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Resonances in the two centers Coulomb system

Presentata da: Marcello Seri

Coordinatore Dottorato:
Alberto Parmeggiani

Relatori:
Mirko Degli Esposti
Andreas Knauf

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Sunto

La tesi è incentrata sulla comprensione delle risonanze quantistiche per il sistema coulombiano a due centri fissi in due e tre dimensioni.

L'operatore di Schrödinger semiclassico

$$-\frac{h^2}{2}\Delta - \frac{Z_1}{|q-s_1|} - \frac{Z_2}{|q-s_2|}$$

in $L^2(\mathbb{R}^2)$ (o in $L^2(\mathbb{R}^3)$) descrive la funzione d'onda di una particella in un campo generato da due cariche coulombiane fisse Z_1 e Z_2 nello spazio bi- e tridimensionale. Le cariche sono considerate con valori arbitrari.

Seppure semplificato, il problema coulombiano a due centri fissi rappresenta un modello per lo studio di ioni molecolari con un elettrone (ad esempio l'idrogeno molecolare ionizzato H_2^+).

Il problema, che risale alla fine del 1800, è stato studiato classicamente da Jacobi in meccanica celeste e introdotto come modello quantistico da Pauli nella sua tesi di dottorato nel 1922. La letteratura è vasta e si protrae fino a questo decennio ma riguarda quasi esclusivamente l'analisi del problema classico e quantistico per energie negative.

Il caso dei due centri è particolarmente interessante in quanto rappresenta il modello molecolare non banale più semplice: la dinamica classica è integrabile. In particolare, tramite le coordinate prolate ellittiche è possibile ricondursi allo studio di un sistema di equazioni di Sturm-Liouville accoppiate a cui è possibile applicare solide tecniche di analisi funzionale e teoria semiclassica.

Nella prima parte del lavoro cerchiamo di completare il quadro classico descrivendo il diagramma delle biforcazioni e la struttura del ritratto di fase per energie non negative. Oltre ad essere interessanti di per se, queste sono importanti anche per comprendere se e dove è possibile aspettarsi la presenza di risonanze quantistiche.

Successivamente ci concentriamo sullo studio del problema quantistico, sviluppando gli strumenti e le costruzioni necessari per poter dare una definizione di risonanze e per poter implementare le stime per la loro localizzazione.

Le risonanze corrispondono a stati meta-stabili microlocalizzati nello spazio delle fasi sulla varietà (in)stabile dell'orbita classica che oscilla tra i due centri.

In quersto lavoro le risonanze sono definite come autovalori complessi generalizzati con parte immaginaria piccola. Tramite diverse tecniche di approssimazione le risonanze sono enumerate in termini di 2 o 3 parametri (per il problema in $\mathbb{R}^2$ e in $\mathbb{R}^3$ rispettivamente) e localizzate in modo esplicito con un errore dell'ordine di

$h^{\frac{3}{2}}$ (eventualmente migliorabile usando una espansione asintotica) e in diversi regimi asintotici dei parametri.

Rispetto al caso bidimensionale, in cui le risonanze descrivono un reticolo ben separato nella fascia del piano complesso vicina all'asse reale, il caso tridimensionale presenta un'ulteriore difficoltà data dalla possibile presenza di valori degeneri.

Zusammenfassung

In dieser Doktorarbeit wurden die Resonanzen für das quantenmechanische Zweizentren-Problem in zwei und drei Dimensionen studiert.

Der semiklassische Schrödinger-Operator, definiert durch

$$-\frac{h^2}{2}\Delta - \frac{Z_1}{|q-s_1|} - \frac{Z_2}{|q-s_2|}$$

auf $L^2(\mathbb{R}^2)$ (oder auf $L^2(\mathbb{R}^3)$), beschreibt die Dynamik der Wellenfunktion eines Teilchens in einem Feld, das durch zwei Coulomb-Zentren beliebiger elektronischer Ladungen Z_1 und Z_2 erzeugt ist.

Obwohl vereinfacht, ist das Zweizentren-Problem ein realistisches Modell zur Untersuchung der molekularen Ionen mit einem Elektronenstrahl (z.B. das ionisierte Wasserstoffmolekül H_2^+).

Das klassische Problem ist von Jacobi am Ende des neunzehnten Jahrhunderts in der Himmelsmechanik studiert werden, und das quantenmechanische Modell hat Pauli in seiner Dissertation im Jahr 1922 eingeführt. Die Literatur ist groß, mit Veröffentlichungen bis in den letzten Jahren, aber sie behandelt ausschließlich die klassischen und quantenmechanische Analyse des Problems für negative Energien.

Das Zweizentren-Problem ist besonders interessant, denn es stellt das einfachste nicht triviale molekulare Modell dar, denn die klassischen Dynamik ist integrierbar. Insbesondere kann das Modell anhand der prolat elliptischen Koordinaten auf ein System von Sturm-Liouville-Gleichungen reduziert werden. Und für dieses System kann man starke Techniken aus Funktionalanalysis und semiklassischer Theorie anwenden.

Im ersten Teil der Arbeit vervollständigen wir das klassische Bild mit dem Verzweigungsdiagramm und dem Phasenportrait für positive Energien. Das ist für sich genommen interessant, aber es ist auch wichtig zu verstehen, ob quantenmechanische Resonanzen existieren, und wo sie sich befinden.

Dann konzentrieren wir uns auf die Untersuchung des quantenmechanischen Modells. In diesem Teil entwickeln wir die Techniken und die Strukturen, um eine Definition der Resonanzen bereitzustellen und die Abschätzungen für ihre Lokalisierung auszuführen.

Die Resonanzen entsprechen metastabilen Zuständen, die im Phasenraum auf der (in-)stabilen Mannigfaltigkeit des zwischen den Zentren oszillierenden geschlossenen Orbits mikrolokalisiert sind.

Die Resonanzen werden als verallgemeinerte komplexe Eigenwerte mit kleinen Imaginärteilen definiert. Sie werden durch verschiedene Approximationstechniken aufgezählt und in verschiedenen asymptotischen Regimen von Parametern mit einem Fehler der Ordnung $\hbar^{\frac{3}{2}}$ explizit lokalisiert.

In die zweidimensionalen Fall beschreiben die Resonanzen ein reguläres Gitter im Bereich der komplexen Ebene in der Nähe der reellen Achse. Andererseits hat der dreidimensionale Fall eine schwierigere Struktur und möglicherweise degenerierte Resonanzen.

CHAPTER 1

Introduction

Our work mainly concerns the study of the quantum mechanical two fixed center Coulomb system in two and three dimensions. The setting will be defined in the next sections, but before entering into details we would like to give an overview on the problem and his history and describe the structure of the thesis.

The classical motion of a test particle in the field of two fixed centers was first considered by Euler in 1760 and it represents one of the most famous integrable problem of classical mechanics [Kna11]. It was Jacobi that in 1884 proved its integrability and gave explicit solutions of the equations of motion in terms of elliptic functions [Jac84].

The first development of the corresponding quantum mechanical model is due to Pauli that, in 1922, even before the Schrödinger formulation of quantum mechanics, applied it to the semi-classical hydrogen molecular ion H_2^+ [Pau22]. Ten years after Pauli's dissertation, the Schrödinger equation was applied to the problem by Jaffé [Jaf34] and Baber and Hassé [BH35] that described the system in its modern form. Starting from this moment, the two-center problem is fully considered in molecular physics as the simplest model for one-electron diatomic molecules.

There has always been a deep connection between classical mechanics and quantum mechanics. The understanding of the classical picture is essential for the comprehension of the semi-classical and the quantum mechanical ones. For classical coulombic problems (including the two-centers one) the literature goes from Jacobi up to the recent years with the work of [WDR04] that gives a complete picture of the phase-space structure for negative energies and [KK92, Kna02] that gives a geometrical description of the classical scattering.

Like for the classical model, there is a huge amount of literature related to the quantum counterpart. Despite this fact, the understanding of the system is far from being complete and a lot is known only for what concerns the discrete spectrum (i.e. negative energies) or in some special limits in which the two-center potential converges to a one-center one [Har80, GGHS85, BHL06, LKJ04, SAFG06]. Of major interest are the works of Strandt and Reinhardt [SR79] that gave an excellent semi-classical description of the model for the hydrogen ion and of its boundstates and [Cha90] that studied the low-lying eigenvalues for the semi-classical two-dimensional problem.

The results related to the quantum or semi-classical scattering are really few and the most important advances can be found in [Lea86, GG76] and [Liu92][1]. In fact most of the results in the literature are related to the hard problem of finding an

[1]Notice that in this paper the computation of the Green's function is known to be wrong.

algorithm to obtain numerical approximations of the scattering solutions. In contrast, nothing or really few is known on the regularity of the solutions with respect to the parameters of the system and the problem of resonances.

Quantum resonances are a key notion of quantum physics: roughly speaking they are scattering states (i.e. states of the essential spectrum) that for long time behave like bound states (i.e. eigenfunctions). They are usually defined as poles of a meromorphic function, but there is not really a unique way to study and define them [Zwo99]. On the other hand, it is known that their many definitions coincide in some settings [HM87] and that their existence is related to the presence of some classical orbits "trapped" by the potential.

If a quantum systems has a potential presenting a positive local minimum above its upper limit at infinity, for example, it is usually possible to find quantum resonances, called shape resonances. They are related to the classical bounded trajectories around the local minimum [HS96]. They are not the only possible ones, in fact it has been proved in [BCD87b, BCD88, Sjö87, GS87] that there can be resonances generated by closed hyperbolic trajectories or by a non-degenerate maximum of the potential. The main difference is that the shape resonances appear to be localized much nearer to the real axis with respect to this last one.

Even the presence or absence of the resonances is strictly related to the classical picture. In fact it is possible to use some classical estimates, called non-trapping conditions, to prove the existence of resonance free regions (see for example [BCD87a, Mar02, Mar07]).

In this work we want to investigate the existence of resonances for two-centers Coulomb systems with arbitrary charges, defining them in terms of generalized complex eigenvalues of a non-selfadjoint deformation of the two-center Schrödinger operator. The fact that the non-trapping condition does not hold for the two centers problem [CJK08], and the presence of a single bounded hyperbolic orbit for big positive energies (see [KK92, Theorem 6.9] and [Kna02, Theorem 12.8]) suggests that resonances are likely to be present. In view of the last two theorems is even clear that the two-centers system is a good model to perform this study, furthermore it is known there that in presence of more coulombic singularities the system is no more integrable and there is a Cantor set of hyperbolic trapped orbits [KK92, Kna02].

The thesis is structured as follows. The rest of this chapter is used to define the three dimensional two-centers Coulomb system and show how its differential equation separates in prolate elliptic coordinates.

In Chapter 2 we integrate the description of the classical bifurcation diagram initiated by [WDR04]. Namely we add the bifurcation diagram of the planar two-centers system for positive energies and identify the "trapped" trajectories.

In Chapter 3 we analyze the separation of the operator in $\mathbb{R}^3$ from an operator theoretical point of view and we clarify formally how we want to define the resonances and the main problems arising.

In Chapter 4 we concentrate on the two-centers problem in $\mathbb{R}^2$. In the first part we analyze the separation of the problem in its radial and an angular part. We then perform an analytic continuation of the eigenvalues of the angular part in the complex plane and we study the asymptotic form of the radial solutions and their analyticity with respect to the energy parameter. With these we define the resolvent kernel (the Green's function), the generalized eigenfunctions (scattering states) and the scattering matrix and show that all these objects admit an analytic continuation in the energy parameter suitable to define the resonances of the system. Finally we compute some approximations of the resonances and perform a numerical investigation of their structure.

In Chapter 5 we relate the results of Chapter 4 and of a paper of Agmon and Klein [AK92] to describe the resolvent kernel (the Green's function), the generalized eigenfunctions (the scattering states) and the scattering matrix for the operator in three dimensions and define its resonances.

In Chapter 6 we summarize the results of the thesis and describe the main open problems and further direction of work.

The main theories and tools needed for the work are described and referenced in the appendices.

1.1. The two-center Coulomb system

We consider the operator in $L^2(\mathbb{R}^3)$, given for $h>0$ by

$$\mathscr{H} := -h^2\Delta + V(q) \quad \text{with} \quad V(q) := \frac{-Z_1}{|q-s_1|} + \frac{-Z_2}{|q-s_2|}. \tag{1.1.1}$$

This describes the motion of an electron in the field of two nuclei of charges $Z_i \in \mathbb{R}^* := \mathbb{R}\setminus\{0\}$, fixed at positions $s_1 \neq s_2 \in \mathbb{R}^3$, taking into account only the electrostatic force. By the unitary realization $Uf(x) := |\det A|^{-1/2} f(Ax+b)$ of an affinity of $\mathbb{R}^d$ we assume that the two centers are at $s_1 := a := \left(\begin{smallmatrix}1\\0\\0\end{smallmatrix}\right)$ and $s_2 := -a$.

REMARK 1.1. *For $Z_1 = Z_2 = 0$ or in case only one of the charges is zero, the problem would reduce respectively to the free Laplacian or the one-center problem. In particular it would not be a two centers problem anymore. Therefore the restriction $Z_i \in \mathbb{R}^*$.*

REMARK 1.2. *Notice that if we set $Z_1 = Z_2 = 1$ in the operator in (1.1.1), we get the Schrödinger operator for the simply ionized hydrogen molecule H_2^+* [SR79]. *In the same way, if $Z_1 = 1 = -Z_2$, it describes an electron moving in the field of a proton and an anti-proton* [GGHS85].

Another important example covered by the operator is the doubly charged helium-hydride molecular ion HeH^{++}, in this case Z_1 and Z_2 are both positive but of different magnitude [WDR04].

REMARK 1.3. *Even if* (1.1.1) *doesn't directly describe the diatomic molecular scattering, it is strictly related to it: the molecular scattering is generally studied by the Thomas Fermi approximation* [LS77]. *The resulting equation appears as a perturbation of a purely Coulombic potential V by a smooth term W. The Coulombic potential then represents the heavy atoms as fixed while the smooth perturbation represents the cloud of electrons of the molecule.*

REMARK 1.4. *In this thesis we use mathematicians' notation h for what the physicists call $\hbar$. It means that for us h is generally a small parameter for asymptotic analysis and it is not necessarily interpreted as the Planck constant.*

1.2. Separation in prolate elliptic coordinates

We define $M := \mathbb{R}_+ \times (0,\pi) \times [0,2\pi)$. The restriction to M of the map from

$$\begin{pmatrix} \xi \\ \eta \\ \phi \end{pmatrix} \in \overline{M} \mapsto \begin{pmatrix} \cosh(\xi)\cos(\eta) \\ \sinh(\xi)\sin(\eta)\cos(\phi) \\ \sinh(\xi)\sin(\eta)\sin(\phi) \end{pmatrix} \in \mathbb{R}^3$$

defines a C^∞ diffeomorphism

$$G : M \to G(M) \tag{1.2.1}$$

whose image $G(M) = \mathbb{R}^3 \setminus (\mathbb{R} \times \{0\} \times \{0\})$ is dense in $\mathbb{R}^3$, therefore it defines a change of coordinate from $q \in \mathbb{R}^3$ to $(\xi,\eta,\phi) \in M$. The new coordinates (ξ,η,ϕ) are called *prolate elliptic coordinates.*

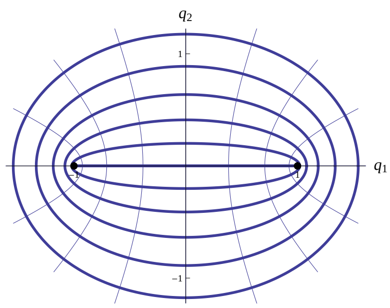


FIGURE 1.1. Prolate elliptic coordinate for $\phi \in \{0,\pi\}$.

REMARK 1.5. *The curve $\phi = c$ describes a half plane, in particular $\phi = 0$ ($\phi = \pi$) is the (q_1,q_2)-half-plane with $q_2 > 0$ ($q_2 < 0$).*

In the (q_1,q_2)-plane the curves $\xi = c$ are half ellipses with foci at $\pm a$ while the curves $\eta = c$ are confocal half hyperbolas.

REMARK 1.6. *The Jacobian determinant*

$$\det(DG(\xi,\eta,\phi)) = \sin(\eta)\sinh(\xi)(\sin^2(\eta) + \sinh^2(\xi)),$$

thus the change of coordinates is degenerate for $\eta \in \{0,\pi\}$ or $\xi = 0$. This happens because the q_1 axes is pointwise invariant under rotations of angle ϕ, in fact for the values $\xi = 0$ the η coordinate would parametrize the q_1-axis interval between the two centers, and for $\eta = 0$ ($\eta = \pi$) the ξ coordinate would parametrize the positive (negative) q_1-axis with $|q_1| > 1$.

The importance of this change of coordinate is clarified by the following theorem (see e.g. [BH35]).

THEOREM 1.7. *Let*

$$u \in C_a(\mathbb{R}^3) := \left\{ C(\mathbb{R}^3) \mid u\restriction_{\mathbb{R}^3\setminus\{\pm a\}} \text{is twice continuously differentiable} \right\}.$$

The eigenvalue equation

$$\left(-\hbar^2\Delta + V(q)\right) u(q) = E u(q), \quad E \in \mathbb{R},$$

transformed to prolate elliptic coordinates, *separates with the ansatz*

$$u \circ G(\xi,\eta,\phi) = f(\xi)g(\eta)e^{i\lambda\phi}$$

into the decoupled system of ordinary differential equations

$$\begin{cases} \left(-\hbar^2\partial_\xi^2 - \hbar^2\coth(\xi)\partial_\xi + \frac{\hbar^2\lambda^2}{\sinh^2(\xi)} - Z_+\cosh(\xi) - E\cosh^2(\xi) + \mu\right) f(\xi) = 0 \\ \left(-\hbar^2\partial_\eta^2 - \hbar^2\cot(\eta)\partial_\eta + \frac{\hbar^2\lambda^2}{\sin^2(\eta)} + Z_-\cos(\eta) + E\cos^2(\eta) - \mu\right) g(\eta) = 0 \\ \left(-\partial_\phi^2 - \lambda^2\right) e^{i\lambda\phi} = 0. \end{cases}$$

Here $\lambda \in \mathbb{Z}$, $\mu \in \mathbb{C}$ *and*

$$\begin{aligned} &f \in C_N^2(\mathbb{R}_+^0) := \left\{ h \in C^2(\mathbb{R}_+^0) \mid h'(0) = 0 \right\}, \\ &g \in C_{\text{per}}^2([0,\pi]) := \left\{ h \in C^2([0,\pi]) \mid h^{(k)}(0) = h^{(k)}(\pi) \text{ for } k = 0,1,2 \right\}, \\ &\phi \in [0,2\pi) \end{aligned}$$

and we have set $Z_\pm := Z_2 \pm Z_1$ *and* $\partial_\alpha := \frac{\partial}{\partial\alpha}$.

REMARK 1.8. *Without restriction we may assume* $Z_- \in \mathbb{R}_+^0$ *and* $Z_+ \in \mathbb{R}$, $Z_+ \neq Z_-$, *i.e.* $Z_2 \geq Z_1$.

PROOF OF 1.7. We set $r_1 := |q - s_1|$, $r_2 := |q - s_2|$ and transform to *prolate elliptic coordinates*. We have

$$\begin{aligned} r_{2,1}^2 &= (q_1 \pm 1)^2 + q_2^2 + q_3^2 \\ &= (\cosh(\xi)\cos(\eta) \pm 1)^2 + \sinh^2(\xi)\sin^2(\eta)\left(\cos^2(\phi) + \sin^2(\phi)\right) \\ &= \cosh^2(\xi)\left(\cos^2(\eta) + \sin^2(\eta)\right) \pm 2\cosh(\xi)\cos(\eta) + (1 - \sin^2(\eta)) \\ &= (\cosh(\xi) \pm \cos(\eta))^2. \end{aligned}$$

Thus the distances from the centers equal

$$r_1 = \cosh\xi - \cos\eta \quad \text{and} \quad r_2 = \cosh\xi + \cos\eta.$$

Defined the function F by

$$F(\xi,\eta) := \sinh^2(\xi) + \sin^2(\eta) = \cosh^2(\xi) - \cos^2(\eta), \tag{1.2.2}$$

we obtain

$$\begin{aligned} V(\xi,\eta,\phi) &= -\frac{Z_1}{r_1} - \frac{Z_2}{r_2} = -\frac{1}{2}\frac{Z_+(r_2 + r_1) + Z_-(r_1 - r_2)}{r_1 r_2} \\ &= -\frac{Z_+\cosh(\xi) - Z_-\cos(\eta)}{F(\xi,\eta)}, \end{aligned} \tag{1.2.3}$$

and the Laplacian is given by

$$\begin{aligned}\Delta &= \frac{1}{F(\xi,\eta)}\left\{\partial_\xi^2 + \coth(\xi)\,\partial_\xi + \partial_\eta^2 + \cot(\eta)\,\partial_\eta + \right.\\ &\qquad \left. + \left(\frac{1}{\sin^2(\eta)} + \frac{1}{\sinh^2(\xi)}\right)\partial_\phi^2\right\}\\ &= \frac{1}{F(\xi,\eta)}\left\{\frac{1}{\sinh(\xi)}\partial_\xi\left(\sinh(\xi)\,\partial_\xi\right) + \frac{1}{\sin(\eta)}\partial_\eta\left(\sin(\eta)\,\partial_\eta\right) + \right.\\ &\qquad \left. + \left(\frac{1}{\sin^2(\eta)} + \frac{1}{\sinh^2(\xi)}\right)\partial_\phi^2\right\}.\end{aligned} \tag{1.2.4}$$

Let $u \in C_a(\mathbb{R}^3)$. We first consider the ansatz

$$u \circ G(\xi,\eta,\phi) = \widetilde{u}(\xi,\eta)e^{i\lambda\phi}$$

where to preserve the continuity and differentiability of the u we have to assume

$$\begin{aligned}\widetilde{u} \in \Big\{ h \in C^2(\mathbb{R}_+ \times [0,\pi]) \mid h \text{ is } \eta\text{-periodic},\\ \partial_\xi h(\xi,\eta)|_{\xi=0} = 0 \text{ for } \eta \in (0,\pi)\Big\}\end{aligned}$$

and $\phi \in [0,2\pi)$. The eigenvalue equation

$$\left(-h^2\Delta - V \circ G\right) u \circ G = E\, u \circ G$$

separates in the form

$$\begin{cases}\left(-h^2\frac{h^2\partial_\xi\left(\sinh(\xi)\,\partial_\xi\right)}{\sinh(\xi)} - h^2\frac{h^2\partial_\eta\left(\sin(\eta)\,\partial_\eta\right)}{\sin(\eta)} + \frac{h^2\lambda^2}{\sin^2(\eta)} + \frac{h^2\lambda^2}{\sinh^2(\xi)} + \widetilde{V}(\xi,\eta)\right)\widetilde{u} = 0\\ \left(-\partial_\phi^2 - \lambda^2\right)e^{i\lambda\phi} = 0\end{cases}$$

where $\widetilde{V}(\xi,\eta) := -Z_+\cosh(\xi) + Z_-\cos(\eta) - E\cosh^2(\xi) + E\cos^2(\eta)$. Then, with the ansatz

$$\widetilde{u}(\xi,\eta) = f(\xi)g(\eta) \quad \text{with} \quad f \in C_N^2(\mathbb{R}_+) \text{ and } g \in C_{\text{per}}^2([0,\pi])$$

the first equation separates and we obtain the decoupled system of ordinary differential equations

$$\begin{cases}-h^2\frac{1}{\sinh(\xi)}\partial_\xi\left(\sinh(\xi)\,\partial_\xi\right)f(\xi) + \left(V_\xi^\lambda(\xi) + \mu\right)f(\xi) = 0\\ -h^2\frac{1}{\sin(\eta)}\partial_\eta\left(\sin(\eta)\,\partial_\eta\right)g(\eta) + \left(V_\eta^\lambda(\eta) - \mu\right)g(\eta) = 0\\ \left(-\partial_\phi^2 - \lambda^2\right)e^{i\lambda\phi} = 0\end{cases} \tag{1.2.5}$$

where

$$V_\xi^\lambda(\xi) := -Z_+ \cosh(\xi) - E\cosh^2(\xi) + \frac{\hbar^2\lambda^2}{\sinh^2(\xi)}, \tag{1.2.6a}$$

$$V_\eta^\lambda(\eta) := Z_- \cos(\eta) + E\cos^2(\eta) + \frac{\hbar^2\lambda^2}{\sin^2(\eta)}. \tag{1.2.6b}$$

□

REMARK 1.9. *Here the separation constant μ plays the role of the spectral parameter in time independent Schrödinger equations, and the original energy E plays the role of a coupling constant.*

CHAPTER 2

The classical problem of two Coulomb centers

In this section we want to extend the results of [WDR04] and the discussions of [Kna02, Kna11] to the case of positive energies and general values of the charges.

2.1. Hamiltonian setting

We consider the classical Hamiltonian function on the cotagent bundle $T^*(\mathbb{R}^3 \setminus \{\pm a\})$ relative to the 2-center potential of (1.1.1), where we have alerady rescaled the two centers to be in $\pm a$:

$$H(p,q) := -\frac{|p|^2}{2} + \frac{-Z_1}{|q-a|} + \frac{-Z_2}{|q+a|}.$$

THEOREM 2.1. *The Hamiltonian $H(p,q)$ restricted to $T^*(\mathbb{R}^3 \setminus (\mathbb{R},0,0))$ is transformed by the prolate elliptic coordinates into the Hamiltonian*

$$H(p_\xi, p_\eta, p_\phi, \xi, \eta, \phi) := \frac{1}{F(\xi,\eta)}(H_1(p_\xi, p_\phi, \xi) + H_2(p_\eta, p_\phi, \eta)) \tag{2.1.1}$$

where F is defined in (1.2.2) and

$$\begin{aligned} H_1(p_\xi, p_\phi, \xi) &:= \frac{p_\xi^2}{2} + \frac{p_\phi^2}{2\sinh^2(\xi)} - Z_+ \cosh(\xi), \\ H_2(p_\eta, p_\phi, \eta) &:= \frac{p_\eta^2}{2} + \frac{p_\phi^2}{2\sin^2(\eta)} + Z_- \cos(\eta). \end{aligned} \tag{2.1.2}$$

There are three independent constants of motion H, $L := H_1 - \cosh^2(\xi)H$ and p_ϕ with values E, K and l respectively.

PROOF. If we apply to $H(p,q)$ the canonical transformation induced by the prolate elliptic coordinates (1.2.1), the potential is transformed as in (1.2.3) and the impulses $p = (p_1, p_2, p_3)$ are transformed according to

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = (DG(\xi,\eta,\phi)^{-1})^t \begin{pmatrix} p_\xi \\ p_\eta \\ p_\phi \end{pmatrix}.$$

From $(DG(\xi,\eta,\phi)^{-1})(DG(\xi,\eta,\phi)^{-1})^t = (DG(\xi,\eta,\phi)^t DG(\xi,\eta,\phi))^{-1}$ and

$$(DG(\xi,\eta,\phi)^t DG(\xi,\eta,\phi)) = \begin{pmatrix} F(\xi,\eta) & 0 & 0 \\ 0 & F(\xi,\eta) & 0 \\ 0 & 0 & \sinh^2(\xi)\sin^2(\eta) \end{pmatrix}$$

we get that the Hamiltonian is transformed into (2.1.1).

The angular momentum p_ϕ around the q_1-axis is a constant of motion, in fact $p_\phi = q_2 p_3 - q_3 p_2$ and for a solution of the Hamilton's equations

$$\begin{aligned}\frac{d}{dt} p_\phi &= \dot{q}_2 p_3 - \dot{q}_3 p_2 + q_2 \dot{p}_3 - q_3 \dot{p}_2 \\ &= p_2 p_3 - p_3 p_2 + (q_2 q_3 - q_3 q_2) r \frac{\partial W}{\partial r}(q_1, r) = 0.\end{aligned}$$

Here we have defined

$$r := \sqrt{q_2^2 + q_3^2} \quad \text{and} \quad W(q_1, r) := \frac{-Z_1}{\sqrt{(q_1 - 1)^2 + r^2}} + \frac{-Z_2}{\sqrt{(q_1 + 1)^2 + r^2}}.$$

Given an initial condition $x_0 \in T^*(\mathbb{R}^3 \setminus \{\pm a\})$ we set $l := p_\phi(x_0)$ and $E := H(x_0)$.

Equation (2.1.1) can be again separated [**Kna11**, Lemma 10.38] passing to the extended phase space and using a new time parameter s defined by

$$\frac{dt}{ds} = F(\xi, \eta).$$

We obtain the new hamiltonian

$$\widetilde{H} := F(\xi, \eta)(H - E) = H_\xi + H_\eta$$

where

$$H_\xi := H_1 - \cosh^2(\xi) E \quad \text{and} \quad H_\eta := H_2 + \cos^2(\eta) E, \tag{2.1.3}$$

then on the submanifold $\widetilde{H}^{-1}(0)$, $\widetilde{H}$ describes the time evolution of $H^{-1}(E)$ up to a time reparametrization. Therefore have a third constant of motion other than H and p_ϕ:

$$L := H_1 - \cosh^2(\xi) H = -(H_2 + \cos^2(\eta) H). \tag{2.1.4}$$

Setting $K := H_\xi(x_0) = -H_\eta(x_0)$ we have three constants of motion H, H_ξ and p_ϕ whose values are denoted respectively E, K and l. Notice that these functions are generally independent in the following sense. Being real analytic functions, the subset of phase space where independence is violated, is of Lebesgue measure zero. □

REMARK 2.2. *By the separation of ϕ and the constancy of $p_\phi = l$ we can restrict the analysis for a given l to a reduced phase space $T^*(\mathbb{R}^2 \setminus \{\pm a\})$ with Hamiltonian*

$$\widehat{H}_l(p_\xi, p_\eta, \xi, \eta) = H_\xi(p_\xi, \xi) + H_\eta(p_\eta, \eta),$$

where the H_ξ and H_η are the one defined in (2.1.3) and have the form

$$H_\xi(p_\xi, \xi) := \frac{p_\xi^2}{2} + V_\xi(\xi), \qquad H_\eta(p_\eta, \eta) := \frac{p_\eta^2}{2} + V_\eta(\eta). \tag{2.1.5}$$

Here V_ξ and V_η are formally the one defined by (1.2.6) with $\lambda = l$ and $\hbar = 1$.

If $l \neq 0$ the effective potential $V_\xi(\xi)$ ($V_\eta(\eta)$) becomes infinite as $\xi \to 0$ ($\eta \to 0$, $\eta \to \pi$) thus the trajectory can never leave $\mathbb{R}^3 \setminus (\mathbb{R} \times \{0\} \times \{0\})$. Therefore on

$T^*(\mathbb{R}^3 \setminus (\mathbb{R} \times \{0\} \times \{0\}))$, the Hamiltonian H generates a complete vector field and the flow exists for all times.

It will be computationally useful for what follows to introduce a new coordinate change. The restriction to $M^2 := (1,\infty) \times (-1,1)$ of the map

$$\begin{pmatrix} x \\ y \end{pmatrix} \in \overline{M^2} \mapsto \begin{pmatrix} \operatorname{arccosh}(x) \\ \arccos(y) \end{pmatrix} \in \mathbb{R}^2$$

defines a C^∞ diffeomorphism

$$G^2 : M^1 \to G^2(M^2) \tag{2.1.6}$$

with image $G^2(M^2) = \mathbb{R}_+ \times (0,\pi)$, therefore it defines a change of coordinates from $(\xi,\eta) \in \mathbb{R}_+ \times (0,\pi)$ to $(x,y) \in M^2$.

THEOREM 2.3. *The diffeomorphism defined in (2.1.6) induces an hamiltonian symplectomorphism $\widehat{G}^2 : T^*(\mathbb{R}_+ \times (0,\pi)) \to T^*M^2$.*

PROOF. It is enough to choose the generating function

$$S_2(\xi,\eta,p_x,p_y) := (\cosh(\xi),\cos(\eta)) \begin{pmatrix} p_x \\ p_y \end{pmatrix}.$$

It induces a canonical transformation [Kna11, Chapter 10.5]

$$\widehat{G}^2 : (p_\xi, p_\eta, \xi, \eta) \mapsto (p_x, p_y, x, y)$$

where

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \frac{\partial S_2}{\partial p_x} \\ \frac{\partial S_2}{\partial p_y} \end{pmatrix} = \begin{pmatrix} \cosh(\xi) \\ \cos(\eta) \end{pmatrix},$$

$$\begin{pmatrix} p_\xi \\ p_\eta \end{pmatrix} = \begin{pmatrix} \frac{\partial S_2}{\partial \xi} \\ \frac{\partial S_2}{\partial \eta} \end{pmatrix} = \begin{pmatrix} \sinh(\xi) p_x \\ \sin(\eta) p_y \end{pmatrix}$$

□

REMARK 2.4. *The change of variable defined in the previous theorem corresponds to the change of variables defined by the restriction to $M^3 := (1,\infty) \times (-1,1) \times [0,2\pi)$ of*

$$\overline{G^3} : \begin{pmatrix} x \\ y \\ \phi \end{pmatrix} \in \overline{M^3} \mapsto \begin{pmatrix} xy \\ \sqrt{(x^2-1)(1-y^2)}\cos(\phi) \\ \sqrt{(x^2-1)(1-y^2)}\sin(\phi) \end{pmatrix} \in \mathbb{R}^3.$$

The Jacobian determinant $\det(D\overline{G^3}(x,y,\phi)) = x^2 - y^2$ is singular only at the two centers $(x,y) = (1,\pm 1)$, thus we can extend it to the whole $\overline{M^3} \setminus (1,\pm 1,[0,2\pi))$.

If $l = 0$ the motion is effectively planar, thus we can restrict it to be in the (q_1, q_2)-plane. In this case the trajectories are allowed to pass through the q_1-axis (where the prolate elliptic coordinate are singular) and even collide with the two centers at $\pm a = (\pm 1, 0)$. There are some different ways to regularize the motion both in the planar and spatial cases (and with an arbitrary number of centers), we refer the reader to [Kna02, Chapter 4-5], [KK92, Chapter 3] and [Kna11, Remark 11.24] for more details and references. We are going to use the regularization scheme of [KK92] for the planar two-center case, extended to the case of repelling centers.

Let $O := \mathbb{R}^2$ and $\hat{O} := \mathbb{R}^2 \setminus \{\pm a\}$ be the configuration space, let $R_E := \{q \in \hat{O} \mid V(q) \geq E\}$ be the complement of the Hill's region for a given energy E and let $\hat{O}_E := \hat{O} \setminus R_E$ be the Hill's region for a given energy E. Notice that for $E > 0$ the set R_E is bounded, and it is nonempty in case there is a repelling singularity ($Z_\# < 0$). Denoted $\hat{g}$ the restriction to $\hat{O}$ of the euclidean metric on $\mathbb{R}^2$, we introduce the *Jacobi metric* $\hat{g}_E$:

$$\hat{g}_E(q) := \left(1 - \frac{V(q)}{E}\right) \hat{g}(q), \quad q \in \hat{O}, \tag{2.1.7}$$

where E is the energy of the particle whose motion we want to analyze. The solutions of the geodesic motion with unit velocity on $(\hat{O}_E, \hat{g}_E)$ coincide, up to a time reparametrization, with the flow on the configuration space Φ^t_E generated by the Hamiltonian H for initial conditions with energy E [Kna11, Section 8.5].

On the other hand $(\hat{M}_E, \hat{g}_E)$ is not geodesically complete. Therefore we identify $q \in O$ with $q \in \mathbb{C}$ and consider the Riemann surface

$$\mathbb{O} := \left\{(q, Q) \in \mathbb{C} \times \mathbb{C} \mid Q^2 = (q - a)(q + a)\right\} \tag{2.1.8}$$

as branched covering surface for O, in fact if $\pi : \mathbb{O} = O$ is the projection on the first coordinate $\pi(q, Q) \to q$, it is a two-sheeted branched covering whose branch points $\pm \mathbf{a} := (\pm a, 0)$ are of order one and project on the positions $\pm a$ of the nuclei. Denoting

$$\hat{\mathbb{O}}_E := \pi^{-1}(\hat{O}_E),$$

the restriction of π to $\hat{\mathbb{O}}_E$ leads to a two-fold unbranched covering $\hat{\pi}_E : \hat{\mathbb{O}}_E \to \hat{O}_E$ and we can lift the Jacobi metric $\hat{g}_E$ to the metric $\hat{\mathbf{g}}_E := \hat{\pi}^*_E \hat{g}_E$ on $\hat{\mathbb{O}}_E$. In this way we obtain an incomplete geodesic motion on the unit tangent bundle $S\hat{\mathbb{O}}_E := \{X \in T\hat{\mathbb{O}}_E \mid \hat{\mathbf{g}}_E(X, X) = 1\}$ that can be related to the restriction of the flow of the Hamiltonian restricted to the energy shell $\hat{S}_E := \{(p, q) \in T^*\hat{O}_E \mid H(p, q) = E\}$ by a two-sheeted unbranched covering $\tilde{\pi}_E : S\hat{\mathbb{O}}_E \to \hat{S}_E$

$$(\dot{q}, q) \mapsto \left(\sqrt{2E}(1 - V(\pi(q))/E)\, T_q\pi(\dot{q}), \pi(q)\right).$$

THEOREM 2.5. *For $Z_\pm > 0$, $\hat{\mathbf{g}}_E$ extends uniquely to a smooth metric $\mathbf{g}_E$ on $\mathbb{O}_E := \pi^{-1}\left(\overline{\hat{O}_E}\right)$ defining a complete Riemann surface $(\mathbb{O}_E, \mathbf{g}_E)$.*

PROOF. With analytic changes of chart we can write near each of the centers $q = Q^2$, then the metric $\hat{\mathbf{g}}_E$ can be explicitly computed showing that it is non degenerate on the singularity and thus can be easily extended.

In case R_E is not empty the trajectory must be regularized on its boundary, for this purpose the regularization technique by Seifert [Sei48] can be applied to obtain geodesic segments of finite length that reaches the boundary of R_E perpendicularly and that can be continued by reflection on the boundary.

The rest follows as in [KK92, Theorem 3.1]. □

REMARK 2.6. *If Z_1 and Z_2 are both negative, the flow Φ_E^t is already complete since the particle with finite energies cannot reach the centers.*

On the other hand, if there is only one index $i_+ \in \{1,2\}$ such that $Z_{i_+} > 0$, the particle is still able to reach the center at s_{i_+}: if we are in one of the case not described by the previous theorem, the motion must be regularized. One of the many ways in which this can be done to extend it by reflecting the particle backward when it collides with the nucleus s_{i_+}. In this way the continuity with respect to the initial conditions is preserved.

To implement rigorously the regularization, it is enough to parametrize the state of the particle with its energy and its incoming and outgoing directions. The completion of the phase space is then obtained adjoining to it the cylinder $\mathbb{R} \times S^1$, see for example [Kna11, Theorem 11.23] *or* [KK92, Proposition 2.3].

2.2. Bifurcation diagrams

The topological structure of a Hamiltonian motion can be described by means of the constants of motion of the system. Taken together, the constants of motion define a vector valued function on the phase space of the Hamiltonian. We can study the structure of the preimages of this function (its levelsets) and how the constants of motion relate together. In the simplest and rather untypical case the levelsets are diffeomorphic manifolds. The general picture is local and can be described through the following local structures [Kna11, Section 7.3].

Given two manifold M and N let $f \in C^\infty(M,N)$. We say that f is *locally trivial* at $y_0 \in N$ if there exists a neighborhood $V \subseteq N$ of y_0 such that $f^{-1}(y)$ is a smooth submanifold of M for all $y \in V$ and there there is a map $g \in C^\infty(f^{-1}(V), f^{-1}(y_0))$ such that $f \times g : f^{-1}(V) \to V \times f^{-1}(y_0)$ is a diffeomorphism. Notice that if f is locally trivial, the restriction $g\restriction_{f^{-1}(y)} : f^{-1}(y) \to f^{-1}(y_0)$ is a diffeomorphism for every $y \in V$.

The *bifurcation set* of f is the set

$$\mathscr{B}(f) := \{y_0 \in N \mid f \text{ is not locally trivial at } y_0\}.$$

REMARK 2.7. *It is not difficult to prove that the critical point of f are points of $\mathscr{B}(f)$ (see* [Kna11, Lemma 7.24]*), on the other hand the converse is true only in the case f is proper (i.e. it has compact preimages).*

A simple counterexample is given by $f : \mathbb{R} \to \mathbb{R}$, $f(q) := -e^{-q^2}$. In its case the minimum -1 is the only singular point of f but $\mathscr{B}(f) = \{0, -1\}$.

Define the function on the phase space as follows

$$\mathscr{F} := \begin{pmatrix} H \\ H_\xi \\ p_\phi \end{pmatrix} : T^*(\mathbb{R}^3 \setminus \{\pm a\}) \to \mathbb{R}^3. \tag{2.2.1}$$

In what follows we want to characterize the bifurcation set $\mathscr{B}(\mathscr{F})$.

2.3. Bifurcations for planar motions

We consider here the case $l = 0$, corresponding to the planar motions on the (q_1, q_2)-plane, define $\mathscr{F}_0$ the restriction of $\mathscr{F}\restriction_{p_\phi^{-1}(0)}$. We have already discussed the regularizability of the problem, for what follows we proceed similarly as [WDR04] but we consider the energy range $E \geq 0$.

To cover the (q_1, q_2)-plane of the configuration space $Q_2 := \mathbb{R}^2 \setminus \{\pm a\}$ we need two half strips $[1, \infty) \times [-1, 1]$ with $\phi = 0$ and $\phi = \pi$ (i.e. one for each sign of q_2). Alternatively we can take the cylinder

$$(\xi, \eta) \in \mathbb{R} \times [-\pi, \pi]$$

as the modified configuration space $\overline{Q}_2$: it is a two-sheeted cover with branch points at the foci that could remind the previous section. The two sheets are related by the involution $I : (\xi, \eta) \mapsto (-\xi, -\eta)$ leaving the cartesian coordinates (q_1, q_2) unchanged. The symplectic lift of I to the phase space $T^*\overline{Q}_2$ equals

$$\widehat{I} : (p_\xi, p_\eta, \xi, \eta) \mapsto (-p_\xi, -p_\eta, -\xi, -\eta).$$

Then T^*Q_2 is obtained from $T^*\overline{Q}_2$ by factorization with respect to I.

