{\Delta x \to 0} \frac{\Delta u}{\Delta x} + i \lim_{\Delta x \to 0} \frac{\Delta v}{\Delta x}.$$

Therefore, if the derivative exists, it will have the value

$$\frac{dw}{dz} = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}.$$
(2.3)

Similarly, if the limit in equation (2.2) exists, it can identically be evaluated by letting $\Delta x \to 0$ first and then $\Delta y \to 0$. Thus

$$\begin{array}{lll} \displaystyle \frac{dw}{dz} & = & \displaystyle \lim_{\Delta y \to 0} \displaystyle \lim_{\Delta x \to 0} \displaystyle \frac{\Delta u + i\Delta v}{\Delta x + i\Delta y} \\ & = & \displaystyle \lim_{\Delta y \to 0} \displaystyle \frac{\Delta u + i\Delta v}{i\Delta y} \\ & = & -i \displaystyle \lim_{\Delta y \to 0} \displaystyle \frac{\Delta u}{\Delta y} + \displaystyle \lim_{\Delta y \to 0} \displaystyle \frac{\Delta v}{\Delta y}, \end{array}$$

and if the derivative exists, it has the value

$$\frac{dw}{dz} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}.$$
(2.4)

Now, if the derivative exists throughout some region including the point z, equations (2.3) and (2.4) must then be identical in that region, u and v being real functions of the real variables x and y, it is possible to equate real and imaginary parts in the equations (2.3) and (2.4). This yields

$$\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = -i\frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}.$$
(2.5)

Then, if the first derivatives of u and v with respect to x and y are continuous at a point, a necessary and sufficient condition for the existence of the derivative at the given point is that u and v satisfy the Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \tag{2.6}$$

$$\frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}, \qquad (2.7)$$



throughout some neighbourhood of the point.

From this, it can be inferred that a function is analytic at the point $z = z_0$ if and only if the above derivative exits at each point in some neighbourhood of the point. A function that is analytic at every point of a region is said to be analytic in that region.

2.1.2 Single-valued and many-valued functions

In defining the analytic function of a complex variable z, we have considered a function f(z) that has assigned to it a definite value for each point z of a connected region, such that f(z) has a continuous derivative in the region. These conditions led to the definition of a single-valued analytic function of z in the domain. It follows that

$$e^z, \cos z, \sin z, \cosh z, \sinh z,$$
 (2.8)

are single-valued analytic functions in the entire plane, as they all have continuous derivative for any z [28]. In the same way,

$$\frac{1}{z^2 - 1}$$
 (2.9)

for instance, is a single-valued analytic function in a region formed by the whole z-plane except the zeros of the denominator $z = \pm 1$, and $\tan z$ is single-valued analytic on a region formed by the whole plane except the infinite point set

$$\dots; -7\frac{\pi}{2}; -5\frac{\pi}{2}; -3\frac{\pi}{2}; -\frac{\pi}{2}; \frac{\pi}{2}; 3\frac{\pi}{2}; 5\frac{\pi}{2}; \dots$$
 (2.10)

Suppose now that f(z) has in general more than one value assigned to it for the points of the region. f(z) is then said to be a many-valued analytic function if its values can be grouped in *branches*, each of which is a singlevalued analytic function about each point of the region [28].

To understand the nature of a many-valued function, we can use the fact that an analytic function is necessarily continuous at all points at which it is analytic. Using a geometrically suggestive approach, the idea of continuity can be expressed by taking into consideration the fact that the value of a function of the variable z does not always depend entirely upon the value of z alone, but to a certain extent also upon the successive values assumed by the z, when going from the initial value to the actual value in consideration [32], in other words, upon the path taken by the variable z.

This leads to a new definition: an analytic function f(z) is said to be singlevalued in a region when all paths in that region which go from a point z_0

17



to any other point z lead to the same final value for f(z). When on the other hand, the final value of f(z) is not the same for all possible paths in the region, the function is said to be many-valued. An important statement in connection with this is found in [32]: a function that is analytic at every point of a region is necessarily single-valued in that region.

Now, if the path from z_0 to z describes a closed circuit, and we return to our point of departure after having gone through the path, there are two possibilities: either we arrive again at the same value of the function, and we there have a necessary and sufficient condition for a function to be singlevalued analytic at every point of a region, or we do not. In this case, we have many-valued function and $f(z_0)$ will have at least two different meanings.

As an example, we will consider the logarithmic function $\log z$. Using polar coordinates r, θ , it can be shown [30] that

$$\log z = \log r + i(\theta + 2\pi n), \qquad n = 0, \pm 1, \pm 2, \dots$$
(2.11)

It is easy to verify that this expression satisfies the Cauchy-Riemann equations, and therefore that $\log z$ as expressed in equation (2.11) is an analytic function of z. The following equation

$$\frac{d}{dz}\left\{\log z\right\} = \frac{1}{z} \tag{2.12}$$

shows that the derivative of $\log z$ is not defined for z = 0. The origin is thus a point where the derivative of the function and the function itself cease to be continuous. It is called a *singular point* of the function.

Equation (2.11) seems to imply that there exists an infinite number of different logarithmic functions, each of them having a different value of n. In reality, they are all branches of one and the same function, and the integer nmerely accounts for the function to be many-valued. Indeed, let the value of n be arbitrarily taken as zero, and let z move in the positive direction along the circle |z| = r, starting from the point (r, 0). log r will remain constant and θ will grow continuously. When z will return to its original position, the function log z will therefore not return to its original value. Instead, we will have

$$\log z = \log r + i2\pi. \tag{2.13}$$

If starting from this value again, describing a complete circular path along |z| = r in the positive direction, the new value obtained will be

$$\log z = \log r + i4\pi. \tag{2.14}$$



The process can be repeated until a value $\log z = \log r + i2\pi n$ is obtained. This indicates that the different values of $\log z$ which are associated with the different values of n in equation (2.11) all belong to the same analytic function.

The *infinite-valued* analytic function $\log z$ can be decomposed into branches, all of which are single-valued, by restricting the value of θ to an interval of length 2π . For instance, by imposing the condition $-\pi < \theta < \pi$, a branch called the *principal value* of $\log z$ can be obtained. This would mean that the logarithmic function cannot cross the negative axis. Crossing the cut will just be like going from one branch to the other.

Another example is the function $f(z) = z^{\alpha}$, which can also be written as

$$e^{\alpha \log z}.$$
 (2.15)

The multi-valuedness of z^{α} can be observed by expressing the principal value of the logarithm as $\log z$ and writing $\log z = \log z + 2i\pi n$. Then from equation

$$e^{\alpha \log z} = e^{\alpha \log z} e^{2in\alpha\pi} = \mathbf{P}\left[\mathbf{z}^{\alpha}\right] e^{2i\alpha n\pi},\tag{2.16}$$

where $P[z^{\alpha}]$ is the principal part of the function z^{α} . The values of z^{α} are then obtained by multiplying the principal value with the factor $e^{2i\alpha n\pi}$. This shows that z^{α} will have infinitely many values. In particular, when α is a rational number of the form $\frac{m}{n}$, with m and n having no common factor and $n \geq 1$, then the set $e^{2i\alpha n\pi}$ becomes

$$e^{2\pi i \left(\frac{m}{n}\right)k},\tag{2.17}$$

contains n different numbers. This is obtained by choosing k = 0, 1, 2, ..., n-1 [30].

Geometrically, it is interesting to see how the values of z^{α} change when the point z describes a circle about the origin. Recalling the example of the logarithmic function, a given value of log z continuously changes into log $z + 2\pi i$ if z returns to its former position after describing a complete circle about the origin in the positive direction. Accordingly, a given value of z^{α} will also change into $z^{\alpha}e^{2i\alpha\pi}$. Repeating the process will yield $z^{\alpha}e^{4i\alpha\pi}$, $z^{\alpha}e^{6i\alpha\pi}$, ..., and we see that z^{α} can take any particular value from any other one when z moves around a closed curve which surrounds the origin in a suitable way. Just like in the case of the logarithmic function, the origin is a singular point of z^{α} , for the function is not single-valued in the neighborhood of z = 0 for all values of α .



2.1.3 Riemann surfaces

In the study of the logarithmic function $f(z) = \log z$ and of the function $f(z) = z^{\alpha}$, two mathematical tools were used in order to better understand the nature of many-valued functions. The first concept was the branchcut, that enables to single out one single-valued branch of the many-valued analytic function. The second was the geometrically suggestive idea of observing how f(z) changes when z starts at a given point and returns to the same point after describing a closed contour. Both ideas can be combined into a single method for visualising the behaviour of a many-valued function through a geometric construction called the *Riemann surfaces*.

