Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering
Department of Mathematics

Spectral Analysis of Two-Dimensional Quantum Models

DOCTORAL THESIS

September 2009

Ing. Matěj Tušek

Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering
Department of Mathematics

Spectral Analysis of Two-Dimensional Quantum Models

by

Ing. Matěj Tušek

Supervisor: Prof. Ing. Pavel Šťovíček, DrSc.

Consultants: Prof. Pierre Duclos
Prof. Vladimir Geyler

Dissertation submitted to
the Faculty of Nuclear Sciences and Physical Engineering of
Czech Technical University in Prague
in partial fulfillment of the requirements
for the degree of

Doctor of Philosophy

in the branch of study Mathematical Physics
of the study program Mathematical Engineering

Prague, September 2009

Contents

List of Notation

We use the bold face for vectors in $\mathbb{R}^n$ and we follow the convention that the appropriate standard face letter stands for the radius of a vector, e.g., $|\mathbf{p}| = p$. If a function f on $\mathbb{R}^n$ acts like a function of the radius only we abuse the notation a little and write $f(\mathbf{p}) = f(p)$. In the most cases, we follow the notation of the fundamental series by Reed and Simon [1, 2, 3, 4], and the notation of [5, 6] if special functions are concerned. For clarity, we attach the following table.

Symbol	**Meaning**
$A \dotplus B$	s.a. operator defined as a form sum of A and B according to the KLMN theorem (see [2, 7])
$A^\dagger$	operator adjoint to A
$\hat{f}$	(generalized) Fourier transform of a function f, we work with the unitary Fourier transform
$\check{f}$	inverse (generalized) Fourier transform of a function f
$\\|\cdot\\|_{1+}$	quadratic form norm
$\\|\cdot\\|_1$	Hilbert Schmidt (operator) norm
$\\|\cdot\\|_p$	norm on $L^p(\Omega, \mathrm{d}\mu)$
$\vert\vert\vert\cdot\vert\vert\vert$	norm on $\mathcal{H}^1(\Omega)$
$\partial\Omega$	boundary of a set Ω
$B_\delta(\mathbf{x})$	$B_\delta(\mathbf{x}) := \{\mathbf{y} \in \mathbb{R}^n : \ \vert\mathbf{x} - \mathbf{y}\vert < \delta\}$
$\mathbb{C}$	the complex numbers
$C_0^\infty(\bar{\Omega})$	linear space of smooth functions with $f\vert_{\partial\Omega} = 0$ and $f\vert_{\mathrm{ext}\Omega} = 0$ whose partial derivatives may be continuously extended to $\bar{\Omega}$
$C_C^\infty(\Omega)$	linear space of smooth functions with a compact support in Ω
dist	distance
Dom	domain
e.s.a.	abbreviation for 'essentially selfadjoint'
ext	exterior
${}_1F_1(a, b, z)$	Kummer confluent hypergeometric function
γ	Euler's constant, $\gamma \simeq 0.5772$
$\Gamma(z)$	gamma function
$H_n(z)$	Struve function
$H_\nu^{(i)}(z)$	Hankel function of the ith kind, $i = 1, 2$

Symbol	Meaning
$\mathcal{H}^m(\Omega)$	Sobolev space $H^{m,2}(\Omega)$
$\mathcal{H}^{m,k}(\Omega)$	Sobolev space
$\mathcal{H}_0^m(\Omega)$	closure of $C_C^\infty(\Omega)$ with respect to the norm of $\mathcal{H}^m(\Omega)$
$I_\nu(z)$	modified Bessel function of the first kind
Id	identity mapping
$\Im z$	imaginary part of a complex number z
int	interior
$J_\nu(z)$	Bessel function of the first kind
$K_\nu(z)$	modified Bessel function of the second kind
$K_\nu^\mu(\theta)$	spheroidal joining factor
$\ker A$	kernel of a linear mapping A
$L_n^{(m)}$	associated Laguerre polynomial
$L^p(\Omega, \mathrm{d}\mu)$	usual L^p space
$(L^\infty(\Omega))_\epsilon + L^2(\Omega)$	linear space of functions such that $f \in (L^\infty(\Omega))_\epsilon + L^2(\Omega) \Leftrightarrow \forall \epsilon :\ \exists$ decomposition $f = f_{0,\epsilon} + f_{1,\epsilon} :\ f_{0,\epsilon} \in L^2(\Omega) \wedge \|f_{1,\epsilon}\|_\infty < \epsilon$
$M(\nu, \mu, z)$	Whittaker function
$\mathbb{N}$	the positive integer numbers
$\mathbb{N}_0$	the non-negative integer numbers
$P_\nu^\mu(z)$	associated Legendre function of the first kind
$Ps_\nu^\mu(z, \theta)$	angular spheroidal function of the first kind
$\Psi(z)$	digamma function
$Q(A)$	form domain of an operator A
$Q_\nu^\mu(z)$	associated Legendre function of the second kind
$Qs_\nu^\mu(z, \theta)$	angular spheroidal function of the second kind
$\mathbb{R}$	the real numbers
$\mathbb{R}^+$	the positive real numbers
$\mathbb{R}^-$	the negative real numbers
Ran	range
Rank	rank=dimension of Ran
$\Re z$	real part of a complex number z
$\mathrm{Res}\, A$	resolvent set of an operator A
S^1	unit circle
$S_\nu^{\mu(j)}(z, \theta)$	radial spheroidal function of the jth kind
$\sigma(A)$	spectrum of an operator A
$\sigma_{ac,ess,pp}(A)$	absolutely continuous, essential, and pure point part of the spectrum of an operator A
s.a.	abbreviation for 'selfadjoint'
span	linear span
$\mathrm{Tr}\, A$	trace of an operator A
$W(\nu, \mu, z)$	Whittaker function
$\mathscr{W}(f, g)$	Wronskian of functions f and g

I. Introduction

This thesis is devoted to the spectral analysis of three non-relativistic quantum mechanical systems. The three systems have several characteristics in common. Two of them are two-dimensional and the last may be considered to be effectively two-dimensional too. All the systems are then rotationally symmetric which substantially simplifies our treatment since the partial wave decomposition may be involved. Furthermore, each of the system studied is a nontrivial modification of a very well known and fundamental quantum mechanical system, either the harmonic oscillator or the hydrogen atom. Namely, the thesis deals with the isotropic harmonic oscillator with the point interaction in the Lobachevsky plane, the two-dimensional hydrogen-like atom with the point interaction, and the hydrogen-like atom in a thin plane-parallel slab.

Chapter II is devoted to the study of the isotropic harmonic oscillator with the point interaction in the Lobachevsky plane. In the three-dimensional Euclidean space, the Hamiltonian of the isotropic harmonic oscillator with the point interaction was used to model the so-called quantum dot with a short-range impurity. The detailed analysis can be found in [8]. Therein, harmonic oscillator potential was used to introduce the confinement, and the point interaction (δ potential) was used to model the impurity. For a physical essence of quantum dots we refer reader to [9]. Just in brief, we may say that the quantum dots are nanostructures with a charge carriers confinement in all space directions. They have an atom-like energy spectrum which can be modified by adjusting geometric parameters of the dots as well as by the presence of an impurity.

An influence of the hyperbolic geometry on properties of quantum mechanical systems is a subject of continual theoretical interest for at least two decades. Numerous models have been studied so far, let us mention just few of them [10, 11, 12, 13]. Naturally, the quantum harmonic oscillator is one of the analyzed examples [14, 15]. It should be stressed, however, that the choice of an appropriate potential on the hyperbolic plane is ambiguous in this case, and several possibilities have been proposed in the literature. With our choice, that will be discussed bellow, we will introduce an appropriate Hamiltonian and derive an explicit formula for the corresponding Green function. In this sense, our model is solvable, and thus its properties may be of interest also from the mathematical point of view.

The spectral problem for the the model leads to a differential equation which is well known from the theory of special functions, namely, to the differential equation of spheroidal functions. It should be stressed, however, that the history of spheroidal functions is much more recent than that of more traditional special functions, like Bessel functions or Legendre polynomials. For example, one of the basic monographs devoted to spheroidal functions appeared only in the fifties of the last century [16], and the notation is still not fully uniform. One can compare, for example, [16] with [6]. Here we follow the latter source. Furthermore, there are values of parameters on which the spheroidal functions depend that have not been fully investigated. In this connection, note that the very values of parameters which are of interest for our model are treated in the textbooks in a rather marginal way. Effective numerical algorithms to evaluate spheroidal functions seem to be rather tedious to create and not available for all cases either. These circumstances make the numerical and qualitative analysis of the spectrum more complicated than one might expect at first glance. The numerical results were derived with the aid of the computer algebra system *Mathematica 6.0* which was the very last version at the time of the computation and the first version where the spheroidal functions were implemented. Those results comprise plots of the eigenvalues as functions of the curvature and plots of the respective eigenfunctions. Beside the numerical results, an asymptotic expansion of the eigenvalues as the curvature radius tends to infinity (the flat limit case) is given, although it was derived in a rather formal way.

The text of Chapter II is essentially a compilation of three successive papers on the topic, namely

- V. Geyler, P. Šťovíček, and M. Tušek. A quantum dot with impurity in the Lobachevsky plane. *Operator Theory: Advances and Applications*, 188:135-148. Birkhäuser Basel, 2009.
- P. Šťovíček and M. Tušek. On the harmonic oscillator on the Lobachevsky plane. *Russian J. Math. Phys.*, 14:493–497, 2007.
- P. Šťovíček and M. Tušek. On the spectrum of the quantum dot in the Lobachevsky plane. To appear in *Operator Theory: Advances and Applications*, 198:291-304. Birkhäuser Basel.

The problem and the model for the quantum dot with an impurity in the Lobachevsky plane was suggested by Vladimir Geyler, the coauthor of the first paper but primarily our dear colleague who, to our great sorrow, passed away very unexpectedly in 2007. It was a great pleasure and honor to collaborate with him.

In Chapter III, we examine the two-dimensional hydrogen atom. Let us point out that the word 'two-dimensional' only indicates that the motion of the electron around a positive point charge is constrained in the plane. In this case the central force between the electron and the nucleus is determined by the attractive Coulomb potential

$$V(\varrho) = -\frac{C}{\varrho}, \ \varrho = \sqrt{x^2 + y^2} \tag{I.1}$$

which we will call the two-dimensional Coulomb potential. A detailed analytic analysis of this system was given in [17]. The two-dimensional Coulomb Green function was derived even earlier in [18]. It is a recently reviewed fact that the Schrödinger equation for the two-dimensional hydrogen atom is separable and integrable in circular, parabolic, and elliptical coordinates [19]. The two-dimensional hydrogen atom was recently investigated in various non-trivial modifications: confined in a subset of the plane [20], in a strong magnetic field [21] or with spin-orbit Rashba interaction [22]. The problem was also reformulated in the momentum space in the source [23].

Our contribution to the problem involves setting the domain of definition of the respective Hamiltonian. To do so, selfadjoint extensions methods will be applied. As a result we shall obtain not only the Hamiltonian for the two-dimensional hydrogen atom itself but Hamiltonians with a one-center point interaction too. An explicit formula for the Green function of the two-dimensional hydrogen atom with the point interaction will be derived and the energy spectrum will be analyzed.

Let us remark that if a hydrogen atom is considered to be two-dimensional in the strict sense, i.e. that all fields including electromagnetic fields, the angular momentum, and the spin are confined to a plane, which will not be our case, then (I.1) is no longer referred as the two-dimensional Coulomb potential. Indeed, the Coulomb law may be derived from the first Maxwell's equation (Gauss's law for electrostatics) that states

$$\operatorname{div}\mathbf{E} = \sigma$$

where, in our case, σ stands for the (planar) charge density, $E_z = 0$, and the electric field is supposed to be rotationally symmetric. Integration of this equation over a disk of radius r together with application of Green's theorem gives the following result for the potential

$$V(r) = const.\, \log r.$$

The Schrödinger equation for this potential was studied in [24]. The spectrum was shown to be purely discrete and bounded bellow. Nevertheless, for a quantitative determination of the eigenvalues, numerical methods had to be involved.

Chapter IV is devoted to the study of the last system, the hydrogen atom in a thin plane-parallel slab of the width a. The problem and the respective model was suggested by Pierre Duclos from Universite du Sud, Toulon. We constrain the atom in the slab simply by an appropriate choice of the domain of definition, namely we set the domain to be $\mathcal{H}_0^1(\Omega_a) \cap \mathcal{H}^2(\Omega_a) \subset L^2(\Omega_a)$. This choice, in principle, corresponds to the Dirichlet boundary condition on the parallel planes. The resulting Hamiltonian seems to be resistant to a direct analytic treatment. Nevertheless, our results implies that it is possible to turn attention to a two-dimensional model described by the so-called effective Hamiltonian.

The adjective 'effective' should be understood in the following way: the eigenvalues (at least these at a bottom of the spectrum) of the exact atomic Hamiltonian tend to the eigenvalues of the effective one as $a \to 0$. The effective Hamiltonian is a Schrödinger operator acting on a Hilbert space that is isomorphic to $L^2(\mathbb{R}^2)$ but its potential part is rather complicated and the respective model is still barely solvable. However, we have proved that the norm resolvent limit of the effective Hamiltonian as $a \to 0$ is nothing but the two-dimensional hydrogen atom Hamiltonian (or shortly Coulomb Hamiltonian) plus the energy of the lowest transversal mode. The latter model is exactly solvable as is demonstrated in Chapter III. Consequently, we will use an exact knowledge of the eigenvalues of the two-dimensional Coulomb Hamiltonian to approximate the eigenvalues of the original exact Hamiltonian. Moreover, we will set the rate and the accuracy of this approximation as $a \to 0$, and compute several terms in a perturbation expansion for the lowest eigenvalue of the effective Hamiltonian. Note that the effective Hamiltonian is not holomorphic in a zero neighborhood of the complex a-plane, as there are powers of $\log a$ in the expansion.

From the perspective of future research, the last system studied seems very promising. First of all, one may look for a Hamiltonian that approximates the effective Hamiltonian better than the Coulomb one but is still solvable. For sure, this Hamiltonian is not the Coulomb one with a one-center point interaction since the addition of the point interaction results in the appearance of an eigenvalue below the spectrum of the pure Coulomb Hamiltonian (see Section III.2.5) whereas the spectrum of the effective Hamiltonian (minus the energy of the lowest transversal mode) always lies above it. Next, generalizations of the system are of interest. Natural question arises whether the norm resolvent limit of the Hamiltonian of a multi-electron atom in a thin slab is just the Hamiltonian of the two-dimensional analogue. It seems so, since the methods and proofs for the single-electron case may be modified to be applicable in the multi-electron case too. One may also ask what happens with the energy spectrum if a slab of a different shape is considered.

For the reader's convenience and a transparency of the document, we supply several appendices. Appendix A comprises plots of the functions that are outputs of our numerical computations. In Appendix B, we not only supply several auxiliary results but we also review and extend some of the standard facts on the Dirichlet Schrödinger operators. Appendix C is devoted exclusively to the spheroidal functions. It contains basic definitions and results which are necessary for our approach.

II. Quantum Dot with Impurity in the Lobachevsky Plane

II.1 Model

Denote by (ϱ, ϕ), $0 \leqslant \varrho < \infty$, $0 \leqslant \phi < 2\pi$, the geodesic polar coordinates in the Lobachevsky plane. Then the metric tensor is diagonal and reads

$$(g_{ij}) = \operatorname{diag}\Big(1, a^2 \sinh^2 \frac{\varrho}{a}\Big)$$

where a, $0 < a < \infty$, denotes the so called curvature radius which is related to the scalar curvature by the formula $R = -2/a^2$. Furthermore, the volume form equals $dV = a \sinh(\varrho/a) \mathrm{d}\varrho \wedge \mathrm{d}\phi$. The Hamiltonian for a free particle of mass $m = 1/2$ takes the form

$$H^0 = -\left(\Delta_{LB} + \frac{1}{4a^2}\right) = -\frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} g^{ij} \frac{\partial}{\partial x^j} - \frac{1}{4a^2}$$

where Δ_{LB} is the Laplace-Beltrami operator and $g = \det g_{ij}$. We have set $\hbar = 1$.

The choice of a potential modeling the confinement is ambiguous. We naturally require that the potential takes the standard form of the quantum dot potential in the flat limit ($a \to \infty$). This is to say that, in the limiting case, it becomes the potential of the isotropic harmonic oscillator $V_\infty(\varrho) = \frac{1}{4}\omega^2\varrho^2$. However, this condition clearly does not specify the potential uniquely. Having the freedom of choice let us discuss the following two possibilities:

$$\text{a)} \quad V_a(\varrho) = \tfrac{1}{4}\, a^2\omega^2 \tanh^2 \tfrac{\varrho}{a}, \tag{II.1}$$

$$\text{b)} \quad U_a(\varrho) = \tfrac{1}{4}\, a^2\omega^2 \sinh^2 \tfrac{\varrho}{a}. \tag{II.2}$$

Potential V_a is the same as that proposed in [25] for the classical harmonic oscillator in the Lobachevsky plane. With this choice, it has been demonstrated in [25] that the model is superintegrable, i.e., there exist three functionally independent constants of motion. Let us remark that this potential is bounded, and so it represents a bounded perturbation to the free Hamiltonian. On the other hand, the potential U_a is unbounded. Moreover, as shown below, the stationary Schrödinger equation for this potential leads, after the partial wave decomposition, to the differential equation of spheroidal functions. In what follows, we concentrate exclusively on case b).

The impurity is modeled by a δ-potential which is introduced with the aid of s.a. extensions and is determined by boundary conditions at the base point. We restrict ourselves to the case when the impurity is located in the center of the dot ($\varrho = 0$). Thus we start from the following symmetric operator:

$$H = -\left(\frac{\partial^2}{\partial\varrho^2} + \frac{1}{a}\coth\Big(\frac{\varrho}{a}\Big)\frac{\partial}{\partial\varrho} + \frac{1}{a^2}\sinh^{-2}\Big(\frac{\varrho}{a}\Big)\frac{\partial^2}{\partial\varphi^2} + \frac{1}{4a^2}\right) + \frac{1}{4}\,a^2\omega^2\sinh^2\Big(\frac{\varrho}{a}\Big),$$
$$\operatorname{Dom} H = C_C^\infty((0,\infty)\times S^1) \subset L^2\left((0,\infty)\times S^1, a\,\sinh\Big(\frac{\varrho}{a}\Big)\,\mathrm{d}\varrho\,\mathrm{d}\varphi\right). \tag{II.3}$$

II.2 Selfadjoint extensions

Substituting $\xi = \cosh(\varrho/a)$ we obtain

$$H = \frac{1}{a^2}\left[(1-\xi^2)\frac{\partial^2}{\partial\xi^2} - 2\xi\frac{\partial}{\partial\xi} + (1-\xi^2)^{-1}\frac{\partial^2}{\partial\varphi^2} + \frac{a^4\omega^2}{4}(\xi^2-1) - \frac{1}{4}\right] =: \frac{1}{a^2}\tilde{H},$$
$$\operatorname{Dom} H = C_C^\infty((1,\infty)\times S^1) \subset L^2\left((1,\infty)\times S^1, a^2\mathrm{d}\xi\,\mathrm{d}\varphi\right). \tag{II.4}$$

Using the rotational symmetry which amounts to a Fourier transform in the variable φ, $\tilde{H}$ may be decomposed into a direct sum as follows

$$\tilde{H} = \bigoplus_{m=-\infty}^{\infty} \tilde{H}_m,$$
$$\tilde{H}_m = -\frac{\partial}{\partial\xi}\left((\xi^2-1)\,\frac{\partial}{\partial\xi}\right) + \frac{m^2}{\xi^2-1} + \frac{a^4\omega^2}{4}\,(\xi^2-1) - \frac{1}{4},$$
$$\operatorname{Dom}\tilde{H}_m = C_C^\infty(1,\infty) \subset L^2((1,\infty),\mathrm{d}\xi).$$

Note that $\tilde{H}_m$ is a Sturm-Liouville operator.