REMARK 2.8. *An analysis of the extrema of V_ξ and V_η for $l = 0$ implies that the image $\mathscr{R}$ of (H, H_ξ) in $\mathbb{R}^2$ is bounded by the following curves. From $K = H_\xi \geq V_\xi$ we have $K \geq K_+(E)$ with*

$$K_+(E) := \begin{cases} -\infty, & E > 0 \\ -(Z_+ + E), & E \leq \min\left(-\frac{Z_+}{2}, 0\right) \\ \frac{Z_+^2}{4E}, & 0 \geq E > \min\left(-\frac{Z_+}{2}, 0\right) \end{cases} \tag{2.3.1}$$

and from $-K = H_\eta \geq V_\eta$ we have $K \leq K_-(E)$ with

$$K_-(E) := \begin{cases} Z_- - E, & E \leq \frac{Z_-}{2} \\ \frac{Z_-^2}{4E}, & E > \frac{Z_-}{2} \end{cases}. \tag{2.3.2}$$

The main objects of our analysis are transformed by the hamiltonian symplectomorphism defined in Theorem 2.3 as follows

$$\begin{array}{lcll} F(\xi,\eta) & \mapsto & \hat{F}(x,y) & := & x^2-y^2, \\ V_\xi(\xi) & \mapsto & V_x(x) & := & -Z_+x-Ex^2+\frac{l^2}{2(x^2-1)}, \\ V_\eta(\eta) & \mapsto & V_y(y) & := & Z_-y+Ey^2+\frac{l^2}{2(1-y^2)}, \\ H_\xi(p_\xi,\xi) & \mapsto & H_x(p_x,x) & := & \frac{(x^2-1)p_x^2}{2}+V_x(x), \\ H_\eta(p_\eta,\eta) & \mapsto & H_y(p_y,y) & := & \frac{(1-y^2)p_y^2}{2}+V_y(y). \end{array} \tag{2.3.3}$$

For the rest of the analysis we proceed with these transformed equations (2.3.3) keeping always in mind their relation with the (ξ,η) variables.

THEOREM 2.9. *Let* $(Z_1,Z_2)\in\mathbb{R}^*\times\mathbb{R}^*$, *then*

$$\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0}=\left\{(E,K)\in\mathscr{L}\mid E\geq 0 \text{ and } K_+(E)\leq K\leq K_-(E)\right\}.$$

Here $\mathscr{L}:=\mathscr{L}_0\cup\mathscr{L}_-^1\cup\mathscr{L}_-^2\cup\mathscr{L}_-^3\cup\mathscr{L}_+^2\cup\mathscr{L}_+^3$ *with*

$$\begin{array}{ll} \mathscr{L}_0:=\{E=0\}, & \mathscr{L}_-^1:=\{K=Z_--E\}, \\ \mathscr{L}_+^2:=\{K=-Z_+-E\}, & \mathscr{L}_-^2:=\{K=-Z_--E\}, \\ \mathscr{L}_+^3:=\{4EK=Z_+^2\}, & \mathscr{L}_-^3:=\{4EK=Z_-^2\}, \end{array} \tag{2.3.4}$$

and K_+ *and* K_- *are defined by* (2.3.1) *and* (2.3.2).

PROOF. The fact that $K_+(E)\leq K\leq K_-(E)$ is a consequence of Remark 2.8.

$\{E=0\}$ corresponds to threshold between compact and non compact energy surfaces, therefore it is clear that it belongs to the bifurcation set.

By definition, the critical points of $\mathscr{F}_0$ are in $\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0}$. To compute them we can take advantage of the simple form of the levelset equation in the (x,y) coordinates. To cover the plane we need to consider the two half strips with $\phi=0$ and $\phi=\pi$ (see Remark 1.5). We start assuming $\phi=0$.

We can rewrite

$$\mathscr{F}_0(p_x,p_y,x,y)=\begin{pmatrix} H(p_x,p_y,x,y) \\ H_x(p_x,x)\end{pmatrix}=\begin{pmatrix} E \\ K\end{pmatrix}$$

in the form

$$\begin{pmatrix} f_1(p_y,y) \\ f_2(p_x,x)\end{pmatrix}:=\begin{pmatrix} K+\frac{(1-y^2)p_y^2}{2}+Z_-y+Ey^2 \\ K-\frac{(x^2-1)p_x^2}{2}+Z_+x+Ex^2\end{pmatrix}=\begin{pmatrix} 0 \\ 0\end{pmatrix}$$

and use of this last representation to compute the critical points.

We look for values of (p_x,p_y,x,y) such that

$$D\begin{pmatrix} f_1(p_y,y) \\ f_2(p_x,x)\end{pmatrix}=\begin{pmatrix} -(x^2-1)p_x & 0 \\ 0 & (1-y^2)p_y \\ -xp_x^2+Z_++2Ex & 0 \\ 0 & -yp_y^2+2Ey+Z_- \end{pmatrix}^t$$

has rank smaller than 2. It is then a simple exercise to check that the critical points are given by the values

(1) $(p_x, \pm\sqrt{Z_- \pm 2E}, x, \pm 1)$,
(2) $(p_x, 0, x, -Z_-/2E)$,
(3) $(\pm\sqrt{2E + Z_+}, p_y, 1, y)$,
(4) $(0, p_y, -Z_+/2E, y)$.

Substituting these values in the equations $f_1(p_y, y) = 0$ and $f_2(p_x, x) = 0$ one obtains the following curves in the (E,K) plane

(1) $K \pm Z_- + E = 0$, thus $\mathscr{L}_-^{1,2}$ is in $\mathscr{B}(\mathscr{F}_0)$,
(2) $K - \frac{Z_-^2}{4E} = 0$, thus $\mathscr{L}_-^3$ is in $\mathscr{B}(\mathscr{F}_0)$,
(3) $K + Z_+ + E = 0$, thus $\mathscr{L}_+^2$ is in $\mathscr{B}(\mathscr{F}_0)$,
(4) $K - \frac{Z_+^2}{4E} = 0$, thus $\mathscr{L}_+^3$ is in $\mathscr{B}(\mathscr{F}_0)$.

For what concerns the half strip (x,y) with $\phi = \pi$, it is enough to notice that it corresponds to the strip $\phi = 0$ with the inversion $(p_x, p_y, x, y) \mapsto (p_x, -p_y, x, -y)$. Therefore it reduces to the analysis that we already performed.

We want to show that for energy parameters (E,K) in a connected component of $\mathscr{R} \setminus \mathscr{B}(\mathscr{F}_0)$, the energy levels $\mathscr{F}_0^{-1}(E,K)$ are diffeomorphic. We start discussing a special example.

Let $(Z_+, Z_-) = (0,2)$. Let (E_0, K_0) be in the interior of the region bounded by $\mathscr{L}_-^1$ and $K_-(E)$ (see Figure 2.1, bottom left plot). We will show in Section 2.5 that all the trajectories in configuration space with energy (E_0, K_0) must cross a segment S_0 strictly contained in the segment joining the the two centers (see Figure 2.4, plot 5 and 6 counted from the left). Since $(E_0, K_0) \notin \mathscr{L}$ the crossing must be transversal. Therefore by the linearizability of the vector field we can define a Poincaré section S_0, such that every trajectory is uniquely identified by its crossing point (see [**Kna11**, Satz 3.46 and Definition 7.16]).

Let (E_1, K_1) be another point in the interior of the region containing (E_0, K_0). As before there is a segment S_1 strictly contained in the segment joining the two centers that is crossed transversally by all the trajectories (with energy (E_1, K_1)). Given (E_1, K_1) we can define the Poincaré section S_1 and every point on the levelset is identified by its crossing point and its time, thus the levelset is diffeomorphic to $\mathbb{R} \times S_1$.

Clearly, S_0 and S_1 are diffeomorphic and thus the levelsets of (E_0, K_0) and (E_1, K_1) are diffeomorphic. By the generality of (E_0, K_0) and (E_1, K_1) all the points in the interior of the region bounded by $\mathscr{L}_-^1$ and $K_-(E)$ have diffeomorphic levelsets.

We consider another example, again $(Z_+, Z_-) = (0,2)$. Let (E_0, K_0) be in the interior of the region of $\{E > 0\}$ bounded by $\mathscr{L}_+^2$, $\mathscr{L}_-^1$ (see Figure 2.1, bottom left plot). We continue to refer to Section 2.5 when we show that for such (E,K) all the trajectories in configuration space must cross a line segment L_0 strictly contained in the q_1-axis with $q_1 < -1$ (see Figure 1.1 and the first plot from the right in Figure 2.4).

As in the previous example the trajectories must cross L_0 transversally and we can reduce the phase space to the Poincaré section L_0. If (E_1, K_1) is another point in the same region we can reiterate the procedure to find a Poincaré section L_1 that is diffeomorphic to L_0. And thus all the points in the region have diffeomorphic levelsets.

The argument sketched above can be reproduced in each connected component of $\mathscr{R} \setminus \mathscr{B}(\mathscr{F}_0)$ choosing a proper transversal section. How to make the choice will be clear in the next three sections, where we characterize the motion in configuration space for the energy parameters in each region. □

REMARK 2.10. *Differently from $\mathscr{L}_0 = \{E = 0\}$, the line $\{K = 0\}$ is in the bifurcation set only in the symmetric case $Z_- = 0$. In this case, in fact, it corresponds to the boundary $K_-(E)$ of the Hill's region.*

Of course there may be points $\{K = 0\}$ in the bifurcation set for $Z_- \neq 0$, but these are just the points in which the curves in $\mathscr{L}$ cross transversally $\{K = 0\}$ (see Figures 2.5 and 2.6).

REMARK 2.11. *The characterization of the bifurcation set given in Theorem 2.9 is redundant. Namely some of the curves $\mathscr{L}_*^*$ restricted to the values of (K, E) in the Hill's region could be empty for some values of Z_1 and Z_2.*

For example, being $K \leq K_-(E)$, we can immediately see that the curve $\mathscr{L}_+^3$ will be in the bifurcation diagram for positive E only when $Z_+ < 0$ and $|Z_+| < Z_-$.

In what follows we will describe more precisely the structure of the bifurcation sets and of the trajectories in configuration space in relation to the values assumed by Z_+ and Z_-.

The momenta (p_x, p_y) at given (E, K) are given in general by

$$\begin{aligned} p_x^2 &= \frac{2(x^2-1)(Ex^2 + Z_+ x + K) - l^2}{(x^2-1)^2}, \\ p_y^2 &= \frac{-2(1-y^2)(Ey^2 + Z_- y + K) - l^2}{(1-y^2)^2}. \end{aligned} \tag{2.3.5}$$

The Hill's region is identified by the values of E and K that admits non-negative squared momenta, being the denominator always positive we can discuss them and identify the possible motion types in terms of the zeros of the polynomials

$$P^l(s) := 2(s^2-1)(Es^2 + Z_\pm s + K) - l^2 \tag{2.3.6}$$

where $s \in \{x, y\}$ and the understanding that we choose "$+$" for $s = x$ and "$-$" for $s = y$. The factor $(s^2 - 1)$ is introduced to provide the correct signs and for computational convenience. The momenta can be simply obtained via $(x^2-1)p_x = \pm\sqrt{P^0(x)}$ and

$(1-y^2)p_y = \pm\sqrt{P^0(y)}$. The roots of $P^0_+(x)$ and $P^0_-(y)$ are respectively

$$x_{1,2} = \pm 1, \qquad x_{3,4} = -\frac{Z_+}{2E} \pm \sqrt{\frac{Z_+^2}{4E^2} - \frac{K}{E}}, \tag{2.3.7}$$
$$y_{1,2} = \pm 1, \qquad y_{3,4} = -\frac{Z_-}{2E} \pm \sqrt{\frac{Z_-^2}{4E^2} - \frac{K}{E}},$$

with the convention that the smaller index correspond to the solution with negative sign. In both variables, the polynomials have two fixed roots at ± 1 and two movable roots which depend on the constants of motion. Being $x \in [1,\infty)$, we are going to consider only roots in this region.

The discriminant of P^0 is proportional to

$$\operatorname{discr}(P^0) = (Z_\pm^2 - 4EK)(E+K-Z_\pm)^2(E+K+Z_\pm)^2. \tag{2.3.8}$$

Double roots appear when $\operatorname{discr}(P^0)$ vanishes. For each couple (Z_+, Z_-) this gives six curves in the (K,E)-plane, three for the x variable and three for the y. These are the curves $\mathscr{L}^1_+ := \{K = Z_+ - E\}$ and $\mathscr{L}^1_-$, $\mathscr{L}^{2,3}_\pm$ defined by (2.3.4).

REMARK 2.12. *The zeroes of the discriminant P^0 (2.3.8) corresponds to the double roots of $(Es^2 + Z_\pm s + K)$ and the points in which these roots reach the fixed roots ± 1, that is the q_1-line. The positivity of P^0 and the positions of its roots, as we will see, characterizes the trajectories in configuration space.*

The curve $\mathscr{L}^1_+$ appearing in the discriminant depends from the fact that we considered $x \in \mathbb{R}$. As such it will have no correspondence in the bifurcation set or in the description of the possible motions.

As a first step we consider the cases in which $Z_- = 0$ or $Z_+ = 0$. In these cases the (K,E)-plane is divided by the curves $\mathscr{L}^{1,2,3}_\pm$ into different regions. We will label these regions using roman numbers with a subscript chosen between $>$, $<$ and 0 indicating if $Z_+ > 0$, $Z_+ < 0$ or $Z_+ = 0$ respectively. In Figure 2.1 are shown representative bifurcation diagrams for these three cases with the corresponding enumeration of the regions.

2.4. Motion for $Z_- = 0$

The case $Z_- = 0$ corresponds to two attracting (or repelling) centers with the same charges. We have the following corollary of Theorem 2.9.

COROLLARY 2.13. *Let $Z_- = 0$ and $Z_+ \in \mathbb{R}^*$. With the notation of (2.3.4) we have*

$$\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0} = \left\{(E,K) \in \mathscr{L}_0 \cup \mathscr{L}^1_- \cup \mathscr{L}^2_+ \mid E \geq 0 \text{ and } K_+(E) \leq K \leq 0\right\}.$$

PROOF. In (1.1.1) we assumed $Z_1, Z_2 \neq 0$, therefore $Z_- = 0$ implies $Z_+ \neq 0$. K cannot be positive because $K_-(E) = 0$ for $E \geq 0$. By $\mathscr{L}^1_- = \mathscr{L}^2_-$ and $\mathscr{L}^3_- = \mathscr{L}_0$, it is redundant to add both in the definition of the bifurcation diagram. The fact that $\mathscr{L}^3_+$ is not in the bifurcation set follows from Remark 2.11. Then the claim follows directly from Theorem 2.9. ☐

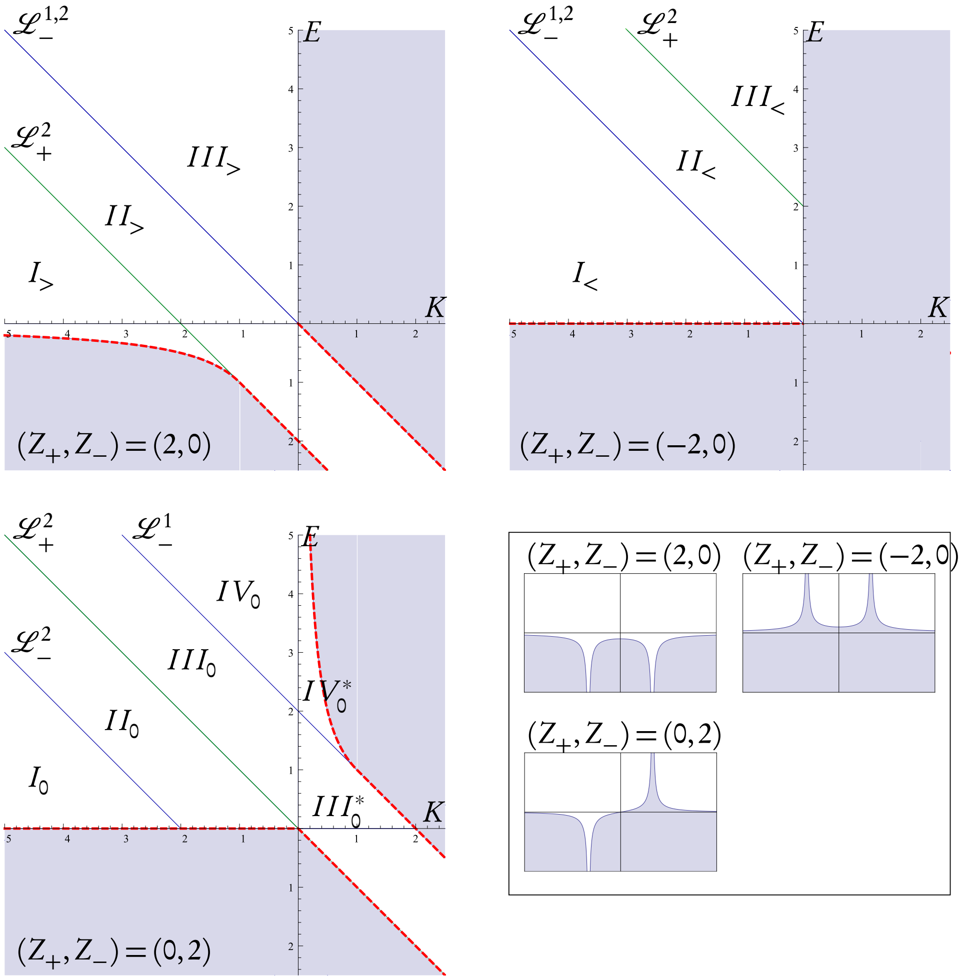


FIGURE 2.1. Examples of bifurcation diagrams for the considered planar cases, the shaded regions identify the complement of the Hill's region, the red dashed curves are K_+ and K_-. The green line $\mathscr{L}_+^2$ parametrized by $K_0(E) = -(Z_+ + E)$ corresponds to the closed orbit wandering between the two centers and having coordinate $x = 1$. The box on the right shows the shape of the potential V on the q_1-axis in the different cases.

Consider the bifurcation diagram for $(Z_+, Z_-) = (\pm 2, 0)$ appearing in Figure 2.1. It is possible to describe the qualitative structure of the motion in configuration space for energy parameters in the different regions by studying the dynamic of the roots (2.3.7) with respect to a walk in the bifurcation diagram. By this we mean fixing a value of E big enough and varying K to move through the regular regions $I_{>,<}$, $II_{>,<}$, $III_{>,<}$ and to cross the bifurcation lines.

A qualitative representation of how the motion changes with respect to the energy parameters is shown in Figure 2.2 for $Z_+ = 2$ and in Figure 2.3 for $Z_+ = -2$. This can be schematically explained through the behavior of the roots (2.3.7) as follows.

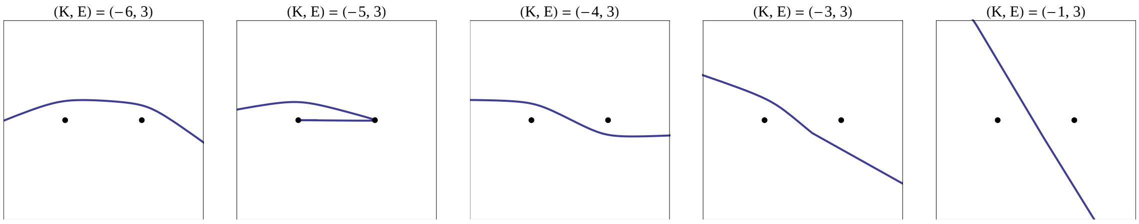


FIGURE 2.2. Example of possible trajectories in the case $Z_+ = 2$, $Z_- = 0$ for $E = 3$ and growing values of K (from left to right) chosen in the different regions of the bifurcation diagram.

- Roots of the polynomial $P^0(y)$.
  - For energies in the regions $I_{>,<}$ and $II_>$ of the bifurcation diagrams, the polynomial $P^0(y)$ is positive for every value of $y \in [-1,1]$ and $|y_{3,4}| > 1$. Thus for energy parameters in these regions, the particle is allowed travel in configuration space everywhere in a region around the centers.
  - Line $\mathscr{L}^1_-$ characterizes the values (E,K) such that the two group of roots of $P^0(y)$ merge: $y_3 = y_1 = -1$ and $y_4 = y_2 = 1$.
  - In the regions $II_<$ and $III_{>,<}$, $|y_{3,4}| < 1$ and the $P^0(y)$ is not negative only if $y \in [y_3, y_4]$. This means that the motion in configuration space can cross the axis between the two centers only passing through the segment joining them centers.
- Roots of the polynomial $P^0(x)$.
  - Notice that x_1 and x_3 are always smaller than 1, thus they won't enter the discussion.
  - In the regions $I_{>,<}$ and $II_<$, the root $x_4 > 1$ and $P^0(x)$ is positive only if $x \in [x_4, \infty)$. Therefore in configuration space, the particle cannot reach the line joining the two centers.
  - For $(E,V) \in \mathscr{L}^2_+$, we have the collision of the solutions $x_4 = x_2 = 1$ and in configuration space the particle can reach the line between the centers.
  - On the right of $\mathscr{L}^2_+$, in the regions $II_>$ and $III_{>/<}$, the root $x_4 < 1$ and $P^0(x)$ is non-negative for $x \in [1, \infty)$. In other words the particle can cross the line in configuration space connecting the centers.

We can now understand the peculiarity of the lines in the bifurcation set.

- For values of the parameters on the singular line $\mathscr{L}^1_-$ we can identify two special trajectories in configuration space. In these, the particle lies in the positive (negative) q_1-axis with $|q_1| > 1$, possibly bouncing against the singularity and being reflected back.
- For (E,V) on $\mathscr{L}^2_+$ we can find the unique periodic orbit of the regularized classical two-centers problem, see [Kna02]. It is the hyperbolic trajectory of a particle bouncing between the centers. Counting from left to right,

the second plot of Figure 2.2 and the fourth plot of Figure 2.3 show the trajectory of a particle on the stable manifold of this special orbit.

- For $K = 0$ ($E > 0$) only one trajectory is possible: the vertical trajectory moving on the line $y = 0$.

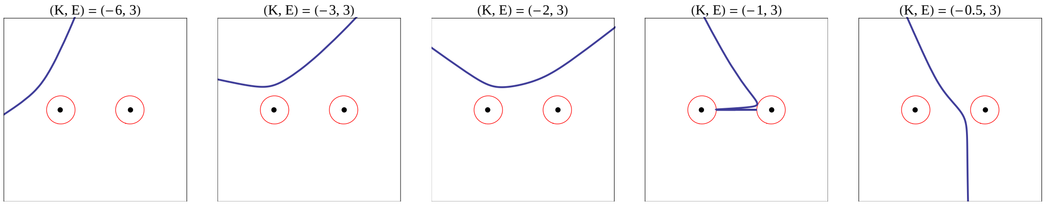


FIGURE 2.3. Example of possible trajectories in the case $Z_+ = -2$, $Z_- = 0$ for $E = 3$ and growing values of K (from left to right) chosen in the different regions of the bifurcation diagram. The red line corresponds to the energy level of the plotted trajectory.

REMARK 2.14. *Notice that the ordering of the singular curves reflects the main difference between the cases $Z_+ > 0$ and $Z_+ < 0$. In the first case (corresponding to the attracting potential) the particle is able to travel arbitrarily near to the centers. In the case $Z_+ < 0$ the centers $\pm a$ have a positive distance from the Hill's region.*

2.5. Motion for $Z_+ = 0$

COROLLARY 2.15. *Let $Z_+ = 0$ and $Z_- > 0$. With the notation of (2.3.4) we have*

$$\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0} = \Big\{(E,K) \in \mathscr{L}_0 \cup \mathscr{L}^1_- \cup \mathscr{L}^2_- \cup \mathscr{L}^3_- \cup \mathscr{L}^2_+ \mid E \geq 0 \text{ and } K_+(E) \leq K \leq K_-(E)\Big\}.$$

PROOF. In (1.1.1) we assumed $Z_1, Z_2 \neq 0$, therefore $Z_+ = 0$ implies $Z_- \neq 0$. We have $\mathscr{L}^3_+ = \mathscr{L}_0$. The claim follows directly from Theorem 2.9. □

As in the previous section we give a qualitative explanation of the possible motions in configuration space through the behavior of the roots (2.3.7). A visual support is provided by Figure 2.4.

- Roots of the polynomial $P^0(y)$.
  - For (E, V) in I_0, the polynomial $P^0(y)$ is not negative for any $y \in [-1, 1]$. Thus in configuration space the particle is free to move around the centers.
  - For energy parameters on $\mathscr{L}^2_-$, two roots collide: $y_4 = y_2 = 1$.
  - The motion in configuration space for (E, V) in II_0 and III_0 is restricted to $y \in [-1, y_4]$. That is, the particle is free to travel around the attracting center but is bounded away from the repelling one.
  - For energies on $\mathscr{L}^1_-$, the other two roots collide: $y_3 = y_1 = -1$ and for $(E, V) \in IV_-$ the only allowed y are restricted in $y \in [y_3, y_4]$:

in configuration space the particle cannot anymore travel around the centers.
  - On the line $K=0$, $y_4=0$ and for bigger values of K (i.e. in the regions III_0^* and IV_0^*) y_4 becomes negative. The particle in configuration space is no more able to flow around the repelling center.
- For the roots of $P^0(x)$ the discussion is similar as before.
  - The roots $x_{1,3}$ are negative. We consider only the roots $x_{2,4}$.
  - For energy parameters in I_0 and II_0 the root $x_4>1$ and the polynomial $P^0(x)$ is positive for $x\in[x_4,\infty)$. Therefore in configuration space the particle cannot reach the line between the centers.
  - For energy parameters on the right of $\mathscr{L}_+^2$ the motion becomes possible for $x\in[1,\infty)$. I.e. the particle can reach the line between the centers.

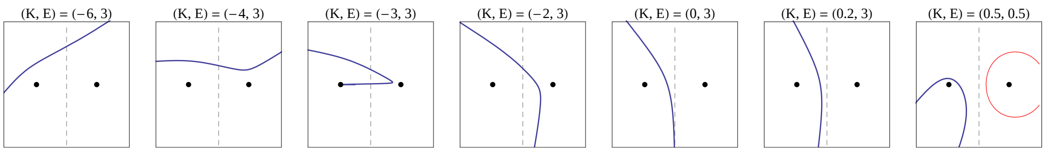


FIGURE 2.4. Example of possible motions in the case $Z_+=0$, $Z_-=2$ for values of E and K in different regions of the bifurcation diagram. The red line is the energy level of the trajectory in the plot.

2.6. The general case

We first describe the bifurcation set for the fully repelling (or attracting) configuration $\mathrm{sign}(Z_1)=\mathrm{sign}(Z_2)$. The picture is similar to the one with $Z_-=0$ (see Section 2.4) with the only difference that some positive values of K are allowed (see Figure 2.5).

COROLLARY 2.16. *Let $|Z_+|>Z_-$, $Z_-\in\mathbb{R}_+^0$. With the notation of (2.3.4) we have*

$$\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0}=\Big\{(E,K)\in\mathscr{L}_0\cup\mathscr{L}_-^1\cup\mathscr{L}_-^2\cup\mathscr{L}_-^3\cup\mathscr{L}_+^2\,|\,E\geq 0,\\ K_+(E)\leq K\leq K_-(E)\Big\}.$$

PROOF. By Remark 2.11, $\mathscr{L}_+^3$ is not in the bifurcation set. The corollary follows immediately from Theorem 2.9. □

The structure of the trajectories and the qualitative behavior of the motion in configuration space for this case is analogous to the one presented in Section 2.4, therefore we will not discuss it.

The case $|Z_+|<Z_-$ looks more complicated and particularly interesting.

COROLLARY 2.17. *Let $|Z_+|<Z_-$, $Z_-\in\mathbb{R}_+^0$. If $Z_+>0$ we have*

$$\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0}=\Big\{(E,K)\in\mathscr{L}_0\cup\mathscr{L}_-^1\cup\mathscr{L}_-^2\cup\mathscr{L}_-^3\cup\mathscr{L}_+^2\,|\\ E\geq 0 \text{ and } K_+(E)\leq K\leq K_-(E)\Big\},$$

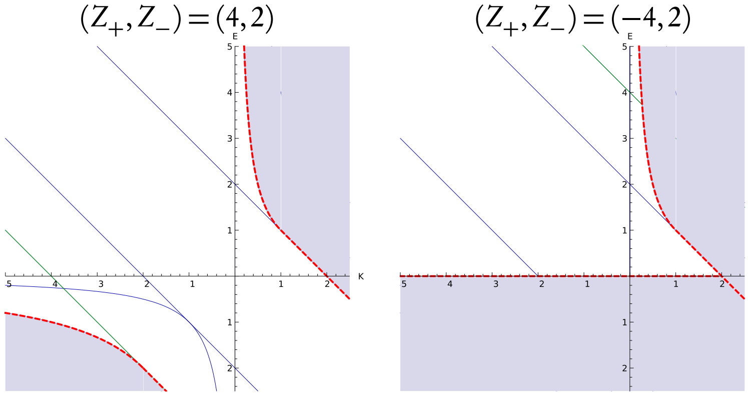


FIGURE 2.5. Bifurcation diagrams for the fully attracting (left) and the fully repelling (right) case respectively. The shaded regions identify the complement of the Hill's region.

while if $Z_+ < 0$ *we have*

$$\mathscr{B}(\mathscr{F}_0)\restriction_{E\geq 0} = \Big\{(E,K) \in \mathscr{L}_0 \cup \mathscr{L}_-^1 \cup \mathscr{L}_-^2 \cup \mathscr{L}_-^3 \cup \mathscr{L}_+^2 \cup \mathscr{L}_+^3 \mid E \geq 0 \text{ and } K_+(E) \leq K \leq K_-(E)\Big\}.$$

PROOF. By Remark 2.11, $\mathscr{L}_+^3$ is not in the bifurcation set. The corollary follows immediately from Theorem 2.9. □

In this case the qualitative behavior of the motion in configuration space is analogous to the one presented in Section 2.5, but for energy parameters in the region $I_<^a$. This region contains the set of energy parameters included in the region bounded above by $\mathscr{L}_+^{3-} := \Big\{(E,K) \in \mathscr{L}_+^3 \;\Big|\; E < \frac{|Z_+|}{2}\Big\}$, on the sides by $\mathscr{L}_+^2$ and $\mathscr{L}_+^1$ and below by $E \geq 0$ (see Figure 2.6).

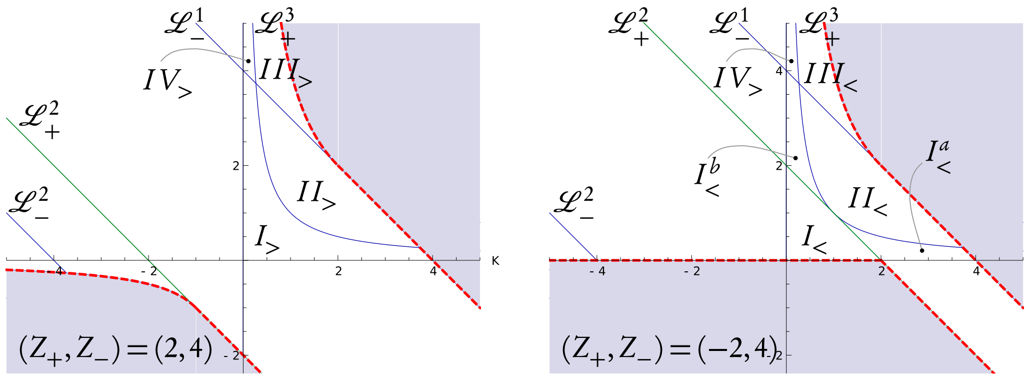


FIGURE 2.6. Bifurcation diagrams and labeled regions for $|Z_+| < Z_-$. The shaded regions identify the complement of the Hill's region.

For (E,V) on $I_<^a$ a new phenomenon appears: both the movable roots of $P^0(x)$ are bigger than one and the polynomial is positive in the union of the two disjoint intervals $[1, x_3]$ and $[x_4, 1]$. On the configuration space they gives rise to an escaping trajectory similar to the previous ones and to a family of bounded trajectories near the attracting center (see Figure 2.7).

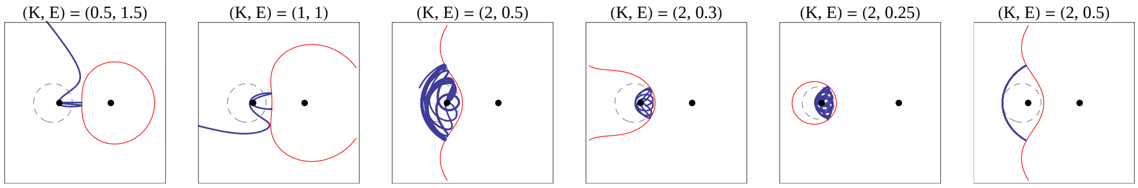


FIGURE 2.7. Bounded motions for $Z_+ < 0$, $|Z_+| < Z_-$ and $E \geq 0$. From left to right: trajectory for energy parameters on the boundary $\mathscr{L}^2_+$ of $I^a_<$, trajectory for energies on the tangency point between $\mathscr{L}^2_+$ and $\mathscr{L}^3_+$, trajectory for energies on the boundary $\mathscr{L}^3_+$ of $I^a_<$ Then follow two trajectories for energies inside $I^a_<$ and the trajectory on $\mathscr{L}^3_+$. The red line is the energy level of the trajectory in the plot, the dotted line is the 0-energy level.

CHAPTER 3

The two-centers system on $L^2(\mathbb{R}^3)$

As a first step we want to analyze from an operator theoretical point of view the separation of variables obtained in the previous section and its consequences on the nature and the properties of the resulting equations.

3.1. First separation from an operator theoretical point of view

We transform by the diffeomorphism G from (1.2.1) into prolate elliptic coordinates (ξ,η,ϕ) with the unitary operator denoted by

$$\mathscr{G}: L^2(\mathbb{R}^3,dq)\to L^2(M,d\chi\, d\phi). \tag{3.1.1}$$

We index the transformed objects by $\mathscr{G}$. Let us write $\chi=(\xi,\eta)$ for the first two prolate elliptic variables and

$$d\widetilde{\chi}:=\sinh\xi\,\sin\eta\, d\xi\, d\eta, \qquad d\chi=F(\xi,\eta)d\widetilde{\chi}, \tag{3.1.2}$$

where $F(\xi,\eta)=\sinh^2(\xi)+\sin^2(\eta)$ is the map given by (1.2.2). The weight in the measure $d\chi$ is nothing else than the Jacobian of the change of coordinate defined by (1.2.1). The weight in the measure $d\widetilde{\chi}$ equals the Jacobian for the planar case. So $d\chi$ is a measure on the domain $R^+\times(0,\pi)$, absolutely continuous with respect to the Lebesgue measure λ^2. Likewise, $d\widetilde{\chi}$ is a measure on M (defined in Section 1.2) absolutely continuous with respect to the Lebesgue measure λ^3

Proposition 3.1. *The operator $\mathscr{H}=-h^2\Delta+V$ on $L^2(\mathbb{R}^3)$ (defined in (1.1.1)) is unitarily equivalent to the operator in $L^2(M,d\chi\, d\phi)$ given by*

$$\mathscr{H}_{\mathscr{G}}:=-h^2\Delta_{\mathscr{G}}+V_{\mathscr{G}}(\xi,\eta)$$

where

$$\Delta_{\mathscr{G}}=\frac{1}{F(\xi,\eta)}\left\{\frac{1}{\sinh(\xi)}\partial_\xi\left(\sinh(\xi)\,\partial_\xi\right)+\right.$$
$$\left.+\frac{1}{\sin(\eta)}\partial_\eta\left(\sin(\eta)\,\partial_\eta\right)+\left(\frac{1}{\sin^2(\eta)}+\frac{1}{\sinh^2(\xi)}\right)\partial_\phi^2\right\}.$$

The potential is given by

$$V_{\mathscr{G}}(\xi,\eta)=-\frac{Z_+\cosh(\xi)-Z_-\cos(\eta)}{F(\xi,\eta)},$$

and F is defined by (1.2.2). $\mathscr{H}_{\mathscr{G}}$ is essentially self-adjoint on

$$\mathscr{G}\left(C_0^\infty(\mathbb{R}^3)\right) = \Big\{ f(\xi,\eta,\phi) \in C_0^\infty\left(\overline{M}\right) \mid \pi\text{-periodic in } \eta, \\ 2\pi\text{-periodic in } \phi \text{ and } \partial_\xi f|_{\xi=0} = 0 \Big\}$$

and self-adjoint on $\mathscr{G}(H^2(\mathbb{R}^3))$.

Proof. It is well known (see for example [**RS75**, Theorem X.15, p. 165] or [**HS96**, Theorem 13.7, p. 136]) that $\mathscr{H}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ (and self-adjoint on $H^2(\mathbb{R}^3)$), see Remark 3.2 below.

It is obvious that the unitarily transformed operator $\mathscr{H}_{\mathscr{G}} := \mathscr{G}\mathscr{H}\mathscr{G}^{-1}$ remains essentially self-adjoint on $\mathscr{G}\left(C_0^\infty(\mathbb{R}^3)\right)$, then the form of the operator $\mathscr{H}_{\mathscr{G}}$ is given by the computations in the proof of Theorem 1.7. □

Remark 3.2. *That $\mathscr{H}$ is self-adjoint on the Sobolev space $H^2(\mathbb{R}^3)$, is a straightforward application of the Kato-Rellich Theorem, see Appendix C. On one hand there is the self-adjointness of the Laplacian on $H^2(\mathbb{R}^3)$, on the other hand there is the Δ-boundedness with relative bound 0 of the potentials $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (see [**RS75**, Theorem X.15]). In this last point is hidden the relevant fact of this proof: if we write $V = V_2 + V_\infty$ and we take $\psi \in D(V)$ we have*

$$\|V\psi\|_2 \le \|V_2\|_2 \cdot \|\psi\|_\infty + \|V_\infty\|_\infty \cdot \|\psi\|_2,$$

*but in principle we have no information on $\|\psi\|_\infty$. Both $D(V)$ and $D(-\Delta)$ contains $C_0^\infty(\mathbb{R}^3)$, then it follows that we can use the characterization of functions in the domain of the laplacian (see [**RS75**, Theorem IX.28]), namely ψ is a bounded continuous function and for any $a > 0$, there is a b, independent of ψ, so that $\|\psi\|_\infty \le a\|\Delta\psi\|_2 + b\|\psi\|_2$ and we have the Δ-boundedness in $L^2(\mathbb{R}^3)$.*

*Notice that the Coulombic potentials are in this class only if the dimension of the space is strictly bigger than 2. In fact for operators in $L^2(\mathbb{R})$ or $L^2(\mathbb{R}^2)$ this is no more true. In particular in dimension 2 the self-adjointness can still be proved using KLMN Theorem [**RS75**, Theorem X.17] and the infinitesimally form boundedness of V w.r.t. Δ [**Agm82**, Theorem 3.2]. In this way the operator is well defined and has form domain $H^1(\mathbb{R}^2)$. In one dimension even this weaker construction fails and it is necessary to remove the singularities from the space and fix proper boundary conditions on the domain.*

Define $M_0 := \mathbb{R}_+^0 \times [0,\pi]$. Let us denote $\mathscr{D}$ the space of finite linear combination of products $f(\chi)w(\phi)$ where

$$f \in \widehat{C}_0^\infty(M_0) := \left\{ f(\xi,\eta) \in C_0^\infty(M_0) \mid \pi\text{-periodic in } \eta,\ \partial_\xi f|_{\xi=0} = 0 \right\} \\ \subset L^2(M_0, d\chi) \tag{3.1.3}$$

and $w \in C^\infty(S^1)$. Due to the factorizability of L^2 spaces (see [**RS80**, Theorem II.10, p. 52]) and the decomposition in prolate elliptic coordinates

$$L^2(M, d\chi\, d\phi) \cong L^2(M_0, d\chi) \otimes L^2(S^1, d\phi),$$

$\mathscr{G}^{-1}\mathscr{D}$ is a dense set in $L^2(\mathbb{R}^3)$.

Furthermore for functions $\psi(\chi,\phi)=f(\chi)w(\phi)$, the operator $\mathscr{H}$ takes the form

$$\mathscr{H}f(\chi)w(\phi)=\left(-h^2A_\chi f(\chi)\right)w(\phi)+\frac{h^2f(\chi)}{\sinh^2(\xi)\sin^2(\eta)}\mathscr{B}w(\phi) \tag{3.1.4}$$

with

$$A_\chi:=\frac{1}{F(\xi,\eta)}\left\{\frac{1}{\sinh(\xi)}\partial_\xi\left(\sinh(\xi)\partial_\xi\right)+\frac{1}{\sin(\eta)}\partial_\eta\left(\sin(\eta)\partial_\eta\right)+\right.$$
$$\left.+h^{-2}Z_+\cosh(\xi)-h^{-2}Z_-\cos(\eta)\right\}$$

acting on $L^2(M_0,d\chi)$ and $\mathscr{B}:=\mathscr{B}_\phi:=-\partial_\phi^2$ the Laplace-Beltrami operator acting on $L^2(S^1,d\phi)$. The operator $\mathscr{B}$ is essentially self-adjoint on $C^\infty(S^1)$ and admits an orthonormal basis of eigenfunctions, namely

$$\mathscr{B}\omega_\lambda(\phi)=\lambda^2\omega_\lambda(\phi),\quad \lambda\in\mathbb{Z},$$

where $\omega_\lambda(\phi)=e^{i\lambda\phi}/\sqrt{2\pi}$. The family of ω_λ defines an orthonormal basis of $L^2(S^1,d\phi)$.