To illustrate this construction, we consider the simplest case, obtained with the mapping of the function $f(z) = z^{\frac{1}{n}}$. As we saw in the preceding section, f(z) will have *n* different values for any given *z* (except for z = 0). In fact, if we rather consider the equation

$$[f(z)]^n = z, (2.18)$$

and if we say

$$z = r(\cos w + i \sin w), \qquad f(z) = \rho(\cos \phi + i \sin \phi), \qquad (2.19)$$

then from the relation (2.19), we can also have the equivalences

$$\rho^n = r, \qquad n\phi = w + 2k\pi, \tag{2.20}$$

where, $\rho = r^{\frac{1}{n}}$ which means that r is the nth arithmetic root of the positive number ρ , and

$$\phi = \frac{\omega + 2k\pi}{n}.\tag{2.21}$$

To obtain all distinct values of f(z), it suffices to give to the arbitrary integer k the n consecutive integral values $1, 2, \ldots, n$; in this way, we obtain expressions for the n roots of the equation (2.18) as

$$f(z) = r^{\frac{1}{n}} \left[\cos \left(\frac{\omega + 2k\pi}{n} \right) + i \sin \left(\frac{\omega + 2k\pi}{n} \right) \right]$$

$$= r^{\frac{1}{n}} e^{\left(i \frac{\omega + 2k\pi}{n} \right)}$$

$$= r^{\frac{1}{n}} e^{\frac{i\omega}{n}} e^{\frac{i2k\pi}{n}}$$

$$= (re^{i\omega})^{\frac{1}{n}} e^{\frac{i2k\pi}{n}}$$

$$= P \left[z^{\frac{1}{n}} \right] e^{\frac{i2k\pi}{n}} \qquad (k = 1, 2, \dots, n), \qquad (2.22)$$



where $P\left[z^{\frac{1}{n}}\right]$ is the principal part of f(z).

Accordingly, f(z) has n branches. Each of these values will be single-valued if z is restricted to the region obtained by cutting the z-plane along the negative axis [30]. The construction of the Riemann surface lies in the idea that to each of the n branches of f(z), will be assigned a replica of the cut plane, in which the function is single-valued. Indeed, this can also be understood thinking that there is a one-to-one correspondence between each angle $(k-1)\frac{2\pi}{n} < \arg z < k\frac{2\pi}{n}, \ k = 1, 2, \dots, n \text{ and } f(z), \text{ except for the positive}$ axis [31]. This is a mere analogy of the single-valued nature of f(z) in each of the n branches on negative axis. Then the image of each angle (or again of each branch) will be obtained by performing a cut that will have an upper and a lower edge, along the positive axis. Corresponding to the n angles (or branches) in the z-plane, there will be n identical copies of the f(z)-plane with the cut. These cut-planes are called the *sheets* of the Riemann surface, and can be distinguished according to the values of $z^{\frac{1}{n}}$ by associating the value $P\left[z^{\frac{1}{n}}\right]e^{\frac{i2k\pi}{n}}$ with the plane of index *n*. Then these Riemann sheets will be placed one upon the other in such a way that the $(k+1)^{\text{th}}$ sheet will be immediately on top of the k^{th} one, and the corresponding point z in each plane have exactly the same position.

If a given point z is now allowed to move along a closed curve which surrounds the origin in a positive direction, the path described will pass from a given branch of the function, say the k^{th} , to another one, say the $(k+1)^{\text{th}}$ one. A geometrical description of the situation is that the upper edge of the cut in the k^{th} plane is attached to the lower edge of the cut in the $(k+1)^{\text{th}}$ plane.

The point z = 0 plays a special role here. Unlike the other points, each of which lies on only one sheet, the origin connects all the sheets of the surface, and a curve must wind n times around the origin before it closes. A point of this kind, which belongs to more than one sheet of the Riemann surface is called a *branch point*.

2.1.4 Factorization revisited

We take a quick break to draw a parallel between the overview of Complex Analysis that has been written up to this point and the process of factorization of the first chapter.

In the first chapter, we introduced the Jost functions as the amplitudes of the incoming and outgoing waves in the asymptotics of the radial wave function

$$u_l(E,r) \to h_l^{(-)}(kr) f_l^{(in)}(E) + h_l^{(+)}(kr) f_l^{(out)}(E).$$
 (2.23)



Furthermore, the Ricatti-Hankel functions $h_l^{(\pm)}(kr)$ were explicitly given as dependent of the momentum k. A few words can be said about the dependence of $f_l^{(in/out)}$ on k and $E = \frac{\hbar^2 k^2}{2\mu}$. Indeed, the momentum can be expressed as $k = \sqrt{\left(\frac{2\mu}{\hbar^2}\right)E}$, and since the energy is complex, it can be put in the exponential form $E = |E|e^{i\theta}$, so that

$$k = \sqrt{\left(\frac{2\mu}{\hbar^2}\right)|E|e^{i\theta}} = \sqrt{\left(\frac{2\mu}{\hbar^2}\right)|E|}e^{i\frac{\theta}{2}},\tag{2.24}$$

where $k = \sqrt{\left(\frac{2\mu}{\hbar^2}\right)|E|}$ will be the positive square root of k. The implication of the exponential complex notation of the energy is that the Jost function will be many-valued. Indeed, as it was seen in the previous section for the types of function studied, the point E = 0 can be considered as a branching point of the functions $f_l^{(in/out)}$. If the variable E describes two full circles about the origin, the functions $f_l^{(in/out)}$ will return to the same values as the original ones. In other words, for any given value of the energy on the circle, the momentum k will have two possible values

$$k = \pm \sqrt{\left(\frac{2\mu}{\hbar^2}\right)E}.$$
(2.25)

The best way to visualise the many-valuedness of $f_l^{(in/out)}$ is to introduce the concept of *energetic Riemann surface*. As we saw in the case of a function z^{α} with non-integral exponents, if $z = \frac{2\mu}{\hbar^2}E$ and $\alpha = \frac{1}{2}$, here we will have a function of the type $E \mapsto \sqrt{E}$ defined by

$$E \mapsto \left[\left(\frac{2\mu}{\hbar^2} \right) E \right]^{\frac{1}{2}}.$$
 (2.26)

Recalling equation (2.22), we can write

$$\left[\left(\frac{2\mu}{\hbar^2} \right) E \right]^{\frac{1}{2}} = \left\{ \left[\left(\frac{2\mu}{\hbar^2} \right) |E| \right]^{\frac{1}{2}} e^{i\frac{\theta}{2}} \right\} e^{2\pi i n \frac{1}{2}}$$
$$= \mathcal{P} \left[E^{\frac{1}{2}} \right] e^{\pi i n} \qquad (n = 0, 1),$$

where $\mathcal{P}\left[E^{\frac{1}{2}}\right]$ is the principal part of the complex function of the energy. The latter can then be expressed as



$$E \mapsto \mathcal{P}\left[E^{\frac{1}{2}}\right]e^{\pi i n}$$
 $(n = 0, 1).$ (2.27)

The geometric construction of the Riemann surface of the energy is done by considering two parallel sheets. When E describes one circle around a branching point, the function of the energy travels on the first sheet, and then continues on the second one until coming back to the first sheet after completing two circles. In quantum theory, such a continuous transition from one sheet to the other is commonly obtained by cutting two exemplars of the complex plane along the positive real axis and gluing the two sheets together in such a way that, if the first sheet is denoted as

$$\Gamma_1 := \left\{ E \in \mathbb{C} : E \mapsto \mathcal{P}\left[E^{\frac{1}{2}}\right] e^{i\alpha}, 0 \le \alpha < 2\pi \right\},$$
(2.28)

and the second sheet as

$$\Gamma_2 := \left\{ E \in \mathbb{C} : E \mapsto \mathcal{P}\left[E^{\frac{1}{2}}\right] e^{i\beta}, 2\pi \le \beta < 4\pi \right\},\tag{2.29}$$

the set (Ω) pictured in Figure (2.3) will represent a neighborhood of the branching point E_R on the Riemann surface. The function of the energy is then single-valued on each sheet.

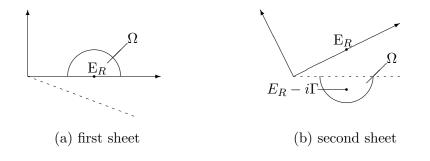


Figure 2.3: The energetic Riemann surface

In the process of factorization discussed in the first chapter, the Jost functions were constructed in such a way that the odd powers of the momentum k were factorised analytically, leaving the other part dependent only of even powers of the momentum k, thus making it a single-valued function of the energy. From this semi-analytic expression of the Jost functions, it was then possible to obtain a system of differential equations where, very conveniently the factorised part that is responsible for the existence of branching points was removed, leading to functions in the set of differential equations that are single-valued functions of the energy.

23



2.1.5 Properties of analytic functions

We briefly discuss some properties of analytic functions that are of interest to us.

Cauchy theorem and Cauchy Integral theorem

Most of the general properties of analytic functions are embedded in two important theorems: the first one is the Cauchy theorem and the second one is the Cauchy integral theorem. Both will be given without proof. Cauchy theorem asserts that if f(z) is a single-valued analytic function of z in a region, then

$$\int_C f(z)dz = 0, \qquad (2.30)$$

for any simple closed curve C in that region. [28] Cauchy integral theorem states that [30] if f(z) is a single-valued analytic function of z in a region bounded by the simple closed curve C, then for any u within C

$$f(u) = \frac{1}{2\pi i} \int_C \frac{f(z)}{z - u} dz.$$
 (2.31)

The second (Cauchy integral) theorem is of a tremendous importance in the theory of Complex Analysis as it basically says that, given a function f(z) that is single-valued in a region C and that has a continuous derivative in that region, if the values of f within the region are not known but are on the edge of C, then it is possible to know the value of f at some interior point u by simply calculating the integral. This means that the values of an analytic function f(z) are completely determined if the values on the boundary C are given.