Proposition II.1 *$\tilde{H}_m$ is e.s.a. for $m \neq 0$, $\tilde{H}_0$ has deficiency indices* $(1,1)$.

Proof. The operator $\tilde{H}_m$ is symmetric and semibounded, and so the deficiency indices are equal. If we set

$$\mu = |m|,\ 4\theta = -\frac{a^4\omega^2}{4},\ \lambda = -z - \frac{1}{4},$$

then the eigenvalue equation

$$\left(-\frac{\partial}{\partial\xi}\left((\xi^2-1)\,\frac{\partial}{\partial\xi}\right) + \frac{m^2}{\xi^2-1} + \frac{a^4\omega^2}{4}\,(\xi^2-1) - \frac{1}{4}\right)\psi = z\psi \tag{II.5}$$

takes the standard form of the differential equation of spheroidal functions (C.1). According to Chapter 3.12, Satz 5 in [16], for $\mu = m \in \mathbb{N}_0$ a fundamental system $\{y_{\mathrm{I}},\ y_{\mathrm{II}}\}$ of solutions to equation (II.5) exists such that

$$y_{\mathrm{I}}(\xi) = (1-\xi)^{m/2}\,\mathfrak{P}_1(1-\xi), \quad \mathfrak{P}_1(0) = 1,$$
$$y_{\mathrm{II}}(\xi) = (1-\xi)^{-m/2}\mathfrak{P}_2(1-\xi) + A_m\,y_{\mathrm{I}}(\xi)\log(1-\xi),$$

where, for $|\xi-1|<2$, $\mathfrak{P}_1$ and $\mathfrak{P}_2$ are analytic functions in ξ, λ, θ; and A_m is a polynomial in λ and θ of total order m with respect to λ and $\sqrt{\theta}$; $A_0=-1/2$.

Suppose that $z\in\mathbb{C}\backslash\mathbb{R}$. For $m=0$, every solution to (II.5) is square integrable near $\xi=1$; while for $m\neq 0$, y_{I} is the only one solution, up to a factor, which is square integrable in a neighborhood of 1. On the other hand, by a classical analysis due to Weyl, there exists exactly one linearly independent solution to (II.5) which is square integrable in a neighborhood of ∞, see Theorem XIII.6.14 in [26]. In the case of $m=0$ this obviously implies that the deficiency indices are $(1,1)$. If $m\neq 0$ then, by Theorem XIII.2.30 in [26], the operator $\tilde{H}_m$ is e.s.a. $\square$

Define the maximal operator associated to the formal differential expression

$$L=-\frac{\partial}{\partial\xi}\left((\xi^2-1)\frac{\partial}{\partial\xi}\right)+\frac{a^4\omega^2}{4}(\xi^2-1)-\frac{1}{4}$$

as follows

$$\begin{aligned}\mathrm{Dom}\ \tilde{H}_{max}=&\Big\{f\in L^2((1,\infty),\mathrm{d}\xi):\ f,f'\in AC((1,\infty)),\\&-\frac{\partial}{\partial\xi}\left((\xi^2-1)\,\frac{\partial f}{\partial\xi}\right)+\frac{a^4\omega^2}{4}\,(\xi^2-1)f\in L^2((1,\infty),\mathrm{d}\xi)\Big\},\\ \tilde{H}_{max}f=&\,Lf.\end{aligned}$$

According to Theorem 8.22 in [27], $\tilde{H}_{max}=\tilde{H}_0^{\dagger}$.

Proposition II.2 *Let $\kappa\in(-\infty,\infty\,]$. The operator $\tilde{H}_0(\kappa)$ defined by the formulae*

$$\mathrm{Dom}\ \tilde{H}_0(\kappa)=\Big\{f\in\mathrm{Dom}\ \tilde{H}_{max}:\ f_1=\kappa f_0\Big\}\,,\ \tilde{H}_0(\kappa)f=\tilde{H}_{max}f,$$

where

$$f_0:=-4\pi a^2\lim_{\xi\to 1+}\frac{f(\xi)}{\log(2a^2(\xi-1))}\,,\ f_1:=\lim_{\xi\to 1+}f(\xi)+\frac{1}{4\pi a^2}\,f_0\log\big(2a^2(\xi-1)\big),$$

is a s.a. extension of $\tilde{H}_0$. There are no other s.a. extensions of $\tilde{H}_0$.

Proof. The methods to treat δ like potentials are now well established [28]. Here we follow an approach described in [29], and we refer to this source also for the terminology and notations. Near the point $\xi=1$, each $f\in\mathrm{Dom}\ \tilde{H}_{max}$ has the asymptotic behavior

$$f(\xi)=f_0\,F(\xi,1)+f_1+o(1)\quad\text{as }\xi\to 1+$$

where $f_0,f_1\in\mathbb{C}$ and $F(\xi,\xi')$ is the divergent part of the Green function for the Friedrichs extension of $\tilde{H}_0$. By formula (II.11) which is derived below,

$$F(\xi,1)=-1/(4\pi a^2)\log\big(2a^2(\xi-1)\big)\,.$$

Proposition 1.37 in [29] states that $(\mathbb{C},\Gamma_1,\Gamma_2)$, with $\Gamma_1 f = f_0$ and $\Gamma_2 f = f_1$, is a boundary triple for $\tilde{H}_{max}$.

According to Theorem 1.12 in [29], there is a one-to-one correspondence between all s.a. linear relations κ in $\mathbb{C}$ and all s.a. extensions of $\tilde{H}_0$ given by $\kappa \longleftrightarrow \tilde{H}_0(\kappa)$ where $\tilde{H}_0(\kappa)$ is the restriction of $\tilde{H}_{max}$ to the domain of vectors $f \in \mathrm{Dom}\,\tilde{H}_{max}$ satisfying

$$(\Gamma_1 f, \Gamma_2 f) \in \kappa. \tag{II.6}$$

Every s.a. relation in $\mathbb{C}$ is of the form $\kappa = \mathbb{C}v \subset \mathbb{C}^2$ for some $v \in \mathbb{R}^2$, $v \neq 0$. If (with some abuse of notation) $v = (1,\kappa)$, $\kappa \in \mathbb{R}$, then relation (II.6) means that $f_1 = \kappa f_0$. If $v = (0,1)$ then (II.6) means that $f_0 = 0$ which may be identified with the case $\kappa = \infty$. □

Remark II.3 *Let $\mathfrak{q}_0$ be the closure of the quadratic form associated to the semibounded symmetric operator $\tilde{H}_0$. Only the s.a. extension $\tilde{H}_0(\infty)$ has the property that all functions from its domain have no singularity at the point $\xi = 1$ and belong to the form domain of $\mathfrak{q}_0$. It follows that $\tilde{H}_0(\infty)$ is the Friedrichs extension of $\tilde{H}_0$ (see, for example, Theorem X.23 in [2] or Theorems 5.34 and 5.38 in [27]).*

II.3 Spectral Analysis

II.3.1 Green function for the unperturbed Hamiltonian

Let us consider the Friedrichs extension of the operator $\tilde{H}$ in $L^2\big((1,\infty)\times S^1, \mathrm{d}\xi\,\mathrm{d}\varphi\big)$ which was introduced in (II.4). The resulting s.a. operator is in fact the Hamiltonian for the impurity free case, let us denote it $\tilde{H}(\infty)$. The corresponding Green function $\mathcal{G}_z$ is the generalized kernel of the Hamiltonian, and it should obey the equation

$$(\tilde{H}(\infty)-z)\mathcal{G}_z(\xi,\varphi;\xi',\varphi') = \delta(\xi-\xi')\delta(\varphi-\varphi') = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}\delta(\xi-\xi')\mathrm{e}^{im(\varphi-\varphi')}.$$

If we suppose $\mathcal{G}_z$ to be of the form

$$\mathcal{G}_z(\xi,\varphi;\xi',\varphi') = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}\mathcal{G}_z^m(\xi,\xi')\mathrm{e}^{im(\varphi-\varphi')}, \tag{II.7}$$

then, for all $m \in \mathbb{Z}$,

$$(\tilde{H}_m(\infty)-z)\mathcal{G}_z^m(\xi,\xi') = \delta(\xi-\xi'), \tag{II.8}$$

where $\tilde{H}_m(\infty)$, $m \in \mathbb{Z}\backslash\{0\}$, is nothing but the closure of $\tilde{H}_m$. From now on, the closure of an e.s.a. operator will be denoted by the same latter as the operator itself.

Let us consider an arbitrary fixed ξ', and set

$$\mu = m,\ 4\theta = -\frac{a^4\omega^2}{4},\ \lambda = -z-\frac{1}{4}.$$

Then for all $\xi \neq \xi'$, the equation (II.8) takes the standard form of the differential equation of spheroidal functions (C.1). As one can see from (C.8), the solution which is square integrable near infinity equals $S_\nu^{|m|(3)}(\xi, -a^4\omega^2/16)$. Furthermore, the solution which is square integrable near $\xi = 1$ equals $Ps_\nu^{|m|}(\xi, -a^4\omega^2/16)$ as one may verify with the aid of the asymptotic formula

$$P_\nu^m(\xi) \sim \frac{\Gamma(\nu + m + 1)}{2^{m/2}\, m!\, \Gamma(\nu - m + 1)}\, (\xi - 1)^{m/2} \quad \text{as } \xi \to 1+, \text{ for } m \in \mathbb{N}_0.$$

We conclude that the mth partial Green function equals

$$\mathcal{G}_z^m(\xi, \xi') = -\frac{1}{(\xi^2 - 1)\mathscr{W}(Ps_\nu^{|m|}, S_\nu^{|m|(3)})}\, Ps_\nu^{|m|}\left(\xi_<, -\frac{a^4\omega^2}{16}\right) S_\nu^{|m|(3)}\left(\xi_>, -\frac{a^4\omega^2}{16}\right) \qquad \text{(II.9)}$$

where the symbol $\mathscr{W}(Ps_\nu^{|m|}, S_\nu^{|m|(3)})$ denotes the Wronskian, and $\xi_<$, $\xi_>$ are respectively the smaller and the greater of ξ and ξ'. By the general Sturm-Liouville theory, the factor $(\xi^2 - 1)\mathscr{W}(Ps_\nu^{|m|}, S_\nu^{|m|(3)})$ is constant. However the value of this constant can not be given as there is no explicit expression for the Wronskian. Nevertheless we will be able to compute the Krein Q-function without this knowledge, just by application of Theorem II.1.

Notice that since $\mathcal{G}_z^m = \mathcal{G}_z^{-m}$, the decomposition (II.7) may be simplified to

$$\mathcal{G}_z(\xi, \varphi; \xi', \varphi') = \frac{1}{2\pi}\, \mathcal{G}_z^0(\xi, \xi') + \frac{1}{\pi} \sum_{m=1}^{\infty} \mathcal{G}_z^m(\xi, \xi') \cos\left[m(\varphi - \varphi')\right]. \qquad \text{(II.10)}$$

II.3.2 Krein Q-function

The Krein Q-function plays a crucial role in the spectral analysis of impurities. It is defined at a point of the configuration space as the regularized Green function evaluated at this point. Here we deal with the impurity located in the center of the dot ($\xi = 1$, φ arbitrary), and so, by definition,

$$Q(z) := \mathcal{G}_z^{reg}(1, 0; 1, 0).$$

Due to the rotational symmetry,

$$\mathcal{G}_z(\xi) := \mathcal{G}_z(\xi, \varphi; 1, 0) = \mathcal{G}_z(\xi, \varphi; 1, \varphi) = \mathcal{G}_z(\xi, 0; 1, 0) = \frac{1}{2\pi}\, \mathcal{G}_z^0(\xi, 1),$$

and hence

$$(\tilde{H}_0(\infty) - z)\mathcal{G}_z(\xi) = 0, \quad \text{for } \xi \in (1, \infty).$$

Let us note that from the explicit formula (II.9), one can deduce that the coefficients $\mathcal{G}_z^m(\xi, 1)$ in the series in (II.10) vanish for $m \in \mathbb{N}$. The solution to this equation is

$$\mathcal{G}_z(\xi) \propto S_\nu^{0(3)}\left(\xi, -\frac{a^4\omega^2}{16}\right).$$

The constant of proportionality can be determined with the aid the following theorem which we reproduce from [29].

Theorem II.1 *Let* $\operatorname{dist}(x,y)$ *denote the geodesic distance between points* x, y *of a two-dimensional manifold* X *of bounded geometry. Let*

$$U \in \mathcal{P}(X) := \Big\{U : \; U_+ := \max\{U,0\} \in L^{p_0}_{loc}(X), \; U_- := \max\{-U,0\} \in \sum_{i=1}^{n} L^{p_i}(X)\Big\}$$

for an arbitrary $n \in \mathbb{N}$ *and* $2 \leqslant p_i \leqslant \infty$. *Then the Green function* $\mathcal{G}_U$ *of the Schrödinger operator* $H_U = -\Delta_{LB} + U$ *has the same on-diagonal singularity as that for the Laplace-Beltrami operator itself, i.e.,*

$$\mathcal{G}_U(\zeta; x, y) = \frac{1}{2\pi} \log \frac{1}{\operatorname{dist}(x,y)} + \mathcal{G}_U^{reg}(\zeta; x, y)$$

where $\mathcal{G}_U^{reg}$ *is continuous on* $X \times X$.

Let us denote by $\mathcal{G}_z^{H(\infty)}$ and $Q^{H(\infty)}(z)$ the Green function and the Krein Q-function for $H(\infty)$, respectively. Since $\tilde{H}(\infty) = a^2 H(\infty)$ and $(\tilde{H}(\infty) - z)\mathcal{G}_z = \delta$, we have

$$\mathcal{G}_z^{H(\infty)}(\xi, \varphi; \xi', \varphi') = a^2 \mathcal{G}_{a^2 z}(\xi, \varphi; \xi', \varphi'), \; Q^{H(\infty)}(z) = a^2 Q(a^2 z).$$

One may verify that

$$\log \operatorname{dist}(\varrho, 0; \vec{0}) = \log \varrho = \log(a \operatorname{arg\,cosh} \xi) = \frac{1}{2} \log\big(2a^2(\xi - 1)\big) + O(\xi - 1)$$

as $\varrho \to 0+$ or, equivalently, $\xi \to 1+$. Finally, for the divergent part

$$F(\xi, \xi') := \mathcal{G}_z(\xi, \varphi; \xi', \varphi) - \mathcal{G}_z^{reg}(\xi, \varphi; \xi', \varphi) = \mathcal{G}_z(\xi, 0; \xi', 0) - \mathcal{G}_z^{reg}(\xi, 0; \xi', 0)$$

of the Green function $\mathcal{G}_z$ we obtain the expression

$$F(\xi, 1) = -\frac{1}{4\pi a^2} \log\big(2a^2(\xi - 1)\big). \tag{II.11}$$

From the above discussion, it follows that the Krein Q-function depends on the coefficients α, β in the asymptotic expansion

$$S_\nu^{0(3)}\left(\xi, -\frac{a^4\omega^2}{16}\right) = \alpha \log(\xi - 1) + \beta + o(1) \quad \text{as } \xi \to 1+, \tag{II.12}$$

and equals

$$Q(z) = -\frac{\beta}{4\pi a^2 \alpha} + \frac{\log(2a^2)}{4\pi a^2}. \tag{II.13}$$

To determine α, β we need relation (C.10) for the radial spheroidal function of the third kind. For ν and $\nu + 1/2$ being non-integer, formula (C.12) implies that

$$\begin{aligned} S_\nu^{0(1)}(\xi, \theta) &= \frac{\sin(\nu\pi)}{\pi} \,\mathrm{e}^{-i\pi(\nu+1)} K_\nu^0(\theta) Qs_{-\nu-1}^0(\xi, \theta), \\ S_{-\nu-1}^{0(1)}(\xi, \theta) &= \frac{\sin(\nu\pi)}{\pi} \,\mathrm{e}^{i\pi\nu} K_{-\nu-1}^0(\theta) Qs_\nu^0(\xi, \theta). \end{aligned} \tag{II.14}$$

Applying the symmetry relation (C.5) for expansion coefficients, we derive that

$$\begin{aligned} Qs^0_{-\nu-1}(\xi,\theta) &= \sum_{r=-\infty}^{\infty} (-1)^r a^0_{-\nu-1,r}(\theta) Q^0_{-\nu-1+2r}(\xi) \\ &= \sum_{r=-\infty}^{\infty} (-1)^r a^0_{\nu,r}(\theta) Q^0_{-\nu-1-2r}(\xi). \end{aligned}$$

Using the following asymptotic formulae (see [6])

$$Q^0_\nu(\xi) = -\frac{1}{2}\log\frac{\xi-1}{2} + \Psi(1) - \Psi(\nu+1) + O((\xi-1)\log(\xi-1))$$

together with the series expansion in (C.11) and formulae (II.14), we deduce that, as $\xi \to 1+$,

$$\begin{aligned} S^{0(1)}_\nu(\xi,\theta) \sim &-\frac{\sin(\nu\pi)}{\pi}\, \mathrm{e}^{-i\pi(\nu+1)} K^0_\nu(\theta) \\ &\times \left[s^0_\nu(\theta)^{-1}\left(\frac{1}{2}\log\frac{\xi-1}{2} - \Psi(1) + \pi\cot(\nu\pi)\right) + \Psi s_\nu(\theta)\right], \\ S^{0(1)}_{-\nu-1}(\xi,\theta) \sim &-\frac{\sin(\nu\pi)}{\pi}\, \mathrm{e}^{i\pi\nu} K^0_{-\nu-1}(\theta) \\ &\times \left[s^0_\nu(\theta)^{-1}\left(\frac{1}{2}\log\frac{\xi-1}{2} - \Psi(1)\right) + \Psi s_\nu(\theta)\right], \end{aligned}$$

where the coefficients $s^\mu_n(\theta)$ are introduced in (C.7),

$$\Psi s_\nu(\theta) := \sum_{r=-\infty}^{\infty} (-1)^r a^0_{\nu,r}(\theta)\Psi(\nu+1+2r),$$

and where we have made use of the following property of the digamma function: $\Psi(-z) = \Psi(z+1) + \pi\cot(\pi z)$.