Call Ω_λ the subspace spanned by ω_λ and define

$$L^2_\lambda:=L^2(M_0,d\chi)\otimes\Omega_\lambda$$

to have

$$L^2(\mathbb{R}^3)\cong\bigoplus_{\lambda\in\mathbb{Z}}L^2_\lambda.$$

Then, if $\mathbb{1}_\lambda$ is the identity operator on Ω_λ, the restriction of $\mathscr{H}$ to $\mathscr{D}_\lambda=\mathscr{D}\cap L^2_\lambda$ is given by $\mathscr{H}\Big|_{\mathscr{D}_\lambda}=\mathscr{H}_\lambda\otimes\mathbb{1}_\lambda$, where

$$\mathscr{H}_\lambda:=\frac{-h^2}{F(\xi,\eta)}\left(\mathscr{A}_\chi-\frac{\lambda^2}{\sinh^2(\xi)}-\frac{\lambda^2}{\sin^2(\eta)}\right) \tag{3.1.5}$$

acts on $L^2(M_0,d\chi)$. This leads to the proposition that follows.

PROPOSITION 3.3. *The operator $\mathscr{H}$ defined in (1.1.1) is unitarily equivalent to the operator $\bigoplus_{\lambda\in\mathbb{Z}}\mathscr{H}_\lambda\otimes\mathbb{1}_\lambda$ acting on $\bigoplus_{\lambda\in\mathbb{Z}}L^2_\lambda$.*

3.2. A remark on the second separation

The problem is now transferred to the study of the self-adjoint extension $\mathscr{H}_\lambda$ of each operator in the new family defined by Proposition 3.3.

Notice that for $\varphi,\psi\in\widehat{C}_0^\infty(M_0)$ we have

$$\langle\psi,\mathscr{H}_\lambda\varphi\rangle_{L^2(M_0,d\chi)}=\langle\psi,K_\lambda\varphi\rangle_{L^2(M_0,d\tilde{\chi})}$$

where $K_\lambda = F(\xi,\eta)\mathscr{H}_\lambda$, i.e.

$$K_\lambda = -h^2\Big(\mathscr{A}_\chi - \frac{\lambda^2}{\sinh^2(\xi)} - \frac{\lambda^2}{\sin^2(\eta)}\Big). \tag{3.2.1}$$

In the same way, if we consider the eigenvalue equation for $\mathscr{H}_\lambda$, we have that for $\psi,\phi \in \widehat{C}_0^\infty(M_0)$

$$\langle \psi,(\mathscr{H}_\lambda - E)\phi\rangle_{L^2(M_0,d\chi)} = \langle \psi,(K_\lambda - EF(\xi,\eta))\phi\rangle_{L^2(M_0,d\widetilde{\chi})},$$

and consequently

$$(\mathscr{H}_\lambda - E)\phi(\xi,\eta)=0 \quad \Longleftrightarrow \quad (K_\lambda - EF(\xi,\eta))\phi(\xi,\eta)=0.$$

The differential equation $(K_\lambda - F(\xi,\eta)E)\psi(\xi,\eta)=0$ can be rewritten as

$$(K_\lambda - F(\xi,\eta)E)\psi(\xi,\eta) = F(\xi,\eta)(H_\lambda - E)\psi(\xi,\eta) = \mathscr{A}^\lambda_{\xi,\eta}\psi(\xi,\eta)=0 \tag{3.2.2}$$

where

$$\mathscr{A}^\lambda_{\xi,\eta}(h) := \mathscr{A}^\lambda_{\xi,\eta,h,E} := (\mathscr{A}^\lambda_{\xi,h,E} + \mathscr{A}^\lambda_{\eta,h,E}) \tag{3.2.3}$$

with

$$\mathscr{A}^\lambda_\xi(h) := -h^2\frac{1}{\sinh(\xi)}\partial_\xi\left(\sinh(\xi)\,\partial_\xi\right) - Z_+\cosh(\xi) - E\cosh^2(\xi) + \frac{h^2\lambda^2}{\sinh^2(\xi)}$$

and

$$\mathscr{A}^\lambda_\eta(h) := -h^2\frac{1}{\sin(\eta)}\partial_\eta\left(\sin(\eta)\,\partial_\eta\right) + Z_-\cos(\eta) + E\cos^2(\eta) + \frac{h^2\lambda^2}{\sin^2(\eta)}.$$

We will call $\mathscr{A}^\lambda_\xi(h)$ *radial* operator and $\mathscr{A}^\lambda_\eta(h)$ *angular* operator, names coming by an obvious comparison with role of the variables ξ and η in the prolate spheroidal coordinate (see Remark 1.5).

In view of this fact, it seems natural to move our point of view from the measure space $L^2(M_0,d\chi)$ to

$$\begin{aligned} L^2(M_0,d\widetilde{\chi}) &= L^2(M_0,\sinh\xi\,\sin\eta\,d\xi\,d\eta) \\ &\cong L^2(\mathbb{R}^0_+,\sinh\xi\;d\xi)\otimes L^2([0,\pi],\sin\eta\,d\eta). \end{aligned}$$

In the next sections we will study these two last operators acting respectively on $L^2(\mathbb{R}^0_+,\sinh(\xi)\,d\xi)$ and $L^2([0,\pi],\sin(\eta)\,d\eta)$ to justify properly the weak separation described in this section.

3.3. Self-adjoint extension and spectrum of the angular operator

Set $I_0 := [-1,1]$. If we apply the unitary transform

$$L^2([0,\pi],\sin\eta\,d\eta) \to L^2(I_0,dx), \quad g(\eta)\mapsto g(\arccos(x)), \tag{3.3.1}$$

the operator $\mathscr{A}^\lambda_\eta(h)$ transforms to

$$\mathscr{A}^\lambda_x(h) := \mathscr{L}^\lambda_x(h) + \mathscr{V}(x) \tag{3.3.2}$$

where

$$\mathscr{L}_x^\lambda(h) := -h^2\partial_x\left((1-x^2)\partial_x\right) + \frac{h^2\lambda^2}{1-x^2}$$

and

$$\mathscr{V}(x) := Ex^2 + Z\_x. \tag{3.3.2a}$$

The eigenvalue equation corresponding to $\mathscr{L}_x^\lambda(1)$

$$\mathscr{L}_x^\lambda(1)u = k(k+1)u$$

is the *associated Legendre equation*. For $k \in \mathbb{N}$ its eigenfunctions are the *associated Legendre function*

$$P_k^\lambda(x) := (-1)^\lambda(1-x^2)^{\lambda/2}\partial_x^\lambda P_k(x), \quad |\lambda| < k,$$

where the $P_k(x)$ are the Legendre polynomials

$$P_k(x) := \frac{1}{2^k k!}\partial_x^k(x^2-1)^k.$$

Another solution, linearly independent from P_k^λ, is given by

$$Q_k^\lambda(x) = P_k^\lambda(x)\int_0^x \frac{dt}{(1-t^2)(P_k^\lambda(x))^2}.$$

If we choose the boundary conditions generated by $P_0(x) = 1$, the following theorem can be proven

THEOREM 3.4. *The operator $\mathscr{L}_x^\lambda(1)$, $\lambda \in \mathbb{Z}$, defined via*

$$D(\mathscr{L}_x^\lambda(1)) = \{f \in L^2(I_0)\,|\, f, f' \in AC(I_0), \mathscr{L}_x^\lambda(1)f \in L^2(I_0), \lim_{x\to\pm 1}(1-x^2)f'(x) = 0 \text{ if } \lambda = 0\}$$

is self-adjoint. Its spectrum is purely discrete, that is

$$\sigma(\mathscr{L}_x^\lambda(1)) = \sigma_d(\mathscr{L}_x^\lambda(1)) = \{k(k+1)\,|\, k \in \mathbb{N}_0, |\lambda| \le k\},$$

and the corresponding eigenfunctions

$$u_{k,\lambda}(x) = \sqrt{\frac{2k+1}{2}\frac{(k-\lambda)!}{(k+\lambda)!}}P_k^\lambda(x), \quad k \in \mathbb{N}_0,\ |\lambda| \le k,$$

form an orthonormal basis for $L^2(I_0)$.

PROOF. The result is standard, one proof can be found in [Tes09, Theorem 10.6, p. 226]. The definition of the domain follows by the fact that $\mathscr{L}_x^\lambda$ is LCC at both -1 and 1 for $\lambda = 0$ and it is LPC in both the points for $\lambda \ne 0$, as one could guess from the presence of the λ dependent singularity at ± 1. □

We need the following Corollary of Theorem 3.4.

COROLLARY 3.5. *The operator $\mathscr{L}_x^\lambda(h)$, $\lambda \in \mathbb{Z}$, defined via*

$$D(\mathscr{L}_x^\lambda(h)) = \{f \in L^2(I_0) \mid f, f' \in AC(I_0),\ \mathscr{L}_x^\lambda(h) f \in L^2(I_0), \lim_{x\to\pm1}(1-x^2)f'(x) = 0 \text{ if } \lambda = 0\}$$

is self-adjoint. Its spectrum is purely discrete, that is

$$\sigma(\mathscr{L}_x^\lambda(h)) = \sigma_d(\mathscr{L}_x^\lambda(h)) = h^2 \sigma_d(\mathscr{L}_x^\lambda(1)),$$

and the corresponding eigenfunctions

$$u_{k,\lambda}^h(x) \quad \text{with} \quad k \in \mathbb{N},\ k(k+1)h^2 \in \sigma(\mathscr{L}_x^\lambda(h)),$$

form an orthonormal basis for $L^2(I_0)$.

THEOREM 3.6. *The operator $\mathscr{A}_x^\lambda(h)$ with domain $D(\mathscr{A}_x^\lambda(h)) = D(\mathscr{L}_x^\lambda(h))$ is self-adjoint and its essential spectrum is empty.*

PROOF. We know from Theorem A.5 that the resolvent of $\mathscr{L}_x^\lambda(h)$ is a Hilbert-Schmidt operator and thus is compact.

In our domain the multiplication operator $\mathscr{V}$ is bounded by

$$|\mathscr{V}(x)| \le |E| + |Z_-|,$$

thus it is only a bounded perturbation of the operator $\mathscr{L}_x^\lambda(h)$. It follows directly that $\mathscr{V} \cdot (\mathscr{L}_x^\lambda(h) - i)^{-1}$ is compact (for more details see [RS80, Theorem VI.12, p.200]) and thus $\mathscr{V}$ is relatively compact with respect to $\mathscr{L}_x^\lambda(h)$.

Therefore by Theorem C.2 follows that $\mathscr{A}_x^\lambda(h)$ is self-adjoint on $D(\mathscr{L}_x^\lambda)(h)$ and $\sigma_{ess}(\mathscr{L}_x^\lambda(h)) = \sigma_{ess}(\mathscr{A}_x^\lambda(h)) = \emptyset$. □

THEOREM 3.7 (min-max principle, operator form). *Let H be a self-adjoint operator that is bounded from below, i.e., $H \ge cI$ for some c. Define*

$$\mu_n(H) := \sup_{\varphi_1,\ldots,\varphi_{n-1}} U_H(\varphi_1,\ldots,\varphi_{n-1})$$

where

$$U_H(\varphi_1,\ldots,\varphi_m) = \inf_{\substack{\psi\in D(H):\|\psi\|=1 \\ \psi\in[\varphi_1,\ldots,\varphi_m]^\perp}} \langle \psi, H\psi\rangle$$

and $[\varphi_1,\ldots,\varphi_m]^\perp$ is a shorthand for $\{\psi | \langle \psi, \varphi_i\rangle = 0, i = 1,\ldots,m\}$. Note that the φ_i are not necessarily independent.

Then, for each fixed n, either*:*

(a) *there are n eigenvalues (counting degenerate eigenvalues a number of times equal to their multiplicity) below the bottom of the essential spectrum, and $\mu_n(H)$ is the nth eigenvalue counting multiplicity;*

or

(b) *μ_n is the bottom of the essential spectrum, i.e. $\mu_n = \inf\{\lambda | \lambda \in \sigma_{ess}(H)\}$ and in that case $\mu_n = \mu_{n+1} = \mu_{n+2} = \cdots$ and there are at most $n-1$ eigenvalues (counting multiplicity) below μ_n.*

PROOF. The proof of the min-max principle and its consequences are in [RS78, Section XIII.1 p. 75]. □

Given the fact that all the operators are defined on the same domain, one has

$$U_{\mathscr{L}_x^\lambda(h)} + m(Z_-, E) \le U_{\mathscr{A}_x^\lambda(h)} \le U_{\mathscr{L}_x^\lambda(h)} + M(Z_-, E), \tag{3.3.3}$$

where

$$m := m(Z_-, E) := \min_{x\in[-1,1]} \mathscr{V}(x) \quad \text{and} \quad M := M(Z_-, E) := \max_{x\in[-1,1]} \mathscr{V}(x) \tag{3.3.4}$$

are both finite. As a consequence

$$\mu_n(\mathscr{L}_x^\lambda)(h) + h^{-2}m \le \mu_n(\mathscr{A}_x^\lambda(h)) \le \mu_n(\mathscr{L}_x^\lambda(h)) + h^{-2}M, \tag{3.3.5}$$

thus the spectrum of $\mathscr{A}_x^\lambda(h)$ is purely discrete and the eigenvalues accumulate at ∞. Moreover Theorem A.5 tells us that the eigenvalues are simple and that the eigenfunctions define an orthonormal basis for $L^2(I_0, dx)$.

REMARK 3.8. *From Theorem 3.4 and its corollary we have in addition that*

$$h^2 n_\lambda(n_\lambda + 1) + m \le \mu_n(\mathscr{A}_x^\lambda(h)) \le h^2 n_\lambda(n_\lambda + 1) + M$$

where $n_\lambda := n + |\lambda|$ and $n \in \mathbb{N}$, and thus for each fixed value of the small parameter h, if n and/or λ are big enough, we can have some control on the eigenvalues position.

COROLLARY 3.9. *$\mathscr{A}_\eta^\lambda(h)$ is self-adjoint on the transformed domain, its spectrum purely discrete and made of simple eigenvalues accumulating at ∞.*

PROOF. It follows as a direct consequence of the unitary equivalence of the operators $\mathscr{A}_x^\lambda(h)$ and $\mathscr{A}_\eta^\lambda(h)$. □

3.4. Analytic extensions of the eigenvalues of $\mathscr{A}_\eta^\lambda$

We continue the study of the previously defined operator $\mathscr{A}_x^\lambda(h)$. All its properties are preserved by the unitary change of variable defined in (3.3.1).

The fact that $\mathscr{A}_x^\lambda(h)$ is closed and x^2 is infinitesimally $\mathscr{A}_x^\lambda(h)$-bounded guarantees that the β-dependent family of operators on $D(\mathscr{L}_x^\lambda(h))$

$$\mathscr{A}_x^\lambda(\beta) := \mathscr{A}_x^\lambda(h, \beta) := \mathscr{L}_x^\lambda(h) + \mathscr{V}(x) + \beta x^2$$

defines an analytic type-(A) family of self-adjoint operators in the sense of Appendix C. In particular it is an entire family because of the $\mathscr{L}_x^\lambda(h)$-infinitesimally boundedness of the perturbation. Notice that by definition (3.3.2a) of V, β essentially perturbs the parameter E.

In our case we have only non-degenerate, isolated eigenvalues, thus it follows from Theorem C.7 that every eigenvalue $\tilde{\mu}_l$ extends analytically as function of β in the circle of radius

$$r(0, ||\mathscr{V}||, \tilde{\mu}_l, \epsilon) = \frac{\epsilon}{||\mathscr{V}||},$$

where the ϵ is given by the distance with the nearest eigenvalue, thus it is $O(l^2)$ in view of Corollary 3.5.

Then, by unitarity the eigenvalues $\mu_l^\lambda(h)$ of $\mathscr{A}^\lambda_{\eta,\widetilde{E},Z_-}(h)$ extends analytically as function of E in a neighborhood of the real axis of radius $O(l^2)$. By Theorem C.4 the corresponding eigenfunctions extend accordingly.

3.5. Second separation from an operator theoretical point of view

We can use the results of Section 3.3 to partially justify the second separation discussed in Section 3.2.

Let us denote $\mathscr{D}_{\widetilde{\chi}}$ the subspace of finite linear combination of products $f(\xi)g(\eta)$ where $f \in C_0^\infty(\mathbb{R}_+^0) \subset L^2(\mathbb{R}_+^0, \sinh(\xi)d\xi)$ with $f'(0)=0$ and $g \in C^\infty([0,\pi]) \subset L^2([0,\pi], \sin(\eta)d\eta)$ is π-periodic. Due to the isomorphism (see [RS80, Theorem II.10, p. 52])

$$L^2(M_0, d\widetilde{\chi}) \cong L^2(\mathbb{R}_+^0, \sin(\xi)d\xi) \otimes L^2([0,\pi], \sin(\eta)d\eta),$$

and the density of $\widehat{C}_0^\infty(M_0)$ in $L^2(M_0, d\widetilde{\chi})$ (see (3.1.3)), we have that $\mathscr{D}_{\widetilde{\chi}}$ is a dense set in $L^2(M_0, d\widetilde{\chi})$. Then for functions $\psi(\xi,\eta) = f(\xi)g(\eta)$, the operator $\mathscr{A}^\lambda_{\xi,\eta}$ takes the form

$$\mathscr{A}^\lambda_{\xi,\eta} f(\xi)g(\eta) = \left(\mathscr{A}^\lambda_\xi(h)f(\xi)\right) g(\eta) + f(\xi)\left(\mathscr{A}^\lambda_\eta(h)g(\eta)\right).$$

Define

$$\mu_l^\lambda := \mu_l^\lambda(h, E, Z_-) \tag{3.5.1}$$

the l-th eigenvalue of $\mathscr{A}^\lambda_\eta(h)$ and

$$\varphi_l^\lambda := \varphi_l^\lambda(h, E, Z_-) \tag{3.5.2}$$

the relative eigenfunction. Call Φ_l^λ the subspace spanned by φ_l^λ and define

$$L^2_{l,\lambda} := L^2\left(\mathbb{R}_+^0, \sinh(\xi)d\xi\right) \otimes \Phi_l^\lambda$$

to have

$$L^2(M_0, d\widetilde{\chi}) = \bigoplus_{l\in\mathbb{N}} L^2_{l,\lambda}.$$

Then, if $\mathbb{1}_{l,\lambda}$ is the identity operator on Φ_l^λ, the restriction of $\mathscr{A}_\lambda$ to $\mathscr{D}_l^\lambda := \mathscr{D}_{\widetilde{\chi}} \cap L^2_{l,\lambda}$ is given by $\mathscr{A}^\lambda_{\xi,\eta}\Big|_{\mathscr{D}_l^\lambda} = \mathscr{A}_l^\lambda \otimes \mathbb{1}_{l,\lambda}$, where

$$\mathscr{A}_l^\lambda := \mathscr{A}_\xi^\lambda + \mu_l^\lambda. \tag{3.5.3}$$

This leads to the following proposition.

PROPOSITION 3.10. *For each integer value of λ, the operator $\mathscr{A}^\lambda_{\xi,\eta}$ defined in (3.2.3) is unitarily equivalent to the operator in $\bigoplus_{l\in\mathbb{N}} L^2_{l,\lambda}$ given by $\bigoplus_{l\in\mathbb{N}} \mathscr{A}_l^\lambda \otimes \mathbb{1}_{l,\lambda}$.*

3.6. Self-adjoint extensions of the radial operators $\mathscr{A}_l^\lambda$

Let us start analyzing the Weyl criterion at ∞. Set

$$\mathscr{A}_l^\lambda = \mathscr{L}_\xi + \mathscr{V}_l^\lambda(\xi) \tag{3.6.1}$$

where

$$\mathscr{L}_\xi := -h^2 \frac{1}{\sinh(\xi)} \partial_\xi(\sinh(\xi)\partial_\xi)$$

and

$$\mathscr{V}_l^\lambda(\xi) := \mathscr{V}^\lambda(\xi) := \frac{h^2\lambda^2}{\sinh^2(\xi)} - E\cosh^2(\xi) - Z_+\cosh(\xi) + \mu_l^\lambda(E).$$

We generalize a completeness criterion from [RS75, Theorem X.8].

THEOREM 3.11. *Consider the differential equation associated to the Sturm-Liouville operator $H_x := L_x + V(x)$ in $L^2((0,\infty), p(x)dx)$ where*

$$L_x := -\frac{1}{p(x)}\partial_x(p(x)\partial_x) \quad \text{and} \quad \lim_{x\to\infty} p(x) \neq 0.$$

Let $V(x)$ be a continuous real-valued function in $(0,\infty)$ and suppose there exists a positive differentiable function $M : \mathbb{R}_+ \to \mathbb{R}_+$ so that

(1) $V(x) \geq -M(x)$
(2) $\int_1^\infty (M(x))^{-1/2} p(x)dx = \infty$
(3) $M'(x)/(M(x))^{3/2}$ *is bounded near ∞.*

Then H_x is in LPC at ∞.

Proof. We will show that the two solutions of $H_x\phi = 0$ cannot be both in $L^2(p(x)dx)$ around ∞. Consider $0 < c_1 < c < \infty$ and let u be a real solution of the previous equation in $L^2(p(x)dx)$ near ∞. Then we have

$$\begin{aligned} -K_1 &:= -\int_{c_1}^\infty u^2(x)p(x)dx \leq -\int_{c_1}^c u^2(x)p(x)dx \\ &\leq \int_{c_1}^c \frac{V(x)}{M(x)} u^2(x)p(x)dx \\ &= \int_{c_1}^c \frac{\partial_x(p(x)\partial_x u(x))}{M(x)} u(x)dx. \end{aligned}$$

That, via integration by parts, gives

$$\begin{aligned} -\frac{u'(x)u(x)}{M(x)}p(x)\Big|_{c_1}^c + \int_{c_1}^c \frac{(u'(x))^2}{M(x)}p(x)dx \\ - \int_{c_1}^c \frac{u'(x)u(x)M'(x)}{M^2(x)}p(x)dx \leq K_1. \end{aligned} \tag{3.6.2}$$

On the other hand, using 3. and Hölder inequality, we can find K_2 such that

$$\begin{aligned}-\int_{c_1}^{c}\frac{u'(x)u(x)M'(x)}{M^2(x)}p(x)dx\leq\\ \leq K_2\left(\int_{c_1}^{c}\frac{(u'(x))^2}{M(x)}p(x)dx\right)^{1/2}\left(\int_{c_1}^{c}(u(x))^2p(x)dx\right)^{1/2}.\end{aligned}\tag{3.6.3}$$

Suppose that $\int_{c_1}^{\infty}\frac{(u'(x))^2}{M(x)}p(x)dx=\infty$, then by the last two inequalities, the positivity of $p(x)$ for $x>0$ and the hypothesis on u, $u'(x)u(x)$ must be positive near ∞ but this imply that u and its derivative have always the same sign, that is impossible since u is in $L^2(p(x)dx)$ near ∞. As a consequence $\int_{c_1}^{\infty}\frac{(u'(x))^2}{M(x)}p(x)dx<\infty$. Suppose now that ϕ and ψ are two independent solutions of $H_x\psi=0$ and that both are in $L^2(p(x)dx)$ near ∞. Moreover, suppose that they are normalized so that $\psi(x)\phi'(x)-\psi'(x)\phi(x)=1$. Then,

$$\left(\frac{1}{M(x)}\right)^{1/2}=\frac{\phi(x)\psi'(x)}{(M(x))^{1/2}}-\frac{\phi'(x)\psi(x)}{(M(x))^{1/2}}$$

would be in $L^1(p(x)dx)$ near ∞ and this contradicts hypothesis 2. . □

Observe that the λ term in $\mathscr{A}_l^\lambda$ decays fastly at infinity, this should give the hint that it shouldn't affect the nature of the point as it happened in the analysis of $\mathscr{A}_\eta^\lambda$. In fact, this is an easy corollary of the previous theorem:

Corollary 3.12. *The differential equation associated to $\mathscr{A}_l^\lambda$ is in the LPC at ∞ for any value of λ.*

Proof. Clearly

$$\mathscr{V}^\lambda(\xi)\geq -M(\xi)\quad\text{with}\quad M(\xi):=C_{E,Z_+,h,\mu}\cosh^2(\xi),$$

and this function satisfy all the hypotheses of the last theorem for $p(\xi)=\sinh(\xi)$. This shows that for $\mathscr{A}_l^\lambda$ we have LPC at ∞ for every value of λ and μ_l^λ. □

For what concerns the nature of the boundary point $\xi=0$, we will see that the λ term in $\mathscr{A}_l^\lambda$ is central. We proceed in a way similar to the one for $\mathscr{A}_\eta^\lambda$. If we apply the unitary transform

$$L^2(\mathbb{R}_+^0,\sinh(\xi)\,d\xi)\to L^2([1,\infty),dy),\quad g(\xi)\mapsto g(\operatorname{arccosh}(y)),\tag{3.6.4}$$

the operator $\mathscr{A}_l^\lambda$ transforms to

$$\mathscr{A}_y^\lambda=\mathscr{L}_y^\lambda+\mathscr{V}_l(y)\tag{3.6.5}$$

where, as before,

$$\mathscr{L}_y^\lambda:=\mathscr{L}_y^\lambda(h):=-h^2\partial_y\left((y^2-1)\partial_y\right)+\frac{h^2\lambda^2}{y^2-1}$$

and

$$\mathscr{V}_l(y):=-Ey^2-Z_+y+\mu_l^\lambda(E).$$

Near $y=1$, $\mathscr{V}_l(y)$ is a bounded perturbation of the operator $\mathscr{L}_y^\lambda(1)$ in the proper domain. Thus it is enough to analyze the limit circle-limit point problem for $\mathscr{L}_y^\lambda(1)$ instead of $A_y^\lambda(1)$.

Similarly as in Section 3.3, we have that

$$\partial_y\left((1-y^2)\partial_y\right)u+\left(k(k+1)-\frac{\lambda^2}{1-y^2}\right)u=0$$

is solved by

$$u(y):=c_1P_k^\lambda(y)+c_2Q_k^\lambda(y)$$

for all $k\in\mathbb{N}_0$ s.t. $|\lambda|\le k$ where P_k^λ and Q_k^λ are the associated Legendre functions analytically extended to $\mathbb{C}\setminus(-\infty,1]$ (see [EMOT53, pp. 120-]). What remains to understand is if they are both in $L^2([1,\infty))$ or not.

In the case $\lambda=0$, as shown in [Leb72, p.167-], we have that $\lim_{y\to 1^+}P_k^0(y)=1$, thus the function stays bounded even in the closed interval. As a consequence its L^2 norm in every compact interval is finite. On the other hand $\lim_{y\to 1^+}Q_k^0(y)=\infty$ so we have to check the order of this divergence. For $y>1$ (even for $|\arg(y-1)|<\pi$) and $\Re k>-1$, we can represent $Q_k^0(y)$ as follows

$$Q_k^0(y)=\int_0^1 h_k\left(\frac{y-1}{2}\cosh^2\psi\right)d\psi \tag{3.6.6}$$

where

$$h_k(w)=\frac{\left(\sqrt{w+1}+\sqrt{w}\right)^{-1-2k}}{\sqrt{w+1}}.$$

So, considered that h_k is monotonic decreasing, $\frac{y-1}{2}\cosh^2\psi\ge\frac{y-1}{4}e^\psi$ and that

$$\widetilde{Q}_k^0(y):=\int_0^1 h_k\left(\frac{y-1}{4}e^\psi\right)d\psi$$

is explicitly solvable, has a finite L^2 norm near 1 and is such that $Q_k^0(y)\le\widetilde{Q}_k^0(y)$, we have that, in any compact interval of the form $[1,c]$,

$$||Q_k^0||_2\le||\widetilde{Q}_k^0||_2<\infty.$$

Thus, for $\lambda=0$ we are in LCC at 1. In the case $\lambda>0$, on the other hand, we use the following representations ([EMOT53, p. 157]):

$$\begin{aligned}P_k^\lambda(y)&=\frac{\Gamma(k+\lambda+1)}{\pi\Gamma(k+1)}\int_0^\pi(y+\sqrt{(y^2-1)}\cos t)^k e^{i\lambda t}\,dt,\\ Q_k^\lambda(y)&=\frac{e^{2\pi i}}{2^{k+1}}\frac{\Gamma(k+\lambda+1)}{\Gamma(k+1)}(y^2-1)^{-\lambda/2}\int_0^\pi(y+\cos t)^{\lambda-k-1}(\sin t)^{2k+1}\,dt,\end{aligned} \tag{3.6.7}$$

the first equation being valid for $\lambda\in\mathbb{N}_0$, the second for $\Re(k)>-1$, $\Re(k+\lambda+1)>0$.

Taken in account that

$$\lim_{y\to 1^+}\int_0^\pi(y+\cos t)^{\lambda-k-1}(\sin t)^{2k+1}\,dt=\frac{2^{\lambda+k}\Gamma(\lambda)\Gamma(k+1)}{\Gamma(k+\lambda+1)},$$

it is clear that both the integral terms are bounded near 1. It is even evident from the remaining terms that, near 1, P_k^λ is in L^2 while Q_k^λ is not! This means that for $\lambda \neq 0$ the operator $\mathscr{L}_y^\lambda(1)$ and thus $\mathscr{A}_y^\lambda(1)$ is LPC at 1.

In [**EMOT53**, p.161 n.10] is shown that for $z \in \mathbb{C} \setminus (-\infty, 1)$ and every λ and k one has

$$(z^2-1)\partial_z P_k^\lambda(z) = kzP_k^\lambda(z) - (\lambda+k)P_{k-1}^\lambda(z).$$

With the representation (3.6.7) for P_k^λ and this formula for the derivative, it is natural to consider the boundary conditions generated by P_1^0 in 1.

We first consider auxiliary operators $L_{y,c}^\lambda$ on the Hilbert spaces $L^2(I_c)$ for bounded intervals $I_c := [1, c)$.

We are not interested in the conditions on the regular point c: these are treated standardly and well defined, we only need to know that there exist a family of initial conditions that must be imposed on the left boundary point to guarantee the (essential) self-adjointness of the operator. As a reference see [**Zet05**, p. 183-193].

We have proven the following lemma:

LEMMA 3.13. *For $1 < c < \infty$ define the operator $\mathscr{L}_{y,c}^\lambda(1)$, $\lambda \in \mathbb{Z}$, by*

$$D(\mathscr{L}_y^\lambda(1)) = \Big\{ f \in L^2(I_c) \,\big|\, f, f' \in AC(I_c),\ \mathscr{L}_y^\lambda(1) f \in L^2(I_c), \\ \lim_{y\to 1^+}(1-y^2)f'(y) = 0 \text{ if } \lambda = 0,\ BC(f,c) \Big\},$$

where $BC(f,c)$ stands for any separated Boundary Condition for f in the regular point c. Then $\mathscr{L}_{y,c}^\lambda(1)$ is self-adjoint.

We have essentially proved the following theorem.

THEOREM 3.14. *The operator $\mathscr{A}_y^\lambda$ with domain*

$$D(\mathscr{A}_y^\lambda) = \Big\{ f \in L^2(I_\infty) \,\big|\, f, f' \in AC(I_\infty),\ \mathscr{A}_y^\lambda f \in L^2(I_\infty), \\ \lim_{y\to 1^+}(1-y^2)f'(y) = 0 \text{ if } \lambda = 0 \Big\},$$

where $I_\infty := [1, \infty)$, is self-adjoint. And thus $\mathscr{A}_l^\lambda$ is self-adjoint on the domain, transformed by (3.6.4).

PROOF. First of all notice that the multiplication by a positive constant will not affect the properties of the operator, thus everything said for $\mathscr{L}_y^\lambda(1)$ is equally true for $\mathscr{L}_y^\lambda(h) = h^2 \mathscr{L}_y^\lambda(1)$.

One of the main aspects clarified by Theorem A.5 is that the domain of essential self-adjointness of a Sturm Liouville operator depends on the nature of the extremal point of the interval of definition, in this case I_∞.

For what concerns ∞, we have already proven in Corollary 3.12 that we have LPC for any λ, thus we do not need to fix boundary conditions. On the other hand $\mathscr{V}(y)$ is a bounded perturbation of $\mathscr{L}_y^\lambda$ in $[1, c]$, thus we can combine Kato-Rellich

Theorem and Theorem 3.13 to fix the boundary conditions in 1 required for $D(\mathscr{A}_y^\lambda)$ to define a self-adjoint operator in $[1,c]$.

From this two observations it follows that $\mathscr{A}_y^\lambda$ is essentially self-adjoint on $D(\mathscr{A}_y^\lambda)$ as stated in the theorem.

The same can be said on $\mathscr{A}_l^\lambda$ with its transformed domain as a consequence of the unitarity of the transformation. □

3.7. Formal "partial wave expansion" of the Green's function

For real E we know that the spectrum of $\mathscr{A}_\eta^\lambda$ consists of an infinite number of simple eigenvalues

$$\mu_1^\lambda(E) < \mu_2^\lambda(E) < \mu_3^\lambda(E) < \dots$$

tending to infinity. The μ_k^λ extends to analytic functions of E in some neighborhood of the real axis. We denote by $\varphi_{n,E}^\lambda$ the eigenfunctions

$$\mathscr{A}_\eta^\lambda(E)\varphi_{n,E}^\lambda(\eta) = \mu_n^\lambda(E)\varphi_{n,E}^\lambda(\eta) \quad , \quad n \in \mathbb{N}_0,$$

normalized by

$$||\varphi_{n,E}^\lambda||^2 = \int_0^{+\pi} |\varphi_{n,E}^\lambda(\eta)|^2 \sin\eta \, d\eta = 1$$

for $E \in \mathbb{R}_+$ and then extended analytically. We choose $\varphi_{n,E}^\lambda$ real for E real.

Let $f \in L^2(\mathscr{M}_0, d\chi)$. Instead of solving $(H_\lambda - E)u = f$ for $E \in \mathbb{C}\setminus\sigma(H_\lambda)$, we look at the solution of

$$(K_\lambda - EF(\xi,\eta))u(\xi,\eta) = F(\xi,\eta)f(\xi,\eta), \tag{3.7.1}$$

with K_λ from (3.2.1). We already saw that

$$(K_\lambda - EF(\xi,\eta))u(\xi,\eta) = (\mathscr{A}_\xi^\lambda + \mathscr{A}_\eta^\lambda)u(\xi,\eta).$$

Now, using the completeness of the orthonormal base $\{\varphi_{n,E}^\lambda\}_{n\in\mathbb{N}_0}$ for $E \in \mathbb{R}$, u possesses the expansion

$$u(\xi,\eta) = \sum_{n\in\mathbb{N}_0} u_n^\lambda(\xi,\eta) \quad \text{with} \quad u_n^\lambda(\xi,\eta) := \varphi_{n,E}^\lambda(\eta)\psi_{n,E}^\lambda(\xi), \tag{3.7.2}$$

where

$$\psi_{n,E}^\lambda(\xi) := \int_0^{+\pi} \varphi_{n,E}^\lambda(\eta)u(\xi,\eta)\sin\eta\, d\eta.$$

This expansion extends to complex values of E by analyticity (note that no complex conjugate is involved, since $\varphi_{n,E}^\lambda$ is chosen real for $E \in \mathbb{R}$).

Analogously we get

$$F(\xi,\eta)f(\xi,\eta) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}^\lambda(\eta) g_{n,E}^\lambda(\xi), \tag{3.7.3}$$

where

$$g_{n,E}^\lambda(\xi) := \int_0^{+\pi} \varphi_{n,E}^\lambda(\eta)(Ff)(\xi,\eta)\sin\eta\, d\eta.$$

Substituting (3.7.2) and (3.7.3) into (3.7.1) one gets

$$\left[\mathscr{A}_\xi^\lambda + \mathscr{A}_\eta^\lambda\right] \sum_{n\in\mathbb{N}_0} u_n^\lambda(\xi,\eta) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}^\lambda(\eta) g_{n,E}^\lambda(\xi)$$

or equivalently

$$\sum_{n\in\mathbb{N}_0} \varphi_{n,E}^\lambda(\eta)\big(\mathscr{A}_n^\lambda(E)\psi_{n,E}^\lambda(\xi) - g_{n,E}^\lambda(\xi)\big) = 0. \tag{3.7.4}$$

If we can prove that (3.7.4) extends to complex points $E \notin \sigma(H_\lambda)$ where $\mathscr{A}_n^\lambda(E)$ possesses an inverse $G_n^\lambda(E)$, we could rewrite the terms in (3.7.4) as

$$\begin{aligned}\psi_{n,E}^\lambda(\xi) &= G_n^\lambda(E) g_{n,E}^\lambda(\xi) \\ &= \int_{\mathbb{R}_+} G_n^\lambda(\xi,\tilde{\xi};E)\int_0^{+\pi} \varphi_{n,E}^\lambda(\tilde{\eta})(Ff)(\tilde{\xi},\tilde{\eta})\sin\tilde{\eta}\,\sinh\tilde{\xi}\; d\tilde{\eta}\, d\tilde{\xi}.\end{aligned} \tag{3.7.5}$$

Then, combining (3.7.5) and (3.7.2) we would obtain

$$u(\xi,\eta) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}^\lambda(\eta) \iint_{M_0} G_n^\lambda(\xi,\tilde{\xi};E)\varphi_{n,E}^\lambda(\tilde{\eta})(Ff)(\tilde{\xi},\tilde{\eta})\,\sin\tilde{\eta}\,\sinh\tilde{\xi}\; d\tilde{\xi}\, d\tilde{\eta}$$

and for each λ, we could read off the partial wave expansion for the Green function

$$G^\lambda(\xi,\eta;\tilde{\xi},\tilde{\eta};E) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}^\lambda(\eta)\varphi_{n,E}^\lambda(\tilde{\eta}) G_n^\lambda(\xi,\tilde{\xi};E)(\sinh^2\tilde{\xi} + \sin^2\tilde{\eta}) \tag{3.7.6}$$

and try to analyze its convergence and its poles to define the resonances of our problem. The theory of Sturm-Liouville differential equations tells us that the inverse $G_n^\lambda(E)$ of $A_n^\lambda(E)$ depends on special solutions of the equation, namely the "incoming and outgoing waves". These are defined as solutions $v_\pm$ that decay exponentially for $k \in \mathbb{C}_\pm$, where $k^2 = E$ and the solution v_0 that is regular at the finite boundary point 0. If $v_+(\xi;E,n)$ (or $v_+(\xi;k,n)$) extend analytically to the lower half-plane $\{\Im k < 0\}$, then we can use the analyticity of *any* solution of the radial equation in ξ and some asymptotic estimates at ∞ to study the aforementioned Green's function.

It is completely unclear at this point how to study the asymptotic behavior of solutions of $\mathscr{A}_n^\lambda$, but in view of Chapter 2 we may expect that the case $\lambda = 0$, corresponding to the planar situation, could be of help in suggesting how to proceed. Being in itself an interesting problem, we dedicate the next chapter to that topic.

CHAPTER 4

The two-centers system on $L^2(\mathbb{R}^2)$

Let us briefly recall the properties of the two-center coulomb equation in $L^2(\mathbb{R}^2)$. It was already sketched in the previous chapter that it defines a self-adjoint operator bounded from below with form-domain $H^1(\mathbb{R}^2)$ (see [**Kna89**, Prop. 1] or [**Agm82**, Theorem 3.2]).

4.1. Separation of variables

If we define, similarly as before, $M := \mathbb{R}_+ \times (-\pi, \pi)$, the restriction to M of the map

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix} \mapsto \begin{pmatrix} \cosh(\xi)\cos(\eta) \\ \sinh(\xi)\sin(\eta) \end{pmatrix}$$

defines a C^∞ diffeomorphism

$$G : M \to G(M)$$

whose image $G(M)$ is dense in $\mathbb{R}^2$. Moreover it defines a change of coordinate from $q \in \mathbb{R}^2$ to $(\xi, \eta) \in M$, called *prolate elliptic coordinates* as in as (1.2.1). The classical picture and the characterization of the bifurcation digrams for this case coincide with the one for the planar case discussed in Section 2.3.

The following result can be proven in the same way as Theorem 1.7.

THEOREM 4.1. *Let*

$$u \in C_a(\mathbb{R}^2) := \left\{ C(\mathbb{R}^2) \mid u\restriction_{\mathbb{R}^2 \setminus \{\pm a\}} \text{ is twice continuously differentiable} \right\}.$$

The eigenvalue equation

$$(-\hbar^2 \Delta + V(q))u(q) = E u(q), \quad E \in \mathbb{R},$$

transformed to prolate elliptic coordinates, separates with the ansatz

$$u \circ G(\xi, \eta) = f(\xi) g(\eta)$$

into the decoupled system of ordinary differential equations

$$\begin{cases} \left(-\hbar^2 \partial_\xi^2 - Z_+ \cosh(\xi) - E\cosh^2(\xi) + \mu\right) f(\xi) = 0 \\ \left(-\hbar^2 \partial_\eta^2 + Z_- \cos(\eta) + E\cos^2(\eta) - \mu\right) g(\eta) = 0, \end{cases}$$

where $\mu \in \mathbb{C}$ is the separation constant,

$$f \in C_N^2(\mathbb{R}_+^0) := \left\{ h \in C^2(\mathbb{R}_+^0) \mid h'(0) = 0 \right\},$$
$$g \in C_{\mathrm{per}}^2([-\pi, \pi]) := \left\{ h \in C^2([-\pi, \pi]) \mid h^{(k)}(-\pi) = h^{(k)}(\pi) \text{ for } k = 0, 1 \right\}$$

and we have set $Z_\pm := Z_2 \pm Z_1$ *and* $\partial_\alpha = \frac{\partial}{\partial \alpha}$.