Power series expansion

An important property of analytic functions is that they can be expanded in series. In its formal statement, If f(z) is analytic at z_0 , there exists a Taylor expansion

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n$$
, valid in $|z - z_0| < R$, (2.32)

where R is the distance from z_0 to the singularity nearest z_0 .



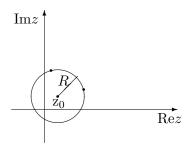


Figure 2.4: Domain of expansion of the analytic function f(z) in power series

Analytic continuation along a path

Up to this point, we have seen that analytic functions are functions differentiable in a region of the complex plane. However, the properties of power series representations aforementioned can be used to extend the domain of definition of an analytic function.

Let f(z) be an analytic function in a connected region of the plane, say a circle of radius R and center z_0 . Then f(z) can be defined at all points within the circle by the Taylor series

$$\sum_{0}^{\infty} a_n (z - z_0)^n.$$
 (2.33)

Consider a path (γ) starting at z_0 , and a point z_1 on the path and inside the circle of radius R centered at z_0 .

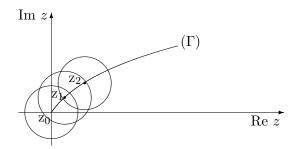


Figure 2.5: Analytic continuation of f(z) along a path

If z_1 is not a singular point of f(z), then the values of f(z) are uniquely

25



determined by the initial conditions at z_0 , and they can themselves be taken as a new set of initial conditions for a new origin at z_1 . Accordingly, we can construct a circle with center z_1 and radius R_1 . There exists a new Taylor series

$$\sum_{0}^{\infty} b_n (z - z_0)^n, \tag{2.34}$$

of radius of convergence R_1 , whose sum is equal to the sum (2.33) at any point of the domain $|z - z_0| \leq R_0$. The sum (2.34) gives the value of f(z)in the circle $|z - z_1| \leq R_1$.

We repeat the same operation from a point z_2 on the path inside the circle $|z - z_1| \leq R_1$, but outside the circle $|z - z_0| \leq R_0$, constructing a circle centered at z_2 and with radius R_2 . It follows that all points that can be attained using all lines (Γ) starting from z_0 provided no singular point is encountered will form a domain, and that a unique value of f(z) at each point z of the domain can be defined. The function f(z) is then analytic in the domain.

This process of finding the value of an analytic function f(z) at a point z, when its value is known at the points of some path (Γ) is called *analytic* continuation [29].

2.2 Existence and nature of solutions of ordinary differential equations

2.2.1 Background

Generally, as an introduction to the study of Ordinary Differential equations of type

$$\frac{dy}{dx} = f(x, y), \tag{2.35}$$

exact solutions can be found using elementary methods of integration, such as the method of separation of variables, or again the method of integrating factors. These types of equations are easily integrable on the account that they belong to certain simple classes. However, it is in general not evident that a differential equation of the type of equation (2.35) will have so elementary a treatment, and very often, the only recourse is to use methods of numerical approximation.

This gives rise to the fundamental question of the existence of solutions of differential questions, and interestingly enough, in the chronology of the theory of Ordinary Differential Equations, existence theorems were established

26



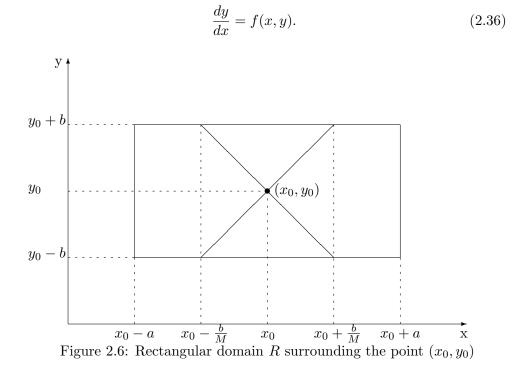
only after the elementary processes of integration aforementioned.

Three proofs of these existence theorems are widely found in the litterature. The first one is the *calculus of limits* credited to Cauchy. Also known as the first rigorous investigation to establish the existence of solutions of a system of ordinary differential equations, the method of calculus of limits proves the existence of solutions for analytic equations through a method of comparison. Cauchy is also at the origin of another method which does not assume the functions to be analytic. Although given by Cauchy and preserved in the lectures of Moigno published in 1844 [32], it was greatly simplified by Lipschitz, who gave an explicit account of the necessary hypotheses or the validity of the proof. For that reason, the proof is called the *Cauchy-Lipschitz* method.

The last of the three existence theorem proofs is the *method of successive* approximations. This method being the one of interest to us, a description of the theory will be given.

2.2.2 The existence theorem

Consider the equation



Let (x_0, y_0) be a pair of values assigned to the real variables (x, y) within a rectangular domain R surrounding the point (x_0, y_0) and defined by the inequalities

27



$$|x - x_0| \le a, \qquad |y - y_0| \le b, \tag{2.37}$$

and f(x, y) a single-valued continuous function of x and y. Let M be the upper boundary of |f(x, y)| in R and let h be the smaller of a and $\frac{b}{M}$ such that if h < a, the following restriction is imposed on x

$$|x - x_0| < h, \tag{2.38}$$

and if (x, y) and (x, Y) are two points within R, of the same abcissa, then

$$|f(x,Y) - f(x,y)| < K|Y - y|,$$
(2.39)

where K is a constant. Inequality (2.39) is known as the Lipschitz condition. These two conditions being satisfied, there exists a unique continuous function of x, say y(x), defined for all values of x such that $|x - x_0| < h$, which satisfies the differential equation and reduces to y_0 when $x = x_0$.

A proof of this existence theorem will now be given using the method of successive approximations.

2.3 The method of successive approximations

The classical theory of Analysis shows that there is a strong relation between differential and integral equations. In fact, most ordinary differential equations can be expressed as integral equations. The converse though is not true. Integral equations are one of the most useful mathematical tools. This is particularly true of problems ranging from both pure and applied mathematical analysis to engineering and mathematical physics, where they are not only useful but indispensable even for numerical computations. Consider the initial value problem

$$\frac{dy}{dx} = f(x, y), \qquad y(x_0) = y_0.$$
 (2.40)

Suppose that a solution of equation is known and that it reduces to y_0 when $x = x_0$. Then the solution clearly satisfies the relation

$$y(x) = y_0 + \int_{x_0}^x f\{s, y(s)\} ds.$$
(2.41)

Indeed, by integrating both sides of the differential equation (2.40), one obtains



$$\int_{x_0}^x y'(s)ds = \int_{x_0}^x f\{s, y(s)\}dy.$$
(2.42)

Then applying the Fundamental Theorem of Calculus to the left side of equation (2.42) yields

$$\int_{x_0}^x y'(s)ds = y(x) - y(x_0) = y(x) - y_0, \qquad (2.43)$$

and we have

$$y(x) - y_0 = \int_{x_0}^x f\{s, y(s)\} ds,$$
(2.44)

which can be arranged into equation (2.41). The initial value problem (2.40) has been reformulated as an equivalent integral equation. Assuming that the function y(x) is unknown, the integral equation can be solve by a method of successive approximation as follows. Observe that the integral equation (2.41) involves the dependent variable in the integrand, hence y(x) occurs on both the left- and right-hand side of the equation. We can use this formula and input y(s) in the integrand $f\{s, y(s)\}$ on the right, and then output the next iteration for y(x) on the left side. This is a type of fixed point iteration, the most familiar form of which is Newton's method for root finding.

Start the iteration with the initial function $y_0(s) = y_0$ and define the next function $y_1(x)$ as

$$y_1(x) = y_0 + \int_{x_0}^x f\{s, y_0(s)\}dt.$$
(2.45)

Then, $y_1(x)$ is used to construct $y_2(x)$ as follows

$$y_2(x) = y_0 + \int_{x_0}^x f\{s, y_1(s)\}dt.$$
 (2.46)

The process is repeated until $y_n(x)$ has been obtained in the recursive equation

$$y_n(x) = y_0 + \int_{x_0}^x f\{s, y_{n-1}(s)\}dt.$$
(2.47)

Following [33], it will then be proved that



- (i) as $n \to \infty$, the sequence of functions $y_n(x)$ tends to a limit which is a continuous function of x,
- (ii) the limit-function satisfies the differential equation and the solution y(x) satisfies the initial condition $y(x_0) = y_0$,
- (iii) the solution thus defined is the only continuous solution.