We conclude that

$$S^{0(3)}_\nu(\xi,\theta) \sim \alpha\log(\xi-1) + \beta + O\left((\xi-1)\log(\xi-1)\right) \quad \text{as } \xi \to 1+, \tag{II.15}$$

where

$$\begin{aligned} \alpha &= \frac{i\tan(\nu\pi)}{2\pi s^0_\nu(\theta)}\left(\mathrm{e}^{i\pi\nu}K^0_{-\nu-1}(\theta) - \mathrm{e}^{-i\pi(2\nu+3/2)}K^0_\nu(\theta)\right), \\ \beta &= \alpha\left(-\log 2 - 2\Psi(1) + 2\Psi s_\nu(\theta) s^0_\nu(\theta)\right) + \mathrm{e}^{-2i\pi\nu} s^0_\nu(\theta)^{-1} K^0_\nu(\theta). \end{aligned} \tag{II.16}$$

Substitution for α, β into (II.13) yields

$$\begin{aligned} Q(z) = &-\frac{1}{4\pi a^2}\left(-\log 2 - 2\Psi(1) + 2\,\Psi s_\nu\!\left(-\frac{a^4\omega^2}{16}\right) s^0_\nu\!\left(-\frac{a^4\omega^2}{16}\right)\right) \\ &+ \frac{1}{2a^2\tan(\nu\pi)}\left(\mathrm{e}^{i\pi(3\nu+3/2)}\,\frac{K^0_{-\nu-1}(-\frac{a^4\omega^2}{16})}{K^0_\nu(-\frac{a^4\omega^2}{16})} - 1\right)^{-1} + \frac{\log(2a^2)}{4\pi a^2} \end{aligned} \tag{II.17}$$

where ν is chosen so that
$$\lambda_\nu^0\left(-\frac{a^4\omega^2}{16}\right) = -z - \frac{1}{4}\,. \tag{II.18}$$

For $\nu = n$ being an integer, we can immediately use the known asymptotic formulae for the spheroidal wave functions (see Section 16.12 in [6]) which give

$$\begin{aligned} S_n^{0(3)}(\xi,\theta) &= \frac{is_n^0(\theta)}{4\sqrt{\theta}K_n^0(\theta)}\,\log(\xi-1) - \frac{is_n^0(\theta)\log 2}{4\sqrt{\theta}K_n^0(\theta)} \\ &\quad + \frac{is_n^0(\theta)^2}{2\sqrt{\theta}K_n^0(\theta)}\sum_{2r\geqslant -n}(-1)^r a_{n,r}^0(\theta)h_{n+2r} + \frac{K_n^0(\theta)}{s_n^0(\theta)} + O(\xi-1), \end{aligned}$$

as $\xi \to 1+$. Here, $h_0 = 1, h_k = 1/1 + 1/2 + \ldots + 1/k$. By (II.13), one can calculate the Q-function in this case, too.

II.3.3 Green function for the perturbed Hamiltonian

The Green function of the Hamiltonian describing a quantum dot with an impurity is given by the Krein resolvent formula

$$\mathcal{G}_z^{H(\chi)}(\xi,\phi;\xi',\phi') = \mathcal{G}_z^{H(\infty)}(\xi,\phi;\xi',\phi') - \frac{1}{Q^{H(\infty)}(z)-\chi}\,\mathcal{G}_z^{H(\infty)}(\xi,0;1,0)\mathcal{G}_z^{H(\infty)}(1,0;\xi',0)$$

(recall that, due to the rotational symmetry, $\mathcal{G}_z^H(\xi,\phi;1,0) = \mathcal{G}_z^H(\xi,0;1,0)$). The parameter $\chi := a^2\kappa \in (-\infty,\infty\,]$ determines the corresponding s.a. extension $H(\chi)$ of H. In the physical interpretation, this parameter is related to the strength of the δ interaction. Recall that the value $\chi = \infty$ corresponds to the Friedrichs extension of H representing the case with no impurity.

II.3.4 General discussion on the spectrum

The unperturbed Hamiltonian $H(\infty)$ describes a harmonic oscillator in the Lobachevsky plane. As is well known (see, for example, [30]), for the confinement potential tends to infinity as $\varrho \to \infty$, the resolvent of $H(\infty)$ is compact, and the spectrum of $H(\infty)$ is discrete and semibounded. A similar observation about the basic spectral properties is also true for the operators $H(\chi)$ for any $\chi \in \mathbb{R}$ since, by the Krein resolvent formula, the resolvents for $H(\chi)$ and $H(\infty)$ differ by a rank one operator. Moreover, the multiplicities of eigenvalues of $H(\chi)$ and $H(\infty)$ may differ at most by ± 1 (see [27, Section 8.3]).

Let us denote by H_m, $m \in \mathbb{Z}$, the restriction of $H(\infty)$ to the eigenspace of the angular momentum with eigenvalue m. This means that $H_0 = a^{-2}\tilde{H}_0(\infty)$. From now on, if not otherwise stated, we will write only $\tilde{H}_0$ instead of $\tilde{H}_0(\infty)$ to unify the notation. For quite general reasons, the spectrum of H_m, for any m, is semibounded below, discrete and simple [27]. We denote the eigenvalues of H_m in ascending order by $E_{n,m}(a^2)$, $n \in \mathbb{N}_0$.

The spectrum of the total Hamiltonian $H(\chi)$, $\chi \neq \infty$, consists of two parts (in a full analogy with the Euclidean case [8]):

i. The first part is formed by those eigenvalues of $H(\chi)$ which belong, at the same time, to the spectrum of $H(\infty)$. More precisely, this part is exactly the union of eigenvalues of H_m for m running over $\mathbb{Z}\backslash\{0\}$. Their multiplicities are discussed below in Section II.3.8.

ii. The second part is formed by solutions to the equation

$$Q^{H(\infty)}(z) = \chi \tag{II.19}$$

with respect to the variable z. Let us denote them in ascending order by $\epsilon_n(a^2, \chi)$, $n \in \mathbb{N}_0$. These eigenvalues are sometimes called the point levels and their multiplicities are at least one. In more detail, $\epsilon_n(a^2, \chi)$ is a simple eigenvalue of $H(\chi)$ if it does not lie in the spectrum of $H(\infty)$, and this happens if and only if $\epsilon_n(a^2, \chi)$ does not coincide with any eigenvalue $E_{\ell,m}(a^2)$ for $\ell \in \mathbb{N}_0$ and $m \in \mathbb{Z}$, $m \neq 0$.

Remark II.4 *The lowest point level, $\epsilon_0(a^2, \chi)$, lies below the lowest eigenvalue of $H(\infty)$ which is $E_{0,0}(a^2)$, and the point levels with higher indices satisfy the inequalities*

$$E_{n-1,0}(a^2) < \epsilon_n(a^2, \chi) < E_{n,0}(a^2), \; n = 1, 2, 3, \dots .$$

II.3.5 Spectrum of the unperturbed Hamiltonian

Our goal is to find the eigenvalues of the mth partial Hamiltonian H_m, i.e., to find solutions in Dom H_m to the equation

$$H_m \psi(\xi) = z\psi(\xi),$$

or, equivalently,

$$\tilde{H}_m \psi(\xi) = a^2 z \psi(\xi). \tag{II.20}$$

As already stated above, this equation coincides with the equation of the spheroidal functions provided we set $\mu = |m|$, $\theta = -a^4\omega^2/16$, and the characteristic exponent ν is chosen so that

$$\lambda_\nu^m\left(-\frac{a^4\omega^2}{16}\right) = -a^2 z - \frac{1}{4}\,.$$

The only solution (up to a multiplicative constant) that is square integrable near infinity is $S_\nu^{|m|(3)}(\xi, -a^4\omega^2/16)$.

Proposition C.1 describes the asymptotic expansion of this function at $\xi = 1$ for $m \in \mathbb{N}$. It follows that the condition on the square integrability is equivalent to the equality

$$\mathrm{e}^{i(3\nu+1/2)\pi} K_{-\nu-1}^m\left(-\frac{a^4\omega^2}{16}\right) + K_\nu^m\left(-\frac{a^4\omega^2}{16}\right) = 0. \tag{II.21}$$

Furthermore, as deduced in (II.15), $S_\nu^{0(3)}(\xi, -a^4\omega^2/16)$ has logarithmic divergency at $\xi = 1$ that disappears just for those values of ν for which (II.21) holds (see (II.16)). Taking into account that the Friedrichs extension has continuous eigenfunctions we conclude that equation (II.21) guarantees existence of the solution to (II.20) in Dom $\tilde{H}_m$.

As far as we see it, the equation (II.21) can be solved only by means of numerical methods. For this purpose we made use of the computer algebra system *Mathematica 6.0*. For the numerical computations we set $\omega = 1$. As an illustration, Figures A.1 and A.2 depict several first eigenvalues of the Hamiltonian H_0 and H_1, respectively, as functions of the curvature radius a. The dashed asymptotic lines correspond to the flat limit ($a \to \infty$).

Remark II.5 *In numerical computations, the following form of the condition (II.21) proved to be rather effective:*

$$\lim_{\xi \to 1+} (\xi - 1)^{|m|/2+1} \frac{\partial S^{|m|(3)}_{-1/2+it}\left(\xi, -\frac{a^4}{16}\right)}{\partial \xi} = 0.$$

This equation was solved with respect to $t \in \mathbb{R}$.

Denote the nth normalized eigenfunction of the mth partial Hamiltonian $\tilde{H}_m$ by $\tilde{\psi}_{n,m}(\xi)$. Obviously, the eigenfunctions for the values of the angular momentum m and $-m$ are the same and are proportional to $S^{|m|(3)}_{\nu}(\xi, -a^4\omega^2/16)$, with ν satisfying the equation (II.21). Let us return to the original radial variable ϱ and, moreover, regard $\tilde{H}_m$ as an operator acting on $L^2(\mathbb{R}^+, \mathrm{d}\varrho)$. This amounts to an obvious isometry

$$L^2(\mathbb{R}^+, a^{-1}\sinh(\varrho/a)\mathrm{d}\varrho) \to L^2(\mathbb{R}^+, \mathrm{d}\varrho): \ f(\varrho) \mapsto a^{-1/2}\sinh^{1/2}(\varrho/a) f(\varrho).$$

The corresponding normalized eigenfunction of $\tilde{H}_m$, with an eigenvalue $a^2 z$, equals

$$\psi_{n,m}(\varrho) = \left(\frac{1}{a}\sinh\left(\frac{\varrho}{a}\right)\right)^{1/2} \tilde{\psi}_{n,m}\left(\cosh\left(\frac{\varrho}{a}\right)\right). \tag{II.22}$$

At the same time, relation (II.22) gives the normalized eigenfunction of H_m (considered on $L^2(\mathbb{R}^+, \mathrm{d}\varrho)$) with the eigenvalue z. The same Hilbert space may be used also in the limiting Euclidean case ($a = \infty$). The eigenfunctions in the flat case, $\Phi_{n,m}$, are well known and satisfy

$$\Phi_{n,m} \propto \varrho^{|m|+1/2} \mathrm{e}^{-\omega\varrho^2/4} {}_1F_1\left(-n, |m|+1, \frac{\omega\varrho^2}{2}\right). \tag{II.23}$$

The fact that we stick to the same Hilbert space in all cases facilitates the comparison of eigenfunctions for various values of the curvature radius a. We present plots of several first eigenfunctions of H_0 (Figures A.3, A.4, and A.5) and H_1 (Figures A.6, A.7, and A.8) for the values of the curvature radius $a^2 = 1$ (the solid line), 10 (the dashed line), and ∞ (the dotted line). Note that, in general, the smaller is the curvature radius a the more localized is the particle in the region near the origin.

II.3.6 Point levels

As has been stated, the point levels are solutions to the equation (II.19) with respect to the spectral parameter z. In general, $Q(\bar{z}) = \overline{Q(z)}$ and so the function $Q(z)$ takes real values on the real axis. Since we know the explicit expression for the Krein Q-function as a function of the characteristic exponent ν rather than of the spectral parameter z itself it is of importance to know for which values of ν the spectral parameter z is real. Propositions C.2 and C.3 give the answer. For $\nu \in \mathbb{R}$ and for ν of the form $\nu = -1/2 + it$ where t is real, the spheroidal eigenvalue $\lambda_\nu^m(-a^4\omega^2/16)$ is real, and so the same is true for z. Moreover, these values of ν reproduce the whole real z axis. With this knowledge, one can plot the Krein Q-function as a function of z for an arbitrary value of the curvature radius a. Note that for $a = \infty$, the Krein Q-function is well known as a function of the spectral parameter z (see [31] or [32]) and equals (setting $\omega = 1$)

$$Q(z) = \frac{1}{4\pi}\left(-\Psi\left(\frac{1-z}{2}\right) + \log(2) + 2\Psi(1)\right).$$

Next, in Figure A.9, we present plots of the Krein Q-function for several distinct values of the curvature radius a. Moreover, in Figure A.10, one can compare the behavior of the Krein Q-function for a comparatively large value of the curvature radius ($a^2 = 24$) and for the Euclidean case ($a = \infty$).

Again, the equation (II.19) can be solved only numerically. Fixing the parameter χ one may be interested in the behavior of the point levels as functions of the curvature radius a. See Figures A.11 and A.12 for the corresponding plots, with $\chi = 0$ and 0.5, respectively, where the dashed asymptotic lines again correspond to the flat case limit ($a = \infty$). Note that for the curvature radius a large enough, the lowest eigenvalue is negative provided χ is chosen smaller than $Q(0) \simeq 0.1195$.

II.3.7 Variational approach for large values of a

The mth partial Hamiltonian H_m, if considered on $L^2(\mathbb{R}^+, \mathrm{d}\varrho)$, acts like

$$H_m = -\frac{\partial^2}{\partial\varrho^2} + \frac{m^2 - \frac{1}{4}}{a^2\sinh^2(\frac{\varrho}{a})} + \frac{1}{4}\,a^2\omega^2\sinh^2\left(\frac{\varrho}{a}\right) =: -\frac{\partial^2}{\partial\varrho^2} + V_m(a,\varrho).$$

For a fixed $\varrho \neq 0$, one can easily derive that

$$V_m(a,\varrho) = \frac{m^2 - \frac{1}{4}}{\varrho^2} + \frac{1}{4}\omega^2\varrho^2 + \frac{\frac{1}{4} - m^2}{3a^2} + \frac{\omega^2\varrho^4}{12a^2} + O\left(\frac{1}{a^4}\right) \quad \text{as } a \to \infty.$$

Recall that the mth partial Hamiltonian of the isotropic harmonic oscillator on the Euclidean plane, H_m^E, also considered on $L^2(\mathbb{R}^+, \mathrm{d}\varrho)$, has the form

$$H_m^E := -\frac{\partial^2}{\partial\varrho^2} + \frac{m^2 - \frac{1}{4}}{\varrho^2} + \frac{1}{4}\omega^2\varrho^2.$$

Table II.1: Comparison of numerical and asymptotic results for the eigenvalues, $a^2 = 24$

	$E_{0,0}$	$E_{1,0}$	$E_{2,0}$	$E_{0,1}$	$E_{1,1}$	$E_{2,1}$
numerical	1.0265	3.162	5.42	2.060	4.259	6.58
asymptotic	1.0268	3.169	5.46	2.058	4.258	6.59
error (%)	-0.03	-0.22	-0.74	0.10	0.02	-0.15

This suggests that it may be useful to view the Hamiltonian H_m, for large values of the curvature radius a, as a perturbation of H_m^E,

$$H_m \sim H_m^E + \frac{1}{12a^2}(1 - 4m^2 + \omega^2\varrho^4) =: H_m^E + \frac{1}{12a^2}U_m(\varrho).$$

The eigenvalues of the compared Hamiltonians have the same asymptotic expansions up to the order $1/a^2$ as $a \to \infty$.

Let us denote by $E_{n,m}^E$, $n \in \mathbb{N}_0$, the nth eigenvalue of the Hamiltonian H_m^E. It is well known that

$$E_{n,m}^E = (2n + |m| + 1)\,\omega$$

and that the multiplicity of $E_{n,m}^E$ in the spectrum of H^E equals $2n + |m| + 1$. The asymptotic behavior of $E_{n,m}(a^2)$ may be deduced from the standard perturbation theory and is given by the formula

$$E_{n,m}(a^2) \sim E_{n,m}^E + \frac{1}{12a^2}\frac{\langle \Phi_{n,m}, U_m\Phi_{n,m}\rangle}{\langle \Phi_{n,m}, \Phi_{n,m}\rangle} \quad \text{as } a \to \infty, \tag{II.24}$$

where $\Phi_{n,m}$ is given by (II.23). The scalar products occurring in formula (II.24) can be readily evaluated in $L^2(\mathbb{R}^+, \mathrm{d}\varrho)$ with the help of Proposition B.1. The resulting formula takes the form

$$E_{n,m}(a^2) \sim (2n + |m| + 1)\,\omega + \left(2n(n + |m| + 1) + |m| + \frac{3}{4}\right)\frac{1}{a^2} \tag{II.25}$$

as $a \to \infty$. This asymptotic approximation of eigenvalues has been tested numerically for large values of the curvature radius a. The asymptotic eigenvalues for $a^2 = 24$ are compared with the precise numerical results in Table II.1. It is of interest to note that the asymptotic coefficient in front of the a^{-2} term does not depend on the frequency ω.

II.3.8 Discussion on the degeneracy

Since $H_{-m} = H_m$ the eigenvalues $E_{n,m}(a^2)$ of the total Hamiltonian $H(\infty)$ are at least twice degenerated if $m \neq 0$. From the asymptotic expansion (II.25) it follows, after some straightforward algebra, that no additional degeneracy occurs and thus these eigenvalues are exactly twice degenerated at least for sufficiently large values of a. Similarly, the eigenvalues $E_{n,0}(a^2)$ are non-degenerated in the spectrum of $H(\infty)$.

Applying the methods developed in [8] one may complete the analysis of the spectrum of the total Hamiltonian $H(\chi)$ for $\chi \neq \infty$. Namely, the spectrum of $H(\chi)$ contains eigenvalues $E_{n,m}(a^2)$, $m > 0$, with multiplicity 2 if $Q^{H(\infty)}(E_{n,m}(a^2)) \neq \chi$, and with multiplicity 3 if $Q^{H(\infty)}(E_{n,m}(a^2)) = \chi$. Let us remark that the absence of the eigenvalues $E_{n,0}(a^2)$ in the spectrum of $H(\chi)$ is a consequence of the fact that these eigenvalues are simultaneously poles of the Krein Q-function. The rest of the spectrum of $H(\chi)$ is formed by those solutions to the equation (II.19) which do not belong to the spectrum of $H(\infty)$. The multiplicity of all these eigenvalues in the spectrum of $H(\chi)$ equals 1.