In fact, if $F(\xi,\eta)$ is the function defined in (1.2.2) we have

PROPOSITION 4.2. *The operator* $\mathscr{H}$ *on* $L^2(\mathbb{R}^2)$ *defined as in (1.1.1) is unitarily equivalent to the operator in* $L^2(M, d\chi)$ *given by*

$$\mathscr{H}_{\mathscr{G}} := -h^2 \Delta_{\mathscr{G}} + V_{\mathscr{G}}(\xi,\eta)$$

where $d\chi := F(\xi,\eta)\, d\xi\, d\eta$,

$$\Delta_{\mathscr{G}} := \frac{1}{F(\xi,\eta)} \left(\partial_\xi^2 + \partial_\eta^2 \right)$$

and

$$V_{\mathscr{G}}(\xi,\eta) := -\frac{Z_+ \cosh(\xi) - Z_- \cos(\eta)}{F(\xi,\eta)}.$$

$\mathscr{H}_{\mathscr{G}}$ *has form core*

$$\mathscr{G}\left(C_0^\infty(\mathbb{R}^2)\right) = \left\{ f(\xi,\eta) \in C_0^\infty\left(\overline{M}\right) \mid f \text{ is } 2\pi\text{-periodic in } \eta \text{ and } \partial_\xi f|_{\xi=0} = 0 \right\}$$

and admits a unique self-adjoint realization with domain $\mathscr{G}(D(\mathscr{H}))$ *where* $D(\mathscr{H})$ *is given by* (4.1.1).

PROOF. The transformation to prolate elliptic coordinates (ξ,η) defines a unitary operator that we denote by

$$\mathscr{G} : L^2(\mathbb{R}^2, dq) \to L^2(M, d\chi).$$

It is well known that $\mathscr{H}$ has a self-adjoint realization on $L^2(\mathbb{R}^2)$ with domain

$$D(\mathscr{H}) := \left\{ u \in L^2(\mathbb{R}^2) \mid Vu \in L^1_{\mathrm{loc}}(\mathbb{R}^2),\ u \in H^1(\mathbb{R}^2),\ \mathscr{H} u \in L^2(\mathbb{R}^2) \right\}, \tag{4.1.1}$$

where $\mathscr{H} u$ is to be understood in distributional sense (see [**Agm82**, Theorem 3.2] and Remark 3.2). The domain of the unitarily transformed $\mathscr{H}_{\mathscr{G}} := \mathscr{G} \mathscr{H} \mathscr{G}^{-1}$ is then transformed to $\mathscr{G}(D(\mathscr{H}))$.

Finally $C_0^\infty(\mathbb{R}^2)$ is a form core for the quadratic form associated to $\mathscr{H}$, therefore it is unitarily transformed to a form core for the quadratic form associated to $\mathscr{H}_{\mathscr{G}}$. See [**RS80**, Section VIII.6] for the appropriate definitions.

Then the form of the operator is given by Theorem 4.1. □

As discussed in Section 3.2 for the three dimensional case, we would like to move our point of view from the study of $\mathscr{H}_{\mathscr{G}} - E$ on $L^2(M, d\chi)$ to the study of the separable operator

$$K_E := K_\xi \otimes \mathbb{1} + \mathbb{1} \otimes K_\eta$$

acting on

$$L^2(M, d\xi\, d\eta) = L^2(R_+^0, d\xi) \otimes L^2([-\pi,\pi], d\eta).$$

Here

$$\begin{aligned} K_\xi(h) &:= K_{\xi,E,h} := -h^2 \partial_\xi^2 - Z_+ \cosh(\xi) - E \cosh^2(\xi), \\ K_\eta(h) &:= K_{\eta,E,h} := -h^2 \partial_\eta^2 + Z_- \cos(\eta) + E \cos^2(\eta). \end{aligned} \tag{4.1.2}$$

The separation reduces the problem to the study of two Sturm-Liouville equations

$$(K_\xi + \mu)f(\xi) = 0 \quad \text{and} \quad (K_\eta - \mu)g(\eta) = 0$$

of the form (A.1) with $p = r = 1$ (see Theorem 4.1). As for the three dimensional problem, we call the first equation *angular equation* and the second equation *radial equation*. In particular they define essentially self-adjoint operators if we assume the proper boundary conditions on $L^2(R^0_+, d\xi)$ and $L^2([-\pi,\pi], d\eta)$ respectively.

More in details the eigenvalue equation of $K_\eta(h)$ is in the class of the so called Hill's equation. In view of Proposition 4.2, we are interested in the 2π-periodic solutions of the equation, i.e. we look for $\varphi \in [-\pi,\pi]$ such that

$$\varphi(-\pi) = \varphi(\pi) \text{ and } \varphi'(-\pi) = \varphi'(\pi).$$

For $K_\xi(h)$ it is clear that 0 is a regular point, we will see later how to treat the singular point ∞. For what concerns the boundary conditions in 0 we will require

$$\phi'(0) = 0 \tag{4.1.3}$$

as suggested by Proposition 4.2.

4.2. Spectrum of the angular equation and its analytic continuation

Let us shortly turn the attention to the angular equation. We will consider separately the case $Z_- = 0$ and $Z_- \neq 0$.

In the simplest case $Z_- = 0$, K_η can be written in the form of a Mathieu equation

$$-\partial^2_\eta \psi(\eta) - \frac{2\mu - E}{2h^2}\psi(\eta) + 2\frac{E}{4h^2}\cos(2\eta)\psi(\eta) = 0 \tag{4.2.1}$$

with periodic boundary conditions in $[-\pi,\pi]$. The potential $V(\eta) := \cos(2\eta)$ being even, it follows from Floquet theory (see [Tes00], [MW79], [MS54], [Eas75]), using the fundamental matrix

$$\mathscr{F}(\alpha,\delta) := \begin{pmatrix} f_1 & f_2 \\ f_1' & f_2' \end{pmatrix}(\pi;\lambda,\delta), \qquad \lambda := \frac{2\mu - E}{2h^2},\ \delta := \frac{E}{4h^2}, \tag{4.2.2}$$

built from the fundamental system

$$f_1(0;\lambda,\delta) = 1 = f_2'(0;\lambda,\delta) \quad , \quad f_2(0;\lambda,\delta) = 0 = f_1'(0;\lambda,\delta), \tag{4.2.3}$$

that all the 2π-periodic solutions must be either π-periodic or π-antiperiodic in $[0,\pi/2]$ (or $[-\pi/2,0]$).

In general the structure of the periodic solutions and their eigenvalues can be inferred by Theorem A.6. For the Mathieu equation, in particular, much more is known (see [MS54, Chapter 2]): for each integer $n \geq 0$ we can find two solutions $\mathrm{ce}_n(x;\delta)$ and $\mathrm{se}_{n+1}(x;\delta)$ that have exactly n zeroes in $(0,\pi)$ and that are π-periodic for even n and π-antiperiodic for odd n, the corresponding eigenvalues being $\lambda_n^+(\delta)$ and $\lambda_{n+1}^-(\delta)$ respectively. For every $\delta \in \mathbb{R}_+$ we have that λ_n^+ and λ_{n+1}^- are real and

$$\lambda_0^+ < \lambda_1^+ < \lambda_1^- < \lambda_2^- < \lambda_2^+ < \cdots.$$

The following fact are proved in [Kat95, Chapter VII.3.3], [MS54, Chapter 2.2], [MSW80, Chapter 2.4] and [Vol98].

(1) The eigenvalues of the Mathieu operators are analytic functions in δ with algebraic singularities.
(2) The number of branch points is infinite, but countable, and there are no finite limit points.
(3) They can be defined uniquely as functions $\lambda_n^{\pm}(\delta)$ of δ by introducing suitable cuts in the δ-plane, moreover they admit an expansion in powers of δ with finite convergence radius $r_n \geq 2.04\, n^2$.
(4) For $\delta \in \mathbb{R}$ no branch point is present and the eigenvalues are well defined real analytic functions of δ.
(5) The number of branch points is infinite, but countable, and there are no finite limit points.
(6) The operator T associated to (4.2.1) can be decomposed according to

$$L^2(-\pi,\pi) = L_0^+ \oplus L_1^+ \oplus L_0^- \oplus L_1^-$$

where the superscripts $\pm$ denote respectively the sets of even and odd functions and where the subscripts 0 and 1 denote respectively the sets of functions symmetric and antisymmetric with respect to $x = \pi/2$.
(7) Each part of T is self-adjoint on the subset $L_{01}^{\pm}$ to which it is restricted and has only simple eigenvalues as given by the following schema:

$$\begin{aligned}
L_0^+ &: \lambda_0, \phi_0 \text{ and } \lambda_n^+, \phi_n^+, \qquad n = 2,4,6,\dots;\\
L_1^+ &: \lambda_n^+, \phi_n^+, \qquad n = 1,3,5,\dots;\\
L_0^- &: \lambda_n^-, \phi_n^-, \qquad n = 1,3,5,\dots;\\
L_1^- &: \lambda_n^-, \phi_n^-, \qquad n = 2,4,6,\dots.
\end{aligned}$$

(8) All the eigenvalues in each of the four groups of the previous remark belong to the same analytic function, i.e. the eigenvalues in the same group lie on the same Riemann surface.
(9) The eigenfunctions $\phi_n^{\pm}(x)$ are called Mathieu Cosine and Mathieu Sine and are themselves analytic functions of x and δ.

Despite the completeness and the clarity of perturbation theory for one-parameter analytic families of self-adjoint operators, the situation is much more intricate and much less complete in presence of more parameters. And we cannot apply the theory as is (see Remark C.11). On the other hand we can use our restrictions on the parameters and the special symmetry of the potential to play in our favor.

We know that Z_- will be a real parameter, thus let us consider the equation

$$-\partial_\eta^2 \psi(\eta) + \left(\frac{E - 2\mu}{2h^2} + \frac{Z_-}{h^2} \cos(\eta) + \frac{E}{2h^2} \cos(2\eta) \right) \psi(\eta) = 0 \tag{4.2.4}$$

with periodic boundary conditions on $[-\pi,\pi]$ where $E \in \mathbb{R}_+$. Let us call

$$\lambda := \frac{E - 2\mu}{2h^2}, \qquad \gamma_1 = \frac{Z_-}{h^2}, \qquad \gamma_2 = \frac{E}{2h^2}.$$

Notice that the main difference between this case and the previous one is that now the period of the potential is no more smaller than the length of the considered interval, then by Floquet theory we look for solutions of period π instead of $\pi/2$.

REMARK 4.3. *We already know from Theorem A.6 that for every choice of γ_1 and γ_2 the spectrum is discrete, at most double degenerate and accumulates at infinity. Anyhow it follows from* [MW79, Theorem 7.10, p. 108] *using a change of variable that in this case there cannot be coexistence of 2π-periodic eigenfunctions for the same eigenvalue. Thus the spectrum will be non-degenerate.*

In accord with the weaker result given in Theorem C.9, it is proved in [Str44] that, for E and Z_- real valued, the eigenvalues are real and form a countably infinite set $\{\lambda_n(\gamma_1,\gamma_2)\}_{n\geq 0}$ of transcendent real analytic (actually entire) functions of the parameters $\gamma_1,\gamma_2 \in \mathbb{R}$, so that in the $(\gamma_1,\gamma_2,\lambda)$ space the sets

$$\{(\gamma_1,\gamma_2,\lambda_n(\gamma_1,\gamma_2)) \mid (\gamma_1,\gamma_2)\in\mathbb{R}\}$$

define a countably infinite number of uniquely defined analytic surfaces.

If we call $K_\eta(E,Z_-,h)$ the left hand side of (4.2.4), we can apply the results of Appendix C to

$$T(\beta) := K_\eta(E,Z_-,h) + \beta(1+\cos(2\eta))$$

where β is supposed to be defined by the real parameters E_{im} and h as follows

$$\beta(E_{\mathrm{im}},h) := i\frac{E_{\mathrm{im}}}{2h^2} \qquad (\text{with } i=\sqrt{-1}).$$

Therefore $T(\beta)$ is nothing else that (4.2.4) with complex E. It is evident that $T(\beta)$ defines a self-adjoint analytic family of type (A). Therefore it follows from Theorem C.7 and Remark C.10 that each $\lambda_n(\gamma_1,\gamma_2,\beta)$ admits an analytic extension on the complex plane around each real E that can be expanded in series of $E_{\mathrm{im}}/2h^2$ with an n-dependent convergence radius. Remark 4.3 concerning the simplicity of the spectrum and the construction described at point (7) keep to hold, therefore we may continue to regard each eigenvalue as simple restricted on its proper subspace and consider the lower bound of the convergence radius in terms of the eigenvalues spacing in the proper subspace. These distances are known to be at least of the order $O(n)$ [Kat95, Chapter VII.2.4].

In the particular case considered, we can use the ansatz given by Theorem A.9 to bound the distance between the periodic solutions with a boundary value problem. To this end we can use the discussion of [Vol96, Section 5] and apply it to our case to obtain the following rough estimate generalizing point (3).

THEOREM 4.4. *Let $E > |2Z_-|$. Then the convergence radii $\rho_n^{D,N}$ associated with (4.2.4) with Dirichlet (resp. Neumann) boundary conditions satisfy*

$$\liminf_{n\to\infty} \frac{\rho_n}{n^2} \geq \frac{6}{13},$$

$$\liminf_{n\to\infty} \frac{\rho_n}{(n-1)^2} \geq \frac{6}{13}.$$

Proof. This is nothing else than Theorem 5.1 of [Vol96] where the estimate $|2\cos(2x)| \leq 2$ (the Mathieu potential) is replaced by a corresponding estimate for $\cos(2x) + \frac{Z_-}{2E}\cos(x)$: if $E \gg |2Z_-|$, then

$$\left|\cos(2x) + 2\frac{Z_-}{E}\cos(x)\right| \leq 2.$$

Then the proof coincides with the proof in [Vol96] and the theorem follows. □

Remark 4.5. *The estimates given in the previous theorem are underestimating the real convergence radius and could be improved upon, the main point for this section is to stress that the series expansion of the λ_n in term of the complex perturbation is likely to converge in a disk of radius of order $O(n^2)$.*

4.3. Asymptotic behavior of solution of the radial Schrödinger equation and their analytic extensions

In this section we want to discuss some general estimates that we will need in order to justify the formal step in the separation of variables and the construction of the Green functions. We proceed similarly as in [AK92].

Consider the equation

$$v''(\xi,k) + h^{-2}\left(k^2\cosh^2(\xi) + Z_+\cosh(\xi) - \mu\right)v(\xi,k) = 0 \qquad (4.3.1)$$

where $\xi > 0$, $h > 0$ and $k \in \mathbb{C}$ are arbitrary, and $\mu := \mu_l$ is the l^{th}-eigenvalue of $\mathscr{A}_\eta$ for some $l \in \mathbb{N}$ (counted in ascending order for real parameters and then extended analytically). We assume w.l.o.g. that $h = 1$, since h can be absorbed in the other parameters.

We will be interested in the solutions $v_\pm(\xi,k) := v_\pm(\xi,k,\mu)$ of (4.3.1) which decay as $\xi \to \infty$ for k in the upper, resp. lower, half-plane $\mathbb{C}_\pm = \{\Im(k) \lessgtr 0\}$. We call them, following [AK92] "outgoing", resp. "incoming", and we will make a specific choice of such a family of solutions by fixing the behavior of $v_\pm(\xi,k)$ as $\xi \to \infty$.

We want to construct a phase function that approximates the eikonal equation of the Schrödinger equation (4.3.1) up to a small error, that is characterized by a particular asymptotic behavior and that is analytic in k. We would like to consider something of the form

$$\phi(\xi,k) \sim \int_0^\xi \sqrt{k^2\cosh^2(t) + Z_+\cosh(t) - \mu}\, dt. \qquad (4.3.2)$$

Sadly this gives a well defined analytic function only for $|k|^2 > |Z_+ - \mu|$. For our analysis it will be essential that the phase function is analytic in $k \in \mathbb{C}\setminus\{0\}$. To construct it we reconsider the previous ansatz and perform a change of variables. If we call $\tau = \sinh(t)$, the above equation is transformed into

$$\phi(\xi,k) \sim \int_0^{\sinh(\xi)} \sqrt{k^2 - q(\tau)}\, d\tau. \quad \text{with} \quad q(\tau) := \frac{\mu}{1+\tau^2} - \frac{Z_+}{\sqrt{1+\tau^2}}.$$

If we call $r = \sinh(\xi)$, we can imagine this $\phi(r)$ as being the usual phase function asymptotic to kr (the phase function for the zero potential).

To start the construction of the proper phase function, we choose for every $j \in \mathbb{N}$ a decomposition

$$q(\tau) = s_j(\tau) + l_j(\tau), \tag{4.3.3}$$

where $s_j(\tau) \in L_1(\mathbb{R}_+)$ and $l_j \in C^2(\mathbb{R}_+)$ verifies

$$\sup_{r>0} l_j(\tau) \leq 1/j \quad \text{and} \quad l_j(\tau) = -\frac{Z_+}{\sqrt{1+\tau^2}} \text{ for } \tau > R_j,$$

where R_j is some sequence of increasing positive numbers. Then the sequence of phase functions

$$\phi_j(\xi, k) = \int_0^{\sinh(\xi)} \sqrt{k^2 - l_j(\tau)}\, d\tau \tag{4.3.4}$$

is analytic in

$$k \in \Omega_j := \{k \in \mathbb{C} \mid |k|^2 > 1/j\}$$

and of class C^2 in $\xi \in \mathbb{R}_+$. In (4.3.4) we have taken the principal branch of the square root, i.e. the uniquely determined analytic branch of $\sqrt{z}$ that maps $\mathbb{R}_+$ into itself. We want to show now that these analytic functions can be modified by analytic functions of k alone such that they all patch together to define a "global" phase function $\phi(\xi, k)$ which is analytic in $k \in \mathbb{C} \setminus \{0\}$ and assigns to each k a germ of a function of ξ at infinity. To this end we want to make use of the following theorem (see [Hör73, Theorem 1.4.3]).

THEOREM 4.6 (Mittag-Leffler Theorem). *Let $\Omega = \cup_j \Omega_j$, where the Ω_j are open sets in $\mathbb{C}$, and let there be given meromorphic functions g_j, respectively, on the sets Ω_j, where the differences $g_j - g_k$ are analytic functions on the intersections $\Omega_j \cap \Omega_k$ for all j and k. Then there is on Ω a meromorphic function f such that the differences $f - g_j$ are analytic on Ω_j for all j.*

In fact we have the following theorem.

THEOREM 4.7. *There is a global phase function $\phi(\xi, k)$ such that for all $j \in \mathbb{N}$ there is a g_j in the space $A(\Omega_j)$ of analytic functions in Ω_j, such that*

$$\phi(\xi, k) = \phi_j(\xi, k) + g_j(k) \qquad \text{for } \xi > \tilde{R}_j,\ k \in \Omega_j, \tag{4.3.5}$$

and

$$\phi(\xi, -k) = -\phi(\xi, k) \qquad \text{for } k \in \mathbb{C} \setminus \{0\}. \tag{4.3.6}$$

PROOF. It follows from the definition given in (4.3.4) that the function

$$g_{jl}(k) = \phi_j(r, k) - \phi_l(r, k) \qquad \text{for } r > \operatorname{arcsinh}(R_{\max\{j,l\}}) \tag{4.3.7}$$

is analytic in $k \in \Omega_{\min\{j,l\}}$. By definition, these functions satisfy the *cocycle condition*

$$g_{jl} = -g_{lj}, \quad g_{jl} + g_{lh} + g_{hj} = 0 \quad \text{in } \Omega_j \cap \Omega_l \cap \Omega_h, \quad \forall j, k, h \in \mathbb{N}. \tag{4.3.8}$$

In view of (4.3.8), we can remove an index using the Mittag-Leffler Theorem 4.6. In fact it implies that for all $j \in \mathbb{N}$ there is $g_j \in A(\Omega_j)$ such that

$$g_{jl} = g_l - g_j \quad \text{in } \Omega_j \cap \Omega_l. \tag{4.3.9}$$

Since $\phi_j(r,-k) = -\phi_j(r,k)$, it follows from (4.3.9) and (4.3.7) that

$$\phi_j(\xi,k) + \frac{1}{2}(g_j(k) - g_j(-k)) = \phi_l(\xi,k) + \frac{1}{2}(g_l(k) - g_l(-k))$$

in the common domain of definition. Thus the local data $\phi_j + \frac{1}{2}(g_j(k) - g_j(-k))$ patch together to define a global phase function satisfying (4.3.5) and (4.3.6). $\square$

Henceforth we will refer to the $\phi(\xi,k)$ defined in Theorem 4.7 as a *global phase function.*

REMARK 4.8. *Choosing in (4.3.3) a different decomposition of $q(\tau)$ into a short range and long range part, keeping $l(\xi)$ fixed near infinity, modifies $\phi(\xi,k)$ by an analytic function of k alone. In particular the term $s(\tau) := \frac{\mu}{1+\tau^2}$ being in the short range component s_j of (4.3.3) will be dropped out for the moment.*

PROPOSITION 4.9. *The phase function $\phi(\xi,k)$ has the asymptotic behavior given by*

$$\phi(\xi,k) = k\sinh(\xi) + \frac{Z_+}{2k}\xi + O(1) = \frac{k}{2}e^{\xi}(1+o(1)) \quad \textit{as} \quad \xi \to \infty. \tag{4.3.10}$$

PROOF. Without losing generality we can suppose $|k| > |Z_+|$ and consider the phase function given by

$$\begin{aligned}\phi(\xi,k) &= \int_0^{\xi} \sqrt{k^2\cosh^2(t) + Z_+\cosh(t)}\,dt \\ &= k\int_0^{\xi} \cosh(t)\sqrt{1 + \frac{Z_+}{k^2\cosh(t)}}\,dt.\end{aligned}$$

We are interested in the asymptotic behavior of $\phi(\xi,k)$ as $\xi \to \infty$. Using

$$\begin{aligned}\phi(\xi,k) &= k\int_0^{\xi} \cosh(t)\left(1 + \frac{Z_+}{2k^2\cosh(t)} + O\left(k^{-2}\cosh^{-2}(t)\right)\right)dt \\ &= k\sinh(\xi) + \frac{Z_+}{2k}\xi - \frac{Z_+^2}{8k^3}\mathrm{gd}(\xi) + O(1),\end{aligned}$$

where $\mathrm{gd}(x) := \arctan\left(\tanh\left(\frac{\xi}{2}\right)\right)$ is the Gudermannian function. Writing $\sinh(\xi) = (e^x - e^{-x})/2$ and collecting the growing term we have the thesis. $\square$

REMARK 4.10. *Notice that all the terms appearing in the $O(1)$ above can be explicitly computed and bounded in terms of a function of k and Z_+.*

The Liouville-Green Theorem B.17 guarantees that for each $k \in \mathbb{C}$ there exist two linearly independent solutions of (4.3.1) such that

$$y_{1,2}(\xi) = \frac{1}{\sqrt{\phi'(\xi,k)}}e^{\pm i\phi(x,k)}(1+o(1)) \quad \text{for } \xi \to \infty.$$

In particular, it follows from the asymptotic estimate of Proposition 4.9 that (4.3.1) must be in the Limit Point Case at infinity – Case I – of Theorem B.3 if we set $r(x) := \cosh^2(x)$, $p := 1$ and $\lambda := k^2$. In what follows we investigate the regularity of the solutions with respect to ξ and k.

THEOREM 4.11. *For each $k \in \mathbb{C} \setminus \{0\}$, equation (4.3.1) has a unique solution $v_\pm(\xi,k)$ verifying the asymptotic relation*

$$v_\pm(\xi,k) = \sqrt{2}e^{-\frac{\xi}{2}}e^{\pm i\phi(\xi,k)}(1+o(1)) \quad \text{as} \quad \xi \to \infty, \tag{4.3.11}$$

where (4.3.11) holds uniformly in any truncated angle $\Lambda_\pm(\eta,\delta) = \{k \in \mathbb{C}\setminus\{0\} \mid \eta \le \arg(\pm k) \le \pi - \eta,\ |k| \ge \delta\}$ with $\eta \ge 0$, $\delta > 0$. The family of solutions defined by (4.3.11) is analytic in $k \in \mathbb{C}_\pm \setminus \{0\} := \{z \in \mathbb{C}\setminus\{0\} \mid \pm\Im z > 0\}$ and extends continuously to $k \in \overline{\mathbb{C}}_\pm \setminus \{0\}$.

REMARK 4.12. *(4.3.6) and the uniqueness of Theorem 4.11 imply that $v_+(\xi,k) = v_-(\xi,-k)$. In particular it suffices to consider v_+.*

PROOF. In view of Theorem 4.7 and the subsequent remark, we can reduce the proof to the case where the phase function is given by

$$\phi(\xi,k) = \int_0^\xi \sqrt{k^2\cosh^2(t) + Z_+\cosh(t)}\,dt \tag{4.3.12}$$

for $\xi > 0$ and $|k|^2 > |Z_+|$. We call this $\phi(\xi,k)$ a *local phase function*.

Let

$$V_\pm(\xi,k) := \left(\frac{k}{\phi'(\xi,k)}\right)^{\frac{1}{2}} e^{\pm i\phi(\xi,k)} \tag{4.3.13}$$

define the approximate solutions of (4.3.1). For $|k| \ge \delta$ the function $V_\pm$ satisfies the comparison equation

$$V_\pm''(\xi,k) + \left(k^2\cosh^2(\xi) + Z_+\cosh(\xi) + \frac{1}{2}S\phi(\xi,k)\right)V_\pm(\xi,k) = 0 \tag{4.3.14}$$

where $S\phi$ denote the Schwarzian derivative

$$S\phi = \frac{\phi'''}{\phi'} - \frac{3}{2}\left(\frac{\phi''}{\phi'}\right)^2. \tag{4.3.15}$$

For $k \in \Lambda_\pm(\eta,\delta)$ the inhomogeneous Volterra Integral Equation [Tri85]

$$v_\pm(\xi,k) = V_\pm(\xi,k) - \int_\xi^\infty K_k(\xi,t)F_k(t)v_\pm(t,k)\,dt \tag{4.3.16}$$

where $F_k(t) = \frac{1}{2}S\phi(t,k) + \mu$ is the function that expresses the difference between the Schrödinger equation (4.3.1) and the comparison equation (4.3.14) and $K(\xi,t)$ is the Green's function associated with equation (4.3.13):

$$K_k(\xi,t) = W(V_-,V_+)^{-1}\{V_+(\xi)V_-(t) - V_+(t)V_-(\xi)\}, \tag{4.3.17}$$

with Wronskian $W(V_-,V_+) := V_-V_+' - V_-'V_+ = 2ik$.

To give (4.3.16) meaning we need to check if the definition makes sense and a solution can be found. From now one we may suppress writing the additional parameter k whenever it is not necessary.

We can explicitly compute $F(t)$ using (4.3.15) obtaining

$$S\phi(\xi) = \frac{10k^4 - Z_+^2 - 2k^4\cosh(2\xi) + Z_+\operatorname{sech}(\xi)\left(12k^2 + 5Z_+\operatorname{sech}(\xi)\right)}{8\left(Z_+ + k^2\cosh(\xi)\right)^2}$$

and thus, for real ξ and for every $k \in \Lambda_+(\eta,\delta)$, we have

$$\lim_{\xi\to\infty} |F(\xi)| = \frac{1}{8} + \mu \quad \text{and} \quad \sup_{\xi\in\mathbb{R}_+} |F(\xi)| =: C_F < \infty. \tag{4.3.18}$$

Of course C_F depends on Z_+, μ and k, thus on η and δ. Moreover from (4.3.13) and (4.3.10), writing $k \in \Lambda_+(\eta,\delta)$ as $k = k_r + ik_i$ (k_r, k_i real), we get

$$\left|V_\pm(\xi,k)\right| = \sqrt{2}e^{-\frac{\xi}{2}}(1+o(1))\left|e^{ik\left(\frac{\phi(\xi,k)}{k}\right)}\right| \le C_V e^{-\frac{\xi}{2}} e^{-\frac{k_i}{2}e^{\xi}(1+o(1))}, \tag{4.3.19}$$

where $C_V(k) := \sup_{\xi\in\mathbb{R}_+}\left(e^{\xi/2}|k/\phi'(\xi,k)|\right) < \infty$. Therefore for $0 < \xi \le t < \infty$ we have

$$\begin{aligned}
|K(\xi,t)| &= \left|\frac{1}{2ik}\sqrt{\frac{k^2}{\phi'(t,k)\phi'(\xi,k)}}\left(e^{i(\phi(\xi,k)-\phi(t,k))} - e^{i(\phi(t,k)-\phi(\xi,k))}\right)\right| \\
&\le \frac{C_V^2}{2}e^{-\frac{\xi+t}{2}}\left|\exp\left(-ik\int_\xi^t \cosh(\tau)\sqrt{1+\tfrac{Z_+}{k^2\cosh(\tau)}}\,d\tau\right)\right. \\
&\qquad \left. - \exp\left(ik\int_\xi^t \cosh(\tau)\sqrt{1+\tfrac{Z_+}{k^2\cosh(\tau)}}\,d\tau\right)\right| \\
&\le \frac{C_V^2}{2}e^{-\frac{\xi+t}{2}} C_K\left|\exp\left(-ik\int_\xi^t \cosh(\tau)\sqrt{1+\tfrac{Z_+}{k^2\cosh(\tau)}}\,d\tau\right)\right|,
\end{aligned} \tag{4.3.20}$$

where

$$C_K(k) := \sup_{t,\xi\in\mathbb{R}^+}\left|1 - \exp\left(2ik\int_\xi^t \cosh(\tau)\sqrt{1+\tfrac{Z_+}{k^2\cosh(\tau)}}\,d\tau\right)\right| \le 2.$$

It follows from (4.3.18), (4.3.19) and (4.3.20) that the Volterra Integral Equation (4.3.16) is well defined as a mapping from the function space

$$\begin{aligned}
\mathscr{C}_\pm(\eta,\delta) := \Big\{ f \in C^2\left(\mathbb{R}_+ \times \Lambda_\pm(\eta,\delta)\right) \,\Big|\, & \forall k \in \Lambda_\pm(\eta,\delta), \\
& \|f\|_k := \sup_{x\in\mathbb{R}_+}\left|f(x,k)e^{\mp i\phi(x,k)}\right| < \infty \Big\}
\end{aligned} \tag{4.3.21}$$

to itself. In particular, being $V_\pm \in \mathscr{C}_\pm(\eta,\delta)$ we can apply the Picard iteration procedure to find a solution of the equation and prove its existence. We claim that the solution must be unique. Suppose there exists two solutions $v_+, w_+ \in \mathscr{C}_+$ of (4.3.16), then

$$\psi(\xi,k) := v_+(\xi,k) - w_+(\xi,k) = -\int_\xi^\infty K(\xi,t)F(t)\psi(t,k)\,dt. \quad (4.3.22)$$

The previous estimates applied to (4.3.22) give

$$\begin{aligned}
|\psi(\xi,k)| &= \left|\int_\xi^\infty K(\xi,t)F(t)\psi(t,k)\,dt\right| \\
&\le \int_\xi^\infty |K(\xi,t)F(t)\psi(t,k)|\,dt \\
&\le \frac{C_K C_F C_\psi}{2}\int_\xi^\infty \left|\sqrt{\frac{k^2}{\phi'(t,k)\phi'(\xi,k)}}\right| \\
&\quad \cdot \left|\exp\left(-ik\int_\xi^t \cosh(\tau)\sqrt{1+\tfrac{Z_+}{k^2\cosh(\tau)}}\,d\tau\right)\right|\left|e^{i\phi(t,k)}\right|\,dt \\
&\le \frac{C_K C_F C_\psi}{2}\left|\sqrt{\frac{k}{\phi'(\xi,k)}}\right|\left|e^{i\phi(\xi,k)}\right|\int_\xi^\infty \left|\sqrt{\frac{k}{\phi'(t,k)}}\right|\,dt \\
&\le \frac{C_K C_F C_\psi C_V}{2}e^{-\frac{\xi}{2}}\left|e^{i\phi(\xi,k)}\right|\int_\xi^\infty \sqrt{2}e^{-\frac{t}{2}}(1+o(1))\,dt \\
&\le \frac{C_K C_F C_\psi C_V C_I}{2}e^{-\frac{\xi}{2}}\left|e^{i\phi(\xi,k)}\right|\int_\xi^\infty e^{-\frac{t}{2}}\,dt \\
&= C_\psi C_{tot}e^{-\xi}\left|e^{i\phi(\xi,k)}\right| \qquad (4.3.23)
\end{aligned}$$

where $C_\psi(k) := \|\psi\|_k$, $C_I := \sup_{\xi\in\mathbb{R}_+}\sqrt{2}\left((1+e^{-2\xi})\sqrt{1+\frac{Z_+}{k^2\cosh(\xi)}}\right)^{-\frac{1}{2}}$ and $C_{tot} := C_K C_F C_V C_I$. Using equations (4.3.22) and (4.3.23)we can reiterate the procedure, in fact defining

$$\begin{aligned}
\psi_1(\xi,k) &:= \int_\xi^\infty K(\xi,t)F(t)\psi(t,k)\,dt, \\
\psi_n(\xi,k) &:= \int_\xi^\infty K(\xi,t)F(t)\psi_{n-1}(t,k)\,dt,
\end{aligned}$$

one can prove by induction that

$$\begin{aligned}
|\psi(\xi,k)| &= |\psi_n(\xi,k)| \\
&\le \frac{C_{tot}^n\,e^{-n\xi}}{(2n-1)(2n-3)\cdots 3\cdot 1}\left|e^{i\phi(\xi,k)}\right| \qquad (4.3.24) \\
&\le C_\psi\frac{C_{tot}^n\,e^{-n\xi}}{n!}\left|e^{i\phi(\xi,k)}\right|
\end{aligned}$$

uniformly in $k \in \Lambda_+(\eta,\delta)$ and for all $n \in \mathbb{N}$. The convergence of

$$\sum_{n=1}^{\infty} C_\psi \frac{C_{tot}^n}{n!} e^{-n\xi} \left| e^{i\phi(\xi,k)} \right| = C_\psi \left| e^{i\phi(\xi,k)} \right| \left(e^{C_{tot} e^{-\xi}} - 1 \right) \tag{4.3.25}$$

implies that $|\psi(\xi,k)| = 0$, i.e. $w_+ = v_+$.

The same inequality implies that after some iterates the homogeneous integral equation is a contraction and coupled with the bounds on V_+ it follows that (4.3.16) has a unique fix point. Thus proving the existence and uniqueness of the solution.

In fact if we define

$$\begin{aligned} v_{0,+}(\xi,k) &:= V_+(\xi,k), \\ v_{n,+}(\xi,k) &:= -\int_\xi^\infty K(\xi,t) F(t) v_{n-1,+}(t,k)\, dt, \end{aligned}$$

the Picard iteration converges to $v_+ = \sum_{n=0}^{\infty} v_{n,+}$, the series converges absolutely uniformly in $k \in \Lambda_+(\eta,\delta)$ with $\left|v_+(\xi,k)\right| \le \left|V_+(\xi,k)\right| e^{Ce^{-\xi}}$ for some positive constant C. Therefore one has

$$v_+(\xi,k) = V_+(\xi,k)(1+o(1)) \quad \text{as} \quad \xi \to \infty$$

and (4.3.11) holds.

The fact that all the bounds are valid for $k \in \mathbb{R}$ completes the proof.

□

REMARK 4.13. *It is possible to compute an explicit bound like* (4.3.24) *using the fact that*

$$\left| v_{n,+} \right| \le C_V e^{-\frac{\xi}{2}} \left| e^{i\phi(\xi,k)} \right| \frac{C_{tot}^n e^{-n\xi}}{2^n n!}.$$

In particular the dependence on the small-range parameter μ appear in the C_{tot} and in view of the previous estimate can be bounded by $|\mu| O(1)$, therefore we can be more precise and say that

$$v_\pm(\xi,k) = \sqrt{2} e^{-\frac{\xi}{2}} e^{\pm i\phi(\xi,k)} \left(1 + M_\pm(\xi, k\mu)\right) \quad \text{as} \quad \xi \to \infty, \tag{4.3.26}$$

where for some constant $C \neq 0$ we have

$$M_\pm(\xi,k,\mu) = e^{C|\mu| e^{-\xi}} o(1).$$

REMARK 4.14. *Let $\tilde{v}$ any other family of solutions of* (4.3.1)*, analytic in $k \in \mathbb{C} \setminus \{0\}$ and satisfying for $k \in \Lambda_+(\eta,\delta)$*

$$\tilde{v}(\xi,k) = o(1) \quad \text{as} \quad \xi \to \infty.$$

Then

$$\tilde{v}(\xi,k) = \gamma(k) v_+(\xi,k),$$

where $\gamma(k)$ is a nowhere-vanishing analytic function of $k \in \Lambda_+(\eta,\delta)$.

In the notation of Appendix B we set $\alpha=\frac{\pi}{2}$, $r(x)=\cosh^2(x)$, $\lambda=k^2$, $p(x)=1$ and $q(x)=\mu-Z_+\cosh(x)$. Let $\mu\in\mathbb{C}_-$, then we have for Q from (B.1)

$$Q\subset\left\{z\in\mathbb{C}\,\middle|\,\Re z\geq\inf_{\xi\geq0}\frac{\Re\mu-Z_+\cosh(\xi)}{\cosh^2(\xi)},\ \Im\mu\leq\Im z\leq0\right\}$$

and $Q_b=\mathbb{R}_+$ for Q_b defined in (B.11). Therefore by Theorem B.9 we have that $m(k^2)$ is defined throughout $\mathbb{C}\setminus Q$, that has a unique connected component, and has a meromorphic extension to $\mathbb{C}\setminus\mathbb{R}_+$ with poles only in $Q\setminus\mathbb{R}_+$.

Let $k^2\in\mathbb{C}\setminus Q$, being $v_+(\xi,k)$ the only integrable solution, it must be up to a constant defined by

$$v_+(\xi,k)=\theta(\xi,k^2)+m(k^2)\phi(\xi,k^2).$$

The fact that the two solution coincide for k in an open subset of the complex plane implies that they must represent the same analytic function, confirming in particular our Theorem 4.7. Notice that in particular this means that $m(k^2)=M(k)$ is a function of the square root of the actual eigenvalue k^2.

For $k^2\in\mathbb{C}\setminus Q$ we can define the Green function as in (B.12)

$$\begin{aligned}G(\xi,\tilde{\xi};k^2)&=\begin{cases}-\phi(\xi,k^2)\psi(\tilde{\xi},k^2), & 0<\xi<\tilde{\xi}<\infty\\ -\psi(\xi,k^2)\phi(\tilde{\xi},k^2), & 0<\tilde{\xi}<\xi<\infty\end{cases}\\ &=\frac{1}{[\phi,v_+]}\begin{cases}-\phi(\xi,k^2)v_+(\tilde{\xi},k), & 0<\xi<\tilde{\xi}<\infty\\ -v_+(\xi,k)\phi(\tilde{\xi},k^2), & 0<\tilde{\xi}<\xi<\infty\end{cases}\end{aligned}\tag{4.3.27}$$

and the resolvent R_λ as in (B.13).

Remark 4.15. *In case $Z_+=0$, the solutions of (4.3.1) are given by linear combinations of the modified Mathieu functions (Mc and Sc) [EMOT55]. In particular, if we look at their asymptotic behavior, we find out that up to a constant factor*

$$v_+(\xi,k)=\mathrm{Mc}\left(\mu-\frac{k^2}{2},\frac{k^2}{4},\xi\right)\tag{4.3.28}$$

where $\mathrm{Mc}(a,q,x)$ is the modified Mathieu cosine, i.e. the solution of

$$y''(x)+(a-2q\cosh(2x))y(x)=0$$

that decays for $\sqrt{q}\in\mathbb{C}_+$. It is well known [MS54, Chapter 2] that the function in the RHS of (4.3.28) admits an analytic continuation through the positive real axis on the negative complex plane for $-\pi/2\leq\arg(k)\leq\pi/2$ and that for $x\to\infty$ and $k\in\mathbb{C}_+$ it has the following asymptotic behavior [MS54, EMOT55]

$$\mathrm{Mc}\left(\mu-\frac{k^2}{2},\frac{k^2}{4},x\right)=e^{-\frac{x}{2}}e^{i\frac{k}{2}e^x(1+o(1))}(1+o(1)),$$

in line with what we expected.

For what follows we will need to work in a slightly different setting. If we perform the change of variable defined by $\xi\mapsto\log(x+1)$ where we consider the principal branch of the logarithm in case of continuation to the complex plane, equation (4.3.1) takes the form

$$\begin{aligned}((x+1)w'(x,k))' + \frac{1}{h^2}\left(\frac{k^2}{4}\left(x+1+(x+1)^{-1}+(x+1)^{-3}\right)\right)w(x,k)\\ +\frac{1}{h^2}\left(\frac{Z_+}{2}\left(1+(x+1)^{-2}\right)-\mu(x+1)^{-1}\right)w(x,k)=0\end{aligned} \tag{4.3.29}$$

where $x>0$, $h>0$ and $k\in\mathbb{C}\setminus\{0\}$. As before we assume $h=1$ for the moment.

Remark 4.16. *In this case Theorem 4.11 and Remark 4.14 is still valid and in accord with the Liouville-Green Theorem B.17 we have two unique solutions that as $x\to\infty$ are asymptotic to*

$$\begin{aligned}w_\pm(x,k) &= \frac{1}{\sqrt{x+1}}e^{\pm i\widetilde{\phi}(x,k)}(1+o(1))\\ &= \frac{1}{\sqrt{x+1}}\exp\left(\pm i\left(\tfrac{k}{2}x+\tfrac{Z_+}{2k}\log(x+1)+\tfrac{k}{2}\right)\right)\\ &\quad\cdot\exp\left(\pm i\left(\tfrac{Z_+^2}{4k^3}(x+1)^{-1}+O\left((x+1)^{-2}\right)\right)\right)(1+o(1))\end{aligned} \tag{4.3.30}$$

where $\widetilde{\phi}(x,k)=\phi(\log(x+1),k)$. The asymptotic behavior (4.3.30) holds uniformly for k in any sector $\Lambda_\pm(\eta,\delta)=\{k\in\mathbb{C}\mid \eta\le\arg(\pm k)\le\pi-\eta,\ |k|\ge\delta\}$ with $\eta\ge 0$ and $\delta>0$. The family of solutions defined by (4.3.30) is analytic in $k\in\mathbb{C}_\pm\setminus\{0\}$ and extends continuously to $k\in\overline{\mathbb{C}}_\pm\setminus\{0\}$.