To prove (i), it will first be shown by induction that, when $x \in (x_0; x_0 + h)$, $|y_n(x)-y_0| \le b$. Suppose that $|y_{n-1}(x)-y_0| \le b$. Then, $|f\{s, y_{n-1}(s)\}| \le M$, and subsequently

$$\begin{aligned} |y_n(x) - y_0| &\leq \int_{x_0}^x |f\{s, y_{n-1}(s)\}| ds \\ &\leq M(x - x_0) \\ &\leq Mh \\ &\leq b. \end{aligned}$$

But clearly

$$|y_1(x) - y_0| \le b. \tag{2.48}$$

Therefore

$$|y_n(x) - y_0| \le b, \qquad \forall n. \tag{2.49}$$

It follows that

$$|f\{s, y_n(s)\}| \le M, \qquad \forall x \in (x_0; x_0 + h).$$
(2.50)

Similarly, it will be shown that

$$|y_n(x) - y_{n-1}(x)| < \frac{MK^{n-1}}{n!} (x - x_0)^n.$$
(2.51)

Suppose that when $x \in [x_0; x_0 + h]$

$$|y_{n-1}(x) - y_{n-2}(x)| < \frac{MK^{n-2}}{(n-1)!}(x - x_0)^{n-1},$$
(2.52)

then



$$|y_n(x) - y_{n-1}(x)| \leq \int_{x_0}^x |f\{s, y_{n-1}(s)\} - f\{s, y_{n-2}(s)\}|ds$$

$$< \int_{x_0}^x K|y_{n-1}(s) - y_{n-2}(s)|ds, \qquad (2.53)$$

by virtue of the Lipschitz condition, so that

$$|y_n(x) - y_{n-1}(x)| < \frac{MK^{n-1}}{(n-1)!} \int_{x_0}^x |s - x_0|^{n-1} ds$$

= $\frac{MK^{n-1}}{n!} |x - x_0|^n.$ (2.54)

Since the inequality (2.54) is true for n = 1 from inequality (2.48), it is also true at level n. The same process can be used for $x \in [x_0 - h : x_0]$, and the inequality (2.54) will hold for $|x - x_0| \le h$. As a result, the series

$$y_0 + \sum_{n=1}^{\infty} \{y_n(x) - y_{n-1}(x)\}$$
(2.55)

is absolutely and uniformly convergent when $|x - x_0| \le h$, and furthermore, each term is continuous in x. Now, since

$$y_n(x) = y_0 + \sum_{n=1}^n \{y_n(x) - y_{n-1}(x)\},$$
(2.56)

 $\forall x \in (x_0 - h; x_0 + h)$ the limit-function

$$y(x) = \lim_{n \to \infty} y_n(x) \tag{2.57}$$

exists and is a continuous function of x. This completes the proof of (i).

(ii) is proved in the following manner

$$\lim_{n \to \infty} y_n(x) = y_0 + \lim_{n \to \infty} \int_{x_0}^x f\{s, y_{n-1}(s)\} ds$$
$$= y_0 + \int_{x_0}^x \lim_{n \to \infty} f\{s, y_{n-1}(s)\} ds.$$
(2.58)



From equation (2.58), it follows that y(x) is a solution of the integral equation (2.41). The inversion of the order between the limit and the integral in equation (2.58) can be explained as follows

$$\left| \int_{x_0}^x \left[f\{s, y(s)\} - f\{s, y_{n-1}(s)\} \right] ds \right| < K \int_{x_0}^x \left| y(s) - y_{n-1}(s) \right| ds < K \epsilon_n |x - x_0| < K \epsilon_n h,$$
(2.59)

where ϵ_n is independent of x and approaches zero when n tends to infinity. Because $f\{s, y(s)\}$ is continuous for $s \in [x_0 - h; x_0 + h]$

$$\frac{dy(x)}{dx} = \frac{d}{dx} \int_{x_0}^x f\{s, y(s)\} ds
= f\{x, y(x)\}.$$
(2.60)

This completes the proof of (ii).

To prove the uniqueness of y(x), consider a solution Y(x) distinct from y(x) and such that $Y(x_0) = y_0$, and continuous for $x \in (x_0; x_0 + h')$, where h' is taken such that

$$\begin{aligned} h' &< h\\ |Y(x) - y_0| &< b. \end{aligned}$$

Y(x) will also satisfy the integral equation

$$Y(x) = y_0 + \int_{x_0}^x f\{s, Y(s)\} ds,$$
(2.61)

giving

$$Y(x) - y_n(x) = \int_{x_0}^x \left[f\{s, Y(s)\} - f\{s, y_{n-1}(s)\} \right] ds.$$
 (2.62)

For n = 1

$$Y(x) - y_1(x) = \int_{x_0}^x \left[f\{s, Y(s)\} - f\{s, y_0\} \right] ds, \qquad (2.63)$$

and from the Lipschitz condition



$$|Y(x) - y_1(x)| < Kk(x - x_0).$$
(2.64)

For n = 2

$$\begin{aligned} |Y(x) - y_2(x)| &< \left| \int_{x_0}^x \left[f\{s, Y(s)\} - f\{s, y_1(s)\} \right] ds \right| \\ &< K \int_{x_0}^x |Y(s) - y_1(s)| ds \\ &< K \int_{x_0}^x Kb(s - x_0) ds = \frac{1}{2} K^2 b(x - x_0)^2. \end{aligned}$$
(2.65)

At level n

$$|Y(x) - y_n(x)| < \frac{K^n b(x - x_0)^n}{n!},$$
(2.66)

thus

$$Y(x) = \lim_{n \to \infty} y_n(x) = y(x), \qquad \forall x \in (x_0; x_0 + h).$$
 (2.67)

The new solution is therefore identical to the original one. This completes the proof of (iii).

2.4 Gronwall inequality

We discuss an inequality that will be useful in facilitating the proof of the uniqueness of solutions of differential equations.

2.4.1 Gronwall Lemma [34]

Let $I = [0; \alpha)$ denote an interval of the real line of the form $[0; \infty)$. Let $f, g : [0; \alpha) \to [0; \infty)$ be real-valued functions. Assume that f and g are continuous and let c be a non-negative number. If

$$f(x) \le c + \int_0^x g(s)f(s)ds, \qquad 0 \le x < \alpha, \tag{2.68}$$

then

$$f(x) \le ce^{\int_0^x g(s)ds}, \qquad 0 \le x < \alpha.$$
(2.69)



To prove the above statement, suppose first that c > 0. Divide both sides of inequality (2.68) by $\left[c + \int_0^x g(s)f(s)ds\right]$, and multiply the result by g(x) to obtain

$$\frac{f(x)g(x)}{c+\int_0^x g(s)f(s)ds} \le g(x). \tag{2.70}$$

Then, integrating from 0 to x yields

$$\ln\{\frac{\left[c + \int_0^x g(s)f(s)ds\right]}{c}\} \le \int_0^x g(s)ds,$$
(2.71)

or

$$f(x) \le c + \int_0^x g(s)f(s)ds \le ce^{\int_0^x g(s)ds}.$$
 (2.72)

If c = 0, the limit as $c \to 0$ can be taken through positive values. This completes the proof.

2.5 On certain methods of successive approximations

In [35], was discussed a method of successive approximations that led to some fundamental theorems on the existence of integrals of the differential equations. In particular, it was noticed that for a linear equation

$$\frac{d^m y}{dx^m} + P_1(x)\frac{d^{m-1}y}{dx^{m-1}} + \dots + P_m(x)y = 0,$$
(2.73)

where the functions $P_i(x)$ on an interval I are continuous functions of x, the method prescribed led to a development in series valid for any value of the variable x in the domain I where the functions P_i are continuous. In the next section, we will see how this general idea of successive approximation can in turn be used, changing the conditions of the problem.

2.6 A general theorem on linear differential equations that depend on a parameter

Here, the method of successive approximations will be used to show an important theorem on linear differential equations [36]. Let a linear differential equation

34



$$\frac{d^m y}{dx^m} + P_1(x,k)\frac{d^{m-1}y}{dx^{m-1}} + \dots + P_m(x,k)y = 0, \qquad (2.74)$$

whose coefficients depend on parameter k, and are *entire* functions of the parameter. Furthermore, the functions $P_i(x, k)$ are x-continuous on an interval I. Then, for x in the interval I, there is a fundamental system of integrals that are entire functions of k, i.e holomorphic on the whole plane of the variable k.

To prove this, if y_n is a sequence of functions, which as defined in section 2.3 tends to y as n approaches infinity, and we represent y_n by the series

$$y_n = y_0 + (y_1 - y_0) + (y_2 - y_1) + \ldots + (y_n - y_{n-1}), \qquad (2.75)$$

each term of the series is an entire function of k, assuming that their initial values are numeric, i.e independent of k. We consider in the plane of the variable k, a circle C. We know that for any x in I, and for any k within the circle C, there exist a fixed number λ such that

$$|y_n - y_{n-1}| < \frac{\lambda^n}{1 \cdot 2 \dots n}.\tag{2.76}$$

This means that we have a series

$$u_0 + u_1 + \dots + u_n + \dots, \qquad (2.77)$$

whose terms u_i are holomorphic functions of k, in the circle C, and that we furthermore have

$$|u_n| < \frac{\lambda^n}{1 \cdot 2 \dots n}.\tag{2.78}$$

It is easy to see that the series of terms u_i will itself be a holomorphic function of k in C. We obtain this by the Cauchy formula

$$u_n(k) = \frac{1}{2\pi i} \oint_C \frac{u_n(z)}{z - k} dz;$$
 (2.79)

The series of general term $u_n(z)$, being uniformly convergent on C, we have

$$u_0(k) + \dots + u_n(k) + \dots = \frac{1}{2\pi i} \oint_C \frac{u_0(z) + \dots + u_n(z) + \dots}{z - k} dz,$$
 (2.80)



and from there, we immediately deduce that the series of terms u is a holomorphic function of k in C, and therefore on the whole plane. We can conclude by saying that the general solution of (2.74) can be put in the form

$$A_1 u_1(x,k) + A_2 u_2(x,k) + \dots + A_n u_n(x,k), \qquad (2.81)$$

with the functions u_i being entire functions of k. This ends the proof.