III. Coulomb Plus One-Center Point Interaction in Two Dimensions

III.1 Selfadjoint extensions

Let $C > 0$. Consider the following symmetric operator acting on $L^2(\mathbb{R}^2, \mathrm{d}x\mathrm{d}y)$:

$$H = -\frac{1}{2}\Delta_{x,y} - \frac{C}{\sqrt{x^2+y^2}}$$
$$\mathrm{Dom}\ H = C_C^\infty(\mathbb{R}^2 \setminus \{0\}).$$

It is convenient to introduce the polar coordinates by $(x, y) = \varrho(\cos\varphi, \sin\varphi)$ and decompose the operator H as follows:

$$H = \bigoplus_{m=-\infty}^{\infty} H_m \otimes Id_{\mathrm{span}\{Y_m\}}$$
$$H_m = -\frac{1}{2}\frac{\partial^2}{\partial\varrho^2} - \frac{1}{2\varrho}\frac{\partial}{\partial\varrho} + \frac{m^2}{2\varrho^2} - \frac{C}{\varrho}$$
$$\mathrm{Dom}\ H_m = C_C^\infty(\mathbb{R}^+),$$

where H_m acts on $L^2(\mathbb{R}^+, \varrho\,\mathrm{d}\varrho)$ and $Y_m(\varphi) := \mathrm{e}^{im\varphi}$ is the angular momentum eigenfunction.

Using the isometry $V : L^2(\mathbb{R}^+, \varrho\,\mathrm{d}\varrho) \to L^2(\mathbb{R}^+, \mathrm{d}\varrho)$, $f(\varrho) \mapsto \sqrt{\varrho}f(\varrho)$, one may eliminate the first derivative in the action of H_m:

$$h_m := V H_m V^{-1} = -\frac{1}{2}\frac{\partial^2}{\partial\varrho^2} + \frac{4m^2-1}{8\varrho^2} - \frac{C}{\varrho}$$
$$\mathrm{Dom}\ h_m = C_C^\infty(\mathbb{R}^+).$$

Note that h_m is a Sturm-Liouville operator.

Let us define the maximal operator $h_{m,max}$ associated to the formal differential expression L_m:

$$L_m = -\frac{1}{2}\frac{\partial^2}{\partial\varrho^2} + \frac{4m^2-1}{8\varrho^2} - \frac{C}{\varrho}$$
$$\mathrm{Dom}\, h_{m,max} = \left\{f \in L^2(\mathbb{R}^+, \mathrm{d}\varrho) :\ f, f' \in AC(\mathbb{R}^+), L_m f \in L^2(\mathbb{R}^+, \mathrm{d}\varrho)\right\}$$

According to Theorem 8.22 in [27], $h_{m,max} = h_m^\dagger$.

Suppose $z \in \mathbb{C}\backslash\mathbb{R}$ and consider the equation

$$(h_m^\dagger - z)y = 0 \tag{III.1}$$

with $m \in \mathbb{N}_0$. The equation (III.1) is nothing but the equation for the Whittaker functions. Therefore, we get

$$y(\varrho) = C_1 M\left(-\frac{iC}{\sqrt{2z}}, m, 2i\sqrt{2z}\varrho\right) + C_2 W\left(-\frac{iC}{\sqrt{2z}}, m, 2i\sqrt{2z}\varrho\right),$$

where we consider $\Im\sqrt{z} \leqslant 0$. Well known asymptotic expansions (see e.g. the source [5]) implie that $W(,,)$ is square integrable near infinity but is not square integrable near zero (except the case $m = 0$) and $M(,,)$ is square integrable near zero but is not square integrable near infinity.

From the discussion above, it follows that for $m \neq 0$, the deficiency spaces contain only the zero vector, whereas $\dim\mathrm{Ker}\,(h_0^\dagger \pm z) = 1$. Hence, for m being non-zero h_m is e.s.a. and h_0 has deficiency indeces $(1,1)$. Every s.a. extension of h_0 can be described by a boundary condition for the domain of definition. To do so, the methods and the language summarized in the extensive source [33] may be involved in the same manner as in Chapter II.

Proposition III.1 *Let $\kappa \in (-\infty, \infty]$. Then the operator $h_0(\kappa)$ defined by the formulae*

$$\mathrm{Dom}\, h_0(\kappa) = \{f \in h_{0,max} :\ f_1 = \kappa f_0 \text{ if } \kappa \in \mathbb{R}, \text{ and } f_0 = 0 \text{ if } \kappa = \infty\}$$
$$h_0(\kappa)f = h_{0,max}f,$$

where

$$f_0 := -\pi \lim_{\varrho\to 0+} \frac{f(\varrho)}{\sqrt{\varrho}\log\varrho}, \quad f_1 := \lim_{\varrho\to 0+}\left(\frac{f(\varrho)}{\sqrt{\varrho}} + \frac{f_0}{\pi}\log\varrho\right)$$

is a s.a. extension of h_0. There are no other s.a. extensions of h_0.

All s.a.extensions of H can be constructed involving the set $\{h_0(\kappa),\ \kappa \in (-\infty, \infty]\}$. We again distinguish them by the index κ. The Hamiltonian $H(\kappa)$ of the two-dimensional hydrogen atom with the point interaction in the origin is then given by the restriction of $H^\dagger$ (easily reconstructed from the known $h_m^\dagger$) to the set of vectors such that

$$f_1 = \kappa f_0 \text{ or } f_0 = 0 \text{ (for } \kappa = \infty)$$

is true for the coefficients in the asymptotic expansion

$$f(\varrho, \varphi) = -\frac{1}{\pi} f_0 \log\varrho + f_1 + o(1) \quad \text{as } \varrho \to 0+.$$

Remark III.2 *There is another way how to describe the domain of $H(\kappa)$. For the domain of the Hamiltonian with no point interaction it holds*

$$\text{Dom } H(\infty) = \left\{ f \in L^2(\mathbb{R}^2), f \in AC^1(\mathbb{R}^2), \left(\bigoplus_{m=-\infty}^{\infty} L_m \right) f \in L^2(\mathbb{R}^2) \right\}.$$

For each $f \in \text{Dom } H(\kappa)$, $f_0 \in \mathbb{C}$ and $F \in \text{Dom } H(\infty)$ exist such that f may be decomposed as $f = f_0 \mathcal{G}_z + F$ in the unique matter. Here, $\mathcal{G}_z(x,y) := \mathcal{G}_z(x,y;\mathbf{0})$, where $\mathcal{G}_z$ stands for the Green function of $H(\infty)$ that is derived bellow. With this decomposition, it holds:

$$f_0 = \frac{F(\mathbf{0})}{\kappa - Q(z)}, \ (H(\kappa) - z)f = (H(\infty) - z)F,$$

where Q denotes the Krein Q-function that is also to be given.

III.1.1 Friedrichs extension

Let us consider the quadratic form q associated with H:

$$\text{Dom } q = \text{Dom } H, \quad q(\psi) = \langle \psi, H\psi \rangle.$$

The closure to this form $\bar{q}$ associates the Hamiltonian $H(\infty)$. Therefore, $H(\infty)$ is the Friedrichs extension of H. To prove it, let us construct $\bar{q}$.

Corollary B.6 states that ϱ^{-1} is $-\Delta$ infinitesimally form bounded. Consequently, q is bounded bellow. Moreover, for the norm induced by q we have:

$$\begin{aligned} &\frac{1}{2}\|\nabla\psi\|^2 + (M+1)\|\psi\|^2 \geqslant \|\psi\|_{1+}^2 = q(\psi) + (M+1)\|\psi\|^2 \\ &\geqslant \left(\frac{1}{2} - \frac{\Gamma\left(\frac{1}{4}\right)^4 C}{8\pi^2 a} \right) \|\nabla\psi\|^2 + \left(M + 1 - \frac{\Gamma\left(\frac{1}{4}\right)^4 Ca}{8\pi^2} \right) \|\psi\|^2, \end{aligned}$$

where $-M,\ M > 0$, is a lower bound of q and $a > 0$. It is easy to find a pair of a and M such that the both expressions in the brackets on the RHS are positive. Therefore, the norm $\|.\|_{1+}$ and the norm on $\mathcal{H}^1(\mathbb{R}^2)$ are equivalent. Consequently, $\bar{q}$ is defined on $\mathcal{H}^1(\mathbb{R}^2)$ because Dom q is a dense subspace of $\mathcal{H}^1(\mathbb{R}^2)$.

The Friedrichs extension of H is the only s.a. extension of H such that its domain is a subset of Dom $\bar{q}$ (see Theorem X.23 in [2]). By Remarks III.2 and III.3, we see that Dom $H(\kappa) \subset$ Dom $\bar{q}$ implies $\kappa = \infty$.

III.2 Spectral analysis

III.2.1 Green function for the unperturbed Hamiltonian

We will find the resolvent kernels for the partial Hamiltonians $\bar{h}_m = h_m^\dagger,\ m \neq 0$, and $h_0(\infty)$, next we will easily use them to construct the resolvent kernel of the Hamiltonian $H(\infty)$. Let us assume

$$(\bar{h}_m - z)y = 0, \quad (h_0(\infty) - z)y = 0.$$

Again we face the equation for the Whittaker functions. The square integrability of these functions has been discussed above. One may use asymptotic expansions for the Whittaker functions to compute their Wronskian because, as a constant, it may be evaluated in an arbitrary point, e.g., $r \to 0+$. After some manipulations, we obtain the following result (verified also in *Mathematica 7.0.0*):

$$\mathscr{W}\left(W\left(-\frac{iC}{\sqrt{2z}}, m, 2i\sqrt{2z}\varrho\right), M\left(-\frac{iC}{\sqrt{2z}}, m, 2i\sqrt{2z}\varrho\right)\right) = \frac{2i\sqrt{2z}(2m)!}{\Gamma\left(\frac{1}{2}+m+\frac{iC}{\sqrt{2z}}\right)}.$$

Finally, by the general Green function theory of the Sturm Liouville operators, for the Green function $\mathcal{G}_z$ of the total Hamiltonian $H(\infty)$, we get

$$\begin{aligned}\mathcal{G}_z(\varrho,\varphi;\varrho',\varphi') =& \frac{1}{2\pi}\sum_{m=-\infty}^{\infty}\frac{\Gamma\left(\frac{1}{2}+|m|+\frac{iC}{\sqrt{2z}}\right)}{i\sqrt{2z}(2|m|)!\sqrt{\varrho\varrho'}}M\left(-\frac{iC}{\sqrt{2z}}, |m|, 2i\sqrt{2z}\varrho_<\right) \\ &\times W\left(-\frac{iC}{\sqrt{2z}}, |m|, 2i\sqrt{2z}\varrho_>\right)\mathrm{e}^{im(\varphi-\varphi')},\end{aligned} \tag{III.2}$$

where $\varrho_<$, $\varrho_>$ denotes smaller, respectively greater out of ϱ, ϱ'.

Remark III.3 *Note that by the definition of the m-th Sobolev space, it may be directly verified that* $\mathcal{G}_z(.\,;\mathbf{0}) \in \mathcal{H}^{1-\epsilon}(\mathbb{R}^2)$ *for every* $\epsilon > 0$ *but* $\mathcal{G}_z(.\,;\mathbf{0}) \notin \mathcal{H}^1(\mathbb{R}^2)$.

Remark III.4 *In [18], it is shown that n-dimensional Coulomb Green's function can be obtained by differentiation of the corresponding functions in the one-dimensional (n odd) or two-dimensional (n even) case. An analytic expression for the two-dimensional case is given but it slightly differs from our result. A factor* $1/(2|m|)!$ *in the sum (III.2) is missing. This misprint is reproduced in the later paper [17] too.*

III.2.2 Eigenvalues of the unperturbed Hamiltonian

The eigenvalues of $H(\infty)$ correspond to the singularities of the respective Green function, i.e., those values of $z \in \mathbb{R}^-$ which $1/2 + |m| + iC/\sqrt{2z} = -n,\ n \in \mathbb{N}_0$, for. This equation implies

$$z = -\frac{C^2}{2(|m|+n+1/2)^2} =: \lambda_{m,n}. \tag{III.3}$$

If we introduce a principal quantum number as $N := |m| + n + 1,\ N \in \mathbb{N}$, then we can denote the eigenvalues by a single index $\lambda_{m,n} \equiv \lambda_N$. The multiplicity of λ_N in the spectrum of $H(\infty)$ is $2N - 1$.

The appropriate unnormalized eigenfunctions are

$$\begin{aligned}\tilde{\psi}_{m,n}(\varrho) &= \varrho^{-1/2}W\left(|m|+n+1/2, |m|, \frac{2C\varrho}{|m|+n+1/2}\right) \\ &= \varrho^{-1/2}\mathrm{e}^{-\frac{C\varrho}{|m|+n+1/2}}\left(\frac{2C\varrho}{|m|+n+1/2}\right)^{|m|+1/2}(-)^n n! L_n^{(2|m|)}\left(\frac{2C\varrho}{|m|+n+1/2}\right),\end{aligned} \tag{III.4}$$

where $L_n^{(2|m|)}$ stands for the associated Laguerre polynomial. With the aid of Proposition B.1, the normalization factor may be deduced to be:

$$\|\tilde{\psi}_{m,n}\|^2 = 2\pi C^{-2}(n + |m| + 1/2)^2 n!(n + 2|m|)!. \qquad \text{(III.5)}$$

The factor 2π comes from integration in the angular variable.

III.2.3 Krein Q-function

The Krein Q-function may be computed as the regularized Green function in the point $(\mathbf{0};\,\mathbf{0})$ (see [33]), i.e., $Q(z) = \mathcal{G}_z^{reg}(\mathbf{0};\,\mathbf{0})$. We will find the asymptotic expansion of $\mathcal{G}_z(\varrho, \varphi;\, 0, \varphi)$ as $\varrho \to 0+$.

Since

$$\frac{1}{\sqrt{\varrho}} M\left(-\frac{iC}{\sqrt{2z}}, |m|, 2i\sqrt{2z}\varrho\right) \propto \varrho^{|m|}$$

as $\varrho \to 0+$, the only term of (III.2) that should be considered is that with the angular momentum $m = 0$. This can be deduced from the rotational symmetry of the model too.

Using the following asymptotic expansions (see [5])

$$\begin{aligned} M(a, 0, x) &= \sqrt{x} + O(x^{3/2}) \quad \text{as } x \to 0 \\ W(a, 0, x) &= \frac{-2\gamma - \log x - \Psi(1/2 - a)}{\Gamma(1/2 - a)}\sqrt{x} + O(x^{3/2}) \text{ as } x \to 0, \end{aligned}$$

one obtains:

$$\mathcal{G}_z(\varrho, \varphi;\, 0, \varphi) = -\frac{1}{\pi}\left(\log \varrho + \log(2i\sqrt{2z}) + 2\gamma + \Psi\left(\frac{1}{2} + \frac{iC}{\sqrt{2z}}\right)\right) + O(\varrho \log \varrho) \text{ as } \varrho \to 0+.$$

Obviously, the divergent part is $-\pi^{-1} \log \varrho$. The general theory treated in [29] gives the same result, although our potential is not in the class of potentials considered in the source. Subtracting the divergent part, we conclude that

$$Q(z) = -\frac{1}{\pi}\left(\log(2i\sqrt{2z}) + 2\gamma + \Psi\left(\frac{1}{2} + \frac{iC}{\sqrt{2z}}\right)\right).$$

III.2.4 Green function for the perturbed Hamiltonian

With the knowledge of the Green function for $H(\infty)$ and the respective Krein Q-function, one may compute the Green function for an arbitrary s.a. extension of H. Denote the Green function of $H(\kappa)$ by the symbol $\mathcal{G}_z^\kappa$. Then the Krein resolvent formula yields

$$\begin{aligned} \mathcal{G}_z^\kappa(\varrho, \varphi;\, \varrho', \varphi') =& \mathcal{G}_z(\varrho, \varphi;\, \varrho', \varphi') - \frac{1}{Q(z) - \kappa}\mathcal{G}_z(\varrho, 0; 0, 0)\mathcal{G}_z(0, 0; \varrho', 0) \\ =& \mathcal{G}_z(\varrho, \varphi;\, \varrho', \varphi') + \frac{1}{Q(z) - \kappa} \frac{\Gamma\left(\frac{1}{2} + |m| + \frac{iC}{\sqrt{2z}}\right)^2}{8\pi^2 z (2|m|)!^2 \sqrt{\varrho\varrho'}} \\ & \times W\left(-\frac{iC}{\sqrt{2z}}, |m|, 2i\sqrt{2z}\varrho\right) W\left(-\frac{iC}{\sqrt{2z}}, |m|, 2i\sqrt{2z}\varrho'\right) \end{aligned}$$

for all $z \in \operatorname{Res} H(\infty) \cap \operatorname{Res} H(\kappa)$.

III.2.5 Eigenvalues of the perturbed Hamiltonian

Note that the set σ of all non-positive poles of the function $Q(z)$ equals

$$\sigma = \left\{-C^2/(2N-1)^2, N \in \mathbb{N}\right\} = \sigma_{pp}(H(\infty)).$$

The following discussion on the eigenvalues and their multiplicities is similar to that of Chapter II. The point part of the spectrum of $H(\kappa)$ contains the eigenvalues λ_N with $N > 1$. The multiplicity of these eigenvalues in the spectrum of $H(\kappa)$ is $2(N-1)$. Additional eigenvalues are solutions to the equation

$$Q(z) = \kappa \tag{III.6}$$

with respect to the spectral parameter z. The multiplicity of these eigenvalues (the so-called point levels) in the spectrum of $H(\kappa)$ is one. Let us denote them in the ascending order by $\epsilon_1(\kappa),\ \epsilon_2(\kappa),\ \epsilon_3(\kappa), \ldots$ Figures A.13, A.14, A.15, and A.16 depict several first point levels as functions of κ with $C = 1$. For $C \neq 1$, the following scaling property may be used:

$$Q^C(z) = Q^1\left(\frac{z}{C^2}\right) - \frac{1}{\pi}\log C.$$

Here the upper index is added to stress the C-dependence. The relation

$$\kappa = Q^C\left(\epsilon_i^C(\kappa)\right) = Q^1\left(\frac{\epsilon_i^C(\kappa)}{C^2}\right) - \frac{1}{\pi}\log C = Q^1\left(\epsilon_i^1\left(\kappa + \frac{1}{\pi}\log C\right)\right) - \frac{1}{\pi}\log C$$

implies

$$\epsilon_i^C(\kappa) = C^2 \epsilon_i^1\left(\kappa + \frac{1}{\pi}\log C\right).$$

IV. Hydrogen Atom in a Thin Slab

IV.1 Exact Hamiltonian

Let us consider a plane parallel slab Ω_a of the width a: $\Omega_a = \mathbb{R}^2 \times (-a/2,\ a/2) \subset \mathbb{R}^3$. It is well known that the hydrogen atom or a hydrogen-like ion (e.g., He^+, $Li^{2+}, \ldots$) is described by the Hamiltonian that in the center of mass coordinate system acts as follows

$$H = -\frac{1}{2}\Delta - \frac{C}{r},$$

where $r := \sqrt{x^2 + y^2 + z^2}$, the reduced mass and the electron charge are set to one, and $C > 0$ stands for the nuclear charge. One of the possibilities how to (mathematically!) constrain the atom in the slab is to choose a proper Hilbert space and the domain of H. It seems natural to set

$$\begin{aligned}
&H^a = -\frac{1}{2}\Delta - \frac{C}{r} = -\frac{1}{2}\Delta_D \dot{+} \left(-\frac{C}{r}\right) \\
&\text{Dom } H^a = \text{Dom } (-\Delta_D) = \mathcal{H}^1_0(\Omega_a) \cap \mathcal{H}^2(\Omega_a) \subset L^2(\Omega_a), \quad Q(H^a) = \mathcal{H}^1_0(\Omega_a),
\end{aligned}$$

where $\mathcal{H}^m(\Omega_a)$ stands for the mth Sobolev space, $H^m_0(\Omega_a)$ denotes the closure of $C^\infty_C(\Omega_a)$ with respect to the norm of $\mathcal{H}^m(\Omega_a)$, and Δ_D is the Dirichlet Laplacian. The selfadjointness of the operator H^a is discussed and proved in Appendix B.2.