Remark 4.17. *From now on we write with an abuse of notation $\phi(x,k)$ in place of $\widetilde{\phi}(x,k)$.*

Before proving the main theorem we need the following lemma.

Lemma 4.18. *Let $\mathscr{K}$ be a compact set in $\mathbb{C}\setminus\{0\}$. Then for any $-\pi<\theta<\pi$, there is a constant A_θ such that any solution of equation (4.3.29) verifies the estimate*

$$|v(x,k)|\le A_\theta(|c|+|c'|)\frac{1}{\sqrt{x}}e^{|\Im\phi(x,k)|} \tag{4.3.31}$$

for $x\in e^{i\theta}[1,\infty)$ and $k\in\mathscr{K}$, where

$$c=v(0,k),\qquad c'=v'(0,k), \tag{4.3.32}$$

denote the initial data at $x=0$.

Proof. We start proving (4.3.31) in the case $\eta\le|\arg k|\le\pi-\eta$ for any $\eta\ge 0$ and $\theta=0$ (i.e. $x\in\mathbb{R}_+$). All the constants that we are going to use without an explicit definition are defined as previously. Using the approximate solutions given by (4.3.13) defined with an abuse of notation by $V_\pm(x,k) := V_\pm(\log(x+1),k)$, we determine a_+ and a_- from the initial data requiring

$$\begin{aligned} c &= a_+ V_+(0,k) + a_- V_-(0,k), \\ c' &= a_+ V_+'(0,k) + a_- V_-'(0,k). \end{aligned} \tag{4.3.33}$$

Then $v(x,k)$ satisfies the Volterra Integral Equation

$$v(x,k) = a_+ V_+(x,k) + a_- V_-(x,k) + \int_0^x K(x,t)F(t)v(t,k)\,\frac{dt}{t+1} \tag{4.3.34}$$

where $K(x,t) := K(\log(x+1), \log(t+1))$ and $F(t) := F(\log(t+1))$ are defined with an abuse of notation from the respective function (4.3.17) and (4.3.16). Notice similarly as in the previous theorem that for $0 \le t \le x$ there exist a constant $C_0(\eta,\delta)$ such that we have

$$\begin{aligned} |K(x,k)| &\le \frac{C_0(\eta,\delta)}{2}\left|\frac{1}{\phi'(x,k)}\right|\left|\frac{1}{\phi'(t,k)}\right| e^{|\Im(\phi(x,k)-\phi(t,k))|} \\ &\le \frac{C_V^2 C_0(\eta,\delta)}{2}\frac{1}{\sqrt{(x+1)(t+1)}} e^{|\Im(\phi(x,k)-\phi(t,k))|}. \end{aligned} \tag{4.3.35}$$

Define now

$$V(x,k) = \sqrt{2}(|a_+| + |a_-|)\frac{1}{\sqrt{x+1}} e^{|\Im\phi(x,k)|}. \tag{4.3.36}$$

The sequence

$$\begin{aligned} v_0(x,k) &:= a_+ V_+(x,k) + a_- V_-(x,k), \\ v_n(x,k) &:= \int_0^x K(x,t)F(t)v_{n-1}(t,k)\,\frac{dt}{t+1}, \end{aligned}$$

is uniformly convergent. In fact, suppressing the dependence of the constant on η and δ, we have $|v_0(x,k)| \le C_V V(x,k)$ and, using the transformed version of (4.3.35), it follows by induction that

$$|v_n(x,k)| \le \frac{1}{n!} V(x,k) L^n(x), \tag{4.3.37}$$

where

$$\begin{aligned} L(x) &:= C_0 \int_0^x \left|\frac{1}{\phi'(t,k)}\right| |F(t)|\,\frac{dt}{t+1} \\ &= C_0 C_V \int_0^x \frac{1}{\sqrt{t+1}}|F(t)|\,\frac{dt}{t+1} \\ &\le C_0 C_V C_F \frac{1}{\sqrt{x+1}} \end{aligned}$$

is uniformly bounded for $x \in \mathbb{R}_+$. Therefore $\sum_{n=0}^\infty v_n(x,k)$ converges uniformly and absolutely and coincides with the given solution $v(x,k)$ of (4.3.34) for $\eta \le |\arg k| \le \pi - \eta$, $\eta \ge 0$. In particular being $a_\pm$ bounded in terms of the initial data c and c', we obtain (4.3.31) for real values of x.

At this point it is enough to notice that as soon as we do not cross the branch cut of the logarithm all the inequalities and the equations written up to this point are valid, therefore the result holds replacing x with $e^{i\theta}x$ for every $-\pi < \theta < \pi$. $\square$

We are ready to prove that the functions $v_\pm$ can be analytically extended in k up to the positive real axis, to this end we consider the transformed $w_\pm$.

REMARK 4.19. *The potential is analytic in $\mathbb{C}\setminus(-\infty,-1]$, therefore its analyticity in the cone*

$$\Sigma_{\alpha,\beta} := \{z \in \mathbb{C} \mid -\alpha < \arg z < \beta, |z| > 0\} \tag{4.3.38}$$

for some $\alpha, \beta \in [0,\pi)$ is clear.

THEOREM 4.20. *Let $w_\pm(x,k)$ be defined as in Remark 4.16. Then $w_+(x,k)$ admits an analytic continuation in k through the positive real k-axis into the region*

$$\{k \in \mathbb{C}\setminus\{0\} \mid -\beta < \arg k < \beta\},$$

$w_-(x,k)$ admits an analytic continuation into

$$\{k \in \mathbb{C}\setminus\{0\} \mid -\alpha < \arg k < \alpha\},$$

for any $\alpha, \beta \in [0,\pi)$ and both verify the asymptotic relation (4.3.11)

$$w_\pm(x,k) = \frac{1}{\sqrt{x}} e^{\pm i\phi(x,k)}(1+o(1)) \quad \text{as} \quad x \to \infty \text{ in } \Sigma_{\alpha,\beta}, \tag{4.3.39}$$

where (4.3.39) holds locally uniformly in k and uniformly in x. Furthermore an analytic continuation of $w_+(x,k)$ and $w_-(x,k)$ through the negative real axis is defined via

$$w_+(x,k) = w_-(x,-k). \tag{4.3.40}$$

REMARK 4.21. *If $\alpha+\beta > \pi$, the analytically continued function $w_\pm(x,k)$ may be double valued for $k \in \mathscr{Z}_\mp$. By an abuse of notation we denote the corresponding possibly self-overlapping domain by*

$$D_\pm(\alpha,\beta) := \{k \in \mathbb{C}\setminus\{0\} \mid -\beta < \arg(\pm k) < \pi + \alpha\} \tag{4.3.41}$$

PROOF. It is well known [**CL55**, Chapter 3.7] that, as solutions of the linear differential equation (4.3.29) with analytic coefficients, $w_\pm(x,k)$ admit an analytic continuation in x into the region $\Sigma_{\alpha,\beta}$. The main point of this proof is to use this information to obtain the analyticity in k via dilation. More in details we plan to resemble the strategy of [**AK92**, Theorem 2.6] refining the crude bound of Theorem 4.18 using the Phragmen-Lindelöf principle. This allows us to identify the dilated solutions with a decaying solution of the dilated equation. In view of Lemma 4.18, this solution is uniquely defined by the asymptotic behavior as x goes to infinity.

Let us consider $w_+(z,k)$ along a ray $\Gamma := \{z \mid \arg z = \gamma\}$ with $0 < \gamma < \beta$. Then for $x > 1$ and $k \in \mathbb{C}_+\setminus\{0\}$, the function

$$\omega(x,k,\gamma) = w_+(e^{i\gamma}x,k) \tag{4.3.42}$$

satisfies the equation

$$\left((e^{i\gamma}x+1)\omega'(x,k)\right)' + \frac{e^{2i\gamma}}{h^2}q(e^{i\gamma}x,k,Z_+,\mu)\omega(x,k) = 0 \tag{4.3.43}$$

where

$$\begin{aligned} q(x,k,Z_+,\mu) := {} & \frac{k^2}{4}\left((x+1)+(x+1)^{-1}+(x+1)^{-3}\right) \\ & + \frac{Z_+}{2}\left(1+(x+1)^{-2}\right) - \mu(x+1)^{-1}. \end{aligned}$$

Moreover the initial data

$$\omega(0,k,\gamma) = w_+(0,k), \quad \omega'(0,k,\gamma) = e^{i\gamma}w_+'(0,k), \tag{4.3.44}$$

are analytic in $k \in \mathbb{C}_+ \setminus \{0\}$.

To obtain an analytic continuation of $w_+(x,k)$ into the lower half-plane first observe that by the Liouville-Green Theorem B.17 and Remark 4.16, equation (4.3.43) has a unique solution $\omega_+(x,k,\gamma)$ in the half-plane $-\gamma < \arg k < \pi-\gamma$ characterized by the asymptotic relation

$$\omega_+(x,k,\gamma) := \frac{1}{\sqrt{e^{i\gamma}x}}e^{i\phi(e^{i\gamma}x,k)}(1+o(1)) \quad \text{as} \quad x\to\infty. \tag{4.3.45}$$

We claim that in fact

$$\omega_+(x,k,\gamma) = \omega(x,k,\gamma) \qquad \text{for } x\in\mathbb{R}_+, \quad 0<\arg k<\pi-\gamma. \tag{4.3.46}$$

Then $\omega_+(1,k,\gamma)$ and $\omega_+'(1,k,\gamma)$ provide the analytic continuation of the initial data for $w_+(x,k)$ into the region $-\gamma < \arg k < 0$, implying that $w_+(x,k)$ can be continued analytically into the lower half-plane.

To prove (4.3.46), we observe that $x \mapsto w_+(x,k)$ is of exponential type for $x\in\Sigma_{\alpha,\beta}$ and decays exponentially for $\Im k>0$. Then it follows from the Phragmen-Lindelöf principle [**Con78**, VI.4] that for fixed $\Im k>0$ the function $w_+(x,k)$ decays exponentially as $x\to\infty$ in a small cone containing $\mathbb{R}_+$.

Therefore Remark 4.16 and Remark 4.14 applied to the dilated function $\omega_+(x,k,\widetilde{\gamma})$ for some small $\widetilde{\gamma}>0$ imply that $\omega_+(x,k,\widetilde{\gamma})$ is a multiple of $\omega(x,k,\widetilde{\gamma})$. This means moreover that it decays at a rate given by the expected function

$$\frac{1}{\sqrt{e^{i\widetilde{\gamma}}x}}e^{i\phi(e^{i\widetilde{\gamma}}x,k)}.$$

We can repeat this procedure a finite number of times and deduce that for fixed k the analytic function

$$g(x,k) := \sqrt{x}e^{-i\phi(x,k)}w_+(x,k) \tag{4.3.47}$$

is uniformly bounded as $x\to\infty$ within an angle $-\epsilon<\arg x<\gamma+\epsilon$ for some $\epsilon>0$. Since

$$\lim_{x\to\infty} g(x,k) = 1,$$

it follows from Montel's theorem [**Con78**, VII.2] that this limit is assumed uniformly as $x\to\infty$ in $0\le\arg x\le\gamma$. This proves (4.3.46). Since $\gamma\in(0,\beta)$ was arbitrary, we obtain an analytic continuation of $w_+(x,k)$ to $-\beta < \arg k < \pi$. It remains to prove (4.3.39).

For $-\alpha < \gamma < \beta$ we can apply Lemma 4.18 to the dilated function $\omega(x,k,\gamma)$ to have

$$g(x,k) = O(1) \quad \text{as} \quad x \to \infty \text{ within } \Sigma_{\alpha,\beta}. \tag{4.3.48}$$

We already know from (4.3.46) that $g(x,k) \to 1$ as $x \to \infty$ along any ray such that $0 < \eta \leq \arg(kx) \leq \pi - \eta$ for some $\eta \geq 0$. Therefore we have that locally uniformly for $k \in \mathbb{C} \setminus \{0\}$, $-\beta < \arg k < \pi$

$$g(x,k) = O(1) \quad \text{as} \quad x \to \infty \text{ within } \Sigma_{\alpha,\beta}$$

and $g(x,k)$ is uniformly bounded along the boundary rays of $\Sigma_{\alpha,\beta}$. That $g(x,k)$ is uniformly bounded in $x \in \Sigma_{\alpha,\beta}$ is now a consequence of the Phragmen-Lindelöf Principle. The fact that $g(x,k)$ tends to 1 as $x \to \infty$ since it does so along some ray contained in its interior, completes the proof of the theorem. □

4.4. Generalized eigenfunctions, Green's function and the scattering matrix

We are now ready to construct the main elements for the partial wave expansion required to give a definition of the resonances of our operator. We considered in the previous section the incoming and outgoing waves as the "regular" solutions at infinity, and because of the fact that they are defined around infinity it required some work to prove that they can be analytically extended to the second Riemann sheet across the positive real axis. The situation is completely different if we consider the solution $w_0(x,k)$ of (4.3.29) (or the corresponding $v_0(\xi,k)$ of 4.3.1) that is regular in 0 in the sense of the boundary conditions derived from (4.1.3), i.e.

$$w_0'(0,k) = 0. \tag{4.4.1}$$

For the moment we can assume that w_0 is normalized so that $w_0(0,k) = 1$. Being the solution of a boundary problem with analytic coefficients and analytic initial conditions, the following theorem follows as a corollary of the standard theory of complex ordinary differential equations (see [**CL55**, Chapter 1.8]).

THEOREM 4.22. *The unique solution $w_0(x,k)$ of (4.3.29) defined by the condition (4.4.1) is analytic in $x \in \Sigma_{\alpha,\beta}$, $k \in \mathbb{C} \setminus \{0\}$ and satisfies*

$$w_0(x,k) = w_0(x,-k). \tag{4.4.2}$$

REMARK 4.23. *Working with (4.3.29) or (4.3.1) is equivalent. We will use each time the representation that makes the proofs and the computations easier. Therefore in what follows we do not continue to remark that the properties are equivalent. It is always possible to understand in which setting we are working, looking at the name of the functions and the variables.*

From now on, we will always assume that the Wronskian is defined it is generalized form given by (A.3).

We are finally ready to introduce the basic elements for scattering theory on the half-line. We call *Jost functions* associated to the radial equation (4.3.29) and our choice of phase function $\phi(x,k)$ the Wronskians

$$f_{\pm}(k) := W(w_{\pm}(x,k), w_0(x,k)). \tag{4.4.3}$$

They connect the regular solution to the incoming and outgoing ones via the identity

$$W(w_-, w_+)w_0 = f_+ w_- - f_- w_+, \qquad W(w_+, w_-) = 2ik, \tag{4.4.4}$$

that follows expanding explicitly the Wronskian and using the asymptotic behavior of the solutions in their domain of analyticity. In particular this implies the following corollary of Theorem 4.22 and Theorem 4.20.

COROLLARY 4.24. *The Jost functions $f_{\pm}(k)$ are analytic in $k \in D_{\pm}(\alpha,\beta)$ defined in* (4.3.41) *and verify*

$$f_{\pm}(k) = \pm(2ik) \lim_{x\to\infty} e^{i\gamma/2}\sqrt{x}\exp\left(\pm i\phi(e^{i\gamma}x,k)\right) w_0(e^{i\gamma}x,k), \tag{4.4.5}$$

where $\gamma \in (-\alpha,\beta)$ satisfies $\gamma \gtrless -\arg(k)$ according to the choice of sign of (4.4.5).

It will be convenient for what follows to change the normalization $w_0(0,k) = 1$ to one at "infinity" in the sense of Corollary 4.24. Namely if $f_+(k) \neq 0$, we define the *generalized eigenfunction* of the radial equation (4.3.29) and our choice of phase function $\phi(x,k)$ the function

$$e(x,k) := f_+(k)^{-1} w_0(x,k). \tag{4.4.6}$$

With this notation we introduce for $k \in \Sigma_{\alpha,\beta}$ with $f_+(k) \neq 0$ the *radial Green's function*

$$G(x,x';k) := e(x_<,k)w_+(x_>,k), \tag{4.4.7}$$

where for $x,x' > 0$, $x_< = \min\{x,x'\}$ and $x_> = \max\{x,x'\}$.

$G(x,x';k)$ is a fundamental solution of the radial Schrödinger equation (4.3.29). In the appropriate coordinate representation it coincides for $\Im k > 0$ with (4.3.27) and therefore with the resolvent kernel (B.12) of the (Z_+,μ)-dependent J-self-adjoint realization of the radial Schrödinger operator associated to the Sturm-Liouville equation (4.3.1) in $L^2(\mathbb{R}_+, \cosh^2(\xi)d\xi)$, described by Theorem B.15.

REMARK 4.25. *We now consider the spectral parameter μ appearing in Equation* (4.3.1) *as a perturbation of the operator K_ξ defined in* (4.1.2). *Consequently we will write*

$$K_\xi(Z_+,\mu) := K_\xi + \mu$$

for the perturbed operator.

REMARK 4.26. *Notice that eventual zeros of $f_+(k)$ for $k \in \mathbb{C}_+ \setminus \{0\}$ correspond to eigenvalues of the operator.*

In view of Theorem 4.20 and 4.22, $G(x,x';k)$ possesses a meromorphic continuation in k into the possibly two-sheeted domain $D_+(\alpha,\beta)$ defined by (4.3.41).

Finally we introduce the so-called *scattering matrix element*

$$s(k) = \frac{f_-(k)}{f_+(k)} \tag{4.4.8}$$

which in lieu of Corollary 4.24 is a meromorphic function of k in $D_+(\alpha,\beta) \cap D_-(\alpha,\beta)$.

LEMMA 4.27. *Let $x, x' > 0$ and $-\beta < \arg(k) < \alpha$.*

(1) *The radial Green's function and the radial generalized eigenfunctions satisfy the functional relation*

$$G(x,x';k) - G(x,x';-k) = 2ik\, e(x,k)e(x,-k). \tag{4.4.9}$$

(2) *The scattering matrix element satisfy the following relation*

$$s(-k) = s(k)^{-1}. \tag{4.4.10}$$

(3) *The scattering matrix elements and the radial generalized eigenfunctions satisfy the functional relation*

$$s(k)e(x,-k) = e(x,k). \tag{4.4.11}$$

PROOF. From (4.3.40) and (4.4.2) we have that

$$f_+(-k) = f_-(k) \tag{4.4.12}$$

for $k \in D_+(\alpha,\beta) \cap D_-(\alpha,\beta)$. Therefore, using (4.4.4) and the definitions of the radial Green's function and the radial generalized eigenfunctions the first part of the lemma is proved.

The second part and the third part follows as a direct application of (4.4.12) to the definition of the scattering matrix elements. □

A first consequence of Lemma 4.27 is that it is enough to discuss the scattering matrix elements in the angle $-\beta < \arg(k) < \alpha$.

With the above definitions we can discuss the notion of eigenvalues for the radial non-selfadjoint Schrödinger operator $K_\xi(Z_+,\mu)$ in $L^2(\mathbb{R}_+, \cosh^2(\xi)d\xi)$. We define

$$\begin{aligned}\mathscr{E}_{Z_+,\mu} := \Big\{ k \in \overline{\mathbb{C}}_+ \setminus \{0\} \mid f_+(k) = 0,& \\ e^{-\xi/2} e^{i\phi(\xi,k)} \in L^2(\mathbb{R}_+, \cosh^2(\xi)d\xi) \Big\}&.\end{aligned} \tag{4.4.13}$$

If $k \in \mathscr{E}$, we call k an *eigenvalue* of this *quadratic eigenvalue problem*. All other zeros of the Jost function $f_+(k)$ are called resonances of $K_\xi(Z_+,\mu)$ and we denote them by

$$\mathscr{R}_{Z_+,\mu} := \big\{ k \in D_+(\alpha,\beta) \setminus \mathscr{E} \mid f_+(k) = 0 \big\}. \tag{4.4.14}$$

REMARK 4.28. *The condition $e^{i\phi(\xi,k)} \in L^2(\mathbb{R}_+, \cosh^2(\xi)d\xi)$ is automatically fulfilled when $k \in \mathbb{C}_+ \setminus \{0\}$ and for it is independent of μ.*

REMARK 4.29. *There cannot be real positive* $k \in \mathscr{E}_{Z_+,\mu}$. *In fact, if there exists* $k \in \mathbb{R}_+$ *in* $\mathscr{E}_{Z_+,\mu}$, *then by Theorem 4.20 we would have* $v_+(x,k) \in L^2(\mathbb{R}_+, \cosh^2(\xi)d\xi)$ *but it is evident from the asymptotic behavior of* v_+ *that this is impossible. On the other hand, we cannot exclude a priori the presence of real* k *in* $\mathscr{R}_{Z_+,\mu}$.

REMARK 4.30. *Two Jost functions cannot vanish simultaneously in* $-\beta < \arg(k) < \alpha$, *otherwise* v_+ *and* v_- *(or* w_+ *and* w_-*) would be linearly dependent in contradiction with their asymptotic behavior. Therefore the points of* $\mathscr{E}_{Z_+,\mu} \cup \mathscr{R}$ *contained in* $-\beta < \arg(k) < \alpha$ *are in one to one correspondence with all the poles of the scattering matrix elements* $s(k)$.

In view of the definitions (4.4.6) *and* (4.4.7), *the set* $\mathscr{E}_{Z_+,\mu} \cup \mathscr{R}_{Z_+,\mu}$ *can be identified with the set of poles of the radial Green's function* $G(\xi,\xi';k)$ *and the poles of the generalized radial eigenfunctions* $e(x,k)$.

REMARK 4.31. *The set* $\mathscr{R}$ *of resonances does not depend on the choice of the phase function which determines the Jost functions* $f_\pm(k)$, *the generalized radial eigenfunctions and the scattering matrix elements.*

4.5. Formal "partial wave expansion" of the Green's function

For real E we know from the previous section that the spectrum of $K_\eta = K_\eta(h,E)$ consists of an infinite number of simple eigenvalues

$$\mu_1(E) < \mu_2(E) < \mu_3(E) < \dots$$

tending to infinity that extends to analytic functions of E in some neighborhood of the real line. We shall denote by $\varphi_{n,E}$ the eigenfunctions

$$K_\eta(E)\varphi_{n,E}(\eta) = \mu_n(E)\varphi_{n,E}(\eta), \quad n \in \mathbb{N}_0,$$

normalized by

$$||\varphi_{n,E}||^2 = \int_{-\pi}^{+\pi} |\varphi_{n,E}(\eta)|^2 \, d\eta = 1$$

for $E \in \mathbb{R}_+$ and then extended analytically. We choose $\varphi_{n,E}$ real for E real.

Define

$$K := F(\xi,\eta)\mathscr{H}_{\mathscr{C}}. \tag{4.5.1}$$

Instead of solving $(\mathscr{H}_{\mathscr{C}} - E)u = f$ in $L^2(M, F(\xi,\eta)d\xi\, d\eta)$ for $E \in \mathbb{C} \setminus \sigma(\mathscr{H}_{\mathscr{C}})$, we look at the solutions of

$$(K - F(\xi,\eta)E)u(\xi,\eta) = F(\xi,\eta)f(\xi,\eta). \tag{4.5.2}$$

We already know (see (4.1.2)) that

$$(K - F(\xi,\eta)E)u(\xi,\eta) = K_E u(\xi,\eta) = (K_\xi + K_\eta)u(\xi,\eta).$$

Now, using the completeness of the orthonormal base $\left\{\varphi_{n,E}\right\}_{n\in\mathbb{N}_0}$ for $E \in \mathbb{R}$, u possesses the expansion

$$u(\xi,\eta) = \sum_{n\in\mathbb{N}_0} u_n(\xi,\eta) \quad \text{with} \quad u_n(\xi,\eta) := \varphi_{n,E}(\eta)\psi_{n,E}(\xi), \tag{4.5.3}$$

where

$$\psi_{n,E}(\xi) = \int_{-\pi}^{+\pi} \varphi_{n,E}(\eta) u(\xi,\eta)\, d\eta.$$

This expansion extends to complex values of E by analyticity (note that no complex conjugate is involved, since $\varphi_{n,E}$ is chosen real for $E \in \mathbb{R}$).

Analogously we get

$$F(\xi,\eta) f(\xi,\eta) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}(\eta) g_{n,E}(\xi), \tag{4.5.4}$$

where

$$g_{n,E}(\xi) := \int_{-\pi}^{+\pi} \varphi_{n,E}(\eta)(Ff)(\xi,\eta)\, d\eta.$$

Substituting (4.5.3) and (4.5.4) into (4.5.2) one gets

$$\left[K_\xi + K_\eta\right] \sum_{n\in\mathbb{N}_0} u_n(\xi,\eta) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}(\eta) g_{n,E}(\xi)$$

or equivalently

$$\sum_{n\in\mathbb{N}_0} \varphi_{n,E}(\eta) \left(\left(K_\xi(E) + \mu_n(E) \right) \psi_{n,E}(\xi) - g_{n,E}(\xi) \right) = 0. \tag{4.5.5}$$

REMARK 4.32. *(4.5.5) extends to complex points $E \notin \sigma(H)$, where $K_\xi(E) + \mu_n(E)$ possesses an inverse $R_n(E)$ similarly as (B.13) by means of the Green's function defined in (4.4.7).*

By (4.5.5):

$$\begin{aligned} \psi_{n,E}(\xi) &= R_n(E) g_{n,E}(\xi) \\ &= \int_{\mathbb{R}_+} G_n(\xi,\tilde{\xi};E) \int_{-\pi}^{+\pi} \varphi_{n,E}(\tilde{\eta})(Ff)(\tilde{\xi},\tilde{\eta})\, d\tilde{\eta}\, d\tilde{\xi}. \end{aligned} \tag{4.5.6}$$

Combining (4.5.6) and (4.5.3) we obtain

$$u(\xi,\eta) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}(\eta) \iint_{M_0} G_n(\xi,\tilde{\xi};E) \varphi_{n,E}(\tilde{\eta})(Ff)(\tilde{\xi},\tilde{\eta})\, d\tilde{\xi}\, d\tilde{\eta}$$

and we read off the partial wave expansion for the Green function

$$G(\xi,\eta;\tilde{\xi},\tilde{\eta};E) = \sum_{n\in\mathbb{N}_0} \varphi_{n,E}(\eta)\varphi_{n,E}(\tilde{\eta}) G_n(\xi,\tilde{\xi};E)(\cosh^2\tilde{\xi} - \cos^2\tilde{\eta}). \tag{4.5.7}$$

It would be of great interest to be able to prove that the sum converges in the sense of distributions in the product space $D'(\mathscr{M}_0) \otimes D'(\mathscr{M}_0)$. Then we could use our results on the analytic continuation of the G_n and of the angular eigenfunctions to give a meromorphic continuation of the $G(\xi,\eta;\tilde{\xi},\tilde{\eta};E)$ in E to the second Riemann sheet (or $k \in \mathbb{C}_-$).

We believe that the lack of this proof is only a matter of time and cannot be included in the thesis just for the imminence of the bureaucratic deadlines.

Nevertheless, for each fixed $N \in \mathbb{N}$, we can consider the restriction K_N of the operator K to the subspace

$$\begin{aligned} \Upsilon_N(E) := & \bigoplus_{n=0}^{N} \Phi_n(E) \otimes L^2(\mathbb{R}_+, \cosh^2(\xi) d\xi) \\ & \subset L^2([-\pi,\pi], d\eta) \otimes L^2(\mathbb{R}_+, \cosh^2(\xi) d\xi) \end{aligned} \tag{4.5.8}$$

where $\Phi_n(E)$ is the subspace spanned by $\varphi_{n,E}$. The relative Green's function

$$G_N(\xi,\eta;\tilde{\xi},\tilde{\eta};E) = \sum_{n=0}^{N} \varphi_{n,E}(\eta)\varphi_{n,E}(\tilde{\eta}) G_n(\xi,\tilde{\xi};E)(\cosh^2\tilde{\xi} - \cos^2\tilde{\eta})$$

is the truncated sum obtained from (4.5.7) and as a finite sum of well defined term is convergent. Moreover it follows from the results of the previous sections that it possesses a meromorphic continuation in E to the second Riemann sheet.

4.6. Resonances for the 2-dimensional problem

The operator K_η defined by (4.2.4) has discrete spectrum $\mu_n(k^2)$ admitting an analytic continuation in $k^2 := E$ in some neighborhood of the real axis. At the same time for each μ, the resolvent of the operator $K_\xi(\mu, Z_+)$ (see Remark 4.32) can be extended in terms of k to the negative complex plane, having there a discrete set of poles $k_m(\mu)$.

With the definitions given in Section 4.4 we set

$$\begin{aligned} \mathscr{E}_n := \{ & k \in \overline{\mathbb{C}}_+ \setminus \{0\} \mid f_+(k, \mu_n(k^2)) = 0, \\ & e^{-\xi/2} e^{i\phi(\xi,k,\mu_n(k^2))} \in L^2(\mathbb{R}_+, \cosh^2(\xi) d\xi) \}. \end{aligned} \tag{4.6.1}$$

If $k \in \mathscr{E}_n$, we call k an *eigenvalue* of the quadratic eigenvalue problem for $K(Z_-, Z_+)$. All other zeros of the Jost function $f_+(k, \mu_n(k))$ are called *resonances* of $K(Z_-, Z_+)$ and we denote them by

$$\mathscr{R}_n := \left\{ k \in D_+(\alpha,\beta) \setminus \mathscr{E}_n \mid f_+(k, \mu_n(k^2)) = 0 \right\}. \tag{4.6.2}$$

Proposition 4.33. *The sets $\mathscr{E}_n$ and $\mathscr{R}_n$ are made by an at most countable number of elements $k_m \in D_+(\alpha,\beta)$ ($m \in I \subseteq \mathscr{N}$) of finite multiplicity such that $f_+(k_m, \mu_n(k_m)) = 0$.*

Proof. $f_+(k)$ and $\mu_n(k^2)$ being analytic functions of k, the statement is clear. □

Remark 4.34. *Notice that if k^2 is an eigenvalue of the full operator K (or its restriction K_N), then it must be an eigenvalue of $K_\xi(Z_+, \mu_n)$ for some $\mu_n(k^2)$ (i.e. an element of $\mathscr{E}_n$).*

Remark 4.35. *By definition it is obvious that $\mathscr{E}_n \cap \mathscr{R}_n = \emptyset$. Furthermore, it is clear looking at the asymptotic behavior of the solutions that it is impossible that $k \in \mathscr{E}_n$ and $k \in \mathscr{R}_{n'}$ for $n \neq n'$.*

Relying on the previous discussion and on Remark 4.29 we can switch from the k^2 plane to the k plane and and refer to

$$\mathscr{E}_N := \bigcup_{n=0}^{N} \mathscr{E}_n, \qquad \mathscr{R}_N := \bigcup_{n=0}^{N} \mathscr{R}_n \tag{4.6.3}$$

as the sets of *eigenvalues* and *resonances* of K_N. Moreover, in view of Remark 4.30, the points of $\mathscr{E}_N \cup \mathscr{R}_N$ contained in $D_+(\alpha,\beta)\cap D_-(\alpha,\beta)$ are in one-to-one correspondence with the poles of the scattering matrix elements $s_n(k) := s(k,\mu_n)$ and with the poles of the Green's functions $G_n(\xi,\tilde{\xi};k) := G(\xi,\tilde{\xi};k,\mu_n(k))$ for $n \in \{0,\dots,N\}$.

Remark 4.36. *If we suppose that* (4.5.7) *is convergent, we can refer to*

$$\mathscr{E} := \bigcup_{n=0}^{\infty} \mathscr{E}_n, \qquad \mathscr{R} := \bigcup_{n=0}^{\infty} \mathscr{R}_n \tag{4.6.4}$$

as the sets of eigenvalues *and* resonances *of K. As for the restricted operator, in view of Remark 4.30, the points of $\mathscr{E}\cup\mathscr{R}$ contained in $D_+(\alpha,\beta)\cap D_-(\alpha,\beta)$ are in one-to-one correspondence with the poles of the scattering matrix elements $s_n(k) := s(k,\mu_n)$ and with the poles of the Green's functions $G_n(\xi,\tilde{\xi};k) := G(\xi,\tilde{\xi};k,\mu_n(k))$.*

4.7. Computation of the resonances of K_ξ

Consider the equation

$$0 = K_\xi(h)\phi(\xi) = -h^2\partial_\xi^2\phi(\xi) - Z_+\cosh(\xi)\phi(\xi) - E\cosh^2(\xi)\phi(\xi) \tag{4.7.1}$$

with the condition $\phi'(0) = 0$. The potential

$$V(\xi;Z_+,E) := -Z_+\cosh(\xi) - E\cosh^2(\xi)$$

has Taylor expansion around $\xi = 0$ given by

$$\begin{aligned}
V(\xi;Z_+,E) &= -\frac{Z_+}{2}\left(e^\xi + e^{-\xi}\right) - \frac{E}{4}\left(e^\xi + e^{-\xi}\right)^2 \\
&= -\frac{Z_+}{2}\left(2+\xi^2+\mathscr{O}(\xi^4)\right) - \frac{E}{4}\left(2+2+(2\xi)^2+\mathscr{O}(\xi^4)\right)^2 \\
&= -Z_+ - E - \left(E + \frac{Z_+}{2}\right)\xi^2 + \mathscr{O}(\xi^4) \\
&= A - \omega^2\xi^2 + \mathscr{O}(\xi^4),
\end{aligned}$$

where $A := -Z_+ - E$ and $\omega = \sqrt{E + \frac{Z_+}{2}}$.

Let now $E + \frac{Z_+}{2} > 0$. We would like to apply the theory [BCD87a, BCD87b, BCD88] and [Sjö87] to get the resonances from the eigenvalues

$$e_n(h) = h(2n+1)\omega \qquad (n \in \mathbb{N})$$

of the harmonic oscillator

$$H_{osc} = -h^2\partial_\xi^2 + \omega^2\xi^2,$$

according to

$$A_n(h,E,Z_+) = -Z_+ - E - ih(2n+1)\omega + \mathcal{O}(h^{3/2}).$$

REMARK 4.37. *In the above discussion there is a major bug: in* [BCD87a, BCD87b, BCD88] *and* [Sjö87] *it is* essential *to assume that the potential is bounded, and this is clearly false in* (4.7.1).

The problem stressed by the previous remark can be solved. With the change of variable given by $y := \sinh(\xi) : \mathbb{R}_+ \to \mathbb{R}_+$ we change the measure from $\cosh^2(\xi)\, d\xi$ to $\sqrt{y^2+1}\, dy$ but at the same time the differential equation of $K_\xi(Z_+,\mu)$ takes the form

$$-h^2(y^2+1)\partial_y^2 u(y) - h^2 y\partial_y u(y) + (\mu - k^2(y^2+1) - Z_+\sqrt{y^2+1})u(y) = 0.$$

Note that μ will correspond to an eigenvalue of the angular equation K_η, and as such it will be an analytic function of E. Moreover it will be real for real values of E (see Section 4.2).

With the ansatz

$$u(y) := \frac{1}{\sqrt[4]{y^2+1}} v(y)$$

we can rewrite the differential equation in Liouville normal form as

$$\frac{y^2+1}{\sqrt[4]{y^2+1}}\left(-h^2\partial_y^2 v(y) + V(k,Z_+,\mu,h;y)v(y)\right) = 0 \tag{4.7.2}$$

where

$$V(k,Z_+,\mu,h;y) := -k^2 - \frac{Z_+}{\sqrt{y^2+1}} + \frac{\mu}{1+y^2} - \frac{y^2-2}{4(y^2+1)^2}h^2.$$

This potential V has the following properties:

- it is smooth in $\mathbb{R}_+$;
- it is bounded;
- it is analytic in a cone centered at the positive real axis;
- it has a non-degenerate global maximum at $y = 0$;
- around the maximum V can be expanded in Taylor series as

  $$V(k,Z_+,\mu,h;y) = A - \omega^2 y^2 + \mathcal{O}(y^4),$$

  where $A := -Z_+ - k^2 + \mu - \frac{h^2}{2}$ and $\omega = \sqrt{\mu + \frac{5}{4}h^2 - \frac{Z_+}{2}}$.

Therefore it satisfies the assumptions of [BCD87a, BCD87b, BCD88] and [Sjö87] and we can use their theories to approximate the resonances through the eigenvalues of the harmonic oscillator according to

$$A_n(h,E,Z_+,\mu) = -Z_+ - k^2 + \mu - ih(2n+1)\omega + \mathcal{O}(h^{3/2}). \tag{4.7.3}$$

This given, we have a zero of (4.7.2) if v is identically 0 or if $A_n=0$, this last condition permits us to identify with some approximation the resonances of our operator $K_\xi(Z_+,\mu)$.

From this first formula one can have a first approximation of the resonances $E_n=k_n^2$ in orders of $\Re(\mu)\gg 0$ as follows

$$\begin{cases} \Im E_n &= (2n+1)h\sqrt{\Re\mu}+\Im\mu+O\left((\Re\mu)^{-1/2}\right) \\ \Re E_n &= \sqrt{\Re\mu-Z_+ +O\left((\Re\mu)^{-1/2}\right)}. \end{cases} \tag{4.7.4}$$

REMARK 4.38. *The approximation (4.7.3) identifies the resonances generated by the top of the potential (at $\xi=0$) and these corresponds to the resonances generated by the classical closed hyperbolic trajectory bouncing between the two centers (see Remark 1.5).*

REMARK 4.39. *In Section 2.6 we have seen that for $Z_+<0$, $|Z_+|<Z_-$, there is for small energies a region of the phase-space characterized by closed orbits related to a local minimum of the potential. We expect in this case the appearance of some shape-resonances at exponentially small distance in h from the real axis (see* [**HS80**, **HCS84**] *and* [**HS96**, Chapter 20]*). We plan to study the existence and the distribution of these other resonances in a future work.*

4.8. Eigenvalues asymptotics and resonant regions for $Z_-=0$ near the bottom of the spectrum

As we did previously, before studying the general system, let us have a look to the simplest case $Z_-=0$. With a proper renaming of the constants and the notation of (4.2.2), in [**MS54**, Section 2.331] it is proved that

THEOREM 4.40. *For $\delta\to+\infty$ and $n\in\mathbb{N}$*

$$\begin{cases} a_n(\delta)=-2\delta+(4n+2)\sqrt{\delta}+\mathcal{O}(1), \\ b_{n+1}(\delta)=-2\delta+(4n+2)\sqrt{\delta}+\mathcal{O}(1). \end{cases}$$

Thus we have as a direct consequence the following theorem.

COROLLARY 4.41. *In the limit $h\searrow 0$ and for every $E>0$ we have*

$$\begin{cases} \mu_n^+(h,E,0)=(2n+1)\sqrt{E}\,h+\mathcal{O}(h^2), \\ \mu_{n+1}^-(h,E,0)=(2n+1)\sqrt{E}\,h+\mathcal{O}(h^2). \end{cases}$$

We can use this result in combination with (4.7.3). We obtain the equation for the resonance energies by setting

$$-A_n(h,E,Z_+,\mu_m^+(h,E,0))=0.$$

Neglecting the error terms and writing $E=k^2$ we have

$$k^2+Z_+-(2n+1)kh+ih(2m+1)\sqrt{(2n+1)kh+\frac{5h^2}{4}-\frac{Z_+}{2}}=0. \tag{4.8.1}$$

4.9. Eigenvalues asymptotics and resonant regions for $Z_- > 0$ near the bottom of the spectrum

Notice that we can always define Z_- in such a way that it is non-negative. In presence of the Z_- term the equation $K_\eta \psi(\eta) = 0$ assumes the form

$$0 = -h^2 \partial_\eta^2 \psi(\eta) + \left(-\mu + Z_- \cos(\eta) + E \cos^2(\eta)\right) \psi(\eta), \tag{4.9.1}$$

with periodic boundary conditions on $[-\pi, \pi]$.

REMARK 4.42. *We can use Corollary 4.41 and the Min-Max principle to compare the eigenvalues obtained for the $Z_- = 0$ case with this more general one, but this is far from giving an accurate estimate.*

LEMMA 4.43. *In the limit $h \searrow 0$ and for $E > 0$ we have*

$$-Z_- + (2n+1)\sqrt{E}\, h + \mathcal{O}(h^2) \leq \mu_n(h, E, Z_-) \leq Z_- + (2n+1)\sqrt{E}\, h + \mathcal{O}(h^2).$$

PROOF. It follows immediately after rewriting $K_\eta \psi(\eta) = 0$ in the Mathieu-like form:

$$0 = -\partial_\eta^2 \psi(\eta) - \frac{2\mu - E}{2h^2} \psi(\eta) + 2\frac{E}{4h^2} \cos(2\eta)\psi(\eta) + \frac{Z_-}{h^2} \cos(\eta)\psi(\eta).$$

$\square$

To obtain better estimates for the spectrum in orders of small h we use the ϵ-quasimodes [AK99, Laz93]. If A is a self-adjoint operator on $D(A)$ in a Hilbert space $\mathcal{H}$, then for $\epsilon > 0$ one can call a pair

$$\left(\widetilde{\psi}, \widetilde{E}\right) \in D(A) \times \mathbb{R},\ ||\widetilde{\psi}|| = 1,\ ||(E - \widetilde{E})\widetilde{\psi}|| \leq \epsilon$$

an *ϵ-quasimode*. Note that with this notation an eigenfunction ψ with eigenvalue E is a 0-quasimode.

The existence of an ϵ-quasimode $\left(\widetilde{\psi}, \widetilde{E}\right)$ implies that the distance between $\widetilde{E}$ and the spectrum of A fulfils

$$\operatorname{dist}\left(\sigma(A), \widetilde{E}\right) \leq \epsilon. \tag{4.9.2}$$

In particular there exist an eigenvalue E of A in the interval $[\widetilde{E} - \varepsilon, \widetilde{E} + \varepsilon]$ for $\varepsilon \leq \epsilon$, if in that interval we know that the spectrum is discrete.