2.7 Extension of the method of successive approximation to a system of differential equations of the first-order; vector-matrix notation

2.7.1 A glance at existence and uniqueness

Let a system of differential equations be in the form

$$\frac{dy_i}{dx} = f_i(x, y_1, y_2, \dots, y_m),$$
 (2.82)

with i = 1, 2, ..., m. If the functions f_i are single-valued and continuous with respect to their m + 1 arguments in a domain R such that

$$\{R = (x, y_1, y_2, \dots, y_n) : |x - x_1^0| \le a, |y - y_2^0| \le b_1, \dots, |y - y_m^0| \le b_m\},\$$

then there exists a unique set of continuous solutions of this system of equations which assume given values $y_1^0, y_2^0, \ldots, y_m^0$ when $x = x_0$. The proof will just be outlined, as the method is similar to the case of a single first order differential equation.

Let M be the greatest of the upper bounds of the functions f_i in the domain R. If h is the least of $a, \frac{b_1}{M}, \ldots, \frac{b_m}{M}$, let x also satisfy the restriction

$$|x - x_0| \le h. \tag{2.83}$$

Moreover, by virtue of the Lipschitz condition

$$|f_r(x, Y_1, Y_2, \dots, Y_m) - f_r(x, y_1, y_2, \dots, y_m)| < K_1 |Y_1 - y_1| + K_2|Y_2 - y_2| + \cdots + K_m|Y_m - y_m|,$$

for r = 1, 2, ..., m. Defining the functions $y_1^n(x), y_2^n(x), ..., y_m^n(x)$ by



$$y_r^n(x) = y_r^0 + \int_{x_0}^x f_r[s, y_1^{n-1}(s), y_2^{n-1}(s), \dots, y_m^{n-1}(s)] ds, \qquad (2.84)$$

it can be shown by induction that

$$|y_r^n(x) - y_r^{n-1}(x)| < M \frac{(K_1 + K_2 + \dots + K_m)^{n-1}}{n!} |x - x_0|^n, \qquad (2.85)$$

and the existence, continuity and uniqueness of the set of solutions can be derived immediately.

2.7.2 Application to linear equations

The preceding results apply in particular to systems of linear equations

$$\frac{dy_i}{dx} = p_{i1}y_1 + p_{i2}y_2 + \dots + p_{im} + r_i, \qquad (2.86)$$

with i = 1, 2, ..., m, and where the coefficients p_{ij} and r_i are functions of x. If all these functions are continuous functions of x in the interval $a \leq x \leq b$, the right-hand side of equation (2.86) is likewise continuous in this interval, and the set of continuous solutions $y_1(x), y_2(x), ..., y_m(x)$ exists and is unique in the interval (a, b). Furthermore, if the coefficients are continuous for all positive and negative values of x, all the solutions are then continuous when x varies from $-\infty$ to $+\infty$. Such a case is found in linear equations in which the coefficients are polynomials functions of x.

2.7.3 Vector-matrix notation

We briefly discuss the use of matrix theory in expressing a linear system of differential equations in a single vector-matrix equation. Consider the the set of equations (2.86), with an associated set of initial conditions $y_i(0) = c_i$ (i = 1, 2, ..., m). To study the system, we introduce the vectors Y and Y_0 , possessing the components y_i and c_i respectively, and the matrix $M = p_{ij}$ [37]. It follows that the derivatives of the vector Y can be expressed as

$$\frac{dY}{dx} = \begin{pmatrix} \frac{dy_1}{dx} \\ \frac{dy_2}{dx} \\ \vdots \\ \frac{dy_m}{dx} \end{pmatrix}, \qquad (2.87)$$

37



and the system of equations can be rewritten as the following initial value problem

$$\frac{dY}{dx} = M(x)Y, \qquad Y_0 = Y(x=0) = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix}.$$
(2.88)

By introducing the (vector) integral equation

$$Y(x) = Y_0 + \int_{x_0}^x M(s)Y(s)ds,$$
(2.89)

where the matrix function M(s) is frequently called the *Kernel*, it can be demonstrated via the method of successive approximations that there exist a unique set of solutions to a system of linear differential equations of the first order, and more importantly to us, that if the coefficients in addition to being continuous functions of x are also analytic functions of a complex parameter, then the solutions are also analytic functions of the parameter.

2.8 Norms of matrices

Let $A = \{a_{jk}\}$ and $B = \{b_{jk}\}$ be the *n* by *n* matrices with respective entries a_{jk} and b_{jk} at the intersection of the jth row and the kth column (j, k = 1, 2, ..., n) [38], and consider the space of all matrices M_n . We call the matrix function $\|\cdot\| : \mathbb{M}_n \to \mathbb{R}$ a matrix norm if for all $A, B \in \mathbb{M}_n$ and $c \in \mathbb{C}$, the following properties are satisfied

- (a) ||A|| = 0 if and only if A = 0,
- (b) If I is the identity matrix, then ||I|| = 1,
- (c) Let c be a complex scalar. Then ||cA|| = |c|||A||,
- (d) $||A + B|| \le ||A|| + ||B||,$
- (e) $||AB|| \le ||A|| ||B||$,
- (f) $\lim_{r\to\infty} A_r = 0$ if and only if $\lim_{r\to\infty} ||A_r|| = 0$.

The norms of A is generally expressed as

$$||A|| = \max_{j} \sum_{k=1}^{n} |a_{jk}|, \qquad (2.90)$$



and likewise for B.

It is worthwhile adding a corresponding definition of the norm of a vector [38]: Let v be the column vector with components v_1, v_2, \ldots, v_n . Then the norm ||v|| is defined by

$$\|v\| = \sum_{k=1}^{n} |v_j|.$$
(2.91)

It has the properties

- (g) v = 0 if and only if ||v|| = 0,
- (h) $||cv|| \le |c|||v||,$
- (i) $||v + w|| \le ||v|| + ||w||$,
- (j) $||Av|| \le ||A|| ||v||$,
- (k) Corresponding to any matrix A, there exist nonzero vectors v such that ||Av|| = ||A|| ||v||.

We will use the notation $\|\cdot\|$ for both vector norm and matrix norm.

2.8.1 An inequality involving norms and integrals

Let $f : \mathbb{R}_n \mapsto \mathbb{R}_n$ be a continuous function. Then

$$\left\|\int_{a}^{b} f(x)dx\right\| \le \int_{a}^{b} \|f(x)\|dx \tag{2.92}$$

To prove this, it can first be noted [39] that

$$\left\|\int_{a}^{b} f(x)dx\right\| = \left(\left\|\int_{a}^{b} f_{1}(x)dx\right\|, \dots, \left\|\int_{a}^{b} f_{n}(x)dx\right\|\right).$$
(2.93)

Then, using the definition of the Riemann integral for a give component function f_i (i = 1, ..., n)

$$\int_{a}^{b} f(x)dx = \lim_{k \to \infty} \sum_{j=1}^{k} f_{i}(x_{j}^{*})\Delta x_{j},$$
(2.94)

with x_j^* as the sample point in the interval $[x_{j-1}, x_j]$ with width Δx_j . Hence



$$\left\| \int_{a}^{b} f_{i}(x) dx \right\| = \left\| \lim_{k \to \infty} \sum_{j=1}^{k} f_{i}(x_{j}^{*}) \Delta x_{j} \right\|$$
$$= \lim_{k \to \infty} \left\| \sum_{j=1}^{k} f_{i}(x_{j}^{*}) \Delta x_{j}^{*} \right\|, \qquad (2.95)$$

since the norm is a continuous function. The result then follows from the triangle inequality.