Due to the form of Ω_a and the Dirichlet boundary condition, the Hamiltonian $-1/2\,\Delta_D$ may be decomposed with respect to the (z-axis) transversal modes as follows

$$-\frac{1}{2}\Delta_D = \bigoplus_{n=1}^{\infty} \left(-\frac{1}{2}\Delta_{x,y} + E^a_n\right) \otimes \langle\ .\ , \chi^a_n\rangle \chi^a_n,$$

with

$$\begin{aligned}
&E^a_n := \frac{n^2\pi^2}{2a^2} \\
&\chi^a_n(z) = \chi_n(z) := \sqrt{\frac{2}{a}} \begin{cases} \cos\frac{n\pi z}{a} & \text{if n is odd} \\ \sin\frac{n\pi z}{a} & \text{if n is even.} \end{cases}
\end{aligned}$$

The projection on the lowest transversal mode is used to introduce the so-called effective Hamiltonian.

Remark IV.1 *Scaling the coordinates as* $\mathbf{x} \to C\mathbf{x}$ *and the energy as* $E \to C^2 E$*, one can see that* H^a_C *is isomorphic to* H^{Ca}_1*, where the lower index is added to* H^a *to stress the charge dependence. More precisely, let us introduce an unitary isomorphisms* $W_C : L^2(\Omega_{Ca}) \to L^2(\Omega_a)$*:*

$$W_C\psi(\mathbf{x}) := C^{3/2}\psi(C\mathbf{x}).$$

Then $W_C\partial_{x_i}W_C^\dagger = \frac{1}{C}\partial_{x_i}$ *and* $W_C V(\mathbf{x})W_C^\dagger = V(C\mathbf{x})$ *for the multiplication by a scalar function* V*. Hence it follows*

$$H^a_C = C^2 W_C H^{Ca}_1 W_C^\dagger.$$

Therefore, from now on we will consider $C = 1$*.*

IV.2 Effective Hamiltonian

Let us denote

$$P^a_n = P_n := Id \otimes \langle\ .\ , \chi_n\rangle\chi_n, \ \ P^a = P := P^a_1.$$

Then we define the effective Hamiltonian H^a_{eff} as a reduction of H^a on the lowest transversal mode:

$$H^a_{\text{eff}} = H_{\text{eff}} := P^a H^a P^a.$$

By this definition, Dom H^a_{eff} = Ran $P^a \cap$ Dom H^a. Using decomposition of $L^2(\Omega_a)$,

$$L^2(\Omega_a) = \bigoplus_{n=1}^{\infty} L^2(\mathbb{R}^2) \otimes \{\chi_n\}_{\text{span}}\,,$$

it may be concluded that Ran $P^a = \left\{f(x,y)\,\chi_1(z) \middle|\ f \in L^2(\mathbb{R}^2)\right\}$. If we want functions from Ran P^a to be in Dom H^a, i.e., in the subset of $\mathcal{H}^2(\Omega_a)$, then it must hold $f \in \mathcal{H}^2(\mathbb{R}^2)$. For such f, the inclusion $f\chi_1 \in \mathcal{H}^1_0(\Omega_a)$ is fulfilled since $\chi_1 \in C_0^\infty\left(\langle -\frac{a}{2}, \frac{a}{2}\rangle\right)$. All in all, we have deduce that

$$\text{Dom } H^a_{\text{eff}} = \left\{f(x,y)\,\chi_1(z),\ \text{where } f \in \mathcal{H}^2(\mathbb{R}^2)\right\}.$$

For the action of H^a_{eff}, one easily derives:

$$H^a_{\text{eff}} = \left(-\frac{1}{2}\Delta_{x,y} + E^a_1 - V^a_{\text{eff}}(x,y)\right) \otimes Id \tag{IV.1}$$

with

$$V^a_{\text{eff}}(x,y) = \frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{\cos^2\left(\frac{\pi z}{a}\right)\mathrm{d}z}{\sqrt{x^2+y^2+z^2}}.$$

Note that in fact V^a_{eff} depends on the radial variable $\varrho := \sqrt{x^2+y^2}$ only, i.e., $V^a_{\text{eff}}(x,y) \equiv V^a_{\text{eff}}(\varrho)$.

The effective Hamiltonian (IV.1) may be viewed as an operator acting on $L^2(\mathbb{R}^2)$. Indeed, if we introduce an unitary isomorphisms $U_z^a: \ L^2(\Omega_1) \to L^2(\Omega_a)$:

$$U_z^a \psi(x,y,z) := a^{-1/2}\psi\left(x,y,\frac{z}{a}\right)$$

then it may be immediately proven that

$$P_n^a = U_z^a P_n^1 U_z^{a\dagger}$$

and consequently

$$H_{\text{eff}}^a = P^a H^a P^a = U_z^a P^1 U_z^{a\dagger} H^a U_z^a P^1 U_z^{a\dagger} = U_z^a \left(-\frac{1}{2}\Delta_{x,y} + E_1^a - V_{\text{eff}}^a(x,y)\right) \otimes Id \ P^1 U_z^{a\dagger}.$$

Therefore H_{eff}^a is unitarilly equivalent to the operator acting on $L^2(\Omega_1)$ with the exactly same action. So one may view H_{eff}^a as an operator acting on Ran P^1 which no longer depends on the parameter a and which we will identify with $L^2(\mathbb{R}^2)$. The same arguments may be applied in the case of V_{eff}^a considered as a multiplication operator.

IV.2.1 Properties of the effective potential

Proposition IV.2 (scaling property) *One immediately sees that*

$$V_{\text{eff}}^a(\varrho) = \frac{1}{a} V_{\text{eff}}^1\left(\frac{\varrho}{a}\right). \tag{IV.2}$$

Proposition IV.3 $V_{\text{eff}}^a \in (L^\infty(\mathbb{R}^2))_\epsilon + L^2(\mathbb{R}^2)$.

Proof. The expression for V_{eff}^a may be easily split into two integrals:

$$V_{\text{eff}}^a(\varrho) = \frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{\mathrm{d}z}{\sqrt{\varrho^2+z^2}} - \frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{\sin^2\left(\frac{\pi z}{a}\right)\mathrm{d}z}{\sqrt{\varrho^2+z^2}}.$$

The first integral may be directly evaluated:

$$\frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{\mathrm{d}z}{\sqrt{\varrho^2+z^2}} = -\frac{4}{a}\log\frac{2\varrho}{a+\sqrt{a^2+4\varrho^2}} =: U^a(\varrho),$$

whereas the second integral is bounded in ϱ:

$$\sup_{\varrho>0}\frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{\sin^2\left(\frac{\pi z}{a}\right)\mathrm{d}z}{\sqrt{\varrho^2+z^2}} = \sup_{\varrho>0}\frac{2}{a}\int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\sin^2(\pi z)\mathrm{d}z}{\sqrt{\frac{\varrho^2}{a^2}+z^2}} = \frac{2}{a}\int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\sin^2(\pi z)\mathrm{d}z}{|z|} =: \frac{C_{(IV.3)}}{a} \tag{IV.3}$$

where $C_{(IV.3)} \simeq 1.6483$. Using the following asymptotic expansions

$$U^a(\varrho) = -\frac{4}{a}\log\frac{\varrho}{a} + O(\varrho^2) \quad \text{as } \varrho \to 0+,$$
$$U^a(\varrho) = \frac{2}{\varrho} + O(\varrho^{-3}) \quad \text{as } \varrho \to \infty,$$

one can conclude that $V_{\text{eff}}^a \in L^\infty(\mathbb{R}^2) + L^2(\mathbb{R}^2)$ with

$$q_0(\varrho) = \theta(\varrho - L)V_{\text{eff}}^a \in L^\infty(\mathbb{R}^2)$$
$$q_1(\varrho) = \theta(L - \varrho)V_{\text{eff}}^a \in L^2(\mathbb{R}^2),$$

where $L > 0$. Moreover, $\lim_{\varrho\to\infty} q_0(\varrho) = 0$, and so $\|q_0\|_\infty$ is arbitrarily small for L large enough. □

Proposition IV.4 (lower bound and essential spectrum) *The effective Hamiltonian H_{eff}^a is lower bounded with a bound $E_1^a - 2$ and $\sigma_{ess}(H_{\text{eff}}^a) = \langle E_1^a, \infty)$.*

Proof. Let h_C stands for the two-dimensional Coulomb Hamiltonian (also denoted $H(\infty)$ in Chapter III). In the form sense, it holds

$$-2 + E_1^a \leqslant h_C + E_1^a \leqslant H_{\text{eff}}^a$$

because $\varrho^{-1} \geqslant V_{\text{eff}}^a$. The first assertion is then a consequence of the min-max principle (see [4]).

Due to Proposition IV.3, we may apply Theorem XIII.15 in [4] (a form of the Weyl's theorem) which gives the second assertion of the proposition. □

Proposition IV.5 (Fourier transform)

$$\hat{V}_{\text{eff}}^1(u) = \frac{4\left(u^2 + 2\pi^2(1 - \mathrm{e}^{-u/2})\right)}{u^2(u^2 + 4\pi^2)}. \tag{IV.4}$$

Consequently, by (IV.2), $\hat{V}_{\text{eff}}^a(u) = a\hat{V}_{\text{eff}}^1(au)$. Furthermore, one can easily find asymptotic expansions

$$\hat{V}_{\text{eff}}^1(u) = \frac{1}{u} + \left(-\frac{1}{4} + \frac{1}{\pi^2}\right) + \left(\frac{1}{24} - \frac{1}{4\pi^2}\right)u + O(u^2) \quad \text{as } u \to 0+ \tag{IV.5}$$
$$\hat{V}_{\text{eff}}^1(u) = \frac{4}{u^2} + O(u^{-4}) \quad \text{as } u \to \infty. \tag{IV.6}$$

Proof. By a direct computation, one has

$$\begin{aligned}\hat{V}_{\text{eff}}^1(u) &= \frac{1}{2\pi}\int_{\mathbb{R}^+\times S^1} \mathrm{e}^{-iu\varrho\cos\varphi} V_{\text{eff}}^1(\varrho)\varrho\,\mathrm{d}\varrho\,\mathrm{d}\varphi = \int_{\mathbb{R}^+} J_0(u\varrho)V_{\text{eff}}^1(\varrho)\varrho\,\mathrm{d}\varrho \\ &= 4\int_0^{\frac{1}{2}} \cos^2(\pi z)\left(\int_{\mathbb{R}^+} \frac{J_0(u\varrho)}{\sqrt{\varrho^2 + z^2}}\varrho\,\mathrm{d}\varrho\right)\mathrm{d}z = 4\int_0^{\frac{1}{2}} \cos^2(\pi z)\frac{\mathrm{e}^{-u/2}}{u}\mathrm{d}z \\ &= \frac{4\left(u^2 + 2\pi^2(1 - \mathrm{e}^{-u/2})\right)}{u^2(u^2 + 4\pi^2)},\end{aligned}$$

where J_0 stands for the Bessel function of the first kind. □

Corollary IV.6 *The function:* $u \mapsto u^{-1} - \hat{V}^1_{\text{eff}}(u)$ *is positive and decreasing on* $\mathbb{R}^+$ *with*

$$\lim_{u\to 0+}\left(u^{-1} - \hat{V}^1_{\text{eff}}(u)\right) = \frac{1}{4} - \frac{1}{\pi^2}, \quad \lim_{u\to\infty}\left(u^{-1} - \hat{V}^1_{\text{eff}}(u)\right) = 0,$$

which implies

$$\|u^{-1} - \hat{V}^a_{\text{eff}}\|_\infty = a\left(\frac{1}{4} - \frac{1}{\pi^2}\right). \tag{IV.7}$$

IV.2.2 Selfadjointness

It is well known that the two-dimensional free particle Hamiltonian $-\Delta/2$ is defined on Dom $(-\Delta/2) = \mathcal{H}^2(\mathbb{R}^2)$ with the form domain being $Q(-\Delta/2) = \mathcal{H}^1(\mathbb{R}^2)$. We will prove that $V^a_{\text{eff}} << -\Delta/2$.

Let us assume that $f \in \mathcal{H}^2(\mathbb{R}^2)$, i.e., $(1+|k|^2)\hat{f}(k) \in L^2(R^2)$. Following a similar line of reasoning as in the three-dimensional case (see [2]), we conclude that $\hat{f}$ is an integrable function and consequently that f is bounded and continuous. Concerning the continuity of f precisely, we have obtained a stronger property, namely:

$$|f(\mathbf{x}) - f(\mathbf{y})| \leqslant C_\gamma |\mathbf{x}-\mathbf{y}|^\gamma \left(\alpha^{2\gamma-2}\|-\Delta f\|^2 + \alpha^{2+2\gamma}\|f\|^2\right),$$

where $\alpha > 0,\ \gamma \in (0,1)$, and C_γ stands for a constant that depends on the choice of γ.

Now, let Q_0 and Q_1 be operators of multiplication by a function q_0 and q_1, respectively, with the maximal domain of definition. Consider $q_0 \in L^\infty(\mathbb{R}^2)$ and $q_1 \in L^2(\mathbb{R}^2)$, and define $Q = Q_0 + Q_1$. For $f \in \mathcal{H}^2(\mathbb{R}^2)$, we may estimate:

$$\begin{aligned} &\|Q_0 f\| \leqslant \|q_0\|_\infty \|f\| \\ &\|Q_1 f\| \leqslant \|q_1\|\|f\|_\infty \leqslant \frac{1}{2\sqrt{\pi}}\|q_1\|\left(\frac{1}{\alpha}\|-\Delta f\| + \alpha\|f\|\right). \end{aligned}$$

The last estimate is a by-product of proving that $\hat{f}$ is integrable. All in all, we have

$$\|Qf\| \leqslant \frac{1}{\sqrt{\pi}\alpha}\|q_1\|\|-(\Delta/2)f\| + \left(\frac{\alpha}{2\sqrt{\pi}}\|q_1\| + \|q_0\|_\infty\right)\|f\|.$$

Since α may be arbitrarily small, we conclude that $Q << -\Delta/2$. The Kato Rellich theorem now implies that $-\Delta/2 + Q$ is s.a. on $\mathcal{H}^2(\mathbb{R}^2)$ and e.s.a. on every core of $-\Delta/2$, e.g., $C^\infty_C(\mathbb{R}^2)$. Hence it follows that H^a_{eff} is s.a. on Dom $H^a_{\text{eff}} = \mathcal{H}^2(\mathbb{R}^2)$ by Proposition IV.3.

IV.2.3 Convergency to the Coulomb Hamiltonian

A proof that the Hamiltonian $H^a_{\text{eff}} - E^a_1 = -\Delta/2 - V^a_{\text{eff}}$ converges to the two-dimensional Coulomb Hamiltonian h_C (denoted by $H(\infty)$ within Chapter III) in the norm resolvent sense as $a \to 0+$ will be given. It consists of several lemmas. Lemmas IV.7 and IV.8 deal only with properties of h_C. Lemma IV.9 provides the rate of convergency of the effective potential to the Coulomb one. In Lemma IV.10, a wide class of potentials that converge to the Coulomb potential is considered. Lemma IV.12 provides a lower bound for the rate of this convergency. The main statement of this section is given in Theorem IV.1.

Lemma IV.7 *Let $h_0 := -\Delta/2$ be the two-dimensional free particle Hamiltonian. Then $(h_C+3)^{-1/2}(h_0+3)^{1/2}$ is bounded with the upper bound $C_{(IV.9)}$ that is defined bellow.*

Proof. Throughout the proof, let us denote $L := (h_C+3)^{-1/2}(h_0+3)^{1/2}$. Then $L^\dagger$ is closed and everywhere defined, and consequently bounded by the closed graph theorem. Since $L \subset \bar{L} = L^{\dagger\dagger}$, L is bounded too by the boundness of $L^{\dagger\dagger}$.

To find an upper bound, we start with the following decomposition:

$$\begin{aligned} LL^\dagger &= (h_C+3)^{-1/2}\left(h_0 - \frac{1}{\varrho} + \frac{1}{\varrho} + 3\right)(h_C+3)^{-1/2} \\ &= 1 + (h_C+3)^{-1/2}(h_0+3)^{1/4}(h_0+3)^{-1/4}\frac{1}{\varrho}(h_0+3)^{-1/4}(h_0+3)^{1/4}(h_C+3)^{-1/2}. \end{aligned}$$

By the Kato inequality (B.4) and the functional calculus, one obtains

$$\begin{aligned} &\langle (h_0+3)^{-1/4}\varrho^{-1}(h_0+3)^{-1/4}\psi,\ \psi\rangle = \langle \varrho^{-1}(h_0+3)^{-1/4}\psi,\ (h_0+3)^{-1/4}\psi\rangle \\ &\leqslant \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\|h_0^{1/4}(h_0+3)^{-1/4}\psi\|^2 \leqslant \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\|\psi\|^2. \end{aligned} \tag{IV.8}$$

Therefore, we may continue estimating $LL^\dagger$ as follows

$$LL^\dagger \leqslant 1 + \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}L(h_C+3)^{-1/2} \leqslant 1 + \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}L.$$

In the last inequality, we made use of the fact that $h_C \geqslant -2$ (see (III.3)).