In our case we want to replace A with an operator of the form

$$P_h := -h^2 \frac{d^2}{dx^2} + V(x) \tag{4.9.3}$$

on an interval $[-a, b] \subseteq \mathbb{R}$ $(a, b > 0)$ and with $V(x) := \frac{x^2}{4} + W(x)$ and $W(x) := \sum_{m=m_0}^{\infty} a_m x^m$ $(m_0 > 2)$ entire of order 1 and finite type.

REMARK 4.44. *The assumptions on V imply that it has a global non-degenerate minimum in 0.*

It is a well known fact that for $W = 0$

$$P_1 D_n^1 = E_n^1 D_n^1$$

with $E_n^1 := n + \frac{1}{2}$ and D_n^1 the normalized Hermite Polynomials

$$D_n^1(x) := \frac{(-1)^n}{n!\sqrt{2\pi}}\, e^{\frac{x^2}{4}} \frac{d^n}{dx^n} e^{-\frac{x^2}{2}}, \qquad n \in \mathbb{N}. \tag{4.9.4}$$

It is equally well known that

$$P_h D_n^h = E_n^h D_n^h \tag{4.9.5}$$

with $E_n^h := h E_n^1$ and $D_n^h := h^{-\frac{1}{4}} D_n^1\left(h^{-\frac{1}{2}} x\right)$.

LEMMA 4.45. *(D_n^h, E_n^h) are $O(h^{m_0/2})$-quasimodes for P_h.*

PROOF. By assumption $V(x) = \frac{x^2}{4} + W(x)$. We need to prove that

$$\|W \cdot D_n^h\| = O\left(h^{\frac{m_0}{2}}\right).$$

Before entering in the details of the computation we want to remark that the space of entire functions of order 1 and of finite type forms an algebra and that we can always write D_n^1 as $P_n(x) e^{-\frac{x^2}{2}}$ for an appropriate polynomial $P_n(x)$ of degree n.

$$\begin{aligned}
\|W \cdot D_n^h\|^2 &= \int_{-a}^{b} \left(W(x)\, h^{-\frac{1}{4}} P_n\left(h^{-\frac{1}{2}} x\right) e^{-\frac{x^2}{2h}}\right)^2 dx \\
&\le 2h^{-\frac{1}{2}} \int_0^\infty W^2(x)\, P_n^2\left(h^{-\frac{1}{2}} x\right) e^{-\frac{x^2}{h}}\, dx \\
&\le \underbrace{2 \int_0^\infty W^2\left(h^{\frac{1}{2}} y\right) P_n^2(y) e^{-y^2}\, dy}_{=: I_h}.
\end{aligned}$$

We can rewrite $W^2(x) = \sum_{m=2m_0}^{\infty} b_m x^m$ with the appropriate b_m. W^2 being and entire function, we can bound the coefficients b_m using the following lemma [Lev96, Lemma 1, p. 5]:

LEMMA 4.46. *If $f(z) = \sum_{m=0}^{\infty} c_m z^m$ is an entire function and for r big enough*

$$\max_{|z|=r} f(z) < e^{A r^K}$$

is fulfilled, then for m big enough

$$|c_m| < \left(\frac{eAK}{m}\right)^{\frac{m}{K}}.$$

In particular, for an entire function of order 1 and finite type σ, one has $K = 1$ and $A = \sigma$, and the inequality reads: For all $m > M$

$$|c_m| < \left(\frac{\sigma e}{m}\right)^m \tag{4.9.6}$$

Moreover, for each $k \in \mathbb{N}$ one has

$$2\int_0^\infty y^k e^{-y^2} dy = \Gamma\left(\frac{k+1}{2}\right),$$

and thus

$$\begin{aligned} I_h &= \lim_{M\to\infty} 2\int_0^\infty \left(\sum_{m=m_0}^{M} h^m b_m y^m\right) P_n^2(y) e^{-y^2} dy \\ &= \lim_{M\to\infty} 2\sum_{m=m_0}^{M} h^m b_m \left(\int_0^\infty C\left(y^{m+2n} + O\left(y^{m+2n-1}\right)\right) e^{-y^2} dy\right) \\ &= \lim_{M\to\infty} 2\sum_{m=m_0}^{M} h^m b_m \left(C\,\Gamma\left(\frac{m+2n+1}{2}\right) + O\left(\Gamma\left(\frac{m+2n}{2}\right)\right)\right) \end{aligned}$$

For $m > M$ we can apply (4.9.6) and Stirling formula

$$\Gamma(n) = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n e^{\frac{\delta}{12n}}, \quad 0 < \delta < 1,$$

to obtain for $m > M_1 \geq M$

$$\begin{aligned} |C\, b_m|\Gamma\left(\frac{m+2n+1}{2}\right) &< |C|\left(\frac{\sigma e}{m}\right)^m \Gamma\left(\frac{m+2n+1}{2}\right) \\ &= \sqrt{2\pi}\,|C|\left(\frac{\sigma e}{m}\right)^m \left(\frac{\frac{m+1}{2}+n}{e}\right)^m e^{\frac{\delta}{6(m+2n+1)}} \\ &= C_1\sigma^m \left(\frac{1}{2} + \frac{2n+1}{2m}\right)^{\frac{m}{2}} \left(\frac{e}{m}\right)^{\frac{m}{2}-(n+1)} e^{\frac{\delta}{6(m+2n+1)}} \\ &= C_1\sigma^m \gamma_1^{\frac{m}{2}} \gamma_2^{\frac{m}{2}-(n+1)} e^{\frac{\delta}{6(m+2n+1)}} \underset{m\to\infty}{\longrightarrow} 0. \end{aligned}$$

Thus in particular the sum converges absolutely and we have

$$I_h = h^{m_0} \sum_{m=m_0}^{\infty} b_m h^{m-m_0}\left(C_2\,\Gamma\left(\frac{m+2n+1}{2}\right)\right) = h^{m_0} C_3,$$

and consequently

$$||W \cdot D_n^h|| = O\left(h^{\frac{m_0}{2}}\right). \tag{4.9.7}$$

□

Sadly our potential has in general two non-degenerate minima at the points

$$\pm\eta_* := \pm\arccos\left(-\frac{Z_-}{2E}\right) \in [-\pi/2, \pi/2]$$

where the potential reaches the value $-\frac{Z_-^2}{4E}$, thus we cannot directly apply the previous strategy as is (see Figure 4.1). Pushed by the intuition that the eigenvalues will be moved toward $\min V$ for h becoming small, we construct our quasimodes to be concentrated near one of the minima. Let the intervals Δ_o^+ and Δ_i^+ be two open neighborhoods of the rightmost minima such that $\overline{\Delta_i^+} \subset \Delta_o^+$ and Δ_o^+ is contained in

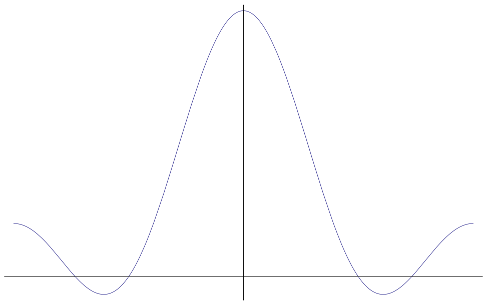


FIGURE 4.1. Shape of $Z_- \cos(\eta) + E\cos^2(\eta)$ in $[-\pi, \pi]$.

the positive axis and is strictly separated from 0. Fix $\chi_+ \in C_0^\infty(\mathbb{R})$ such that $\chi_+ = 1$ in Δ_i^+ and $\chi_+ = 0$ in $\mathbb{R} \setminus \Delta_o^+$.

LEMMA 4.47. *Let P_h be as in (4.9.3) but with $V(x) := \frac{(x-x_*)^2}{4} + W(x)$ and $W(x) := \sum_{m=m_0}^\infty a_m (x - x_*)^m$ $(m_0 > 2)$ entire of order 1 and finite type. Define*

$$\psi_n^h(x) := h^{-\frac{1}{4}} D_n \left(h^{-\frac{1}{2}}(x - x_*)\right) \chi_+(x) = D_n^h(x - x_*)\chi_+(x),$$

where χ_+ is the characteristic function defined in the previous paragraph. Then $(\psi_n^h(x), E_n^h)$ is an $O\left(h^{3/2}\right)$-quasimode for P_h.

PROOF. Applying the operator to ψ_n^h we have

$$\begin{aligned}
P_h \psi_n^h &= -h^2 \psi_n^{h\,\prime\prime} + \frac{(x - x_*)^2}{4} \psi_n^h + W\, \psi_n^h \\
&= \left(-h^2 D_n^{h\,\prime\prime} + \frac{(x - x_*)^2}{4} D_n^h + W\, D_n^h\right) \chi_+ \\
&\quad - h^2 \left(2h^{-\frac{1}{2}} D_n^{h\,\prime} \chi_+' + D_n^h \chi''\right) \\
&\overset{(4.9.3)}{=} E_n^h \psi_n^h + W\, \psi_n^h - h^2 \left(2h^{-\frac{1}{2}} D_n^{h\,\prime} \chi_+' + D_n^h \chi''\right).
\end{aligned}$$

For what concerns $W\, \psi_n^h$ we are in the situation of Lemma 4.45, thus we can use equation (4.9.7) as bound to obtain

$$||W \cdot \psi_n^h|| = O\left(h^{\frac{m_0}{2}}\right).$$

We need now to take care of the last error term. For this last term the inequality

$$\left|h^2 \left(2h^{-\frac{1}{2}} D_n^{h\,\prime} \chi_+' + D_n^h \chi''\right)\right| \leq h c_1 e^{-\frac{c_2}{h}}$$

holds with proper $c_1, c_2 > 0$ (that depend only on n and χ_+). Thus this term integrated on $[a, b]$ will give an error that can be bounded with any polynomial order of decay, in particular we can choose it to be

$$\left\|h^2 \left(2h^{-\frac{1}{2}} D_n^{h\,\prime} \chi_+' + D_n^h \chi''\right)\right\| = O\left(h^{\frac{m_0}{2}}\right).$$

$\square$

We need now to transform our equation into something like $V(x)$ in the previous theorem. We already know the two minima $\pm\eta_*$. If we expand $V(\eta) := Z_-\cos(\eta) + E\cos^2(\eta)$ in the neighborhood of those minima we obtain

$$V(x) = -\frac{Z_-^2}{4E} + E\left(1 - \frac{Z_-^2}{4E^2}\right)(\eta \pm \eta_*)^2 + W(\eta \pm \eta_*) \tag{4.9.8}$$

for a suitable entire W with $m_0 = 3$ and of order 1 and finite type.

To simplify a bit the notation let us call

$$A := -\frac{Z_-^2}{4E}, \qquad B := \sqrt{E\left(1 - \frac{Z_-^2}{4E^2}\right)}.$$

We focus for the moment only the localization near the rightmost minima, i.e. we choose $(\eta - \eta_*)$. With the unitary transformation $\mathscr{X}$ defined by change of variable

$$z(\eta) := \sqrt{2B}(\eta - \eta_*),$$

the eigenvalue equation (4.9.1) is transformed into

$$0 = K_z\psi(z) := 2B\left(-h^2\partial_\eta^2\psi(z) + \left(\widetilde{\mu} + \frac{z^2}{4} + \widetilde{W}(z)\right)\psi(z)\right), \tag{4.9.9}$$

where

$$\widetilde{\mu} = \frac{1}{2B}(-\mu + A)$$

and $\widetilde{W}$ is entire with $m_0 = 3$ and of order 1 and finite type. If in the spirit of the previous lemmas we define

$$\widetilde{\psi}_n^h(z) := D_n^h(z)\chi(z), \qquad \widetilde{\mu}_n^h := A + 2B\left(n + \frac{1}{2}\right)h,$$

where $\chi(z)$ is the transformed of the cut-off localized in the neighborhood of η_*, then the couple $(\widetilde{\psi}_n^h, \widetilde{\mu}_n^h)$ is an $O(h^{3/2})$-quasimode for K_z and thus if

$$\psi_n^h(\eta) := \left(\mathscr{X}^{-1}\widetilde{\psi}_n^h\mathscr{X}\right)(\eta),$$

the couple $(\psi_{n\pm}^h, \widetilde{\mu}_n^h)$ defines an $O(h^{3/2})$-quasimode for K_η.

Exactly the same happens if we look near the other minimum, i.e. if we choose the case $(\eta + \eta_*)$. In other words in the limit of $h \searrow 0$ the spectrum of K_η consists of pairs $\mu_n^-(h)$, $\mu_n^+(h)$ with the same asymptotics $\widetilde{\mu}_n^h$ in the limit.

We have proved the following.

THEOREM 4.48. *Let $E > \frac{Z_-}{2} > 0$. Define*

$$\widetilde{\mu}_n^h := -\frac{Z_-^2}{4E} + \sqrt{E\left(1 - \frac{Z_-^2}{4E^2}\right)}(2n+1)h. \tag{4.9.10}$$

There exists an eigenvalue μ_n^h of K_η and a constant c such that

$$\left|\widetilde{\mu}_n^h - \mu_n^h\right| = ch^{3/2}.$$

Moreover, the interval $\left[\widetilde{\mu}^h_n - 2ch^{3/2}, \widetilde{\mu}^h_n + 2ch^{3/2}\right]$ *contains at least two eigenvalues of* K_η.

REMARK 4.49. *It can be proved by standard methods involving the IMS formula* [**CFKS87**, Chapter 3.1] *and Agmon estimates* [**Agm82**] *that the distance between the eigenvalues in each pair is of the order* $\exp(-C/h)$ *with* $C \in \mathbb{R}_+$.

We can use this result in combination with (4.7.3). Neglecting the error terms, we obtain the equation for the resonance energies by setting

$$A_n(h,E,Z_+,\mu^+_m(h,E)) = 0. \tag{4.9.11}$$

They are given by the solutions of

$$\begin{aligned} -E - Z_+ - \frac{Z_-^2}{4E} + \sqrt{E - \frac{Z_-^2}{4E}}(2m+1)h \\ + ih(2n+1)\sqrt{\sqrt{E - \frac{Z_-^2}{4E}}(2m+1)h - \frac{Z_-^2}{4E} - \frac{Z_+}{2}} = 0. \end{aligned} \tag{4.9.12}$$

REMARK 4.50. *For* $Z_- = 0$ *we recover* (4.8.1) *of the previous section. In Section* (4.8) *on the other hand the approximation error is of order* $O(h^2)$ *instead of* $O(h^{3/2})$.

For $0 < E < \frac{Z_-}{2}$ the bottom of the potential is reached at π and thus we expand the potential around this other point. It turns out that in this case the eigenvalues are approximated by

$$\widehat{\mu}^h_n := E - Z_- + \sqrt{\frac{Z_-}{2} - E}\,(2n+1)h. \tag{4.9.13}$$

And the resonances in this range can be computed accordingly from the equation $A_n(h,E,Z_+,\widehat{\mu}^+_m(h,E)) = 0$.

REMARK 4.51. *This approach gives good results if we stay localized near the bottom of the potential: in this case we can find an approximation for the eigenvalue up to an order of any integer power of* h.

The deficiency of this approach lies in the fact that we have no control on the relative error between n *and* h. *We need therefore to find a different approximation scheme that keeps track of the mutual relation between the parameters.*

4.10. High energy estimates

We consider the potential in the form $V(x) = E\cos^2(x) + Z_-\cos(x)$. Substituting this value in the formulae given in Theorem D.4 we have

$$\int_{-\pi}^{\pi} V(x)dx = E\pi \quad \text{and} \quad \int_{-\pi}^{\pi} V^2(x)dx = \frac{3E^2\pi}{4} + \pi Z_-^2$$

and thus the eigenvalues μ_{2m+1} and μ_{2m+2} can be represented as

$$\begin{aligned}\sqrt{\mu} = {} & (m+1)h + \frac{E}{4(m+1)h} + \left(Z_-^2 - \frac{E^2}{4}\right)\frac{1}{16(m+1)^3h^3} \\ & + O\left(\frac{1}{m^5h^5}\right) + o\left(\frac{1}{m^3h}\right).\end{aligned} \tag{4.10.1}$$

Therefore we can estimate μ_{2m+1} and μ_{2m+2} with

$$\begin{aligned}\mu = {} & (m+1)^2h^2 + \frac{E}{2} + \left(Z_-^2 + \frac{E^2}{4}\right)\frac{1}{8(m+1)^2h^2} \\ & + O\left(\frac{1}{m^4h^4}\right) + o\left(\frac{1}{m^2}\right).\end{aligned} \tag{4.10.2}$$

We can thus approximate the resonances $E_{n,2m+1}$ and $E_{n,2m+2}$ solving

$$A_n(h, E, Z_+, \mu_{2m+1}(h,E)) = 0. \tag{4.10.3}$$

More explicitly, for fixed n and up to errors of orders

$$h^{\frac{3}{2}}, \qquad (mh)^{-4} \quad \text{and} \quad m^{-2},$$

we get the expression

$$\begin{aligned}& -\frac{E}{2} - Z_+ + (m+1)^2h^2 + \frac{Z_-^2 + \frac{E^2}{4}}{8(m+1)^2h^2} \\ & \qquad + i(2n+1)h\sqrt{(m+1)^2h^2 + \frac{E - Z_+}{2} + \frac{Z_-^2 + \frac{E^2}{4}}{8(m+1)^2h^2}} = 0.\end{aligned}$$

Remark 4.52. *We cannot hide the term $(m+1)^2h^2$ in the error term of order $h^{3/2}$ because we want to analyze the asymptotic behavior for $m \geq C/h$ ($C \in \mathbb{R}_+$) and that term is rather big compared with h.*

4.11. Numerical investigations

In the previous sections we have explicitly written three implicit equations to approximate the value of the resonances in terms of the atomic numbers n and m (and of course of the parameters h, Z_+ and Z_-).

Modern symbolic algebra software like Mathematica, Maple and SAGE are often able to find explicit solutions of implicit equations. These are generally incredibly long and complex but easily computable and plottable. In this section we want to investigate the qualitative structure of the resonances using the approximations given by (4.9.11) and (4.10.3).

In view of Remark 4.38 and Remark 4.39 we know that at least for certain values of the charges Z_i we are not describing all the resonances of the system, on the other hand the additional resonances should appear only for small $\Re(E)$. Therefore we want to consider $\Re(E)$ big enough to be sure that we are considering an energy region in which all the resonances are generated by the classical closed hyperbolic trajectory between the centers.

In this case equation (4.7.4) implies that $\Re(\mu_m)$ must be big and thus it is evident from (4.9.10), (4.9.13) and (4.10.2) that m must be big. The quasi-mode approximation obtained in Section 4.8 and 4.9 are valid only for small values of m and $\hbar$, therefore they are automatically excluded from the analysis.

In some sense we are lucky because it was not possible to solve Equation (4.9.11) (algebraically or numerically) for small $\hbar$, arbitrary Z_+ and $Z_- \neq 0$.

In Figure 4.2(a) and 4.2(b) we plotted all the approximated resonances obtained from (4.9.11) setting $Z_- = 0$. We plotted all the values including the one in not allowed regions of energies or where we have no control on the error. In these picture we can see a particularly interesting behavior. In particular for big values of m we recover the structure shown by the resonances approximated with (4.10.3): see Figure 4.3(a) and Figure 4.3(b).

The physically interesting resonances are the one nearer to the real axis, this because they can be measured in experiments. Thus to keep $\Im(E)$ as small as possible we will consider small values of n (see (4.7.4)).

REMARK 4.53. *Unless differently specified, in the plots we consider* $n = 0,1,2,3$ *and* $m \in \{\lceil C/\hbar \rceil + k \mid k = 0,1,2,\ldots,20\}$. *The values of* Z_+, Z_-, $\hbar$ *and* C *will be specified in the title or in the caption of the plots. For practical reasons we will plot the resonances in the plane* $(\Re(E), -\Im(E))$.

The software used for the simulations is Wolfram Mathematica 8.

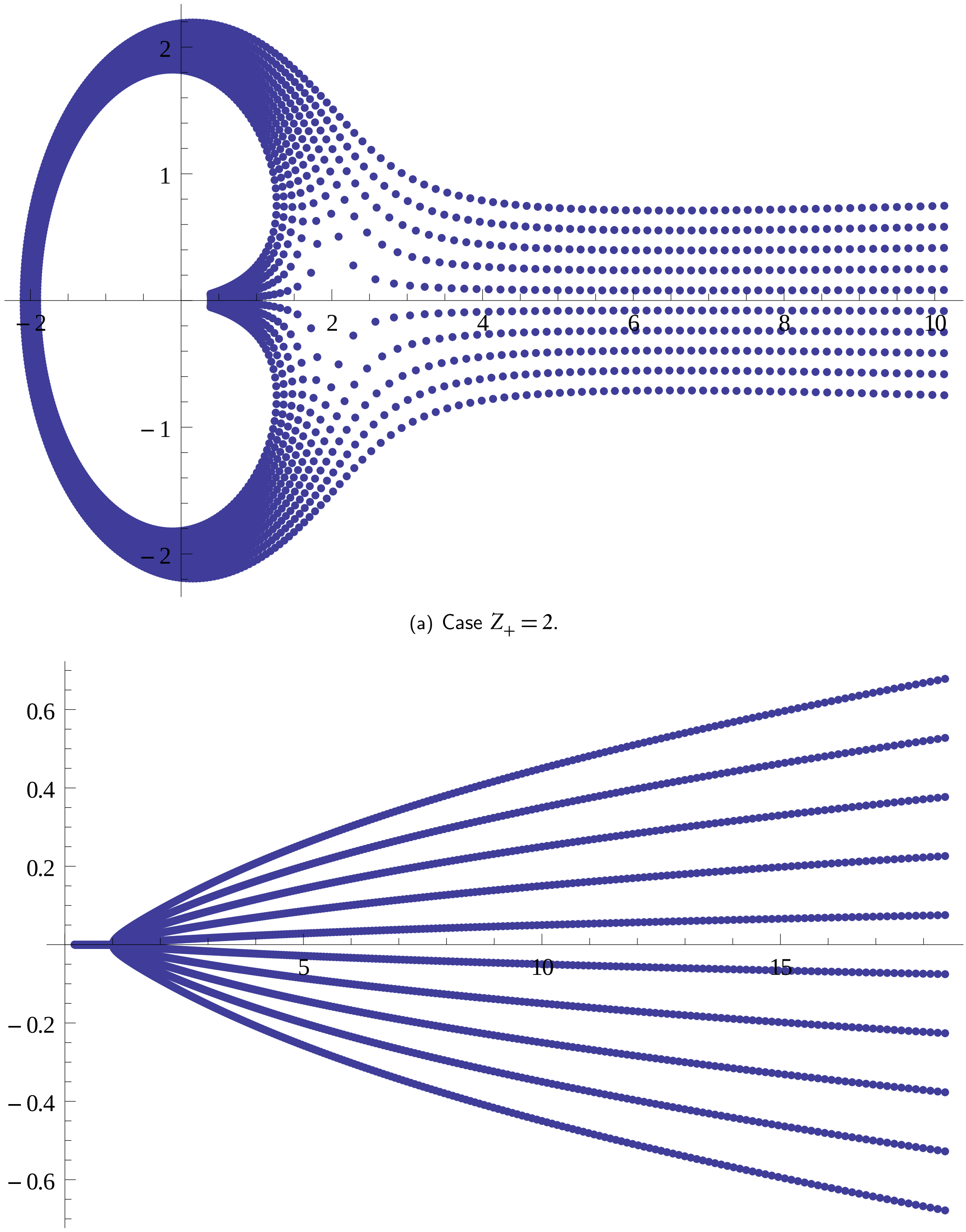
Equation (4.10.3) has two couples of solutions (S_+, L_+) and (S_-, L_-), specular w.r.t. the real axis. They correspond respectively to the resonances and the anti-resonances, i.e. the resonances defined inverting the roles of the incoming and outgoing waves $v_\pm$ in the construction of Section 4.4.

We restrict our analysis to the resonances (S_+, L_+). The two sets $S_+, L_+ \in \mathbb{C}_-$ characterize two different energy regions, this meaning that the resonances in S_+ have relatively small real part if compared to the resonances in L_+ (see Figure 4.3(a) and Figure 4.3(b)).

The structure that we find is extremely regular and the first question that arises is if we are really computing the resonances associated with energy values on the critical line $\mathscr{L}^2_+$ discussed in Section 2.3.

For each computed resonance $E_{n,m}$ we can use the approximation obtained in (4.10.2) to estimate the associated constant of motion $K_{n,m}$. We can thus superimpose the points $(\Re(E), \Re(K))$ to the bifurcation diagram and visualize how they are related. As shown in Figure 4.4, the energy parameters appear to lay exactly upon $\mathscr{L}^2_+$, giving a strong hint on the correctness of the result.

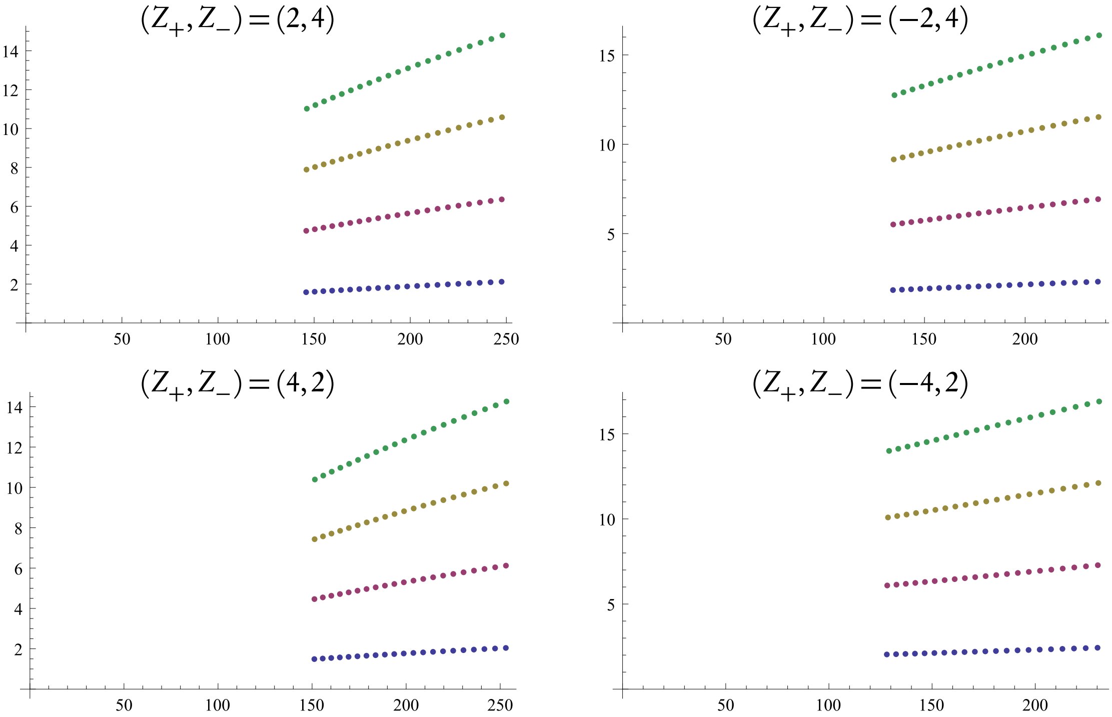
Another reasonable question at this point regards the order of growth of the resonances in n and m. For a system that is classically hyperbolic we can borrow an ansatz from physics. In scattering physics the study of quantum resonances is generally performed with the Gutzwiller trace formula. One of the standard results is that the imaginary part of the energy is proportional to the sum of the Lyapunov exponents of the closed hyperbolic trajectories [GAB95]. It is well known that the Lyapunov exponent of the bounded orbits of a Coulombic two-centers system diverges



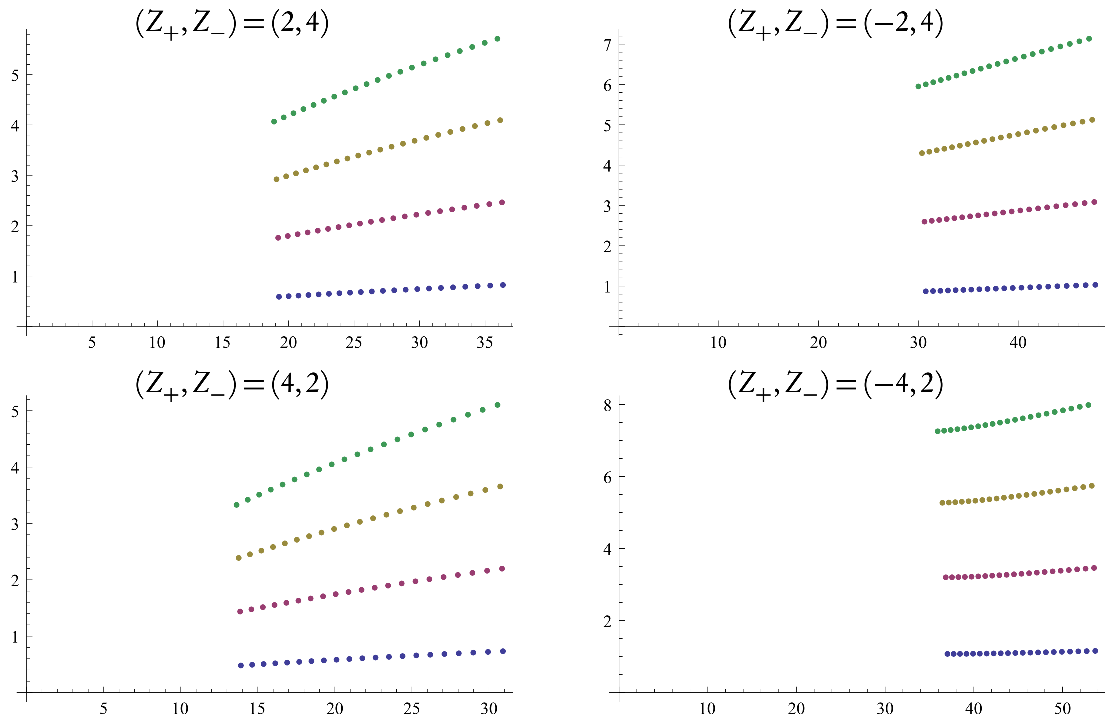
(a) Case $Z_+ = 2$.

(b) Case $Z_+ = -2$.

FIGURE 4.2. Solutions of (4.9.11) with $Z_- = 0$, $h = 0.01$, $n = 0, \ldots, 4$, $m = 1, \ldots, 250$.



(a) Resonances in L_+.



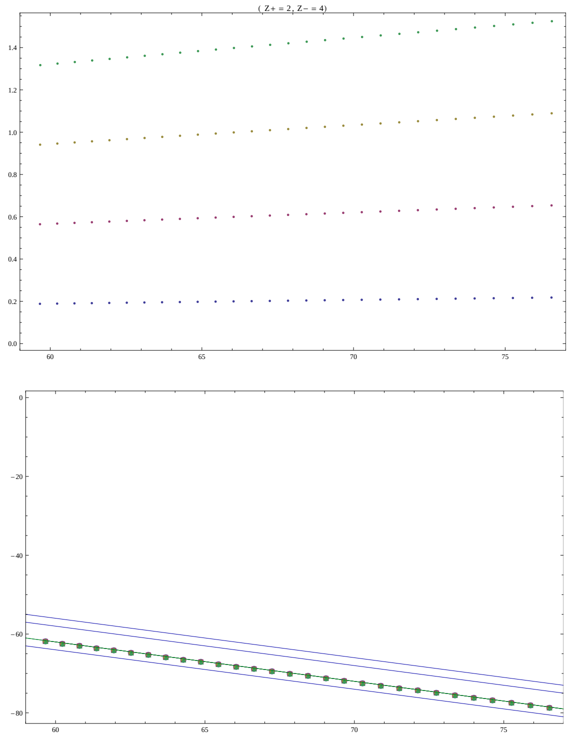
(b) Resonances in S_+.

FIGURE 4.3. Resonances for $h = 0.05$ and $C = 10$.

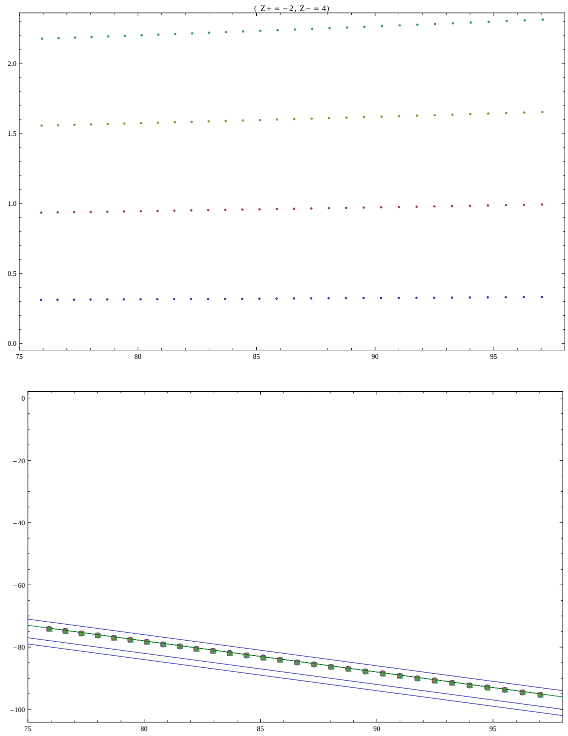
like $\ell(E) = \sqrt{E}\ln(E)$ (see [KK92, Proposition 5.6]). In this sense it is reasonable to normalize the real and imaginary part of the resonances in L_+ (or S_+) dividing them by $\ell(\Re(E))$. In this way it is possible to investigate, at least qualitatively the formally expected behavior.

The numerics confirms the expected behavior. It is evident from Figure 4.5(a) and 4.5(b) that the renormalized resonances look like distributed on a regular lattice of points with (almost perfectly) aligned and equispaced real and imaginary parts.

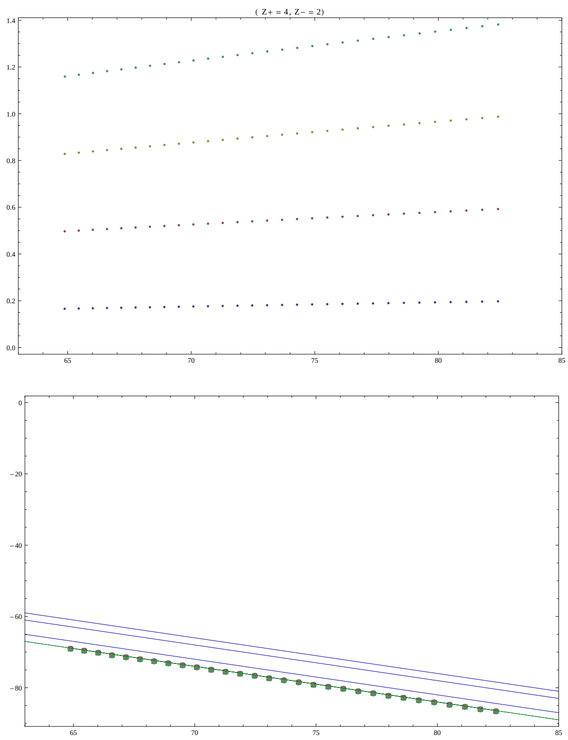
Notice moreover that the vertical spacing of the imaginary parts is $d = O(h)$ and the distance between the real axis and the resonances with smaller imaginary part is approximately $d/2$, as expected from the harmonic oscillator perturbation used to approximate the resonances.



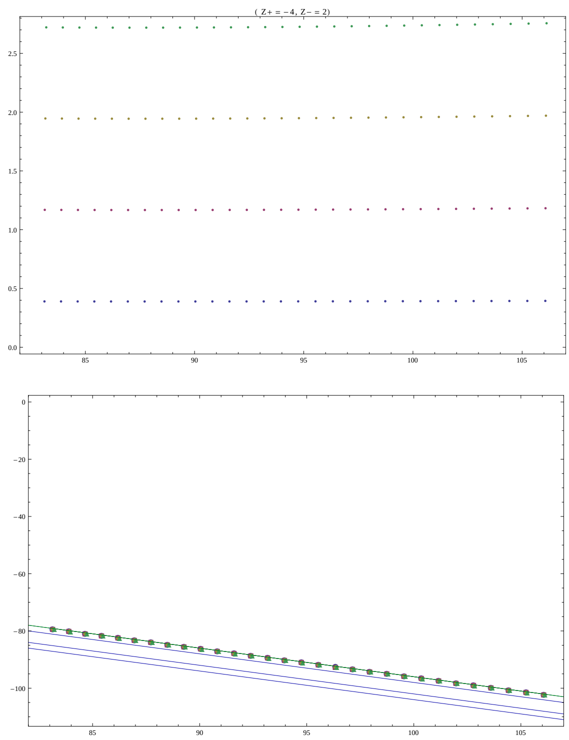
(a) $(Z_+, Z_-) = (2, 4)$, $C = 4$, $m = 400, \ldots, 430$.



(b) $(Z_+, Z_-) = (-2, 4)$, $C = 7$, $m = 700, \ldots, 730$.

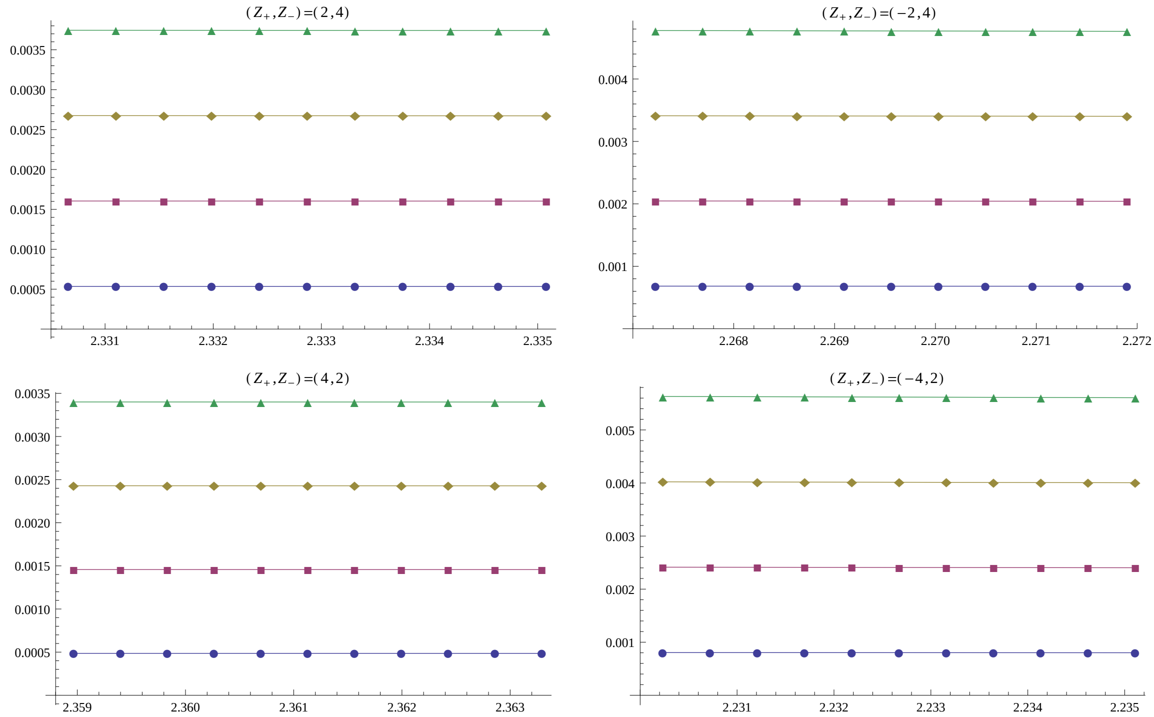


(c) $(Z_+, Z_-) = (4, 2)$, $C = 4$, $m = 400, \ldots, 430$.

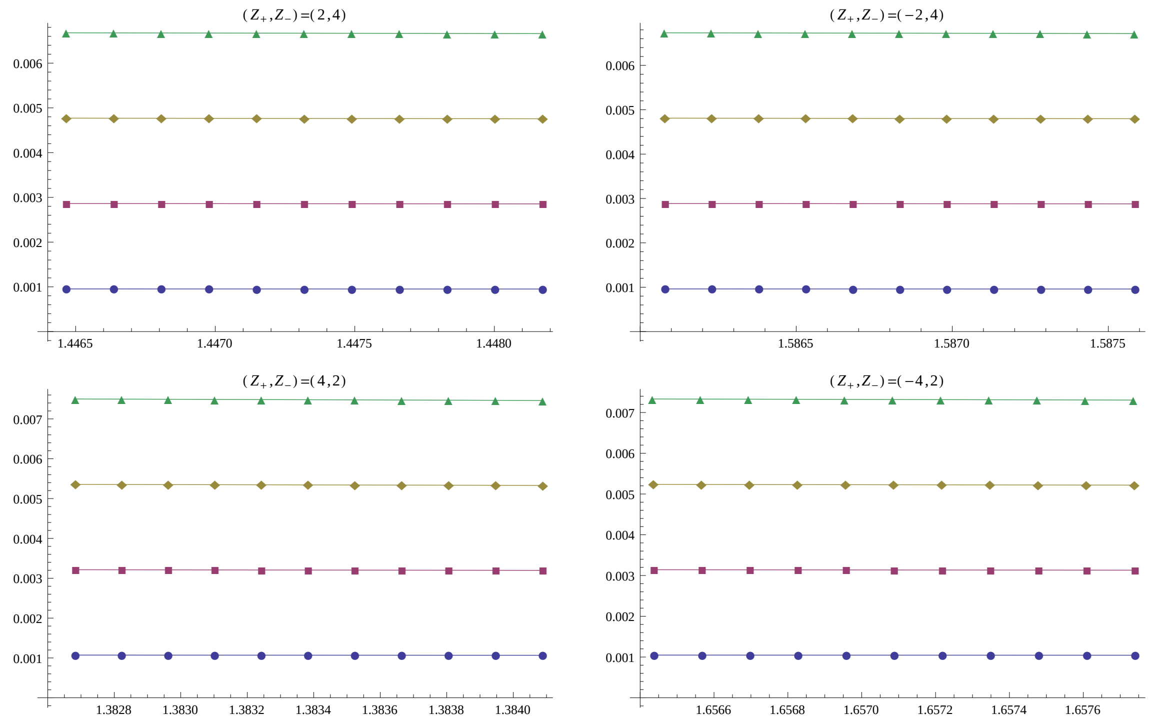


(d) $(Z_+, Z_-) = (-4, 2)$, $C = 7$, $m = 700, \ldots, 730$.