Chapter 3

Analyticity of the functions $\tilde{A}_{l}\left(E,r\right)$ and $\tilde{B}_{l}\left(E,r\right)$

We start with the system of first order differential equations derived from the radial Schrödinger equation in the first chapter

$$\begin{cases} \partial_r \tilde{A}_l(E,r) &= -\tilde{y}_l(E,r)V(r) \left[\tilde{j}_l(E,r)\tilde{A}_l(E,r) - \tilde{y}_l(E,r)\tilde{B}_l(E,r) \right] \\ \partial_r \tilde{B}_l(E,r) &= -\tilde{j}_l(E,r)V(r) \left[\tilde{j}_l(E,r)\tilde{A}_l(E,r) - \tilde{y}_l(E,r)\tilde{B}_l(E,r) \right], \end{cases}$$
(3.1)

and for which the coefficients and solutions are single-valued functions of the energy. The system can be rewritten in the following form

$$\begin{cases} \partial_r \tilde{A} = -\tilde{y}V\tilde{j}\tilde{A} + \tilde{y}V\tilde{y}\tilde{B} \\ \partial_r \tilde{B} = -\tilde{j}V\tilde{j}\tilde{A} + \tilde{j}V\tilde{y}\tilde{B}, \end{cases}$$
(3.2)

devoid of arguments. Equation (3.2) can be recast in matrix form

$$\partial_r \begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix} = \begin{pmatrix} -\tilde{y}V\tilde{j} & \tilde{y}V\tilde{y} \\ -\tilde{j}V\tilde{j} & \tilde{j}V\tilde{y} \end{pmatrix} \begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix}$$
(3.3)

which in turn can be rewritten as

$$\partial_r \begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix} = M \begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix}, \qquad (3.4)$$

or again

$$X' = MX. \tag{3.5}$$

41



3.1 Existence and uniqueness

The matrix M being defined and continuous for $r \ge 0$, then there exists a unique solution to the differential equation (3.5). To set the proof, we proceed in the following way. In place of the differential equation, we consider the integral equation

$$X = \begin{pmatrix} 1\\0 \end{pmatrix} + \int_0^r M X \mathrm{d}r', \tag{3.6}$$

or more formally

$$X(E,r) = {\binom{1}{0}} + \int_0^r M(E,r')X(E,r')dr'.$$
 (3.7)

We then define a sequence of vector-functions $\{X_n\}$ by

$$X_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
 and $X_n = X_0 + \int_0^r M X_{n-1} dr',$ (3.8)

and we show by induction that each $X_n(E, r)$ is defined for $r \ge 0$, and is continuous. Let $m = \max_{o \le r \le r_1} ||M(E, r)||$, where ||M(E, r)|| represents the norm of matrix M(E, r), and consider the series

$$X_0(E,r) + \sum_{n=1}^{\infty} \left(X_n(E,r) - X_{n-1}(E,r) \right), \qquad (3.9)$$

whose partial sum is $X_n(E, r)$. We show by induction that

$$||X_n(E,r) - X_{n-1}(E,r)|| \le \frac{m^n r^n}{n!}.$$
(3.10)

We start by writing

$$\begin{aligned} \|X_{1} - X_{0}\| &= \left\| \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \int_{0}^{r} M(E, r') X_{0} dr' - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\| \\ &= \left\| \int_{0}^{r} M(E, r') \begin{pmatrix} 1 \\ 0 \end{pmatrix} dr' \right\| \\ &\leq \int_{0}^{r} \left\| M(E, r') \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\| dr' = \int_{0}^{r} \|M(E, r')\| \left\| \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\| dr' \\ &= \int_{0}^{r} \|M(E, r')\| dr' \\ &\leq mr = \frac{m^{1} r^{1}}{1!}, \end{aligned}$$



so that inequality (3.10) is true for n = 1. We then assume the same inequality to be true at level n, and show that it is therefore also true at level n + 1

$$||X_{n+1} - X_n|| = \left\| \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \int_0^r M X_n dr' \right] - \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \int_0^r M X_{n-1} dr' \right] \right\|$$

$$= \left\| \int_0^r M (X_n - X_{n-1}) dr' \right\|$$

$$\leq \int_0^r ||M|| ||X_n - X_{n-1}|| dr'$$

$$\leq m \int_0^r ||X_n - X_{n-1}|| dr',$$

and from inequality (3.10)

$$||X_{n+1} - X_n|| \le m \int_0^r \frac{m^n r^n}{n!} = m \left(\frac{1}{n+1} \frac{m^n r^{n+1}}{n!}\right)$$
$$= \frac{m^{n+1} r^{n+1}}{(n+1)!},$$

as required.

But $\frac{(mr)^n}{n!}$ is the typical term of a Taylor series of e^{mr} that converges uniformly and absolutely on a finite interval. Therefore, (3.9) also converges uniformly on the interval, to a continuous limit-function, say X(E, r). We may then take the limit as $n \to \infty$ and pass it through the integral obtaining expression (3.7) by writing

$$X(E,r) = \lim_{n \to \infty} X_n(E,r), \qquad (3.11)$$

so that the limit-function X(E, r) is a solution of the initial value problem. Since by assumption, M(E, r) is continuous for $r \ge 0$, we may take r arbitrarily large. We may thus obtain a solution valid for $r \ge 0$.

To see that X(E, r) is the only solution, suppose that there are two solutions, say $X_1(E, r)$ and $X_2(E, r)$, on the finite interval, then from expression (3.7)

$$\|X_1 - X_2\| = \left\| \int_0^r M(X_1 - X_2) dr' \right\|$$

 $\leq m \int_0^r \|X_1 - X_2\| dr'.$

This is of the form



$$||X_1 - X_2|| \le C + \int_0^r m ||X_1 - X_2|| dr', \qquad (3.12)$$

with C = 0. By Gronwall inequality

$$||X_1 - X_2|| \leq C e^{mr} = 0, (3.13)$$

hence

$$X_1 = X_2. (3.14)$$

This completes the proof of the existence and uniqueness of X(E, r).

3.2 Analyticity

We now use the method of successive approximations to show that X is an analytic function of E. By iteration of equation (3.6), we obtained a formal series

$$X(E,r) = \sum_{n=0}^{\infty} X_n(E,r),$$
 (3.15)

where

$$X_0(E,0) = \begin{pmatrix} 1\\0 \end{pmatrix}, \tag{3.16}$$

and

$$X_n(E,r) = \int_0^r M(E,r') X_{n-1}(E,r') \mathrm{d}r'.$$
 (3.17)

We consider a circle C in the plane of the variable E. We show by induction that for any x in an interval I, and for any k within the circle C, we have

$$||X_n|| \le \frac{\left[\int_0^r ||M|| \mathrm{d}r'\right]^n}{n!}.$$
(3.18)



This is true at level 1. Indeed

$$X_1 = \int_0^r M X_0 dr' = \int_0^r M \begin{pmatrix} 1 \\ 0 \end{pmatrix} dr'.$$
 (3.19)

If follows that

$$\|X_1\| = \left\| \int_0^r M\begin{pmatrix}1\\0\end{pmatrix} dr' \right\| \leq \int_0^r \left\| M\begin{pmatrix}1\\0\end{pmatrix} \right\| dr'$$
$$= \int_0^r \|M\| \left\| \begin{pmatrix}1\\0\end{pmatrix} \right\| dr'$$
$$= \int_0^r \|M\| dr', \qquad (3.20)$$

and therefore

$$||X_1|| \le \frac{\left[\int_0^r ||M|| \mathrm{d}r'\right]^1}{1!}.$$
(3.21)

We then assume inequality (3.18) true at level n, and we show that it is also true at level n+1. From

$$X_{n+1}(E,r) = \int_0^r M(E,r') X_n(E,r') dr', \qquad (3.22)$$

Follows

$$||X_{n+1}|| = \left\| \int_{0}^{r} MX_{n} dr' \right\| \leq \int_{0}^{r} \left\| MX_{n} \right\| dr'$$

$$\leq \int_{0}^{r} ||M| \left\| \frac{\left[\int_{0}^{r'} ||M| ||dr'' \right]^{n}}{n!} dr'$$

$$= \frac{1}{n!} \int_{0}^{r} ||M| \left[\int_{0}^{r'} ||M| ||dr'' \right]^{n} dr'$$

$$= \frac{\left[\int_{0}^{r'} ||M| ||dr'' \right]^{n+1}}{(n+1)!}. \quad (3.23)$$

Hence, X_n converges absolutely in the interval I, and in the circle C. It is easy to see that the series of terms X_n will be a holomorphic function of Ein C. We obtain this by making use of the Cauchy formula



$$X_n(E) = \frac{1}{2\pi i} \oint_C \frac{X_n(r)}{r-E} \mathrm{d}r, \qquad (3.24)$$

for any complex variable r.

The series of general terms $X_n(r)$ being uniformly convergent on C, we will obtain

$$X_0(E) + X_1(E) + \ldots + X_n(E) = \frac{1}{2\pi i} \oint_C \frac{X_0(r) + X_1(r) + \ldots + X_n(r)}{r - E} dr,$$
(3.25)

and from there, we immediately deduce that the series

$$\sum_{n=0}^{\infty} X_n,\tag{3.26}$$

is a holomorphic function of E in C and therefore in the whole plane by using the principle of analytic continuation along a path.

We conclude by saying that the solutions $A_l(E, r)$ and $B_l(E, r)$ can be expanded in the form

$$\tilde{A}_{l}(E,r) = \sum_{n=0}^{\infty} \alpha(E,r)(E-E_{0})^{n}$$
 (3.27)

$$\tilde{B}_{l}(E,r) = \sum_{n=0}^{\infty} \beta(E,r)(E-E_{0})^{n}.$$
(3.28)



Chapter 4

Analyticity of the functions $\tilde{A}_{l}(E,\infty)$ and $\tilde{B}_{l}(E,\infty)$

So far, we have established that the solutions of equation (1.43), namely $\tilde{A}_l(E,r)$ and $\tilde{B}_l(E,r)$, are entire (analytic single-valued) functions of the complex variable E only for finite values of the variable r. But we ought to remember that in order to establish the analytic properties of the Jost functions, we must also and in particular, consider what happens asymptotically, *i.e.* when r approaches infinity.