The estimate above implies

$$\|LL^\dagger\| = \|L\|^2 \leqslant 1 + \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\|L\|.$$

Hence, we can proceed to the so-called quadratic estimate that yields

$$\|L\| \leqslant \frac{1}{2}\left(\frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2} + \sqrt{\frac{\Gamma\left(\frac{1}{4}\right)^8}{8\pi^4} + 4}\right) =: C_{(IV.9)}. \tag{IV.9}$$

□

Lemma IV.8 *Let $\xi \in \operatorname{Res} h_C \cap \mathbb{R}$. Then*

$$\|(h_C-\xi)^{-1}(h_C+3)\| \leqslant \max\left\{\frac{3}{d_C(\xi)},\ 1\right\},$$

where $d_C(\xi) := \operatorname{dist}\{\xi,\ \sigma(h_C)\}$.

Proof. One can follow the same line of reasoning as in [34]. Let us recall that $\sigma(h_C)$ consists of the continuous part formed by the positive half-axis and of the pure point part formed by countable many values in the interval $\langle -2,\ 0)$. Hence, for $\xi \in \mathbb{R}$, three cases may occur:

i. $\xi \in (\xi^-,\ \xi^+),\ \xi^\pm \in \sigma_{pp}(h_C)$. Then by the functional calculus,

$$\|(h_C - \xi)^{-1}(h_C + 3)\| = \sup_{x \in \sigma(h_C)} \frac{|x+3|}{|x-\xi|}.$$

It may be directly verified that for $x < \xi^-$, the function $x \to \frac{|x+3|}{|x-\xi|}$ is increasing, whereas for $x > \xi^+$ is decreasing. So its supremum is taken in ξ^+ or ξ^-, which implies

$$\|(h_C - \xi)^{-1}(h_C + 3)\| \leqslant \frac{3}{d_C(\xi)}.$$

ii. $-3 \leqslant \xi < -2$. Then the estimate above may be used too.

iii. $\xi < -3$. Then the supremum is taken in $x = \infty$ and its value equals 1.

□

Lemma IV.9 *For all $a > 0$, it holds*

$$\|(h_0+3)^{-1/2}\left(\varrho^{-1} - V_{\mathrm{eff}}^a\right)(h_0+3)^{-1/2}\|^2 \leqslant 4\left(\frac{1}{4} - \frac{1}{\pi^2}\right)^2 a^2 \log^2 a - 4a^2 \log a + 2a^2. \quad \text{(IV.10)}$$

Proof. Throughout the proof, let $T_a := \left(\varrho^{-1} - V_{\mathrm{eff}}^a\right)^{1/2}(h_0+3)^{-1/2}$. Furthermore, let us remind that the (generalized) Fourier transform of ϱ^{-1} is p^{-1}. Then the operator $T_a^\dagger T_a$ considered in 'the momentum representation' acts like an integral operator with the kernel

$$\frac{1}{2\pi}\frac{1}{\sqrt{\frac{1}{2}\mathbf{p}^2+3}}\left(\frac{1}{|\mathbf{p}-\mathbf{q}|} - \hat{V}_{\mathrm{eff}}^a(|\mathbf{p}-\mathbf{q}|)\right)\frac{1}{\sqrt{\frac{1}{2}\mathbf{q}^2+3}}$$

(the factor $(2\pi)^{-1}$ arises from the convolution). By the unitarity of the Fourier transform, the operator norm remains the same and may be bounded above by the Hilbert-Schmidt norm which is denoted $\|.\|_1$ within this text. The change of variables gives

$$\|T_a^\dagger T_a\|_1^2 = \frac{1}{\pi^2}\int_{\mathbb{R}^2\times\mathbb{R}^2} \frac{1}{(\mathbf{p}+\mathbf{q})^2+6}\left(\frac{1}{|\mathbf{p}|} - \hat{V}_{\mathrm{eff}}^a(|\mathbf{p}|)\right)^2 \frac{1}{\mathbf{q}^2+6}\,\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q},$$

where the integration in $\mathbf{q}$ may be done:

$$\int_{\mathbb{R}^2} \frac{1}{(\mathbf{p}+\mathbf{q})^2+6}\,\frac{1}{\mathbf{q}^2+6}\,\mathrm{d}\mathbf{q} = \int_{\mathbb{R}^+\times S^1} \frac{1}{p^2+q^2+2pq\cos\theta+6}\,\frac{1}{q^2+6}\,q\mathrm{d}q\mathrm{d}\theta$$
$$= \pi\int_{\mathbb{R}^+}\left((t+p^2+6)^2 - 4p^2 t\right)^{-1/2}\frac{1}{t+6}\,\mathrm{d}t$$
$$= \frac{\pi}{p\sqrt{p^2+24}}\log\left[1 + \frac{p}{72}\left(12\sqrt{p^2+24} + p\left(24 + p(p+\sqrt{p^2+24})\right)\right)\right] =: \pi F(p).$$

For the asymptotic behavior of the function F, we get

$$F(p) = \frac{1}{6} - \frac{p^2}{216} + O(p^4) \quad \text{as } p \to 0+ \tag{IV.11}$$

$$F(p) = \frac{4\log p}{p^2} - \frac{\log 36}{p^2} + O\left(\frac{\log p}{p^4}\right) \quad \text{as } p \to \infty.$$

Moreover, it is not difficult to verify that F is positive decreasing on $\mathbb{R}^+$ and that for $p \geqslant 5$:

$$0 \leqslant F(p) \leqslant \frac{4\log p}{p^2}. \tag{IV.12}$$

Splitting the integral for $\|T_a^\dagger T_a\|_1^2$ into three parts:

$$I(\mathbb{R}^+) = \|T_a^\dagger T_a\|_1^2 = I((0,5)) + I((5,R)) + I((R,\infty)),$$

where

$$I(A) := 2\int_A F(p)\left(\frac{1}{p} - \hat{V}_{\text{eff}}^a(p)\right)^2 p\,\mathrm{d}p,$$

each part may be estimated separately. For the first integral, we make use of (IV.7) and (IV.11) together with the monotonicity of F to estimate

$$I((0,5)) \leqslant \frac{5}{3}\left(\frac{1}{4} - \frac{1}{\pi^2}\right)^2 a^2.$$

The second integral may be estimated in the similar manner, but we can bound F as in (IV.12):

$$I((5,R)) \leqslant 2\int_5^R \frac{4\log p}{p^2}\, a^2 \left(\frac{1}{4} - \frac{1}{\pi^2}\right)^2 p\mathrm{d}p = 4\left(\frac{1}{4} - \frac{1}{\pi^2}\right)^2 (\log^2 R - \log^2 5)a^2.$$

Since, by the results of Corollary IV.6,

$$0 \leqslant \frac{1}{p} - \hat{V}_{\text{eff}}^a(p) \leqslant \frac{1}{p},$$

we get

$$I((R,\infty)) \leqslant 2\int_R^\infty \frac{4\log p}{p^2}\,\frac{1}{p^2} p\mathrm{d}p = \frac{2 + 4\log R}{R^2}$$

for an upper bound of the third integral. To optimize the total bound, we set $R = a^{-1}$ which leads to (IV.10). $\square$

Lemma IV.10 *Let $W \in L^1(\mathbb{R}^+ \times S^1, \mathrm{d}\varrho\mathrm{d}\varphi)$ such that*

$$\sup_{\varrho\in\mathbb{R}^+,\,\varphi\in S^1} \int_{\max\{-1,-\varrho\}}^1 |W(v+\varrho,\varphi)| \log^2|v|\,\mathrm{d}v =: K_W < \infty. \tag{IV.13}$$

Let us set $V(\varrho,\varphi) := \varrho^{-1}(1 - W(\varrho,\varphi))$ *and* $V^a(\varrho,\varphi) := a^{-1}V(a^{-1}\varrho,\varphi)$ *for* $\varrho \in \mathbb{R}^+$, $\varphi \in S^1$. *Then for any* $a < \frac{1}{2}$, *it holds*

$$\|(h_0+3)^{-1/2}\left(\varrho^{-1} - V^a\right)(h_0+3)^{-1/2}\|^2 \leqslant \frac{12}{\pi^2}a^2\log^2 a\left(\int_{\mathbb{R}^+\times S^1}|W(\varrho,\varphi)|\,\mathrm{d}\varrho\mathrm{d}\varphi\right)^2 + \frac{16}{\pi}K_W a^2\int_{\mathbb{R}^+\times S^1}|W(\varrho,\varphi)|\,\mathrm{d}\varrho\mathrm{d}\varphi. \tag{IV.14}$$

Proof. Throughout the proof, let $T_a := \left|\varrho^{-1} - V^a\right|^{1/2}(h_0+\frac{1}{2})^{-1/2}$. Then

$$\|(h_0+\tfrac{1}{2})^{-1/2}\left(\varrho^{-1} - V^a\right)(h_0+\tfrac{1}{2})^{-1/2}\| = \|T_a^\dagger\,\mathrm{sgn}\,W T_a\| \leqslant \|T_a^\dagger\|\|T_a\| = \|T_a T_a^\dagger\|$$

since $\mathrm{sgn}\,W$ is an isometry and $\|T_aT_a^\dagger\| = \|T_a\|^2 = \|T_a^\dagger\|^2$. Therefore, we will consider W to be non-negative and make use of $\|T_aT_a^\dagger\|^2$ to majorize the LHS of (IV.14).

For the Green function $\mathcal{G}_z$ of h_0, it may be deduced that

$$\mathcal{G}_z(\mathbf{x_1},\mathbf{x_2}) = \frac{i}{2}H_0^{(1)}(i\sqrt{-2z}|\mathbf{x_1}-\mathbf{x_2}|) = \frac{1}{\pi}K_0(\sqrt{-2z}|\mathbf{x_1}-\mathbf{x_2}|),$$

with $z < 0, \Im\sqrt{z} > 0$ (see e.g. for [32] the derivation) from which it follows that the integral kernel of $T_aT_a^\dagger$ is

$$\mathcal{K}(\mathbf{x_1},\mathbf{x_2}) := \frac{1}{\pi}\sqrt{\varrho_1^{-1}W\left(\frac{\varrho_1}{a},\varphi_1\right)}K_0(|\mathbf{x_1}-\mathbf{x_2}|)\sqrt{\varrho_2^{-1}W\left(\frac{\varrho_2}{a},\varphi_2\right)},$$

where $\mathbf{x_i} = \varrho_i(\cos\varphi_i,\sin\varphi_i)$. Let us find an upper estimate for the Hilbert-Schmidt norm of $T_aT_a^\dagger$. Since the modified Bessel function K_0 is positive and strictly decreasing on R^+, we get

$$\|T_aT_a^\dagger\|_1^2 \leqslant \frac{1}{\pi^2}I(R^+\times S^1\times R^+\times S^1)$$

with

$$I(M) := \int_M W\left(\frac{\varrho_1}{a},\varphi_1\right)K_0(|\varrho_1-\varrho_2|)^2 W\left(\frac{\varrho_2}{a},\varphi_2\right)\,\mathrm{d}\varrho_1\mathrm{d}\varphi_1\mathrm{d}\varrho_2\mathrm{d}\varphi_2.$$

K_0 has the following asymptotic expansion

$$K_0(\varrho) = -\log\varrho + \log 2 - \gamma + O(\varrho^2\log\varrho) \quad \text{as } \varrho \to 0+.$$

Consequently, for any $C > 1$, there is R such that $K_0(a) \leqslant -C\log a$ for all $a < R$. To arrive to an explicit estimate, set $C = 2$. Then we may consider $R = 1/2$. If $|\varrho_1 - \varrho_2| > a < 1/2$ then

$$K_0(|\varrho_1-\varrho_2|) < K_0(a) < -2\log a$$

and

$$I(\{|\varrho_1-\varrho_2| > a\}) \leqslant 4a^2\log^2 a\left(\int_{\mathbb{R}^+\times S^1}W(\varrho,\varphi)\,\mathrm{d}\varrho\mathrm{d}\varphi\right)^2.$$

If $|\varrho_1 - \varrho_2| < a < 1/2$ then

$$K_0(a|\varrho_1 - \varrho_2|)^2 < (-2\log(a|\varrho_1 - \varrho_2|))^2 \leqslant 8\log^2 a + 8\log^2|\varrho_1 - \varrho_2|$$

from which it follows

$$\begin{aligned} I(\{|\varrho_1 - \varrho_2| < a\}) &\leqslant 8a^2\log^2 a \left(\int_{\mathbb{R}^+\times S^1} W(\varrho,\varphi)\,\mathrm{d}\varrho\mathrm{d}\varphi\right)^2 \\ &+ 8a^2\int_{|\varrho_1-\varrho_2|<1} W(\varrho_1,\varphi_1)\log^2|\varrho_1-\varrho_2| W(\varrho_2,\varphi_2)\,\mathrm{d}\varrho_1\mathrm{d}\varphi_1\mathrm{d}\varrho_2\mathrm{d}\varphi_2 \\ &\leqslant 8a^2\log^2 a\left(\int_{\mathbb{R}^+\times S^1} W(\varrho,\varphi)\,\mathrm{d}\varrho\mathrm{d}\varphi\right)^2 + 16\pi K_W a^2\int_{\mathbb{R}^+\times S^1} W(\varrho,\varphi)\,\mathrm{d}\varrho\mathrm{d}\varphi. \end{aligned}$$

Altogether, we conclude that

$$\|T_a T_a^\dagger\|_1^2 \leqslant \frac{12}{\pi^2}a^2\log^2 a\left(\int_{\mathbb{R}^+\times S^1} W(\varrho,\varphi)\,\mathrm{d}\varrho\mathrm{d}\varphi\right)^2 + \frac{16}{\pi}K_W a^2\int_{\mathbb{R}^+\times S^1} W(\varrho,\varphi)\,\mathrm{d}\varrho\mathrm{d}\varphi.$$

By the functional calculus

$$\|(h_0+3)^{-1/2}(h_0+\tfrac{1}{2})^{1/2}\| = \sup_{x\geqslant 0}\sqrt{\frac{x+\frac{1}{2}}{x+3}} = 1$$

which completes the proof. □

Remark IV.11 *For example, the condition (IV.13) is fulfilled for a function W such that*

$$\exists\epsilon>0,\ \delta>0,\ L>0:\ \forall\mathbf{x}\in\mathbb{R}^2,\ \int_{B_\delta(\mathbf{x})}|W(\varrho,\varphi)|^{1+\epsilon}\,\mathrm{d}\varrho\mathrm{d}\varphi < L$$

which implies that if $W\in L^{1+\epsilon}(\mathbb{R}^+\times S^1,\mathrm{d}\varrho\mathrm{d}\varphi)$ or W is bounded then (IV.13) holds.

In particular, $W_{\mathrm{eff}}(\varrho) := 1-\varrho V^1_{\mathrm{eff}}(\varrho)$ is bounded, more precisely $0\leqslant W_{\mathrm{eff}}(\varrho)\leqslant 1$. A numerical calculation yields approximately 1.061 *for the constant in front of the $a^2\log^2 a$ term in the estimate (IV.14). Actually, this constant may be pushed down to its quarter (setting $C\to 1+$ and $R\to 0+$ in the proof of Lemma IV.10). In the case of non-generic estimate (IV.10), the constant in front of the same term has a smaller numerical value, namely approximately* 0.088.

Lemma IV.12 *Let $W\in L^1(\mathbb{R}^+,\mathrm{d}\varrho)$, $W(\varrho)\geqslant 0$; and $V(\varrho)$, $V^a(\varrho)$, and T_a be defined in the same manner as in Lemma IV.10. Then*

$$\|(h_0+3)^{-1/2}\left(\varrho^{-1}-V^a\right)(h_0+3)^{-1/2}\| \geqslant 2\left(\int_0^R W(\varrho)\mathrm{d}\varrho\right)\log\frac{1}{aR}a$$

whenever $a<1$ and $1<R<a^{-1}$.

Proof. If $f \in L^2(\mathbb{R}^2, \mathrm{d}\mathbf{x})$, $f \neq 0$, then $\|T_a T_a^\dagger\| \geqslant \langle f, T_a T_a^\dagger f\rangle / \|f\|^2$. We choose

$$f(\mathbf{x}) = \frac{1}{\sqrt{\varrho}} W\Big(\frac{\varrho}{a}\Big)^{1/2} \ \text{ with } \varrho := |\mathbf{x}|.$$

Then

$$\|f\|^2 = 2\pi a \int_0^\infty W(\varrho)\mathrm{d}\varrho$$

and

$$\begin{aligned}\langle f, T_a T_a^\dagger f\rangle =& \frac{1}{\pi}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} K_0(|\mathbf{x}_1 - \mathbf{x}_2|)\frac{1}{\varrho_1} W\left(\frac{\varrho_1}{a}\right)\frac{1}{\varrho_2} W\left(\frac{\varrho_2}{a}\right)\mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_2\\ =& \frac{1}{\pi}\int_{\mathbb{R}^+\times S^1}\int_{\mathbb{R}^+\times S^1} K_0\left(\left(\varrho_1^2 + \varrho_2^2 - 2\varrho_1\varrho_2\cos(\varphi_1 - \varphi_2)\right)^{1/2}\right)\\ &\times W\left(\frac{\varrho_1}{a}\right) W\left(\frac{\varrho_2}{a}\right)\mathrm{d}\varrho_1\mathrm{d}\varphi_1\mathrm{d}\varrho_2\mathrm{d}\varphi_2.\end{aligned}$$

Let us notice that by the formula 11.4.44 in [5]

$$K_0\left(\left(\varrho_1^2 + \varrho_2^2 - 2\varrho_1\varrho_2\cos\varphi\right)^{1/2}\right) = \int_0^\infty J_0\left(\left(\varrho_1^2 + \varrho_2^2 - 2\varrho_1\varrho_2\cos\varphi\right)^{1/2} t\right)\frac{t}{t^2+1}\,\mathrm{d}t.$$

Integrating Graf's formula (see [5]) for the Bessel functions we obtain

$$\frac{1}{2\pi}\int_0^{2\pi} J_0\left(\left(\varrho_1^2 + \varrho_2^2 - 2\varrho_1\varrho_2\cos\varphi\right)^{1/2} t\right)\mathrm{d}\varphi = J_0(\varrho_1 t) J_0(\varrho_2 t).$$

Since

$$\int_0^\infty J_0(\varrho_1 t) J_0(\varrho_2 t)\frac{t}{t^2+1}\mathrm{d}t = I_0(\varrho_<) K_0(\varrho_>),$$

where $\varrho_<$, $\varrho_>$ denotes smaller, respectively greater out of ϱ_1, ϱ_2; we conclude that

$$\frac{1}{2\pi}\int_0^{2\pi} K_0\left(\left(\varrho_1^2 + \varrho_2^2 - 2\varrho_1\varrho_2\cos\varphi\right)^{1/2}\right)\mathrm{d}\varphi = I_0(\varrho_<) K_0(\varrho_>).$$

Also recall that $I_0(\varrho) \geqslant 1$ and $K_0(\varrho) \geqslant \log(2/\varrho) - \gamma \geqslant \log(1/\varrho)$.