FIGURE 4.4. Comparison of the resonances in L_+ for $h = 0.001$ (plot above) and their projection on the bifurcation diagram (plot below).



(a) Plot for for $E \in L_+$.



(b) Plot for $E \in S_+$.

FIGURE 4.5. Renormalized resonances $E/\ell(\Re(E))$ with parameters $h = 0.001$, $C = 9$ and $m = 9000, \ldots, 9010$.

CHAPTER 5

Back to the three dimensional problem

5.1. Asymptotic analysis of the solutions of $\mathscr{A}_l^\lambda$

In view of the results of the preceding chapter, we rewrite the radial equation (3.6.1) of the three dimensional problem in normal form. For the moment we don't worry about the domains of definition of the operator. With the definition

$$u(\xi) := \frac{1}{\sqrt{\sinh(\xi)}} v(\xi), \tag{5.1.1}$$

the differential equation $\mathscr{A}_l^\lambda u = 0$ takes the following form

$$-h^2 v''(\xi) + \left(\mu + \frac{h^2}{4} + \frac{h^2\lambda^2}{\sinh^2(\xi)} - k^2\cosh^2(\xi) - Z_+\cosh(\xi)\right) v(\xi) = 0. \tag{5.1.2}$$

Clearly, for $\lambda = 0$ equation (5.1.2) has the same form of (4.3.1) and all the asymptotic results of Section 4.3 can be applied. The radial incoming and outgoing waves of (3.6.1) can be thus defined for $k \in \mathbb{C}_\pm$ by

$$u_\pm(\xi,k) := \frac{1}{\sqrt{\sinh(\xi)}} v_\pm(\xi,k) \tag{5.1.3}$$

where $v_\pm(\xi,k)$ is given by Theorem 4.11 with properly redefined constants. For $u_\pm(\xi,k)$ we have up to a constant factor the asymptotic expansion

$$u_\pm(\xi,k) = e^{-\xi} e^{\pm i\phi(\xi,k/h)}(1+o(1)) \quad \text{as} \quad \xi \to \infty. \tag{5.1.4}$$

The existence of an analytic continuation in k through the positive real axis follows then by Theorem 4.20.

Remark 5.1. *The first description of (5.1.4) for the general two-center problem is given in [Lea86] and [MS54]. The solutions $u_\pm$ are explicitly represented of as slowly convergent sums of special functions. In this way the authors had a deep control on the regularity of $u_\pm$ for complex ξ and could use the known asymptotic form of the considered special functions to estimate the asymptotic behavior of the $u_\pm$. With these methods, on the other hand, the regularity of $u_\pm$ with respect to k, μ and Z_+ was inaccessible.*

Remark 5.2. *The asymptotic expansions of [Lea86] confirms that the asymptotic (5.1.4) continues to hold in the case $\lambda \neq 0$, but we cannot apply Theorem 4.20 or extend its proof in a straightforward way because of the singularity of $\frac{h^2\lambda^2}{\sinh^2(\xi)}$ at the origin. We shall thus find a way to regularize the equation or transform it in a more manageable one.*

We proceed like in (4.7.2) and apply the change of variables induced by $y = \sinh(\xi)$. Then (5.1.2) transforms to

$$-h^2(y^2+1)\partial_y^2\tilde{v}(y) - h^2 y\partial_y\tilde{v}(y) + \left(\mu + \frac{h^2}{4} + \frac{h^2\lambda^2}{y^2} - k^2(y^2+1) - Z_+\sqrt{y^2+1}\right)\tilde{v}(y) = 0,$$

and with the ansatz

$$\tilde{v}(y) = \frac{1}{\sqrt[4]{y^2+1}}w(y)$$

we get

$$-h^2\frac{y^2+1}{\sqrt[4]{y^2+1}}\left(\partial_y^2 + \frac{k^2}{h^2} + \frac{Z_+/h^2}{\sqrt{y^2+1}} - \frac{\mu+\frac{h^2}{4}}{y^2+1} - \frac{\lambda^2}{y^2(y^2+1)}\right)w(y) = 0.$$

If we get rid of the term outside the brackets, we obtain the equation

$$\partial_y^2 w(y) + \left(\frac{k^2}{h^2} + \frac{Z_+/h^2}{\sqrt{y^2+1}} - \frac{\mu+\frac{h^2}{4}}{y^2+1} - \frac{\lambda^2}{y^2(y^2+1)}\right)w(y) = 0. \quad (5.1.5)$$

(5.1.5) is particularly helpful because it fits in the framework considered by [AK92, Sections 3,4,5]. In particular in [AK92] it is proved that for $k \in \mathbb{C}_\pm$ the incoming and outgoing waves are well defined functions, are uniquely determined by the asymptotic behavior

$$w_\pm(y,k) = \exp\left(\pm i\frac{k}{h}y(1+o(1))\right)(1+o(1)) \quad \text{as} \quad y \to \infty,$$

and admit an analytic extension in the energy parameter k through the real axis for $\arg \pm k < \pi$.

If we apply the transformations needed to obtain (5.1.5) in the opposite direction we get that $w_\pm(y,k)$ are transformed to $u_\pm(\xi,k)$ having exactly the asymptotic form (5.1.4) and admitting an analytic extension in k through the positive real axis.

REMARK 5.3. *The fact that for $\lambda \neq 0$ there exists only one regular solution in 0 that is identified (up to a constant) by decaying at 0 like $|y|^\lambda$ and that is entire in k and μ is a standard consequence of Frobenius theory* [Tes00, p. 105]. *Additionally, in* [AK92] *are given explicit asymptotic bounds for the decay rates of $u_\pm$ and u_0 in term of big values of λ.*

Now, for $k \in \mathbb{C}_\pm$ the waves $u_\pm$ are in $L^2(\mathbb{R}_+, \cosh^2(\xi)\sinh(\xi)d\xi)$ and thus for $\lambda \neq 0$ and any fixed μ it is possible to give a rigorous definition of the radial Green's function, the scattering elements and the generalized eigenfunctions exactly as in Section 4.4. Moreover, if $\mu_n(\lambda,k)$ ($n \in \mathbb{N}_0$) are the eigenvalues of the angular operator, for each fixed λ and n we can define the sets $\mathscr{E}_{n,\lambda}$ and $\mathscr{R}_{n,\lambda}$ respectively of eigenvalues and of resonances of the radial Schrödinger operator $\mathscr{A}_n^\lambda$ defined by (3.5.3). These definition can be given exactly as in Section 4.6, with the care of using $\cosh^2(\xi)\sinh(\xi)d\xi$ instead of $\cosh^2(\xi)d\xi$ as measure of the L^2 space.

Moreover for every λ and n the remarks and the propositions of Section 4.6 continue to hold and we can define

$$\mathscr{E}_\lambda := \bigcup_{n=0}^{\infty} \mathscr{E}_{n,\lambda}, \qquad \mathscr{R}_\lambda := \bigcup_{n=0}^{\infty} \mathscr{R}_{n,\lambda}, \tag{5.1.6}$$

as the sets of *eigenvalues* and *resonances* of the Schrödinger operators K_λ defined in (3.2.1).

We only have to prove the convergence of the partial wave expansion (3.7.6) for a fixed λ, in particular we can choose $\lambda = 0$. Then the convergence of the sum (3.7.6) would result estimating the decay of the Green's function in λ using the decay at 0 of the regular solutions as in [**AK92**] (compare with Remark 5.3).

This would give meaning to the second separation discussed in Section 3.2 and therefore we could define the sets of *eigenvalues* and *resonances* of the two-center Schrödinger operator $\mathscr{H}$ by means of

$$\mathscr{E} := \bigcup_{\lambda \in \mathbb{Z}} \mathscr{E}_\lambda \quad \text{and} \quad \mathscr{R} := \bigcup_{\lambda \in \mathbb{Z}} \mathscr{R}_\lambda. \tag{5.1.7}$$

REMARK 5.4. *As for the planar case (see (4.5.8)), we can define a truncated operator in some subspace depending on a finite number of values of n and λ with convergent partial wave expansion (3.7.6). Its resonances belong to a subset of $\mathscr{R}$ and its eigenvalues to a subset of $\mathscr{E}$. On the other hand, our approximations in this case are not as good as for the planar case. In fact the singularity appearing in equation (5.1.5) for $\lambda \neq 0$ prevented us from giving a good numerical description of the resonances.*

REMARK 5.5. *Using the estimates developed in* [**AK92**, Sections 3, 4 and 5] *is it possible to define a truncated operator depending only on a finite number of values of n and with convergent partial wave expansion. As in the previous remark its resonances belong to a subset of $\mathscr{R}$ and its eigenvalues to a subset of $\mathscr{E}$.*

Nevertheless, we expect that the structure of the resonances set for the three dimensional problem will be more involved than for the two dimensional one. In particular it is not possible to exclude the degeneracy of the resonances. A main intuition on this problem could be given by the description of the bifurcation diagrams for non planar motions. Sadly this was not developed in the thesis even if we hope to complete the puzzle adding the analysis of this last case in the next future.

The following two sections present the estimates of the eigenvalues of the angular operator that we were able to find.

5.2. Estimate for the eigenvalues in the case $Z_- = 0$

REMARK 5.6. *We want to approximate the eigenvalues and the eigenfunctions of*

$$\mathscr{A}_x^\lambda y(x) = \frac{\mu}{h^2} y(x).$$

With the following ansatz, coming from Frobenius theory of regular singular points [Tes00, p.105],

$$y(x) = (1-x^2)^{\lambda/2} u(x),$$

one finds for the u

$$-(1-x^2)^{\frac{\lambda}{2}}\Big[(1-x^2)u''(x) - 2x(\lambda+1)u'(x) \\ + \left(\frac{\mu}{h^2} - \lambda(\lambda+1) - \frac{E}{h^2}x^2 - \frac{Z_-}{h^2}x\right)u(x)\Big] = 0.$$

Let $Z_- = 0$. *If we set*

$$\gamma := \frac{\sqrt{E}}{h}, \quad z := \sqrt{2\gamma}x, \quad v(z) := u(x), \quad L := \frac{h^{-2}\mu - \lambda(\lambda+1)}{2\gamma},$$

we get the following equation for the v*:*

$$\left(1 - \frac{z^2}{2\gamma}\right)v''(z) - 2(\lambda+1)\frac{z}{2\gamma}v'(z) + \left(L - \frac{z^2}{4}\right)v(z) = 0.$$

Thus, formally setting $1/\gamma = h/\sqrt{E} = 0$*, we get a Quantum Harmonic Oscillator like equation, i.e.*

$$v''(z) + \left(L - \frac{z^2}{4}\right)v(z) = 0.$$

Let us proceed now rigorously. Let

$$\mathscr{R} := \left\{ y \in D(\mathscr{A}_x^{\lambda}(h)) \,\middle|\, f(x) = (1-x^2)^{\lambda/2}u(x) \text{ with } u \text{ entire} \right\}. \tag{5.2.1}$$

The eigenvalue differential equation

$$\mathscr{A}_x^{\lambda}(h)y(x) = \frac{\mu_n^{\lambda}(h)}{h^2}y(x).$$

for $0 \neq y \in \mathscr{R}$ then reads

$$-(1-x^2)^{\frac{\lambda}{2}}\Big[(1-x^2)u''(x) - 2x(\lambda+1)u'(x) \\ + \left(\frac{\mu_k^{\lambda}}{h^2} - \lambda(\lambda+1) - \frac{E}{h^2}x^2 - \frac{Z_-}{h^2}x\right)u(x)\Big] = 0. \tag{5.2.2}$$

For the moment we follow [MS54, Chapter 3.25] and study the symmetric problem, thus we set $Z_- = 0$. We consider only $\lambda \geq 0$. For $\lambda < 0$ is enough to replace all the appearences of λ with $|\lambda|$.

Thinking to the previous remark, we set

$$y_p^{\lambda}(x) := (1-x^2)^{\lambda/2} D_p(\sqrt{2\gamma}\, x) \quad \text{and} \quad M_p^{\lambda}(\gamma) := (2p+1)\gamma + \lambda(\lambda+1) \tag{5.2.3}$$

where

$$\gamma := \gamma(E,h) := \frac{\sqrt{E}}{h},$$

and for $p \in \mathbb{N}$

$$D_p(x) := (-1)^p e^{\frac{x^2}{4}} \frac{d^p}{dx^p} e^{-\frac{x^2}{2}} \tag{5.2.4}$$

are the Parabolyc Cylinder Functions.

REMARK 5.7. *Notice that $h \to 0$ implies $\gamma \to \infty$*

REMARK 5.8. *The $'$ appearing in what follows means that we are taking the derivative with respect to the explicitly written variable.*

Using the fact that

$$D_p''(x) + \left(p + \frac{1}{2} - \frac{x^2}{4}\right) D_p(x) = 0,$$

we have $\mathscr{A}_x^\lambda(h) y_p^\lambda + M_p^\lambda(h) y_p^\lambda = f_p$ where

$$f_p^\lambda = -\left(1-x^2\right)^{\frac{\lambda}{2}} \left(z^2 D_p{}''(z) + 2z(\lambda+1) D_p{}'(z)\right), \qquad z = \sqrt{2\gamma}\, x.$$

THEOREM 5.9.

$$\frac{\|f_p^\lambda\|}{\|y_p^\lambda\|} = \mathcal{O}(1) \qquad (\gamma \to \infty).$$

PROOF. First of all we have that

$$z^2 D_p{}''(z) = x^2 D_p{}''(\sqrt{2\gamma}\, x) \quad \text{and} \quad z D_p{}'(z) = x D_p{}'(\sqrt{2\gamma}\, x),$$

thus

$$\frac{\|f_p^\lambda\|}{\|y_p^\lambda\|} = \frac{\left\| -\left(1-x^2\right)^{\frac{\lambda}{2}} \left(x^2 D_p{}''(\sqrt{2\gamma}\, x) + 2x(\lambda+1) D_p{}'(\sqrt{2\gamma}\, x)\right)\right\|}{\left\|\left(1-x^2\right)^{\frac{\lambda}{2}} D_p(\sqrt{2\gamma}\, x)\right\|}.$$

By means of the binomial formula we can perform the expansion

$$\left(1 - \left(\frac{z}{\sqrt{2\gamma}}\right)^2\right)^\lambda = \sum_{n=0}^{\lambda} \binom{\lambda}{n} \left(-\frac{z^2}{2\gamma}\right)^{\lambda-n} = 1 - \frac{z^2}{2\gamma} + \mathcal{O}\left(\frac{1}{\gamma^2}\right)$$

Writing $x = \frac{z}{\sqrt{2\gamma}}$, we have

$$\begin{aligned}
\|f_p^\lambda\|^2 &= \frac{1}{\sqrt{2\gamma}} \int_{-\sqrt{2\gamma}}^{\sqrt{2\gamma}} \left(1 - \left(\frac{z}{\sqrt{2\gamma}}\right)^2\right)^\lambda z^2 \left(zD_p''(z) + 2(\lambda+1)D_p'(z)\right)^2 dz \\
&= \frac{1}{\sqrt{2\gamma}} \int_{-\sqrt{2\gamma}}^{\sqrt{2\gamma}} \left(1 + \mathcal{O}\left(\frac{1}{\gamma}\right)\right) z^2 \left(zD_p''(z) + 2(\lambda+1)D_p'(z)\right)^2 dz \\
&= \frac{1}{\sqrt{2\gamma}} \int_{-\infty}^{+\infty} z^2 \left(zD_p''(z) + 2(\lambda+1)D_p'(z)\right)^2 dz + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right) \\
&= \frac{C_1}{\sqrt{2\gamma}} + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right).
\end{aligned}$$

where C_1 is a finite positive constant and we used the fact that the tails are given by a bounded integral that decays exponentially in γ and that we are computing the integral of a positive even function.

In the same way we have

$$\|y_p^\lambda\|^2 = \frac{1}{\sqrt{2\gamma}} \int_{-\sqrt{2\gamma}}^{\sqrt{2\gamma}} \left(1 - \left(\frac{z}{\sqrt{2\gamma}}\right)^2\right)^\lambda D_p(z)\,dz = \frac{\|D_p\|^2}{\sqrt{2\gamma}} + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right),$$

where $\|D_p\|^2$ is finite, strictly positive and exactly computable.

Thus, when $\gamma \to \infty$

$$\frac{\|f_p^\lambda\|}{\|y_p^\lambda\|} \to \frac{\sqrt{C_1}}{\|D_p\|} < \infty.$$

□

We need the following theorem.

THEOREM 5.10. *Let $\mathscr{R}$ be a complex linear space with an Hermitian positive-defined scalar product. Let F be a linear operator defined on $D(F) \subset \mathscr{R}$ dense. Let its discrete spectrum is given by a countable set of simple eigenvalues*

$$\lambda_n = P_2(n) + \mathcal{O}(1),$$

where $n \in \mathbb{N}_0$ or $n \in \mathbb{Z}$ and P_2 a polynomial of degree exactly 2 s.t. for $n_1 \neq n_2$ it is $P_2(n_1) \neq P_2(n_2)$. The corresponding eigenvalues build an orthonormal system in $\mathscr{R}$

$$\langle y_i, y_k^* \rangle = \delta_{ik},$$

and there exist two constants α, β ($+\infty > \alpha > \beta > 0$) such that for every function f in the space

$$\beta^2 \sum_n |\langle f, y_n^* \rangle|^2 \le \langle f, f \rangle \le \alpha^2 \sum_n |\langle f, y_n^* \rangle|^2.$$

For $z \in D(F)$ and arbitrary λ

$$Fz + \lambda z = f$$

with $f \in \mathscr{R}$. Moreover if $\lambda = \lambda_m$ is an eigenvalue of F, then

$$\langle f, y_m^* \rangle = 0$$

and

$$||z|| \leq \frac{\alpha}{\beta} \frac{1}{\min_{\lambda_n \neq \lambda} |\lambda_n - \lambda|} ||f||.$$

PROOF. This theorem is a particular case of [MS54, Chapter 1.5, Satz 1], we refer the reader to the reference for the proof. □

It follows from Theorem 5.10 that, in the limit $\gamma = \frac{\sqrt{E}}{h} \to +\infty$, we have

$$\min_n \left| M_p^\lambda(E,h) - \frac{\mu_n^\lambda(E,h)}{h^2} \right| = \mathcal{O}(1).$$

Thus in particular there exist a constant C such that

$$p = n - \lambda + C.$$

THEOREM 5.11. *Thus there exist C such that for $n \geq \lambda$ and for every $E > 0$,*

$$\lim_{h \searrow 0} \frac{\mu_n^\lambda(E,h)}{h} = \sqrt{E}(2(n - \lambda + C) + 1)$$

PROOF. It follows directly from the fact that

$$\frac{\mu_n^\lambda(Z_-,E,h)}{h^2} = (2(n-\lambda+C)+1)\gamma(E,h) + \lambda(\lambda-1) + \mathcal{O}(1).$$

□

REMARK 5.12. *In principle, one expects the eigenvalues to be quadratic in n, what happens in fact is that in the semi-classical limit only the Harmonic Oscillator like part of the potential becomes relevant, hiding this relation. In fact for $\frac{E}{h^2} \ll 1$, see* [MS54, Chapter 3.24], *in the limit $n \to \infty$ one finds*

$$\frac{\mu_n^\lambda(Z_-,E,h)}{h^2} = n(n+1) - \frac{1}{2}\frac{E}{h^2} + \mathcal{O}\left(\frac{1}{n^2}\right),$$

where one recalls the quadratic dependence in n of the eigenvalues and its independence from the h dependent factor.

5.3. Estimate for the eigenvalues in the case $Z_- \neq 0$

Like in the previous subsection, we set

$$y_p^\lambda(x) := (1-x^2)^{\lambda/2} F_p^\delta(\sqrt{2\gamma}\, x) \quad \text{and} \quad M_p^\lambda(\gamma) := (2p+1)\gamma + \lambda(\lambda+1), \tag{5.3.1}$$

where

$$\gamma := \gamma(E,h) := \frac{\sqrt{E}}{h}, \qquad \delta := \delta(Z_-,E,h) := \frac{Z_-}{2E}\sqrt{\frac{\gamma}{2}} = \frac{Z_-}{2\sqrt{2hE\sqrt{E}}},$$

and

$$F_p^\delta(x) := D_{p+[\delta^2]}(x+2\delta), \qquad D_p(x) := (-1)^p e^{\frac{x^2}{4}} \frac{d^p}{dx^p} e^{-\frac{x^2}{2}}. \quad (5.3.2)$$

REMARK 5.13. *Notice that $\delta = 0$ corresponds to $Z_- = 0$.*

Using the fact that

$$\left(F_p^\delta\right)''(x) + \left(p + \frac{1}{2} - \frac{x^2}{4} - \delta x - \{\delta^2\}\right) F_p^\delta(x) = 0,$$

where $\{\cdot\} \in [0,1)$ is the fractional part function, we have

$$\mathscr{A}_x^\lambda(h) y_p^\lambda + M_p^\lambda(h) y_p^\lambda = f_p$$

where for $z = \sqrt{2\gamma}\, x$

$$f_p^\lambda = -\left(1-x^2\right)^{\frac{\lambda}{2}} \left(z^2 \left(F_p^\delta\right)''(z) + 2z(\lambda+1)\left(F_p^\delta\right)'(z) - \{\delta^2\} F_p^\delta(z)\right).$$

THEOREM 5.14. *For $E > Z_-/2$*

$$\frac{\|f_p^\lambda\|}{\|y_p^\lambda\|} = \mathscr{O}(1) \qquad (\gamma \to \infty).$$

PROOF. First of all we have that

$$z^2 \left(F_p^\delta\right)''(z) = x^2 \left(F_p^\delta\right)''(\sqrt{2\gamma}\, x) \quad \text{and} \quad z\left(F_p^\delta\right)'(z) = x\left(F_p^\delta\right)'(\sqrt{2\gamma}\, x),$$

thus

$$\frac{\|f_p^\lambda\|}{\|y_p^\lambda\|} = \frac{\left\| -\left(1-x^2\right)^{\frac{\lambda}{2}} \left(x^2 \left(F_p^\delta\right)''(\sqrt{2\gamma}\, x) + 2x(\lambda+1)\left(F_p^\delta\right)'(\sqrt{2\gamma}\, x) - \{\delta^2\} F_p^\delta(\sqrt{2\gamma}\, x)\right)\right\|}{\left\|\left(1-x^2\right)^{\frac{\lambda}{2}} F_p^\delta(\sqrt{2\gamma}\, x)\right\|}.$$

By means of the binomial formula we can expand

$$\begin{aligned}\left(1 - \left(\frac{z-2\delta}{\sqrt{2\gamma}}\right)^2\right)^\lambda &= \sum_{n=0}^{\lambda} \binom{\lambda}{n} \left(1 - \frac{Z_-^2}{4E^2} + \frac{Z_-}{E} z\right)^n \left(-\frac{z^2}{2\gamma}\right)^{\lambda-n} \\ &= \left(1 + \frac{zZ_-}{E} - \frac{Z_-^2}{4E^2}\right) + \mathscr{O}\left(\frac{1}{\gamma}\right),\end{aligned}$$

and writing $x = \frac{z-2\delta}{\sqrt{2\gamma}}$, we have

$$
\begin{aligned}
\|f_p^\lambda\|^2 &= \frac{1}{\sqrt{2\gamma}} \int_{-\sqrt{2\gamma}+2\delta}^{\sqrt{2\gamma}+2\delta} \left(1 - \left(\frac{z-2\delta}{\sqrt{2\gamma}}\right)^2\right)^\lambda \Xi^2(z,p,\delta,\lambda)\, dz \\
&= \frac{1}{\sqrt{2\gamma}} \int_{-\sqrt{2\gamma}+2\delta}^{\sqrt{2\gamma}+2\delta} \left(1 + \frac{zZ_-}{E} - \frac{Z_-^2}{4E^2} + \mathcal{O}\left(\frac{1}{\gamma}\right)\right) \Xi^2(z,p,\delta,\lambda)\, dz \\
&= \frac{1}{\sqrt{2\gamma}} \left(1 - \frac{Z_-^2}{4E^2}\right) \int_{-\infty}^{\infty} \Xi^2(z,p,\delta,\lambda)\, dz \\
&\quad + \frac{1}{\sqrt{2\gamma}} \frac{Z_-}{E} \int_{-\infty}^{\infty} z\Xi^2(z,p,\delta,\lambda)\, dz + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right) \\
&= \left(1 - \frac{Z_-^2}{4E^2}\right) \frac{C_2}{\sqrt{2\gamma}} + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right)
\end{aligned}
$$

where C_2 is a finite positive constant and

$$
\Xi(z,p,\delta,\lambda) := z^2 D''_{p+[\delta^2]}(z) + 2z(\lambda+1) D'_{p+[\delta^2]}(z) - \{\delta^2\} D_{p+[\delta^2]}(z).
$$

To perform this computation we used the following facts:

(1) $\lim_{\gamma\to+\infty} (\pm\sqrt{2\gamma} + 2\delta) = \lim_{\gamma\to\infty} \sqrt{2\gamma}\left(\pm 1 + \frac{Z_-}{2E}\right) = \pm\infty$ iff $E > \frac{Z_-}{2}$ so that the integral over the tails is exponentially decaying in γ;

(2) $\Xi^2(z,p,\delta,\lambda)$ is even, thus $z\Xi^2(z,p,\delta,\lambda)$ integrated on a symmetric interval gives a vanishing term;

(3) C_2 is non negative because it is the integral of a positive even function on a symmetric interval.

In the same way we have

$$
\begin{aligned}
\|y_p^\lambda\|^2 &= \frac{1}{\sqrt{2\gamma}} \int_{-\sqrt{2\gamma}+2\delta}^{\sqrt{2\gamma}+2\delta} \left(1 - \left(\frac{z-2\delta}{\sqrt{2\gamma}}\right)^2\right)^\lambda D^2_{p+[\delta^2]}(z)\, dz \\
&= \frac{1}{\sqrt{2\gamma}} \int_{-\infty}^{\infty} \left(1 + \frac{zZ_-}{E} - \frac{Z_-^2}{4E^2}\right) D^2_{p+[\delta^2]}(z)\, dz + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right) \\
&= \frac{1}{\sqrt{2\gamma}} \left(1 - \frac{Z_-^2}{4E^2}\right) \int_{-\infty}^{\infty} D^2_{p+[\delta^2]}(z)\, dz \\
&\quad + \frac{1}{\sqrt{2\gamma}} \frac{Z_-}{E} \int_{-\infty}^{\infty} z D^2_{p+[\delta^2]}(z)\, dz + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right) \\
&= \left(1 - \frac{Z_-^2}{4E^2}\right) \frac{\left\| D_{p+[\delta^2]} \right\|^2}{\sqrt{2\gamma}} + \mathcal{O}\left(\frac{1}{\gamma^{3/2}}\right).
\end{aligned}
$$

Thus, in the limit $\gamma \to +\infty$ ($h \searrow 0$),

$$\frac{||f_p^\lambda||}{||y_p^\lambda||} \to \frac{\sqrt{C_2}}{||D_{p+[\delta^2]}||}.$$

$\square$

It follows from Theorem 5.10 that, in the limit $\gamma = \frac{\sqrt{E}}{h} \to +\infty$, we have

$$\min_n \left| M_p^\lambda(E,h) - \frac{\mu_n^\lambda(E,h)}{h^2} \right| = \mathscr{O}(1).$$

Therefore there exists a constant C such that

$$p + \left[\delta^2\right] = n - \lambda + C \quad \text{or, equivalently,} \quad p = n - \lambda - \left[\delta^2\right] + C.$$

THEOREM 5.15. *There exists a constant C such that for $n \geq \lambda + \left[\delta^2\right] \geq \lambda + \frac{Z_-^2}{8hE\sqrt{E}}$ and for every $E > \frac{Z_-}{2}$, in the limit $h \searrow 0$*

$$\mu_n^\lambda(E,h) = -\frac{Z_-^2}{4E} + \sqrt{E}\left(2\left(n - \lambda - \{\delta^2\} + C\right) + 1\right) h + \mathscr{O}\left(h^2\right).$$

PROOF. It follows directly from the fact that $\left[\delta^2\right] = \delta^2 - \{\delta^2\}$ and

$$\frac{\mu_n^\lambda(Z_-,E,h)}{h^2} = \left(2(n - \lambda - \left[\delta^2\right] + C) + 1\right)\gamma(E,h) + \lambda(\lambda - 1) + \mathscr{O}(1).$$

$\square$

REMARK 5.16. *Sadly this is a really bad approximation, giving no hope to develop a numerical study of the resonances as in the previous chapter.*

CHAPTER 6

Final considerations

Before discussing the open problems and the possible further directions of work, we want to give a summary of the main results of this thesis.

In the classical picture, the novelty is given by Theorem 2.9 with the description of the bifurcation diagram for the planar motion for positive energies for arbitrary values of the charges. This is integrated in the subsequent section with a detailed analysis of the structure of the trajectories in configuration space.

Most of the operator theoretical analysis of the separated equations of the quantum mechanical problem is new, nevertheless it is based on well established theories presented in the Appendices. The limit point criterion obtained in Theorem 3.11 should be new as far as we know.

A new important results is given by Theorem 4.11 where it is proven that it is possible to define the concept, central in scattering theory, of incoming and outging waves for the radial separated equation. They are characterized by their asymptotic form using a WKB ansatz that involves a unique globally defined phase function. This result is strong in the sense that the approximation is not affected by the Stokes phenomenon near the turning points.

Even more important is Theorem 4.20. In this theorem it is proved that the incoming and outgoing waves admits an analytic extension in the energy parameter to the second Riemann sheet. The major consequence of this theorem is the possibility to extend the Green's function, the generalized eigenfunctions and the scattering matrix elements to the second Riemann sheet, making it possible to define the resonances for the two center system for the first time (see Sections 4.4 and 4.6).

Moreover our construction integrates the one made in [**AK92**] and permits to characterize and define the resonances in the three dimensional case (see Chapter 5).

Of great interest are even the results of Section 4.7, 4.9 and 4.10. Even if we have not a good mathematical control on them, they permit to localize numerically the resonances and give a qualitative description of their structure (see Section 4.11).

Despite our efforts there are still many open question that we would try to address in the future. First of all in this work the proof of the convergence of the partial wave expansion of the Green's function is missing for both the two and the three dimensional case. This is a important step to make the whole analysis completely rigorous. For the moment we only know that at least numerically it seems to converge. It is important to remark here that the missing point to prove the convergence of (3.7.6) is the convergence of the planar partial wave expansion (4.5.7).

Secondly, as stressed in Remark 4.38 and 4.39, we have given a description of the resonances associated to the classical closed hyperbolic trajectory bouncing between the centers. We expect that another class of resonances appear for $Z_+ < 0$, $|Z_+| < Z_-$, namely the shape resonances associated to energy parameter in the region $I^a_<$ described in Section 2.6.

Moving further from the two-centers model, a first interesting question arises from Remark 1.3. A diatomic molecule in Thomas Fermi approximation [**LS77**] looks like the two-centers operator (1.1.1) perturbed by a smooth potential W. In this case it is known that the closed hyperbolic trajectory between the centers is still present [**KK92**, **Kna02**] and the non-trapping condition fails to hold [**CJK08**]. It would be interesting to know if the resonances are still present and share the same structure as the resonances for the two-centers problem. In presence of the perturbation W the system is no more separable, thus we cannot apply the methods of this thesis. One possibility would be to proceed similarly as Gérard and Sjöstrand in [**GS87**].

Another big interesting question is the investigation of the resonances for the n-centers problem for $n \geq 3$. In this case is present a Cantor set of classical hyperbolic trajectories [**KK92**, **Kna02**] and the non-trapping condition fails to hold [**CJK08**]. Therefore one expect the resonances to be present and to be distributed in some complicated way. There are only few known examples presenting a similar structure that have been investigated rigorously (see [**SZ07**] and [**NZ05**]) and they suggests that the resonances are present and are distributed in a fractal set. In this case, anyhow, a huge effort is required to properly extend the techniques needed to deal with the problem.

APPENDIX A

A small introduction to the theory of Sturm-Liouville operators

To proceed we need some theorems and preliminary definitions (cfr. [Wei80, pp. 247-257], [Tes09, pp. 84-85, 181-195]).

Let $I := (a,b) \subset \mathbb{R}$ define an interval (eventually unbounded), moreover set

$$AC(a,b) := \left\{ f \in C(I) \,\middle|\, f(x) = f(c) + \int_c^x g(t)dt,\ c \in I,\ g \in L^1_{loc}(I) \right\}$$

the space of all the absolutely continuous functions. Consider a formal operator of the type

$$\tau f := \frac{1}{r}\{-(pf')' + qf\} \tag{A.1}$$

where the coefficients p, q and r satisfy the following assumptions:

(1) p, q and r are real-valued continuous functions defined on I;
(2) p is continuously differentiable;
(3) $p(x) > 0$ and $r(x) > 0$ for all $x \in I$.

The differential equation $\tau f = 0$ is called *Sturm-Liouville equation*. If a is finite and if p^{-1}, q and r are in $L^1((a,c))$ for some $c \in I$, then the Sturm-Liouville equation (A.1) is called *regular* in a, otherwise is called *singular*. Similarly for b. If it is regular (resp. singular) in both a and b, then it is called *regular* (resp. *singular*).

We call *fundamental solutions* of a Sturm-Liouville differential equation τ on $[a,b]$ the two solutions ϕ_1, ϕ_2 that satisfy the following boundary conditions

$$\phi_1(0) = \phi_2'(0) = 0 \quad \text{and} \quad \phi_1'(0) = \phi_2(0) = 1. \tag{A.2}$$

It is possible to define operators on $L^2(I, r(x)dx)$ using differential equations such as τ. The *maximal* operator T induced by τ is defined by

$$D(T) = \{f \in L^2(I, r(x)dx) \mid f, f' \in AC(a,b),\ \tau f \in L^2(I, r(x)dx)\}$$

$$Tf = \tau f \quad \text{for} \quad f \in D(T).$$

The *minimal* operator T_0 induced by τ is defined by the formula

$$D(T_0) = \{f \in D(T) \mid \operatorname{supp}(f) = K \subset I, K \text{ compact}\}$$

$$T_0 f = \tau f \quad \text{for} \quad f \in D(T_0).$$

REMARK A.1. *When there is no risk of confusion, we will write $L^2(I, r)$ in place of $L^2(I, r(x)dx)$ to shorten the notation.*

THEOREM A.2. *Let τ be as in (A.1). The operator T_0 is symmetric and has equal deficiency indices, i.e., T_0 has self-adjoint extensions.*

THEOREM A.3. *Let τ be as in (A.1). All self-adjoint extensions of T_0 have the same essential spectrum. If T_0 is semibounded, then all self-adjoint extensions of T_0 are semibounded.*

THEOREM A.4 (The Weyl alternative). *Let τ be a Sturm-Liouville differential equation defined on I, and let $c \in I$. Either*

- *every solution u of the equation $(\tau - z)u = 0$ lies in $L^2((c,b), r(x)dx)$ for every $z \in \mathbb{C}$; or*
- *for every $z \in \mathbb{C}$ there exists at least one solution u of the equation $(\tau - z)u = 0$ for which $u \notin L^2((c,b), r(x)dx)$.*

In the second case, for every $z \in \mathbb{C} \setminus \mathbb{R}$ there exists (up to a factor) exactly one solution u of the equation $(\tau - z)u = 0$ for which $u \in L^2((c,b), r(x)dx)$.

According to Weyl we say that in the first case we have the *limit circle case* (LCC) at b and in the second case we have the *limit point case* (LPC) at b. Similarly a corresponding theorem holds for the boundary point a from which the corresponding definitions of limit point case and limit circle case follow.

For $x \in I$ and for $f, g \in C^1(I, \mathbb{C})$, now, we define

$$[f,g]_x := p(x)\left(f'(x)g(x) - f(x)g'(x)\right) = -W(f,g,x) \tag{A.3}$$

where W is the modified Wronskian. In the following theorem, borrowed from [Wei80] (see also [Tes09]), we write LPC for Limit Point Condition and LCC for Limit Circle Condition.

THEOREM A.5. *Let τ be a Sturm-Liouville operator (A.1). Moreover, let $\lambda \in \mathbb{R}$, and let v and w be non-vanishing real solutions of the equation $(\tau - \lambda)u = 0$.*

(1) *The operator $T_{v,w}$ defined using the separate boundary conditions by*
$$D(T_{v,w}) = \{f \in D(T) \mid [v,f]_a = 0 \text{ if LCC at } a,\ [w,f]_b = 0 \text{ if LCC at } b\}$$
$$T_{v,w} f = Tf \quad \text{for} \quad f \in D(T_{v,w}).$$
is a self-adjoint extension of T_0. Note that if we have LPC at a and/or b, then the index v and/or w is meaningless.

(2) *For $z \in \mathbb{C} \setminus \mathbb{R}$ the resolvent $R_z = (z - T_{v,w})^{-1}$ is an Hilbert-Schmidt operator of the c-invariant form*
$$R_z g(x) = \frac{1}{W(u_a, u_b)} \left\{ u_b(x) \int_a^x u_a(y) g(y) r(y)\, dy + u_a(x) \int_x^b u_b(y) g(y) r(y)\, dy \right\},$$
where for some $c \in (a,b)$, u_a and u_b are the solutions of the equation $(\tau - z)u = 0$ uniquely determined up to a factor by the conditions
   - *$[v, u_a]_a = 0$ if we have LCC at a, respectively $u_a \in L^2((a,c), r)$ if we have LPC at a,*

- $[w, u_b]_b = 0$ *if we have LCC at* b*, respectively* $u_b \in L^2((c,b),r)$ *if we have LPC at* b.

(3) *All eigenvalues of* $T_{v,w}$ *are simple.*
(4) *If we have the LCC at both* a *and* b*, then* $T_{v,w}$ *has a pure discrete spectrum and the eigenfunctions form an orthonormal basis.*

Notice that if one defines the operator by means of coupled boundary conditions, the eventual discrete spectrum has at most multiplicity 2 but in general is not simple. In fact the following theorems can be proved.

THEOREM A.6. *Let* τ *be a Sturm-Liouville operator (A.1) with* $p(x) > 0$*. Assume that the self-adjoint realization* T *is defined by means of the boundary conditions*

$$\begin{cases} u(b) = \alpha\, u(a) \\ p(b)u'(b) = \frac{1}{\alpha}\, p(a)u'(a) \end{cases} \quad \text{with} \quad \alpha > 0.$$

By u_j *we denote the eigenfunction corresponding to the eigenvalue* λ_j *(for double-degenerate eigenvalues the choice of the corresponding eigenfunctions is arbitrary).*

- u_0 *has no zero in* $[a,b]$*,* u_{2n+1} *and* u_{2n+2} *both have exactly* $2(n+1)$ *zeros in* $[a,b)$*.*
- *We have*

$$\lambda_0 < \lambda_1 \le \lambda_2 < \ldots \le \lambda_{2n} < \lambda_{2n+1} \le \lambda_{2n+2} < \ldots.$$

PROOF. The proof can be found in [Wei87, Theorem 13.7, p. 206] and [Eas75, Theorem 2.3.1 and Theorem 3.1.2]. □

REMARK A.7. *The periodic boundary conditions are the special case* $\alpha = 1$*.*

As in the separated case, the eigenvalues of Sturm-Liouville problems can be compared to obtain bounds on the spectrum.

THEOREM A.8. *Let* $r(x) = 1$*. Let* $\lambda_{1,n}$ $(n \ge 0)$ *denote eigenvalues in the periodic problem over* $[a,b]$ *when* $p(x)$ *and* $q(x)$ *are replaced by* $p_1(x)$ *and* $q_1(x)$*, where*

$$p_1(x) \ge p(x) \quad \text{and} \quad q_1(x) \ge q(x).$$

Then we have $\lambda_{1,n} \ge \lambda_n$ *for all* n*.*

PROOF. Given in a more general form in [Eas75, Theorem 2.2.2, p. 23] □

For even potentials we can characterize the periodic boundary conditions in terms of separated boundary conditions. In fact the following theorem holds.

THEOREM A.9. *Consider the differential equation*

$$y'' + Q(x)y = 0 \tag{A.4}$$

where $Q(x)$ *is an even (real or complex valued) function of the real variable* x*, piecewise continuous in every finite interval and with minimal period* π*. Let* $\phi_1(x)$ *and* $\phi_2(x)$ *be its fundamental solutions as defined by (A.2). Then there exists a nontrivial periodic solution of (A.4) which is*

(1) *even and of period* π*, if and only if* $\phi_2'(\pi/2) = 0$.
(2) *odd and of period* π*, if and only if* $\phi_1(\pi/2) = 0$.
(3) *even and of period* 2π*, if and only if* $\phi_2(\pi/2) = 0$.
(4) *odd and of period* 2π*, if and only if* $\phi_1'(\pi/2) = 0$.

PROOF. The proof can be found in [MW79, Theorem 1.1] □

APPENDIX B

Singular second-order Sturm-Liouville operators with complex coefficients

The Weyl LPC-LCC classification presented in the previous Appendix can be generalized to Sturm-Liouville problems of the form (A.1) on an interval $[a,b)$, $a < b \leq \infty$, where

(1) $r > 0$, $p \neq 0$ a.e. on $[a,b)$ and $r, 1/p \in L^1_{\mathrm{loc}}([a,b))$;
(2) p, q are complex valued, $q \in L^1_{\mathrm{loc}}([a,b))$ and

$$Q := \overline{\mathrm{co}}\left\{ \frac{q(x)}{r(x)} + \rho p(x) \,\middle|\, x \in [a,b),\, \rho \in (0,\infty) \right\} \neq \mathbb{C}, \tag{B.1}$$

where $\overline{\mathrm{co}}$ denotes the closed convex hull.