4.1 Asymptotics of the Ricatti-Bessel and of the Ricatti-Neumann functions

The Ricatti-Hankel asymptotics are expressed in the following form

$$h_l^{(\pm)}(kr) \xrightarrow{|kr| \to \infty} \mp i e^{\left[\pm i \left(kr \mp l\frac{\pi}{2}\right)\right]}.$$
(4.1)

Recalling the Ricatti-Hankel functions as a linear combination of the Ricatti-Bessel and of the Ricatti-Neumann, it is possible to obtain the two latter in terms of the Ricatti-Hankel functions. The Ricatti-Hankel function reads

$$h_l^{(\pm)}(kr) = j_l(kr) \pm iy_l(kr).$$
(4.2)

From equation (4.2), it is easy to write the Ricatti-Bessel functions as

$$j_l(kr) = \frac{h^{(+)}(kr) + h^{(-)}(kr)}{2},$$
(4.3)

and the Ricatti-Neumann functions as



$$y_l(kr) = \frac{h^{(+)}(kr) - h^{(-)}(kr)}{2i}.$$
(4.4)

Inserting equation (4.1) into the latter expressions of the Ricatti-Bessel and of the Ricatti-Neumann functions will yield their respective asymptotics. The Ricatti-Bessel asymptotics are found by writing

$$j_l(kr) \xrightarrow{|kr| \to \infty} \frac{-ie^{\left(+ikr-il\frac{\pi}{2}\right)} + ie^{\left(-ikr+il\frac{\pi}{2}\right)}}{2} \tag{4.5}$$

which after some algebraic manipulation results into

$$j_l(kr) \xrightarrow{|kr| \to \infty} \frac{1}{2i} \left(e^{ikr} (-i)^l - e^{-ikr} (i)^l \right)$$
(4.6)

Similarly, the Ricatti-Neumann asymptotics are found by writing

$$y_l(kr) \xrightarrow{|kr| \to \infty} \frac{-ie^{\left(+ikr-il\frac{\pi}{2}\right)} - ie^{\left(-ikr+il\frac{\pi}{2}\right)}}{2i}, \qquad (4.7)$$

which in turn gives

$$y_l(kr) \xrightarrow{|kr| \to \infty} -\frac{1}{2} \left(e^{ikr} (-i)^l + e^{-ikr} (i)^l \right).$$

$$(4.8)$$

4.2 The integral equation and its Kernel

The integral equation that is solution of equation (3.5) is of the form

$$X(E,r) = {\binom{1}{0}} + \int_0^r M(E,r')X(E,r')dr',$$
(4.9)

where the matrix M(E, r') is the kernel of the integral equation. For solutions of equation (3.5) to exist, the kernel must be finite. It is expressed in the following matrix form

$$M(E,r) = \begin{pmatrix} \tilde{y}V\tilde{j} & \tilde{y}V\tilde{y} \\ -\tilde{j}V\tilde{j} & \tilde{j}V\tilde{y} \end{pmatrix}, \qquad (4.10)$$

with

$$\tilde{y} = k^l y$$
 and $\tilde{j} = k^{-(l+1)} j.$ (4.11)



For the class of potential (exponential) we are working with, the determination of the expression of the different entries of the matrix M asymptotically gives

$$-\tilde{y}V\tilde{j} = -\left\{ \left[-\left(\frac{e^{ikr}(-i)^{l} + e^{-ikr}(i)^{l}}{2}\right) \right] \left[e^{-\lambda r} \right] \left[\frac{e^{ikr}(-i)^{l} - e^{-ikr}(i)^{l}}{2i} \right] \right\}$$

$$= \frac{(-1)^{l}}{4i} \left[e^{(2ik-\lambda)r} - e^{-(2ik+\lambda)r} \right],$$
(4.12)

$$\tilde{y}V\tilde{y} = \left\{ \left[-\left(\frac{e^{ikr}(-i)^{l} + e^{-ikr}(i)^{l}}{2}\right) \right] \left[e^{-\lambda r} \right] \left[-\left(\frac{e^{ikr}(-i)^{l} + e^{-ikr}(i)^{l}}{2i}\right) \right] \right\} \\ = \frac{1}{4} \left[e^{(2ik-\lambda)r}(-1)^{l} + e^{-(2ik+\lambda)r}(-1)^{l} + 2e^{-\lambda r} \right],$$
(4.13)

$$-\tilde{j}V\tilde{j} = -\left\{ \left[-\left(\frac{e^{ikr}(-i)^l - e^{-ikr}(i)^l}{2i}\right) \right] \left[e^{-\lambda r} \right] \left[\left(\frac{e^{ikr}(-i)^l - e^{-ikr}(i)^l}{2i}\right) \right] \right\}$$
$$= \frac{1}{4} \left[e^{(2ik-\lambda)r}(-1)^l + e^{-(2ik+\lambda)r}(-1)^l - 2e^{-\lambda r} \right],$$
(4.14)

$$-\tilde{j}V\tilde{y} = -\left\{ \left[-\left(\frac{e^{ikr}(-i)^{l} - e^{-ikr}(i)^{l}}{2i}\right) \right] \left[e^{-\lambda r} \right] \left[-\left(\frac{e^{ikr}(-i)^{l} + e^{-ikr}(i)^{l}}{2i}\right) \right] \right\}$$
$$= -\frac{(-1)^{l}}{4i} \left[e^{(2ik-\lambda)r} - e^{-(2ik+\lambda)r} \right],$$
(4.15)

4.3 Restriction on the Kernel

The behaviour of the matrix M(E, r) when the variable r approaches infinity is dictated by the functions $e^{(2ik-\lambda)r}$ and $e^{-(2ik+\lambda)r}$. For these functions and for the matrix to be finite, we must have

$$\operatorname{Re}(2ik - \lambda) < 0$$
 and $\operatorname{Re}(2ik + \lambda) > 0.$ (4.16)

Let k be a complex number that can be written in the form

$$k = u + iv. \tag{4.17}$$

Then

$$e^{(2ik-\lambda)r} = e^{[2i(u+iv)-\lambda]r}$$
$$= e^{2iur}e^{-(2v+\lambda)r}, \qquad (4.18)$$



and

$$e^{-(2ik+\lambda)r} = e^{-[2i(u+iv)+\lambda]r}$$
$$= e^{-2iur}e^{(2v-\lambda)r}.$$
 (4.19)

Hence, from equation (4.18), for the matrix to be finite, we must have the following restriction

$$2v + \lambda > 0, \tag{4.20}$$

or again

$$v > \frac{-\lambda}{2},\tag{4.21}$$

and from equation (4.19), we must have

$$2v - \lambda < 0, \tag{4.22}$$

or again

$$v < \frac{\lambda}{2}.\tag{4.23}$$

v being the imaginary part of k, from the latter two inequalities comes

$$|\mathrm{Im}k| < \frac{\lambda}{2},\tag{4.24}$$

or also

$$(\mathrm{Im}k)^2 < \frac{\lambda^2}{4}.\tag{4.25}$$

It is also known that

$$k = \pm \sqrt{\frac{2\mu E}{\hbar^2}},\tag{4.26}$$

which gives

$$k^2 = \frac{2\mu E}{\hbar^2}.\tag{4.27}$$



If E is a complex number that can be written as E = x + iy, then

$$(u+iv)^2 = \frac{2\mu}{\hbar^2}(x+iy),$$
(4.28)

which in turn gives

$$(u^{2} - v^{2}) + 2iuv = \frac{2\mu}{\hbar^{2}}(x + iy).$$
(4.29)

By identification, the real part and the complex part in the above equation give

$$\begin{cases} u^2 - v^2 = \frac{2\mu}{h^2} x \\ 2uv = \frac{2\mu}{h^2} y. \end{cases}$$
(4.30)

From the second equation of the system (4.30)

$$u = \frac{\mu}{\hbar^2} \frac{y}{v},\tag{4.31}$$

which leads to

$$u^{2} = \left(\frac{\mu}{\hbar^{2}}\right)^{2} \frac{y^{2}}{v^{2}}.$$
 (4.32)

Then in the first equation of the system (4.30)

$$\begin{pmatrix} \frac{\mu}{\hbar^2} \end{pmatrix}^2 \frac{y^2}{v^2} - v^2 = \left(\frac{2\mu}{\hbar^2}\right) x \left(\frac{\mu}{\hbar^2}\right)^2 \frac{y^2}{v^2} = \left(\frac{2\mu}{\hbar^2}\right) x + v^2 y^2 = \frac{\left(\frac{2\mu}{\hbar^2}\right)}{\left(\frac{\mu}{\hbar^2}\right)^2} x v^2 + \frac{1}{\left(\frac{\mu}{\hbar^2}\right)^2} v^4 y^2 = \frac{2\hbar^2}{\mu} v^2 x + \frac{\hbar^4}{\mu^2} v^4.$$
 (4.33)

Previously, it was established that

$$(\mathrm{Im}k)^2 < \frac{\lambda^2}{4},\tag{4.34}$$



which also gives

$$(\mathrm{Im}k)^4 < \frac{\lambda^4}{16}.$$
 (4.35)

This leads to the following set of inequalities

$$(\mathrm{Im}k)^{2} < \frac{\lambda^{2}}{4} \qquad (\mathrm{Im}k)^{4} < \frac{\lambda^{4}}{16} \\ v^{2} < \frac{\lambda^{2}}{4} \qquad v^{4} < \frac{\lambda^{4}}{16} \\ \frac{2\hbar^{2}}{\mu}xv^{2} < \frac{\hbar^{2}}{2\mu}x\lambda^{2} \qquad \frac{\hbar^{4}}{\mu^{2}}v^{4} < \frac{\hbar^{4}}{16\mu^{2}}\lambda^{4} \qquad (4.36)$$

From the set of inequalities (4.36), we can write

$$\frac{2\hbar^2}{\mu}v^2x + \frac{\hbar^4}{\mu^2}v^4 < \frac{\hbar^2\lambda^2}{2\mu}x + \frac{\hbar^4\lambda^4}{16\mu^2}.$$
 (4.37)

This allows us to write

$$y^2 < \left(\frac{\hbar^2 \lambda^2}{2\mu}\right) x + \frac{\hbar^4 \lambda^4}{16\mu^2},\tag{4.38}$$

or again

$$\left(\mathrm{Im}E\right)^2 < \left(\frac{\hbar^2 \lambda^2}{2\mu}\right) \left(\mathrm{Re}E\right) + \frac{\hbar^4 \lambda^4}{16\mu^2}.$$
(4.39)

The inequality is sketched below in the complex E-plane as the shadded area inside the parabolic region.