Now choose $a < 1$ and R, $1 < R < a^{-1}$. We get

$$\begin{aligned}\langle f, T_a T_a^\dagger f\rangle &= 4\pi\int_{\mathbb{R}^+}\int_{\mathbb{R}^+} I_0(\varrho_<) K_0(\varrho_>) W\left(\frac{\varrho_1}{a}\right) W\left(\frac{\varrho_2}{a}\right)\mathrm{d}\varrho_1\mathrm{d}\varrho_2\\ &\geqslant 8\pi a^2\int_0^R\left(\int_{\varrho_2}^R \log\frac{1}{a\varrho_1} W(\varrho_1)\mathrm{d}\varrho_1\right) W(\varrho_2)\mathrm{d}\varrho_2\\ &\geqslant 4\pi a^2|\log a|\left(\int_0^R W(\varrho)\mathrm{d}\varrho\right)^2 - 4\pi a^2\log R\left(\int_0^R W(\varrho)\mathrm{d}\varrho\right)^2\end{aligned}$$

and consequently

$$\|T_a T_a^\dagger\| \geqslant 2\left(\int_0^R W(\varrho)\mathrm{d}\varrho\right) a|\log a| - 2\log R\left(\int_0^R W(\varrho)\mathrm{d}\varrho\right) a.$$

□

Corollary IV.13 *There exist constants $0 < C_1 < C_2$ such that for all sufficiently small a, $1 > a > 0$,*

$$C_1 a|\log a| < \|T_a T_a^\dagger\| < C_2 a|\log a|.$$

Theorem IV.1 *Let $\xi \in \operatorname{Res} h_C \cap \mathbb{R}$ and let $\mathcal{U}(a)$ stands for the square root of the RHS of (IV.10). If $a < a_0$, where a_0 is small enough that it holds*

$$\max\left\{\frac{3}{d_C(\xi)},\ 1\right\} C^2_{(IV.9)}\mathcal{U}(a_0) = \frac{1}{2}, \tag{IV.15}$$

then $\xi \in \operatorname{Res}(H^a_{\text{eff}} - E^a_1)$ and

$$\|(H^a_{\text{eff}} - E^a_1 - \xi)^{-1} - (h_C - \xi)^{-1}\| \leqslant \frac{2}{d_C(\xi)} \max\left\{\frac{3}{d_C(\xi)},\ 1\right\} C^2_{(IV.9)}\mathcal{U}(a).$$

Proof. With the convention that $A^{1/2} := \operatorname{sgn} A|A|^{1/2}$, if A is a s.a. operator; denote

$$K(\xi) := |h_C - \xi|^{-1/2}\left(\frac{1}{\varrho} - V^a_{\text{eff}}\right)(h_C - \xi)^{-1/2}. \tag{IV.16}$$

Then

$$\begin{aligned}\|K(\xi)\| =& \||h_C - \xi|^{-1/2}(h_C+3)^{1/2}(h_C+3)^{-1/2}(h_0+3)^{1/2}(h_0+3)^{-1/2} \\ &\times \left(\varrho^{-1} - V^a_{\text{eff}}\right)(h_0+3)^{-1/2}(h_0+3)^{1/2}(h_C+3)^{-1/2}(h_C+3)^{1/2}(h_C-\xi)^{-1/2}\| \\ \leqslant& \||h_C - \xi|^{-1/2}(h_C+3)^{1/2}\|^2\ \|(h_C+3)^{-1/2}(h_0+3)^{1/2}\|^2 \\ &\times \|(h_0+3)^{-1/2}\left(\varrho^{-1} - V^a_{\text{eff}}\right)(h_0+3)^{-1/2}\|\end{aligned}$$

By Lemmas IV.7, IV.8, and IV.9, we have

$$\|K(\xi)\| \leqslant \max\left\{\frac{3}{d_C(\xi)},\ 1\right\} C^2_{(IV.9)}\mathcal{U}(a).$$

Since $\mathcal{U}(a) \sim \mathit{const.}\, a\log a$ as $a \to 0+$, for any $\xi \in \operatorname{Res} h_C \cap \mathbb{R}$, $\lim_{a\to 0+}\|K(\xi)\| = 0$. Consequently, for such ξ, we can find a_0 such that $\|K(\xi)\| \leqslant 1/2$ for all $a < a_0$. Given ξ and $a < a_0$, one can make the following estimate in the symmetrized resolvent formula (see also the proof of Theorem IV.3)

$$\begin{aligned}\|(H^a_{\text{eff}} - E^a_1 - \xi)^{-1} - (h_C - \xi)^{-1}\| &\leqslant \frac{1}{d_C(\xi)}\frac{\|K(\xi)\|}{1 - \|K(\xi)\|} \leqslant \frac{2}{d_C(\xi)}\|K(\xi)\| \\ &\leqslant \frac{2}{d_C(\xi)} \max\left\{\frac{3}{d_C(\xi)},\ 1\right\} C^2_{(IV.9)}\mathcal{U}(a).\end{aligned}$$

□

IV.3 Relation between the effective and the exact Hamiltonian

The approximation of the exact Hamiltonian H^a by the effective one is discussed in several steps. The main theorem of this section, Theorem IV.4, is just a fusion of Theorems IV.2 and IV.3. It states that H^a tends to H^a_{eff} in the norm resolvent sense linearly in a, as $a \to 0+$.

Let $-\Delta_D/2$, H^a, E^a_n, P, and H^a_{eff} be defined as in the Sections IV.1 and IV.2. Furthermore, let us introduce the following notation:

$$\begin{aligned}
&Q := Id - P\\
&H^a_\perp = H_\perp := QH^aQ,\ V := -\frac{1}{r}\\
&R^a_\perp(\xi) = R_\perp(\xi) = R_\perp := (H^a_\perp - \xi)^{-1}\\
&\mathscr{W}^a(\xi) = \mathscr{W}(\xi) := PVQR_\perp(\xi)QVP\\
&R^{\mathscr{W}}_{\text{eff}}(\xi) = R^{\mathscr{W}}_{\text{eff}} := (H^a_{\text{eff}} - \mathscr{W}(\xi) - \xi)^{-1}\\
&r_{\text{eff}}(\xi) = r_{\text{eff}} := (H^a_{\text{eff}} - \xi)^{-1}\\
&T_\perp := Q(-\Delta_D/2)Q,\ R_0(\xi) = R_0 := (T_\perp - \xi)^{-1}.
\end{aligned}$$

The operator $\mathscr{W}^a$ will be viewed as acting on $L^2(\mathbb{R}^2)$.

With the decomposition

$$H^a = \begin{pmatrix} PH^aP & PH^aQ \\ QH^aP & QH^aQ \end{pmatrix} = \begin{pmatrix} H^a_{\text{eff}} & PH^aQ \\ QH^aP & H^a_\perp \end{pmatrix},$$

it holds that (Feshbach formula)

$$(H^a - \xi)^{-1} = \begin{pmatrix} R^{\mathscr{W}}_{\text{eff}} & -R^{\mathscr{W}}_{\text{eff}}PVQR_\perp \\ -R_\perp QVPR^{\mathscr{W}}_{\text{eff}} & R_\perp + R_\perp QVPR^{\mathscr{W}}_{\text{eff}}PVQR_\perp \end{pmatrix}. \tag{IV.17}$$

Notice that $PH^aQ = PVQ,\ QH^aP = QVP$.

Theorem IV.2 *Let $a < \frac{3\pi}{16}$, $\xi \leqslant E^a_1$, and in the same time $\xi \notin \sigma((H_{\text{eff}} - \mathscr{W}(\xi)) \oplus H_\perp)$. Then $\xi \in \operatorname{Res} H^a$ and*

$$\|(H^a - \xi)^{-1} - R^{\mathscr{W}}_{\text{eff}}(\xi) \oplus R_\perp(\xi)\| \leqslant \frac{1}{d^{\mathscr{W}}_{\text{eff}}(\xi)} \frac{16a}{3\pi}\left(1 + \frac{16a}{3\pi}\right),$$

where $d^{\mathscr{W}}_{\text{eff}}(\xi) := \operatorname{dist}(\xi,\ \sigma(H_{\text{eff}} - \mathscr{W}(\xi)))$.

Proof. To prove the theorem, we will follow the steps of the proof of Theorem 3.1 in [34]. Namely, we will estimate the terms that appear in the decomposition (IV.17).

Let us consider $\xi < E^a_1 = \frac{\pi^2}{2a^2}$. Since $T_\perp = Q\,(-\Delta_{x,y}/2) \otimes Id\ Q + Q\ Id \otimes (-\partial^2_z/2)\ Q \geqslant E^a_2 = 2\pi^2/a^2$, it follows

$$0 \leqslant R_0(\xi) \leqslant (E^a_2 - E^a_1)^{-1} = \frac{2a^2}{3\pi^2}.$$

The symmetrized resolvent formula states that

$$R_\perp(\xi) = (T_\perp + QVQ - \xi)^{-1} = R_0(\xi)^{1/2}\left(1 + R_0(\xi)^{1/2} QVQ R_0(\xi)^{1/2}\right)^{-1} R_0(\xi)^{1/2}. \quad \text{(IV.18)}$$

The upper bound to the middle term in the formula above may be found using the following sequence of estimates:

$$\begin{aligned} 0 &\leqslant \left(R_0^{1/2} QVQ R_0^{1/2}\right)^2 = R_0^{1/2} QVQR_0QVQ R_0^{1/2} \leqslant \frac{2a^2}{3\pi^2} R_0^{1/2} QVQVQ R_0^{1/2} \\ &\leqslant \frac{2a^2}{3\pi^2} R_0^{1/2} QV^2Q R_0^{1/2} \leqslant \{\text{Hardy inequality (B.5)}\} \leqslant \frac{16a^2}{3\pi^2} R_0^{1/2} T_\perp R_0^{1/2} \\ &\leqslant \frac{16a^2}{3\pi^2} R_0^{1/2}(T_\perp - \xi + \xi) R_0^{1/2} \leqslant \frac{16a^2}{3\pi^2}(Q + \xi R_0) \leqslant \frac{16a^2}{3\pi^2}\frac{4}{3} \end{aligned} \quad \text{(IV.19)}$$

which implies

$$\|R_0^{1/2} QVQ R_0^{1/2}\| \leqslant \frac{8a}{3\pi} =: \frac{a}{a_H}$$

because, as can be rather directely verified, if A, B, and C ,$C \geqslant 0$, are s.a. operators then $(ABA)^2 \leqslant C$ implies $\|ABA\| \leqslant \|C\|^{1/2}$. Consequently, if we choose $a < a_H$, it holds

$$\|R_0^{1/2} QVQ R_0^{1/2}\| < 1.$$

Then by the formula (IV.18), the resolvent $R_\perp$ exists and $R_\perp \geqslant 0$. Moreover, we have

$$R_\perp \leqslant \|R_\perp\| \leqslant \|R_0^{1/2}\|^2 \left\| \left(1 + R_0^{1/2} QVQ R_0^{1/2}\right)^{-1} \right\| \leqslant \frac{\|R_0^{1/2}\|^2}{1 - \|R_0^{1/2} QVQ R_0^{1/2}\|}.$$

Since R_0 is positive (even for $\xi < E_2^a$) and s.a., $\|R_0^{1/2}\|^2 = \|R_0\|$ and

$$R_\perp \leqslant \frac{\|R_0\|}{1 - \|R_0^{1/2} QVQ R_0^{1/2}\|} \leqslant \frac{\frac{2a^2}{3\pi^2}}{1 - \frac{a}{a_H}} \leqslant \left\{\text{for } a < \frac{a_H}{2}\right\} \leqslant \frac{4a^2}{3\pi^2}. \quad \text{(IV.20)}$$

From (IV.19), it follows that

$$\|VQR_0^{1/2}\|^2 = \|R_0^{1/2} QV^2 Q R_0^{1/2}\| \leqslant \frac{32}{3}$$

which implies

$$\|VQR_0^{1/2}\| \leqslant 4\sqrt{\frac{2}{3}}.$$

The symmetrized resolvent formula:

$$0 \leqslant VQR_\perp QV = VQR_0^{1/2}\left(1 + R_0^{1/2} QVQ R_0^{1/2}\right)^{-1} R_0^{1/2} QV$$

leads to the estimate:

$$\|VQR_\perp QV\| \leqslant \frac{\|VQR_0^{1/2}\|^2}{1 - \|R_0^{1/2} QVQ R_0^{1/2}\|}$$

which, for $a < a_H/2$, implies

$$\|R_\perp^{1/2} QV\| = \|VQR_\perp^{1/2}\| \leqslant \frac{\|VQR_0^{1/2}\|}{\left(1 - \|R_0^{1/2} QVQR_0^{1/2}\|\right)^{1/2}} \leqslant \sqrt{2}\|VQR_0^{1/2}\| \leqslant \frac{8}{\sqrt{3}}.$$

By the Feshbach formula (IV.17) together with Proposition B.3 we have

$$\begin{aligned}
\|(H^a - \xi)^{-1} - R_{\mathrm{eff}}^{\mathscr{W}}(\xi) \oplus R_\perp(\xi)\| &\leqslant \|R_{\mathrm{eff}}^{\mathscr{W}} PVQR_\perp\| + \|R_\perp QVPR_{\mathrm{eff}}^{\mathscr{W}} PVQR_\perp\| \\
&\leqslant \|R_{\mathrm{eff}}^{\mathscr{W}}\|\|VQR_\perp^{1/2}\|\|R_\perp^{1/2}\| + \|R_{\mathrm{eff}}^{\mathscr{W}}\|\|VQR_\perp^{1/2}\|^2\|R_\perp^{1/2}\|^2 \\
&= \|R_{\mathrm{eff}}^{\mathscr{W}}\|\|VQR_\perp^{1/2}\|\|R_\perp^{1/2}\| \left(1 + \|VQR_\perp^{1/2}\|\|R_\perp^{1/2}\|\right) \\
&\leqslant \|R_{\mathrm{eff}}^{\mathscr{W}}\| \frac{16a}{3\pi}\left(1 + \frac{16a}{3\pi}\right)
\end{aligned}$$

which completes the proof. □

Lemma IV.14 *Let h_0 stands for the two-dimensional free particle Hamiltonian $h_0 = -\Delta_{x,y}/2$ and let $\xi < E_1^a$. Then*

$$\|(h_0 + 3)^{-1/2} \mathscr{W}(\xi)(h_0 + 3)^{-1/2}\| \leqslant \left(\frac{2}{3}\right)^{3/2} \frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3} a.$$

Proof. Within the proof, let $A := (h_0 + 3)^{-1/2}\mathscr{W}(\xi)(h_0 + 3)^{-1/2}$. Using the estimate (IV.20) we get

$$\begin{aligned}
0 \leqslant \mathscr{W}(\xi) = PVQR_\perp(\xi)QVP \leqslant \frac{4a^2}{3\pi^2} PV^2P = \frac{16a}{3\pi^2}\int_0^{\frac{a}{2}} \frac{\cos^2\frac{\pi z}{a}}{\varrho^2 + z^2}\,\mathrm{d}z \leqslant \frac{16a}{3\pi^2}\int_0^{\frac{a}{2}} \frac{\mathrm{d}z}{\varrho^2 + z^2} \\
= \frac{16a}{3\pi^2\varrho} \arctan\frac{a}{2\varrho} \leqslant \frac{8a}{3\pi\varrho}
\end{aligned}$$

from which it follows that

$$A \leqslant \frac{8a}{3\pi}(h_0 + 3)^{-1/2}\frac{1}{\varrho}(h_0 + 3)^{-1/2}.$$

Now one can easily find an upper bound to the latter operator with the aid of the estimate (IV.8) which yields

$$(h_0 + 3)^{-1/4}(h_0 + 3)^{-1/4}\frac{1}{\varrho}(h_0 + 3)^{-1/4}(h_0 + 3)^{-1/4} \leqslant \sqrt{\frac{2}{3}}\frac{\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}.$$

Hence, we conclude that

$$\|A\| \leqslant \left(\frac{2}{3}\right)^{3/2} \frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3} a.$$

□

Lemma IV.15 *Let $\mu := E_1^a - 3$. Then it holds*

$$\|r_{\text{eff}}(\mu)^{1/2}(h_0+3)^{1/2}\| \leqslant C_{(IV.9)}.$$

Proof. Throughout the proof, set

$$A := r_{\text{eff}}(\mu)^{1/2}(h_0+3)^{1/2} = (h_0 - V_{\text{eff}}^a + 3)^{-1/2}(h_0+3)^{1/2}.$$

Then $A^\dagger$ is closed and everywhere defined, and consequently bounded by the closed graph theorem. Since $A \subset \bar{A} = A^{\dagger\dagger}$, A is bounded too by the boundness of $A^{\dagger\dagger}$. To obtain an upper bound, let us proceed as follows:

$$\begin{aligned} AA^\dagger &= (h_0 - V_{\text{eff}}^a + 3)^{-1/2}(h_0 - V_{\text{eff}}^a + 3 + V_{\text{eff}}^a)(h_0 - V_{\text{eff}}^a + 3)^{-1/2} \\ &= 1 + (h_0 - V_{\text{eff}}^a + 3)^{-1/2} V_{\text{eff}}^a (h_0 - V_{\text{eff}}^a + 3)^{-1/2}. \end{aligned}$$

By the obvious observation that $0 \leqslant V_{\text{eff}}^a(\varrho) \leqslant \varrho^{-1}$ and by the inequality (IV.8), we have

$$(h_0+3)^{-1/4} V_{\text{eff}}^a (h_0+3)^{-1/4} \leqslant \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}$$

from which it follows

$$AA^\dagger \leqslant 1 + \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2} A (h_0 - V_{\text{eff}}^a + 3)^{-1/2} \leqslant 1 + \frac{\sqrt{2}\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2} A$$

because $h_0 - V_{\text{eff}}^a \geqslant h_0 - \varrho^{-1} \geqslant -2$.