Similarly as in the real case, the end point b is called *singular* if at least one of $b = \infty$ or

$$\int_a^b \left(r(x) + \frac{1}{|p(x)|} + |q(x)| \right) dx = \infty$$

holds.

The general theory and the proofs of the theorems of this section can be found in [BMEP99] unless a different source is explicitly specified. We will present here only the results that we need and adapt them to our notation. We will continue to denote the Sturm-Liouville differential equation with τ as in (A.1).

The complement in $\mathbb{C}$ of the closed convex set Q has one or two connected components. For $\lambda_0 \in \mathbb{C} \setminus Q$, denote by $K = K(\lambda_0)$ its (unique) nearest point in Q and denote by $L = L(\lambda_0)$ the tangent to Q at K if it exists or otherwise any line touching Q at K. Then if the complex plane is subjected to a translation $z \to z - K$ and a rotation through an appropriate angle $\eta = \eta(\lambda_0) \in (-\pi, \pi]$, the image of L coincides with the imaginary axis and the images of λ_0 and Q lie in the new negative (w.r.t. the real line) and non-negative half-planes respectively: i.e. for all $x \in [a,b)$ and $r \in \mathbb{R}_+$,

$$\Re\left[\left(\rho p(x) + \frac{q(x)}{r(x)} - K \right) e^{i\eta} \right] \geq 0 \quad \text{and} \quad \Re\left[(\lambda_0 - K) e^{i\eta} \right] < 0. \tag{B.2}$$

For such admissible η, K (corresponding to some $\lambda_0 \in \mathbb{C} \setminus Q$), we define the region

$$\Lambda_{\eta,K} := \left\{ \lambda \in \mathbb{C} \mid \Re\left[(\lambda_0 - K) e^{i\eta} \right] < 0 \right\}. \tag{B.3}$$

Then $\mathbb{C} \setminus Q$ is the union of the half-planes $\Lambda_{\eta,K}$ over the set S of admissible η, K.

Let θ, ϕ be the solutions of

$$-(py')' + qy = \lambda r y \tag{B.4}$$

satisfying

$$\begin{cases} \phi(a,\lambda) = \sin(\alpha), & \theta(a,\lambda) = \cos(\alpha), \\ p\phi'(a,\lambda) = -\cos(\alpha), & p\theta'(a,\lambda) = \sin(\alpha), \end{cases} \tag{B.5}$$

where $\alpha \in \mathbb{C}$. In fact we will consider only the case $\alpha = 0$ or $\alpha = \pi/2$, so we suppose from now $\alpha \in \{0, \pi/2\}$ without specifying it all the time unless it is necessary.

REMARK B.1. *The values $\alpha = 0, \pi/2$ correspond respectively to the usual Dirichlet and Neumann problems. For different values of α's the set of admissible η, K and the region Q need to be slightly redefined and the situation can be partially different from the one depicted below, the general theory in detail can be found in* [BMEP99] *and the references therein.*

It is well known that the linearly independent solutions ϕ and θ are at least continuous in (x,λ) and for every fixed x are entire functions of λ with their derivatives [CL55]. Moreover every solution ψ of (B.4) except for ϕ is, up to a constant multiple, of the form

$$\psi(x,\lambda) = \theta(x,\lambda) + m(\lambda)\phi(x,\lambda) \tag{B.6}$$

for some function m depending only of λ in some complex region.

REMARK B.2. *As in the real case one can define LPC and LCC conditions in terms of the number of solutions of* (B.4) *lying in $L^2([a,b), r(x)dx)$. As in the real case, in the LPC the function m is uniquely defined while in the LCC there is a continuous number of possible m lying on some complex circle $C_b(\lambda)$ and being specified uniquely by the boundary conditions at b.*

We want to understand the analytical properties of such an m and its domain of definition. Before doing this we need to state how the Weyl alternative translates in this more general setting.

THEOREM B.3. *For $\lambda \in \Lambda_{\eta,K}$, $(\eta, K) \in S$ the Weyl circles converge either to a limit-point $m(\lambda)$ or a limit-circle $C_b(\lambda)$. The following distinct cases are possible, the first two being sub-cases of the limit-point case.*

Case I: *there exists a unique solution y of* (B.4) *satisfying*

$$\int_a^b \Re\left[e^{i\eta}(p|y'|^2 + (q-Kr)|y|^2\right]dx + \int_a^b |y|^2 r\,dx < \infty, \tag{B.7}$$

and this is the only solution satisfying $y \in L^2([a,b), r(x)dx)$.

Case II: *there exists a unique solution y of* (B.4) *satisfying* (B.7) *but all solutions of* (B.4) *are in $L^2([a,b), r(x)dx)$.*

Case III: *all solutions of* (B.4) *satisfy* (B.7) *and, hence, are in $L^2([a,b), r(x)dx)$.*

Moreover this classification is independent of λ in the sense that

(1) *if all solutions of* (B.4) *satisfy* (B.7) *for some $\lambda' \in \Lambda_{\eta,K}$, then all solutions of* (B.4) *satisfy* (B.7) *for all $\lambda \in \mathbb{C}$;*

(2) *if all solutions of* (B.4) *are in* $L^2([a,b), r(x)dx)$ *for some* $\lambda' \in \mathbb{C}$, *then all solutions of* (B.4) *for all* $\lambda \in \mathbb{C}$.

REMARK B.4. *In cases* II *and* III *the classification appears to depend on the chosen* K, η *even assuming more restrictions on the coefficients of* (B.4).

We are ready to state the results on the regularity properties of the m function.

LEMMA B.5. *In cases I and II,* $m_{\eta,K}$ *is analytic throughout* $\Lambda_{\eta,K}$. *In case I, the function defined by* $m(\lambda) = m_{\eta,K}(\lambda)$ $(\lambda \in \Lambda_{\eta,K})$ *is well defined on each of the possible two connected components of* $\mathbb{C} \setminus Q$; *the restriction to a connected component is analytic on that set.*

In case III, *given* $m_0 \in C_b(\lambda_0)$, $\lambda_0 \in \Lambda_{\eta,K}$, *there exists a function* $m_{\eta,K}$ *that is analytic in* $\Lambda_{\eta,K}$ *and* $m_{\eta,K}(\lambda_0) = m_0$; *moreover, a function* $m_{\eta,K}$ *can be found such that* $m_{\eta,K}(\lambda) \in C_b(\lambda)$ *for all* $\lambda \in \Lambda_{\eta,K}$.

REMARK B.6. *If* $\alpha = 0$ *(or* π*),* $m(\cdot)$ *possesses an analogue of the Nevanlinna representation* [**AG93**, Chapter 2.69, Theorem 2], *like for the Titchmarsh-Weyl function of the symmetric case. That is not the case if* $\alpha = \pi/2$.

LEMMA B.7. *Let* $\lambda, \lambda' \in \Lambda_{\eta,K}$ *and*

$$\psi(\cdot,\lambda) = \theta(\cdot,\lambda) + m(\lambda)\phi(\cdot,\lambda), \tag{B.8}$$

where $m(\lambda)$ *is either the limit-point or an arbitrary point on* $D_b(\lambda)$ *in the LCC. Then*

$$\lim_{\beta \to b} [\psi(\cdot,\lambda), \psi(\cdot,\lambda')](\beta) = 0, \tag{B.9}$$

with the modified Wronskian $[,]$ *from* (A.3). *In case I,* (B.9) *continues to hold for all* $\lambda, \lambda' \in \mathbb{C} \setminus Q$.

THEOREM B.8. *For all* $\lambda, \lambda' \in \Lambda_{\eta,K}$

$$(\lambda' - \lambda) \int_a^b \psi(x,\lambda)\psi(x,\lambda') r(x) dx = m(\lambda) - m(\lambda'); \tag{B.10}$$

this holds for all $\lambda, \lambda' \in \mathbb{C} \setminus Q$ *in case I. Moreover, in cases II and III, for a fixed* $\lambda' \in \Lambda_{\eta,K}$, *the function* $m(\lambda)$ *can be extended as a meromorphic function in* $\mathbb{C}$ *with pole at* λ *if and only if*

$$1 + (\lambda - \lambda') \int_a^b \phi(x,\lambda)\psi(x,\lambda') w(x) dx = 0.$$

THEOREM B.9. *Suppose that* (B.4) *is in case I. Define*

$$Q_c := \overline{\mathrm{co}} \left\{ \frac{q(x)}{r(x)} + \rho p(x) \,\middle|\, x \in [c,b),\ \rho \in (0,\infty) \right\}, \quad Q_b := \bigcap_{c \in (a,b)} Q_c. \tag{B.11}$$

Then $m(\lambda)$ *is defined throughout* $\mathbb{C} \setminus Q$, *and has a meromorphic extension to* $\mathbb{C} \setminus Q_b$, *with poles only in* $Q \setminus Q_b$.

By means of the theory just presented it is possible to define the Green function and the resolvent associated to (B.4). For $\lambda \in \Lambda_{\eta,K}$, $(\eta,K)\in S$, define

$$G(x,y;\lambda)=\begin{cases}-\phi(x,\lambda)\psi(y,\lambda), & a<x<y<b,\\ -\psi(x,\lambda)\phi(y,\lambda), & a<y<x<b,\end{cases} \tag{B.12}$$

where ϕ,ψ are the functions defined in (B.5) and (B.8). For $f\in L^2([a,b),r(x)dx)$ we define

$$R_\lambda f(x):=\int_a^b G(x,y;\lambda)f(y)r(y)\,dy. \tag{B.13}$$

LEMMA B.10. *Let $\lambda\in\Lambda_{\eta,K}$, $(\eta,K)\in S$. For R_λ defined in (B.13) the following properties are satisfied.*

(1) *For $x\in(a,b)$, $[\phi,\psi](x)=[\phi,\psi](a)=1$.*
(2) *For $f\in L^2([a,b),r(x)dx)$, $p(R_\lambda f)'\in AC_{\mathrm{loc}}([a,b))$ and a.e. $x\in(a,b)$*

$$(\tau-\lambda)R_\lambda f(x)=f(x),$$

where τ is the differential equation (A.1) with coefficients fulfilling the conditions described at the beginning of this section.
(3) *For any $\lambda'\in\mathbb{C}$ and for $f\in L^2([a,b),r(x)dx)$*

$$[R_\lambda f,\phi(\cdot,\lambda')](a)=0. \tag{B.14}$$

Moreover, if $\lambda'\in\Lambda_{\eta,K}$

$$[R_\lambda f,\psi(\cdot,\lambda')](b)=0. \tag{B.15}$$

REMARK B.11. *In general m, and hence ψ, depends on (η,K). However Lemma B.5 shows that in Case I the definition properly extends to $\mathbb{C}\setminus Q$.*

REMARK B.12. *In case I, (B.15) holds for all $\lambda,\lambda'\in\mathbb{C}\setminus Q$.*

THEOREM B.13. *Let $f\in L^2([a,b),r(x)dx)$ and $\lambda\in\Lambda_{\eta,K}$, $(\eta,K)\in S$. Then, in every case*

$$\int_a^b \Re\Big(e^{i\eta}(p|\Phi'|^2+(q-Kr)|\Phi|^2)\Big)dx \\ +\Big(\Re((K-\lambda)e^{i\eta})-\epsilon\Big)\int_a^b|\Phi|^2r\,dx\le\frac{1}{4\epsilon}\int_a^b|f|^2r\,dx$$

for any $\epsilon>0$ where $\Phi:=R_\lambda f$ and $\delta=\operatorname{dist}(\lambda,\partial\Lambda_{\eta,K})$. In particular, R_λ is bounded and

$$\|R_\lambda f\|\le\frac{1}{\delta}\|f\| \tag{B.16}$$

where $\|\cdot\|$ is to be intended as the $L^2([a,b),r(x)dx)$ norm.

Moreover in cases II and III, R_λ is Hilbert-Schmidt for any $\lambda\in\Lambda_{\eta,K}$, $(\eta,K)\in S$.

For some $(\eta,K)\in S$ fix a $\lambda'\in\Lambda_{\eta,K}$ and set

$$\begin{aligned} D(\widetilde{\tau}) := \Big\{ u\in L^2([a,b),r(x)dx) \mid & \, u, pu'\in AC_{\text{loc}}([a,b)),\\ & \tau u\in L^2([a,b),r(x)dx),\\ & [u,\phi(\cdot,\lambda')](a)=0=[u,\psi(\cdot,\lambda')](b)\Big\},\\ \widetilde{\tau}u := \tau u, \qquad u\in D(\widetilde{\tau}). \end{aligned} \tag{B.17}$$

In general $D(\widetilde{\tau})$ will depend on λ', but in one case as clarified by the following theorem.

Theorem B.14. *Let*

$$\begin{aligned} D_1 := \Big\{ u\in L^2([a,b),r(x)dx) \mid & \, u, pu'\in AC_{\text{loc}}([a,b)),\\ & \tau u\in L^2([a,b),r(x)dx),\\ & \cos(\alpha)u(a)+\sin(\alpha)p(a)u'(a)=0\Big\}. \end{aligned}$$

Then in Case I one has the equality $D_1=D(\widetilde{\tau})$, while in cases II and III, D_1 is given by the direct sum $D_1=D(\widetilde{\tau})+\operatorname{span}(\phi(\cdot,\lambda'))$.

Let now J be the conjugation operator $u\mapsto\overline{u}$. An operator T is called *J-symmetric* if $JTJ\subset T^*$ and *J-self-adjoint* if $JTJ=T^*$. Moreover T is *m-accretive* if $\Re\lambda<0$ implies that $\lambda\in\rho(T)$, the resolvent set of T, and $\|(T-\lambda\mathbb{1})^{-1}\|\le 1/|\Re\lambda|$. If, for some $K\in\mathbb{C}$ and $\eta\in(-\pi,\pi)$, $e^{i\eta}(T-K)$ is m-accretive, we shall say that T is *quasi-m*-accretive.

Let $\sigma(\widetilde{\tau})$ denote the spectrum of $\widetilde{\tau}$, then the essential spectrum $\sigma_e(\widetilde{\tau})$ is defined as the complement in $\mathbb{C}$ of the set

$$\Delta(\widetilde{\tau}) := \{\lambda\in\mathbb{C} \mid (\widetilde{\tau}-\lambda\mathbb{1}) \text{ is a Fredholm operator and } \operatorname{ind}(\widetilde{\tau}-\lambda\mathbb{1})=0\},$$

where an operator A is called *Fredholm* if its kernel and cokernel are finite-dimensional and its range is closed. The following theorem will give a meaning to the operator defined in (B.17).

Theorem B.15. *The operators defined in* (B.17) *for any $\lambda'\in\Lambda_{\eta,K}$, $(\eta,K)\in S$ are J-self-adjoint and quasi-m-accretive, and $\sigma(\widetilde{\tau})\subseteq\mathbb{C}\setminus\Lambda_{\eta,K}$. For any $\lambda\in\Lambda_{\eta,K}m$ $(\widetilde{\tau}-\lambda\mathbb{1})^{-1}=R_\lambda$.*

In case I, $\sigma(\widetilde{\tau})\subseteq Q$ and $\sigma_e(\widetilde{\tau})\subseteq Q_b$. In $Q\setminus Q_b$, $\sigma(\widetilde{\tau})$ consists only of eigenvalues of finite geometric multiplicity, these points being the poles of the meromorphic extension of m defined in Theorem B.9.

In cases II and II, R_λ is compact for any $\lambda\in\rho(\widetilde{\tau})$ and $\sigma(\widetilde{\tau})$ consists only of isolated eigenvalues (in $\mathbb{C}\setminus\Lambda_{\eta,K}$) having finite algebraic multiplicity.

Remark B.16. *Notice that in case of a real differential equation, everything coincides with the classical theory of Sturm-Liouville Operators with a singular endpoint.*

Despite its length, the following is an extremely useful result to understand in which case one equation belongs is the following theorem on asymptotic solutions of differential equations of the form (A.1).

THEOREM B.17 (Liouville-Green Theorem). *Consider the Sturm-Liouville differential equation* (B.4). *Let p and $Q := q - \lambda r$ be nowhere zero complex valued functions and with locally absolutely continuous first derivatives in $[x_0, \infty)$ for some x_0 in their domain of definition. Assume the following conditions are fulfilled*

- $(pQ)'/pQ = o(\sqrt{Q/p})$ *as* $x \to \infty$,
- $\left(p^{-1/2}Q^{-3/2}(pQ)'\right)' \in L^1(x_0, \infty)$,
- $p^{-3/2}Q^{-5/2}(pQ)'^2 \in L^1(x_0, \infty)$,
- $\Re(\sqrt{Q/p})$ *have one sign in* $[x_0, \infty)$.

Then (B.4) *has solutions y_1 and y_2 such that up to a constant factor*

$$y_1 = (pQ)^{-1/4} \exp\left(\int_{x_0}^{x} \sqrt{Q/p}\, dt\right) \qquad \text{as } x \to \infty, \tag{B.18}$$

$$py_1' = (pQ)^{1/4} \exp\left(\int_{x_0}^{x} \sqrt{Q/p}\, dt\right) \qquad \text{as } x \to \infty, \tag{B.19}$$

with similar formulae for y_2 containing $-\sqrt{Q/p}$ in the exponential term.

PROOF. See [**Eas89**, Corollary 2.2.1, p. 58] □

APPENDIX C

Perturbation theory in a nutshell

This chapter is mainly based on [RS78, Chapter XII.2] unless otherwise stated. A more general version of the theory can be found in [Kat95, Chapter VII]. A simplified reformulation particularly useful for applications to Mathieu and spheroidal operators can be found in [MS54, Chapters 1.4–1.6].

Let A and B be two operators densely defined on an Hilbert space $\mathfrak{H}$ with domains $D(A)$ and $D(B)$ respectively. B is said to be *A-bounded* if

(1) $D(B) \supset D(A)$
(2) For some a and b in $\mathbb{R}$ and all $\phi \in D(A)$,

$$||B\phi|| \le a||A\phi|| + b||\phi||$$

The infimum of such a is called the *relative bound* of B with respect to A. If the relative bound is zero, B is said to be *infinitesimally small* with respect to A ($B \ll A$).

THEOREM C.1 (Kato-Rellich Theorem). *Suppose that A is self-adjoint, B is symmetric, and B is A bounded with relative bound $a < 1$. Then $A+B$ is self-adjoint on $D(A)$. Further, if A is bounded from below, then $A+B$ is bounded from below.*

Let A be a self-adjoint operator. An operator C with $D(A) \subset D(C)$ is called *relatively compact* with respect to A if and only if $C(A+i)^{-1}$ is compact. For this kind of operator one has the following property.

THEOREM C.2. *Let A be a self-adjoint operator and let C be a relatively compact perturbation of A. Then*

(1) *$B = A + C$ defined on $D(B) = D(A)$ is a closed operator;*
(2) *if C is symmetric, B is self-adjoint;*
(3) *$\sigma_{ess}(A) = \sigma_{ess}(B)$.*

Let $R \subseteq \mathbb{C}$ be a connected domain and let $T(\beta)$ be a closed operator with nonempty resolvent set $\rho(T(\beta))$ for each $\beta \in R$.

- We say that $T(\beta)$ is an *analytic family* if and only if for every $\beta_0 \in R$, there is a $\gamma_0 \in \rho(T(\beta_0))$ such that $\gamma_0 \in \rho(T(\beta))$ for β near β_0 and $(T(\beta)-\gamma_0)^{-1}$ is an analytic operator-valued function of β near β_0.
- We say that $T(\beta)$ is an *analytic family of type (A)* if and only if
  (1) the operator domain $D(T(\beta))$ of $T(\beta)$ is some set D independent of β;
  (2) for each $\phi \in D$, $T(\beta)\phi$ is a vector-valued analytic function of β.

REMARK C.3. *The number γ_0 in the above definition plays no special role.*

One of the main properties of the analytic families of operators is clarified by the following theorem.

THEOREM C.4 (Kato-Rellich Theorem). *Let $T(\beta)$ be an analytic family. Let λ_0 be a non-degenerate discrete eigenvalue of $T(\beta_0)$. Then, for β near β_0:*

- *there is exactly one point $\lambda(\beta)$ of $\sigma(T(\beta))$ near λ_0 and this point is isolated and non-degenerate;*
- *$\lambda(\beta)$ is an analytic function of β and has a corresponding analytic eigenvector $\phi(\beta)$.*

Moreover, if $T(\beta)$ is self-adjoint for $\beta - \beta_0$ real, then $\phi(\beta)$ can be chosen to be normalized for $\beta - \beta_0$ real.

The following theorem gives a simple criterion for a family to be type(A).

THEOREM C.5. *Let H_0 be a closed operator with nonempty resolvent set. Define $H_0 + \beta V$ on $D(H_0) \cap D(V)$. Then $H_0 + \beta V$ is an analytic family of type (A) if and only if V is H_0-bounded.*

The main advantage of having an analytic family of closed operators, in particular of a family of type (A), is that it guarantees the existence of an analytic extension of the eigenvalues. In particular the following theorem holds.

THEOREM C.6. *Let $H_0 + \beta V$ be an analytic family of type (A) in a region R. Then if $0 \in R$ and E_0 is an isolated non-degenerate eigenvalue of H_0, then there is a unique point $E(\beta)$ of $\sigma(H_0 + \beta V)$ near E_0 when $|\beta|$ is small which is an isolated non-degenerate eigenvalue. Moreover $E(\beta)$ is analytic near $\beta = 0$.*

The convergence radius can be estimated by means of the following theorem.

THEOREM C.7. *Suppose that $||V\phi|| \leq a||H_0\phi|| + b||\phi||$. Let H_0 be self-adjoint with an unperturbed isolated, non-degenerate eigenvalue λ_0. Define*

$$\epsilon := \epsilon(\lambda_0) := \frac{1}{2}\mathrm{dist}(\lambda_0, \sigma(H_0) \setminus \{\lambda_0\}) \tag{C.1}$$

and

$$r(a, b, \lambda_0, \epsilon) = [a + \epsilon^{-1}[b + a(|\lambda_0| + \epsilon)]]^{-1}. \tag{C.2}$$

Then the eigenvalue $\lambda(\beta)$ of $H_0 + \beta V$ near λ_0 is analytic at least in the circle of radius $r(a, b, \lambda_0, \epsilon)$.

A huge simplification of the general theory can be achieved in presence of a self-adjoint analytic family of operator.

Let $T(\beta)$ be an analytic family of operators for β in a domain $R \subseteq \mathbb{C}$ symmetric with respect to the real axis. Suppose that

(1) $T(\beta)$ densely defined for all $\beta \in R$,

(2) $T(\beta)^* = T(\overline{\beta})$.

Then we call $T(\beta)$ a *self-adjoint analytic family*.

REMARK C.8. *It is clear from this definition that for all $\beta \cap R$, $T(\beta)$ is a closed self-adjoint operator.*

If $T(\beta)$ is a self-adjoint analytic family on a domain R containing 0, any isolated eigenvalue λ of $T(0)$ with finite multiplicity splits in one or more eigenvalues of $T(\beta)$ that are analytic at $\beta = 0$. Every $\lambda(\beta)$ of these analytic functions, with its eigenfunction, can be analytically extended along the real axis representing an eigenvalue of $T(\beta)$ with its eigenfunction and this stays true even when the graph of $\lambda(\beta)$ crosses the graph of another such eigenvalue, as long as the eigenvalue is isolated and has finite multiplicity. This feature is even stronger when the family is of type (A), in fact the following theorem holds [Kat95, Theorem 3.9, Chapter VII.3.5].

THEOREM C.9 (Rellich Theorem). *Let $T(\beta)$ be a self-adjoint analytic family of type (A) defined for β in a neighborhood of an interval I_0 of the real axis. Furthermore, let $T(\beta)$ have compact resolvent. Then all eigenvalues of $T(\beta)$ can be represented by functions which are analytic in I_0. More precisely, there is a sequence of scalar-valued functions $\lambda_n(\beta)$ and a sequence of vector-valued functions $\phi_n(\beta)$, all analytic on I_0, such that for $\beta \in I_0$, the $\lambda_n(\beta)$ represent all the repeated eigenvalues of $T(\beta)$ and the $\phi_n(\beta)$ form a complete orthonormal family of the associated eigenvectors of $T(\beta)$.*

REMARK C.10. ([Kat95, Remark 3.10, Chapter VII.3.5]) *Each $\lambda_n(\beta)$ is analytic in a complex neighborhood of I_0 but this neighborhood will depend on n, so that it is in general impossible to find a complex neighborhood in which* all *the $\lambda_n(\beta)$ exists.*

REMARK C.11. *The statements concerning analyticity are false for two-parameter perturbations. A standard counterexample is given by the following family of linear operators in $\mathbb{R}^2$*

$$T(\alpha, \beta) := \begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix}.$$

APPENDIX D

Generalized Prüfer transformation in the semi-classical limit

The method for establishing estimates is based on a modification of the Prüfer variables described in [Eas75, Chapter 4.1]. Consider a Sturm-Liouville differential equation on $[x_1, x_2]$ of the form

$$(C(x)y'(x))' + D(x)y(x) = 0 \tag{D.1}$$

in which $C(x)$ and $D(x)$ are real-valued, not necessarily periodic, differentiable and with piecewise continuous derivatives. Suppose also that $C(x)$ and $D(x)$ are positive and define $R(x) := \sqrt{C(x)D(x)}$. If y is a non-trivial real-valued solution of (D.1), we can write

$$R(x)y(x) = \rho(x)\sin(\theta(x)), \quad C(x)y'(x) = \rho(x)\cos(\theta(x)), \tag{D.2}$$

where

$$\rho(x) := \sqrt{R^2(x)y^2(x) + C^2(x)y'^2(x)},$$
$$\theta(x) := \arctan\left(\frac{R(x)y(x)}{C(x)y'(x)}\right).$$

Up to now $\theta(x)$ is defined as a continuous function of x only up to a multiple of 2π, to solve this problem we select a point $a_0 \in [x_1, x_2]$ and we stipulate that $-\pi \leq \theta(a_0) < \pi$. Moreover, if $y(a_0) \geq 0$, we have by (D.1) that

$$0 \leq \theta(a_0) < \pi. \tag{D.3}$$

LEMMA D.1. *Let $a_1 \in (a_0, x_2]$ and let the other definitions be the one given above. Then*

$$\theta'(x) = \left(\frac{D(x)}{C(x)}\right)^{1/2} + \frac{1}{4}\frac{(C(x)D(x))'}{C(x)D(x)}\sin(2\theta(x)). \tag{D.4}$$

If $y(x)$ has N zeroes in $(a_0, a_1]$ and $y(a_0) \geq 0$, then

$$N\pi \leq \theta(a_1) < (N+1)\pi. \tag{D.5}$$

PROOF. The theorem is proved in [Eas75, Chapter 4.1]. □

We want to apply (D.2) to equation (4.9.1). In particular we still keep ourselves a bit more general saying that we want to apply the transform to

$$h^2(p(x)y'(x))' + (\mu - V_1(x))y(x) = 0 \tag{D.6}$$

where $V_1(x)$ is not necessarily the potential $V(x)$ that we are analyzing but it does have the same period 2π. Since we are concerned with the limit $\mu \to \infty$ (parametrically depending on h), we can consider μ large enough to have $\mu - V_1(x) > 0$ in $[-\pi, \pi]$. In the new case (D.6) the two functions $\theta(x)$ and $\rho(x)$ will depend on μ and h as well as x. If we write $\theta(x)$ as $\theta_h(x,\mu)$, (D.4) becomes

$$\begin{aligned}\theta_h'(x,\mu) = &\frac{1}{h}\sqrt{\frac{\mu - V_1(x)}{p(x)}} \\ &+ \frac{1}{4}\frac{\mu\, p'(x) - (p(x)V_1(x))'}{(\mu - V_1(x))p(x)}\sin(2\theta_h(x,\mu)).\end{aligned} \tag{D.7}$$

A first consequence of (D.7) is that as $\mu \to \infty$

$$\theta_h'(x,\mu) = \frac{\mu^{\frac{1}{2}}}{h}\sqrt{\frac{1-\widetilde{V}_1(x)}{p(x)}} + O(1), \tag{D.8}$$

where $\widetilde{V}_1(x) := V_1(x)/\mu$. Moreover, if $y(x)$ has period 2π we have

$$\theta_h(\pi,\mu) - \theta_h(-\pi,\mu) = 2k\pi \tag{D.9}$$

for an integer k.

LEMMA D.2. *Let $f(x)$ be integrable over $[-\pi,\pi]$. Let c be a constant. Let $\theta_h(x,\mu)$ satisfy (D.7). Then*

$$\int_{-\pi}^{\pi} f(x)\sin\left(c\,\theta_h(x,\mu)\right)dx \longrightarrow 0$$

as $\mu \to \infty$ (and/or $h \searrow 0$). The same results holds with $\sin\left(c\,\theta_h(x,\mu)\right)$ replaced by $\cos\left(c\,\theta_h(x,\mu)\right)$.

PROOF. To keep the equations compact let's drop the μ dependence of $\theta_h(x,\mu)$ in the rest of the proof. Fix any $\epsilon > 0$. Let $g(x)$ be a continuously differentiable function such that

$$\int_{-\pi}^{\pi} |f(x) - g(x)|\,dx < \epsilon.$$

Then

$$\left|\int_{-\pi}^{\pi} f(x)\sin\left(c\,\theta_h(x)\right)dx\right| < \epsilon + \left|\int_{-\pi}^{\pi} g(x)\sin\left(c\,\theta_h(x)\right)dx\right|. \tag{D.10}$$

Define

$$G(x) := g(x)\sqrt{\frac{p(x)}{1-\widetilde{V}_1(x)}}.$$

Then by (D.8)

$$\begin{aligned}\int_{-\pi}^{\pi} g(x)\sin\left(c\,\theta_h(x)\right)dx &= \frac{h}{\mu^{\frac{1}{2}}}\int_{-\pi}^{\pi} G(x)\sin\left(c\,\theta_h(x)\right)\theta_h'(x)dx + O\left(\frac{h}{\mu^{\frac{1}{2}}}\right)\\ &= \frac{h}{c\,\mu^{\frac{1}{2}}}\Big(\left[G'(x)\cos\left(c\,\theta_h(x)\right)\right]_{-\pi}^{\pi}\\ &\quad - \int_{-\pi}^{\pi} G'(x)\cos\left(c\,\theta_h(x)\right)dx\Big) + O\left(\frac{h}{\mu^{\frac{1}{2}}}\right).\end{aligned}$$

Hence

$$\left|\int_{-\pi}^{\pi} g(x)\sin\left(c\,\theta_h(x)\right)dx\right| \le \frac{h}{\mu^{\frac{1}{2}}}K(\epsilon) < \epsilon$$

if μ is large enough, $K(\epsilon)$ being a number independent of μ. The lemma follows by the genericity of ϵ and (D.10). □

For $\mu \to \infty$, the first term on the right hand side of (D.7) can be rewritten expanding the square root as

$$\begin{aligned}\frac{1}{h}\sqrt{\frac{\mu - V_1(x)}{p(x)}} &= \frac{\mu^{\frac{1}{2}}}{h\sqrt{p(x)}}\left(1 - \frac{V_1(x)}{2\mu} + O\left(\mu^{-2}\right)\right)\\ &= \frac{\mu^{\frac{1}{2}}}{h\sqrt{p(x)}} - \frac{V_1(x)}{2h\mu^{\frac{1}{2}}\sqrt{p(x)}} + O\left(\frac{1}{h\mu^{\frac{3}{2}}}\right).\end{aligned}$$

Then, in the case $p(x) = 1$,

$$\theta_h'(x,\mu) = \frac{1}{h}\sqrt{\mu - V_1(x)} - \frac{1}{4}\frac{V_1'(x)}{\mu - V_1(x)}\sin(2\theta_h(x,\mu)), \tag{D.11}$$

and asymptotically as $\mu \to \infty$ the first term on the right hand side becomes

$$\frac{1}{h}\sqrt{\mu - V_1(x)} = \frac{\mu^{\frac{1}{2}}}{h} - \frac{V_1(x)}{2h\mu^{\frac{1}{2}}} + O\left(\frac{1}{h\mu^{\frac{3}{2}}}\right). \tag{D.12}$$

Let μ_n for $n \in \mathbb{N}$ denote the eigenvalues of the Sturm-Liouville periodic problem (D.1). We know from Appendix A that they exists, are discrete, at most doubly degenerate and accumulate at infinity. Then we have the following theorem.

Theorem D.3. *Let $p(x) = 1$. Then as $m \to \infty$, μ_{2m+1} and μ_{2m+2} both satisfy*

$$\sqrt{\mu} = (m+1)h + \frac{\int_{-\pi}^{\pi} V(x)dx}{4\pi(m+1)h} + o\left(\frac{1}{mh}\right).$$

Proof. Fix an $\epsilon > 0$. Le $V_1(x)$ be a continuously differentiable function with period 2π such that

$$V_1(x) \ge V(x) \tag{D.13}$$

and

$$\int_{-\pi}^{\pi} V_1(x)dx \le \epsilon + \int_{-\pi}^{\pi} V(x)dx. \tag{D.14}$$

Let $\mu_{1,n}$ denote the eigenvalue in the periodic problem associated with $V_1(x)$ (and with $p(x)=1$) and $\psi_{1,n}$ its eigenfunction. Then by Theorem A.8 and (D.13) we have

$$\mu_{1,n} \ge \mu_n.$$

We can assume that $\psi_{1,n}(-\pi)\ge 0$ and we apply the modified Prüfer transformation to $y(x)=\psi_{1,2m+1}(x)$ with $a_0=-\pi$ in (D.3). Now, from (D.3) and (D.9) we have

$$2k\pi \le \theta(\pi,\mu_{1,2m+1}) < (2k+1)\pi$$

for some integer k. For Theorem A.6 we know that $\psi_{1,2m+1}$ has $2(m+1)$ zeroes in $(-\pi,\pi]$, hence by (D.5) with $a_1=\pi$ we have $2k=2(m+1)$ and thus

$$\theta_h(\pi,\mu_{1,2m+1})-\theta(-\pi,\mu_{1,2m+1})=2(m+1)\pi. \tag{D.15}$$

Integrating (D.11) with $\mu=\mu_{1,2m+1}$ over $[-\pi,\pi]$ we obtain

$$2(m+1)\pi = \int_{-\pi}^{\pi} \frac{1}{h}\sqrt{\mu-V_1(x)}dx - \frac{1}{4}\int_{-\pi}^{\pi} \frac{V_1'(x)}{\mu-V_1(x)}\sin(2\theta_h(x,\mu))dx. \tag{D.16}$$

By Lemma D.2 the rightmost term is $o(\mu^{-1})$ as $m\to\infty$ (becoming $o(h/m^2)$ in (D.17) and thus being suppressed from the equation). For the first integral on the right we can use the binomial expansion as in (D.12). Thus (D.16) gives

$$2(m+1)\pi = \frac{\mu^{\frac{1}{2}}}{h}2\pi - \frac{\int_{-\pi}^{\pi}V_1(x)dx}{2h\mu^{\frac{1}{2}}} + O\left(\frac{1}{h\mu^{\frac{3}{2}}}\right)$$

that is

$$\mu-(m+1)h\sqrt{\mu}-\frac{1}{4\pi}\int_{-\pi}^{\pi}V_1(x)dx + O\left(\frac{1}{\mu}\right)=0.$$

Solving for μ one gets

$$\sqrt{\mu}=\frac{1}{2}\left((m+1)h+\sqrt{(m+1)^2h^2+\frac{1}{\pi}\int_{-\pi}^{\pi}V_1(x)dx+O(\mu^{-1})}\right).$$

Extracting $(m+1)h$ and using once more the binomial expansion one gets

$$\sqrt{\mu_{2m+1}}=(m+1)h+\frac{\int_{-\pi}^{\pi}V_1(x)dx}{4\pi(m+1)h}+O\left(\frac{1}{m^2h^2}\right). \tag{D.17}$$

Hence by (D.13), (D.14) and by the fact that ϵ is arbitrarily small

$$\sqrt{\mu_{2m+1}}\le(m+1)h+\frac{\int_{-\pi}^{\pi}V(x)dx}{4\pi(m+1)h}+o\left(\frac{1}{mh}\right).$$

The opposite inequality can be proved in the same way. The result for μ_{2m+1} holds in the same form using the fact that its eigenfunction must have $2(m+1)$ zeroes. $\square$

So far we have not used any differentiability-related property of V. Using the differentiability, we can improve incredibly the previous result.

THEOREM D.4. *Let $p(x) = 1$, let $r \in \mathbb{N}$, and let $\frac{d^r}{dx^r}V(x)$ exist and be piecewise continuous. Then μ_{2m+1} and μ_{2m+2} both satisfy*

$$\sqrt{\mu} = (m+1)h + \sum_{k=1}^{r+1} \frac{A_k}{(m+1)^k h^k} + O\left(\frac{1}{m^{r+2}h^{r+2}}\right) + o\left(\frac{1}{m^{r+1}h^{r-2}}\right)$$

where the A_k are independent of m and involve $q(x)$ and its derivatives up to order $r-1$. In particular,

$$A_1 = \frac{1}{4\pi}\int_{-\pi}^{\pi} V(x)dx,\ A_2 = 0,\ A_3 = \frac{1}{16\pi}\int_{-\pi}^{\pi} V^2(x)dx - A_1^2. \tag{D.18}$$

PROOF. We consider $V_1(x) = V(x)$ in (D.11), then $\mu_{1,n} = \mu_n$ and the case $r = 1$ correspond simply to (D.17). To deal with $r \geq 2$ we reconsider (D.16), which is now

$$2(m+1)\pi = \int_{-\pi}^{\pi} \frac{1}{h}\sqrt{\mu - V(x)}dx - \frac{1}{4}\int_{-\pi}^{\pi} \frac{V'(x)}{\mu - V(x)} \sin(2\theta_h(x,\mu))dx \tag{D.19}$$

and μ is μ_{2m+1} or μ_{2m+2}. By (D.11), with $V_1(x) = V(x)$, the second integral on the right in (D.19) is

$$\begin{aligned}\int_{\pi}^{\pi} \frac{hV'(x)}{(\mu - V(x))^{\frac{3}{2}}} &\left(\theta_h'(x,\mu) + \frac{1}{4}\frac{V_1'(x)}{\mu - V_1(x)}\sin(2\theta_h(x,\mu))\right)\sin(2\theta_h(x,\mu))dx \\ &= \frac{h}{2}\int_{-\pi}^{\pi}\left(\frac{d}{dx}\frac{V'(x)}{(\mu - V(x))^{\frac{3}{2}}}\right)\cos(2\theta_h(x,\mu))dx \\ &\quad + \frac{h}{8}\int_{-\pi}^{\pi}\frac{V'^2(x)}{(\mu - V(x))^{\frac{5}{2}}}dx \\ &\quad - \frac{h}{8}\int_{-\pi}^{\pi}\frac{V'^2(x)}{(\mu - V(x))^{\frac{5}{2}}}\cos(4\theta_h(x,\mu))dx \end{aligned}\tag{D.20}$$

after integrating by parts. The first term on the right here is $o\left(h\mu^{-\frac{3}{2}}\right)$ by Lemma D.2, the last is $o\left(h\mu^{-\frac{5}{2}}\right)$ for the same reason and the central one is $O\left(h\mu^{-\frac{5}{2}}\right)$. This, together with the binomial expansion of $\sqrt{\mu - V(x)}$ in the first term on the right of (D.19) gives

$$2(m+1)\pi = \frac{\mu^{\frac{1}{2}}}{h}2\pi - \frac{\int_{-\pi}^{\pi} V(x)dx}{2h\mu^{\frac{1}{2}}} - \frac{\int_{-\pi}^{\pi} V^2(x)dx}{8h\mu^{\frac{3}{2}}} + O\left(\frac{1}{h\mu^{\frac{5}{2}}}\right) + o\left(\frac{h}{\mu^{\frac{3}{2}}}\right) \tag{D.21}$$

To solve (D.21) for $\mu^{\frac{1}{2}}$ in terms of m, we write it as

$$\mu^{\frac{1}{2}} = M + \mu^{-\frac{1}{2}} A_1 + \mu^{-\frac{3}{2}}(A_3 - A_1^2) + O\left(\frac{1}{m^5 h^5}\right) + o\left(\frac{1}{m^3 h}\right) \tag{D.22}$$

where $M = h(m+1)$. Then, taking the reciprocals we obtain

$$\begin{aligned} \mu^{-\frac{1}{2}} &= M^{-1}\left(1 - \mu^{-\frac{1}{2}} A_1 M^{-1} + O(h^{-4} m^{-4})\right) \\ &= M^{-1} - M^{-3} A_1 + O(h^{-5} m^{-5}). \end{aligned} \tag{D.23}$$

And thus,

$$\mu^{-\frac{3}{2}} = M^{-3} + O(h^{-5} m^{-5}). \tag{D.24}$$

Substituting (D.23) and (D.24) into (D.22) give the result for $r = 2$.

To deal with $r = 3$, we introduce $\theta'(x,\mu)$ into the integrals in (D.20) involving $\cos(2\theta_h(x,\mu))$ and $\cos(4\theta_h(x,\mu))$, exactly as we did for (D.19). Then, if $\frac{d^3}{dx^3}V(x)$ exists and is piecewise continuous we can integrate by parts as before. The binomial expansions of $\frac{1}{h}\sqrt{\mu - V(x)}$ and $(\mu - V(x))^{-\frac{3}{2}}$ extends (D.21) to $o\left(h^2 \mu^{-\frac{5}{2}}\right) + O\left(h^{-1}\mu^{-\frac{7}{2}}\right)$ giving the result for $r = 3$. The process can be continued as long as $q(x)$ is sufficiently differentiable for the integration by parts to be carried out, and the theorem is proved. □

Remark D.5. *We can intend Theorem D.4 as the result of analytic perturbation theory of*

$$h^2(p(x)y'(x))' + y(x) = 0$$

(derived from (D.6)) in terms of the parameter $V_1(x)/\mu$. As a consequence we get $A_{2k} = 0$ for all $k \in \mathbb{N}$.

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