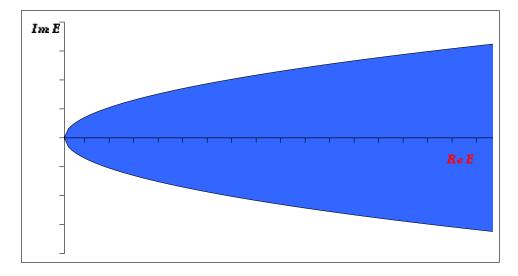


Figure 4.1: Region of analyticity defined by inequality (4.39). The functions $\tilde{A}_l(E,\infty)$ and $\tilde{B}_l(E,\infty)$ are holomorphic inside the parabolic region. The parabola crosses the real axis at $\mathrm{E}=-\frac{\hbar^2\lambda^2}{8\mu}$.



Chapter 5

Conclusion

A novel theory on the Jost functions was developed recently. The originality of the theory is that on one hand it allows for an exact and unified treatment of all bound, scattering and resonant states whereas by the past these different states had to be treated separately. On the other hand, the Jost function had for a long time been regarded as mathematical entities without practical use. The perception changed after the advent of this new method...

The development of the theory was based on the derivation of a system of two ordinary linear differential equations of order one which is equivalent to the Schrödinger equation. The system of equation was derived using a method known as the variation of parameters, from an expression of the solution of the radial Schrödinger equation, in which the coefficients of the solutions are functions of the energy and of r at finite values of r, and become functions of the energy only when r tends to infinity. These functions of the energy when r tends to infinity are the Jost functions.

However, the new method is based on a power series expansion of the Jost function. This implies that the latter must be analytic single-valued. Since it is not the case of the Jost functions, they were split into two parts, one that has factors responsible for all branching points, the other one containing single-valued valued functions of the energy. Conveniently, the factorized part was cancelled in the system of differential equations, leaving it with only the single-valued functions of the energy.

In the present work, we used the method of successive approximations to show that the functions in the system of differential equations are analytic functions of the energy. We firstly established the existence and the uniqueness of these functions in the set of linear differential equations for finite values of r, and then showed their analyticity. These properties were thereafter extended to the asymptotic case. In contrast with the case of finite values of r where the functions are analytic on the whole complex plane, it was interesting to observe that asymptotically, the functions of the dif-



CHAPTER 5. CONCLUSION

ferential equations are analytic on a specific portion of the complex plane. Finally, the domain of analyticity of these functions was explicitly determined.

Note should be taken that we worked with a certain class of potential, shortrange potentials. As another case of study, it would then be interesting to see how well the theory holds with a different type of potential...



Bibliography

- P. Roman, Advanced Quantum Theory, Addison-Wesley Publishing Company, Inc., Reading Massachusetts, 1965.
- [2] M. L. Goldberger and K. M. Watson, *Collision Theory*, John Wiley and Sons, Inc., 1964.
- [3] R. Jost, Helv. Phys. Acta, v. XX, pp. 256-266, 1947.
- [4] S. A. Rakitiansky, Jost Functions in Quantum Mechanics, lectures, 2008.
- [5] R.G. Newton, Scattering Theory of Waves and Particles, Dover Publications, Inc., 2nd Edition, 2002.
- [6] S. A. Rakityansky and S. A. Sofianos, Jost functions for coupled partial waves, Journal of Physics, A31, pp. 5149- 5175 (1998).
- [7] M. Reed and B. Simon, Methods of Modern Mathematical Physics, Vol. 3, American Press, Inc., New York, 1979.
- [8] V. V. Pupyshev and S. A. Rakitiansky, Z. Phys. A348, 227, 1994.
- [9] F. Calogero, Variable phase approach to Potential Scattering, Academic Press, New York, 1967.
- [10] S. A. Rakityansky, S. A. Sofianos, K. Amos, A method for calculating the Jost function for analytic potentials, Nuovo Cim., B111, pp. 363-378, 1996.
- [11] J. Mathews and R. L. Walker, *Mathematical Methods of Physics*, W. A. Benjamin, Inc, New York, 1964.
- [12] The entire special issue of J. Quantum Chem., 14(4), 1978, is devoted to the complex coordinate method. See also the review by Y. K. Ho, Phys. Rep., 99, 1983.
- [13] V. V. Pupyshev and S. A. Rakitiansky, Communication of JINR, E4-91-418, Dubna, 1991.



BIBLIOGRAPHY

- [14] Handbook of Mathematical functions, Eds M. Abramovitz and A. Stegun, NBS, Washington, 1964.
- [15] S. A. Rakitiansky, Unified treatment of bound, scattering, and resonant states in semiconductor nanaostructures, Phys. Rev., B68(19), 195320, 2003.
- [16] S. A. Rakitiansky, Modified Transfer-matrix for nano-structures with arbitrary potential profile, Phys. Rev., B70(20), 205323, 2004.
- S. A. Rakitiansky and N. Elander, Analyzing the contribution of individual resonance poles of the S-matrix to two channel scattering, Int. J. Quantum Chem., Vol.106(5), pp. 1105-1129, 2006.
- [18] H. Friedrich, *Theoretical Atomic Physics*, Third Edition, Springer, 2010.
- [19] L. Brand, Differential and Difference equations, Wiley, New York, 1966.
- [20] S. A. Rakitiansky and N. Elander, Analytic structure and powerseries expansion of the Jost function for the two-dimensional problem, arXiv:1201.0172v1[quant-ph], 2012.
- [21] J. Liouville, J. de Math. (1) 2, p 19, 1838; J. Liouville, J. de Math.
 (1) 3, p 515, 1838.
- [22] J. Caqué, J. de Math. (2) 9, p 185, 1864.
- [23] L. Fuchs, Annali di Mat. (2) 4, p 36 [Ges. Werke I, p 295], 1870.
- [24] G. Peano, Math. Ann. 32, p 450, 1888.
- [25] E. Picard, *Traité d' analyse II*, p 301, Edition Gauthier-Villars, Paris, 1893;
 E. Picard, *Traité d' analyse II*, p 340, Edition Gauthier-Villars, 2nd édition, Paris, 1905.
- [26] E.Picard, Leçons sur quelques problèmes aux limites de la théorie des équations différentielles, p 15, Edition Gauthier-Villars, Paris, 1930.
- [27] H. Poincaré, Sur les groupes des équations linéaires, Acta Math. 4 201-311, 1884.
- [28] J. Pierpont, *Functions of a complex variable*, Ginn and Company, 1914.
- [29] G. Valiron, Equations fonctionnelles Applications, éditions Masson et Cie, Paris, 1945.



BIBLIOGRAPHY

- [30] Z. Nehari, Introduction to Complex Analysis, Allyn and Bacon, Inc., Boston, 1961.
- [31] L. V. Ahlfors, *Complex Analysis*, 3rd Ed., Mc Graw-Hill, Inc., 1979.
- [32] E. Goursat, Cours d' Analyse Mathematique II, Edition Gauthier-Villars, 2nd édition, Paris, 1918.
- [33] E. L. Ince, Ordinary differential equations, Dover Publications, Inc., 2nd edition, 1956.
- [34] T.A. Burton Volterra Integral and Differential Equations, 2nd Ed., Elsevier, 2005.
- [35] E. Picard, Traité d' analyse II, p 340, Edition Gauthier-Villars, 2nd édition, Paris, 1905.
- [36] E. Picard, Traité d' analyse III, pp 88-90, Edition Gauthier-Villars, 2nd édition, Paris, 1908.
- [37] R. E. Bellman, Introduction to Matrix Analysis, Mc Graw-Hill, Inc., 1960.
- [38] W. Wasow, Asymptotic Expansions for Ordinary Differential equations, Dover Publications, Inc., New York, 1965.
- [39] J. Arino, Fundamental Theory Of Ordinary Differential Equations, lecture notes, 2006.