Now we face the exactly same inequality as in the proof of Lemma IV.7, so by the quadratic estimate $\|A\| \leqslant C_{(IV.9)}$. □

Theorem IV.3 *Let us define*

$$C_{(IV.21)} := C_{(IV.9)}^2 \left(\frac{2}{3}\right)^{3/2} \frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3} \tag{IV.21}$$

and $d_{\text{eff}}(\xi) := \operatorname{dist}(\xi,\ \sigma(H_{\text{eff}}^a))$. Furthermore, let

$$a < \min\left\{\frac{1}{2C_{(IV.21)}},\ \frac{d_{\text{eff}}(\xi)}{6C_{(IV.21)}}\right\},$$

and in the same time $\xi \in \operatorname{Res} H_{\text{eff}}^a \cap \mathbb{R}$. Then $\xi \notin \sigma(H_{\text{eff}}^a - \mathscr{W}(\xi))$ and

$$\|R_{\text{eff}}^{\mathscr{W}}(\xi) - r_{\text{eff}}(\xi)\| \leqslant \frac{2C_{(IV.21)}}{d_{\text{eff}}(\xi)} \max\left\{\frac{3}{d_{\text{eff}}(\xi)},\ 1\right\} a.$$

Proof. With the convention that $A^{1/2} := \operatorname{sgn} A|A|^{1/2}$, if A is a s.a. operator, the symmetrized resolvent formula takes the following form

$$R_{\text{eff}}^{\mathscr{W}} = r_{\text{eff}}^{1/2}(1 + |r_{\text{eff}}|^{1/2}\mathscr{W} r_{\text{eff}}^{1/2})^{-1}|r_{\text{eff}}|^{1/2} \tag{IV.22}$$

that implies

$$\|R_{\text{eff}}^{\mathscr{W}}(\xi) - r_{\text{eff}}(\xi)\| \leqslant \frac{1}{d_{\text{eff}}(\xi)} \frac{\|K_{\text{eff}}(\xi)\|}{1 - \|K_{\text{eff}}(\xi)\|} \tag{IV.23}$$

with

$$K_{\text{eff}}(\xi) := |r_{\text{eff}}(\xi)|^{1/2}\mathscr{W}(\xi) r_{\text{eff}}(\xi)^{1/2},$$

whenever $\|K_{\text{eff}}(\xi)\| < 1$.

Following the same line of reasoning as in the proof of Lemma IV.8 with regard to the results of Proposition IV.4, we obtain

$$\|r_{\text{eff}}(\xi)(H_{\text{eff}}^a - \mu)\| \leqslant \max\left\{\frac{E_1^a - \mu}{d_{\text{eff}}(\xi)},\ 1\right\},$$

for $\mu < E_1^a - 2$. This result together with Lemmas IV.14 and IV.15 leads to the following estimate:

$$\begin{aligned} K_{\text{eff}}(\xi) =& |r_{\text{eff}}(\xi)|^{1/2}(H_{\text{eff}}^a - \mu)^{1/2} r_{\text{eff}}^{1/2}(\mu)(h_0+3)^{1/2}(h_0+3)^{-1/2}\mathscr{W}(\xi)(h_0+3)^{-1/2} \\ & \times (h_0+3)^{1/2} r_{\text{eff}}^{1/2}(\mu)(H_{\text{eff}}^a - \mu)^{1/2} r_{\text{eff}}(\xi)^{1/2} \leqslant \max\left\{\frac{3}{d_{\text{eff}}(\xi)},\ 1\right\} C_{(IV.21)} a \end{aligned}$$

where we have set $\mu = E_1^a - 3$. The assumptions of the theorem then imply that $\|K_{\text{eff}}(\xi)\| \leqslant \frac{1}{2}$. The assertion of the theorem is now a direct consequence of the formula (IV.23). □

Remark IV.16 *For a and ξ as in Theorem IV.3, the resolvent formula (IV.22) implies*

$$\|R_{\text{eff}}^{\mathscr{W}}(\xi)\| \leqslant 2\|r_{\text{eff}}(\xi)\|$$

which means

$$\frac{1}{d_{\text{eff}}^{\mathscr{W}}(\xi)} \leqslant \frac{2}{d_{\text{eff}}(\xi)}. \tag{IV.24}$$

Similarly, under the assumptions of Theorem IV.1,

$$\frac{1}{d_{\text{eff}}(\xi + E_1^a)} \leqslant \frac{2}{d_C(\xi)}. \tag{IV.25}$$

Theorem IV.4 *Under the assumptions of Theorem IV.3, i.e.,*

$$a < \min\left\{\frac{1}{2C_{(IV.21)}},\ \frac{d_{\text{eff}}(\xi)}{6C_{(IV.21)}}\right\}, \tag{IV.26}$$

and in the same time $\xi \in \operatorname{Res} H_{\text{eff}}^a \cap \mathbb{R}$; it holds $\xi \in \operatorname{Res} H^a$ and

$$\|(H^a - \xi)^{-1} - r_{\text{eff}}(\xi) \oplus 0\| \leqslant \left(\frac{32}{3\pi} + \max\left\{\frac{3}{d_{\text{eff}}(\xi)},\ 1\right\} C_{(IV.21)}\right)\frac{2a}{d_{\text{eff}}(\xi)} + \frac{4a^2}{3\pi^2}.$$

Proof. If $\xi \in \operatorname{Res} H^a_{\text{eff}} \cap \mathbb{R}$ then, by Proposition IV.4, $\xi < E^a_1$. Furthermore, from Theorem IV.3, it follows $\xi \notin \sigma(H^a_{\text{eff}} - \mathscr{W}(\xi))$. Also remark that, by the fact that $R_\perp(\xi) \geqslant 0$ for any $\xi < E^a_1$, $H_\perp > E^a_1$ (see the proof of Theorem IV.2). Altogether, this implies that $\xi \notin \sigma((H^a_{\text{eff}} - \mathscr{W}(\xi)) \oplus H_\perp)$. Further, it may be directly verified that

$$\frac{1}{2C_{(IV.21)}} < \frac{3\pi}{16}.$$

From above, we conclude that under the assumptions of Theorem IV.3, the assumptions of Theorem IV.2 are fulfilled too. Consequently, we have arrived to the following estimates

$$\begin{aligned} &\|(H^a - \xi)^{-1} - r_{\text{eff}}(\xi) \oplus 0\| \leqslant \|(H^a - \xi)^{-1} - R^{\mathscr{W}}_{\text{eff}}(\xi) \oplus R_\perp(\xi)\| \\ &+ \|R^{\mathscr{W}}_{\text{eff}}(\xi) - r_{\text{eff}}(\xi)\| + \|R_\perp(\xi)\| \leqslant \left(\frac{32}{3\pi} + \max\left\{\frac{3}{d_{\text{eff}}(\xi)},\ 1\right\} C_{(IV.21)}\right) \frac{2a}{d_{\text{eff}}(\xi)} + \frac{4a^2}{3\pi^2}, \end{aligned}$$

where we have used (IV.20) and (IV.24). □

IV.4 Relation between the exact and the two-dimensional Coulomb Hamiltonian

Theorem IV.5 *Let $\xi \in \operatorname{Res}(h_C + E^a_1)$ such that $-3 + E^a_1 < \xi < E^a_1$, and*

$$a < \min\left\{a_0,\ \frac{d_C(\xi - E^a_1)}{12C_{(IV.21)}}\right\},$$

where a_0 is defined by the condition:

$$\frac{3}{d_C(\xi - E^{a_0}_1)}\, C^2_{(IV.9)}\, \mathcal{U}(a_0) = \frac{1}{2}.$$

Then $\xi \in \operatorname{Res} H^a$ and

$$\|(H^a - \xi)^{-1} - (h_C + E^a_1 - \xi)^{-1} \oplus 0\| \leqslant \frac{6\, C^2_{(IV.9)}}{d_C(\xi - E^a_1)^2}\, \mathcal{U}(a) + \frac{30\, C_{(IV.21)}\, a}{d_C(\xi - E^a_1)^2} + \frac{4a^2}{3\pi^2}. \quad \text{(IV.27)}$$

Proof. Let us consider Theorem IV.1 with $\xi - E^a_1$ substituted for ξ. The assumptions of this theorem are fulfilled since $-3 + E^a_1 < \xi < E^a_1$ implies that $d_C(\xi - E^a_1) < 3$, from which it follows

$$\max\left\{\frac{3}{d_C(\xi - E^a_1)},\ 1\right\} = \frac{3}{d_C(\xi - E^a_1)}.$$

Then we have $\xi \in \operatorname{Res} H^a_{\text{eff}}$ and

$$\|r_{\text{eff}}(\xi) - (h_C + E^a_1 - \xi)^{-1}\| \leqslant \frac{6\, C^2_{(IV.9)}}{d_C(\xi - E^a_1)^2}\, \mathcal{U}(a).$$

According to (IV.25), $d_C(\xi - E_1^a) \leqslant 2d_{\text{eff}}(\xi)$, which together with the choice of ξ implies that (IV.26) holds. Hence, the assumptions of Theorem IV.4 are fulfilled too, so $\xi \in H^a$ and we may make the following estimate:

$$\begin{aligned}
&\|(H^a - \xi)^{-1} - (h_C + E_1^a - \xi)^{-1} \oplus 0\| \\
&\leqslant \|(H^a - \xi)^{-1} - r_{\text{eff}} \oplus 0\| + \|r_{\text{eff}}(\xi) - (h_C + E_1^a - \xi)^{-1}\| \\
&\leqslant \frac{4a}{d_C(\xi - E_1^a)} \left(\frac{32}{3\pi} + \frac{6\, C_{(IV.21)}}{d_C(\xi - E_1^a)} \right) + \frac{4a^2}{3\pi^2} + \frac{6\, C_{(IV.9)}^2}{d_C(\xi - E_1^a)^2} \mathcal{U}(a).
\end{aligned}$$

The inequality (IV.27) is then a consequence of the fact that

$$\frac{32}{3\pi} < \frac{1}{4} \frac{6\, C_{(IV.21)}}{d_C(\xi - E_1^a)}.$$

□

Remark IV.17 *Since* $\lim_{a\to 0+} a\,\mathcal{U}(a)^{-1} = 0$*, there exists a constant* a_1 *such that the estimate (IV.27) takes a more closed form:*

$$\|(H^a - \xi)^{-1} - (h_C + E_1^a - \xi)^{-1} \oplus 0\| \leqslant \frac{7\, C_{(IV.9)}^2}{d_C(\xi - E_1^a)^2} \mathcal{U}(a) =: \frac{C_{(IV.28)}}{d_C(\xi - E_1^a)^2} \mathcal{U}(a) \quad \text{(IV.28)}$$

for all

$$a < \min\left\{ a_0,\ a_1,\ \frac{d_C(\xi - E_1^a)}{12 C_{(IV.21)}} \right\}.$$

IV.5 Spectral analysis

IV.5.1 Localization of the point spectrum

Let us consider $\lambda_N \in \sigma_{pp}(h_C)$ and $\xi_+ := E_1^a + \delta$ with $\delta \in \operatorname{Res} h_C$ such that $\lambda_N < \delta < (\lambda_N + \lambda_{N+1})/2$ and $\partial_a \delta = 0$. Moreover, let Γ be the anti-clockwise oriented circle with the center $\lambda_N + E_1^a$ passing the point ξ_+. Notice that the radius of this circle is $d_C(\delta)$. For any $\xi \in \Gamma$, it holds

$$\|(h_C + E_1^a - \xi_+)(h_C + E_1^a - \xi)^{-1}\| = \sup_{x \in \sigma(h_C + E_1^a)} \left| \frac{x - \xi_+}{x - \xi} \right| \leqslant 3.$$

We are almost prepared to show that the projections $\mathcal{P}^a$ and $\mathcal{P}_C^a$ onto the spectrum of H^a and $h_C + E_1^a$, respectively, inside Γ are of the same dimension. To propagate the estimate (IV.28) on all Γ, we use the formula (3.10) of Section IV in [35]:

$$\begin{aligned}
\|(H^a - \xi)^{-1} - (h_C + E_1^a - \xi)^{-1} \oplus 0\| &\leqslant \frac{L\|(h_C + E_1^a - \xi_+)(h_C + E_1^a - \xi)^{-1}\|}{1 - |\xi - \xi_+| L} \\
&\leqslant \frac{3L}{1 - 2d_C(\delta) L}
\end{aligned}$$

with

$$\begin{aligned} L &= \|(h_C + E_1^a - \xi_+)(h_C + E_1^a - \xi)^{-1}\| \|(H^a - \xi_+)^{-1} - (h_C + E_1^a - \xi_+)^{-1} \oplus 0\| \\ &\leqslant 3\|(H^a - \xi_+)^{-1} - (h_C + E_1^a - \xi_+)^{-1} \oplus 0\| \leqslant \frac{3\, C_{(IV.28)}}{d_C(\delta)^2}\,\mathcal{U}(a). \end{aligned} \tag{IV.29}$$

We have arrived at the following estimate

$$\|(H^a - \xi)^{-1} - (h_C + E_1^a - \xi)^{-1} \oplus 0\| \leqslant \frac{9\, C_{(IV.28)} d_C(\delta)^{-2}\,\mathcal{U}(a)}{1 - 6\, C_{(IV.28)} d_C(\delta)^{-1}\,\mathcal{U}(a)}$$

which may be used to find an upper bound for the difference of the eigenprojections:

$$\begin{aligned} \|\mathcal{P}^a - \mathcal{P}_C^a \oplus 0\| &= \frac{1}{2\pi}\left\| \int_\Gamma (H^a - \xi)^{-1} - (h_C + E_1^a - \xi)^{-1} \oplus 0 \, \mathrm{d}\xi \right\| \\ &\leqslant \frac{9\, C_{(IV.28)} d_C(\delta)^{-1}\,\mathcal{U}(a)}{1 - 6\, C_{(IV.28)} d_C(\delta)^{-1}\,\mathcal{U}(a)}. \end{aligned} \tag{IV.30}$$

Obviously, this bound is smaller then one for all

$$a < \min\left\{ a_0,\ a_1,\ a_2,\ \frac{d_C(\delta)}{12 C_{(IV.21)}} \right\}$$

where a_2 is given by the relation:

$$\mathcal{U}(a_2) = \frac{d_C(\delta)}{15\, C_{(IV.28)}}.$$

Since by definition, $a_2 < a_0$, we see that $\|\mathcal{P}^a - \mathcal{P}_C^a \oplus 0\| < 1$, for all $a < a_B$ where

$$a_B := \min\left\{ a_1,\ a_2,\ \frac{d_C(\delta)}{12 C_{(IV.21)}} \right\}$$

Finally, using Lemma B.4, we conclude that for a given δ and the corresponding a_B it holds that if $a < a_B$ then in the $d_C(\delta)$ neighborhood of $\lambda_N + E_1^a$ there is the exactly same number of eigenvalues of H^a as the multiplicity of λ_N in the spectrum of h_C is.

Remark IV.18 *The estimate (IV.30) also provides an information about the closeness of the respective eigenfunctions. If one is only interested in the closeness of the eigenvalues of H^a_{eff} to those of $h_C + E_1^a$ then Lemma B.5 may be used in the straightforward manner.*

IV.5.2 Perturbation expansion

Under the assumptions above, the results of Section B.3 may be used (with $H = h_C + E_1^a$, $H_a = H^a_{\text{eff}}$, and $\mathcal{W} = 3C^2_{(IV.9)}\mathcal{U}$). Namely, let us consider the lowest eigenvalue $\lambda_{0,0} = -2$ of h_C that is non-degenerate. Then the perturbation expansion (of the type (B.7)) for the lowest eigenvalue $\lambda_{0,0}^{\mathrm{eff}}(a)$ of H_{eff}^a converges if $a \leqslant \min\{a_B, a_3\}$ where a_3 is defined by the equality

$$\frac{3C_{(IV.9)}^2 \mathcal{U}(a_3)}{d_C(\delta)} = \frac{1}{13}.$$

However, since it may be easily viewed that $a_3 > a_2$, it suffices to consider $a \leqslant a_B$. The expansion reads

$$\lambda_{0,0}^{\mathrm{eff}}(a) = E_1^a - 2 + \langle W_a \psi_{0,0},\ \psi_{0,0}\rangle - \langle \psi_{0,0}, W_a S(\lambda_{0,0}) W_a \psi_{0,0}\rangle + \mathscr{R}_3(a) \tag{IV.31}$$

with

$$|\mathscr{R}_3(a)| \leqslant 3^6\, 8 \frac{C_{(IV.9)}^6 \mathcal{U}^3(a)}{d_C(\delta)^2} \leqslant const.\, a^3 \log^3 a, \tag{IV.32}$$

where $W_a(\varrho) := \varrho^{-1} - V_{\mathrm{eff}}^a(\varrho)$, $S(\lambda_{0,0})$ stands for the reduced resolvent of h_C in the point $\lambda_{0,0}$, and $\psi_{0,0}(\varrho) = 2\sqrt{\frac{2}{\pi}}\mathrm{e}^{-2\varrho}$ denotes the normalized (in the space $L^2(\mathbb{R}^+ \times S^1, \varrho \mathrm{d}\varrho \mathrm{d}\varphi)$, see (III.4)) eigenfunction of h_C associated with $\lambda_{0,0}$.

Proposition IV.19 *As $a \to 0+$, it holds*

$$\begin{aligned}\langle W_a \psi_{0,0},\ \psi_{0,0}\rangle =& 16\left(\frac{1}{4} - \frac{1}{\pi^2}\right) a + 16\left(\frac{1}{6} - \frac{1}{\pi^2}\right) a^2 \log a + \\ &+ 8\left[(2\gamma - 1 + 2\log 2)\left(\frac{1}{6} - \frac{1}{\pi^2}\right) + 16 C_{(IV.33)}\right] a^2 + O(a^3)\end{aligned}$$

where

$$C_{(IV.33)} := \int_0^{\frac{1}{2}} z^2 \log z \cos^2(\pi z)\, \mathrm{d}z \simeq -0,0115. \tag{IV.33}$$

Proof. By a simple integration, we have

$$\langle W_a \psi_{0,0},\ \psi_{0,0}\rangle = 4 - \langle V_{\mathrm{eff}}^a \psi_{0,0},\ \psi_{0,0}\rangle.$$

Next, we can integrate using the Fubini theorem:

$$\begin{aligned}\langle V_{\mathrm{eff}}^a \psi_{0,0},\ \psi_{0,0}\rangle &= 64 \int_0^{\frac{1}{2}} \cos^2(\pi z) \int_0^\infty \frac{\mathrm{e}^{-4\varrho}\varrho}{\sqrt{\varrho^2 + (az)^2}}\, \mathrm{d}\varrho \mathrm{d}z \\ &= -32\pi a \int_0^{\frac{1}{2}} \cos^2(\pi z) z \big(Y_1(4az) + H_{-1}(4az)\big)\, \mathrm{d}z,\end{aligned}$$

where Y_1 stands for the Bessel function of the second kind and H_{-1} is the Struve function. The following asymptotic expansion (see [5]) together with the term by term integration yields the assertion of the proposition:

$$Y_1(4az) + H_{-1}(4az) = -\frac{1}{2\pi z a} + \frac{2}{\pi} + \frac{4z}{\pi} a \log a + \frac{2}{\pi}\left[(2\gamma - 1 + 2\log 2) z + 2z \log z\right] a + O(a^2)$$

as $a \to 0+$. □

Proposition IV.20 *As $a \to 0+$, it holds*

$$\langle \psi_{0,0}, W_a S(\lambda_{0,0}) W_a \psi_{0,0} \rangle = -32\gamma \left(\frac{1}{4} - \frac{1}{\pi^2} \right)^2 a^2 + O(a^3 \log a).$$

Proof. Due to the rotational symmetry of W_a and $\psi_{0,0}$, only the radial part of the kernel of S contributes to the integral in the scalar product. Let us denote it by $\mathcal{S}_z^{(0)}$, where z stands for the spectral parameter. By the definition of the reduced resolvent and the formula (III.2) for the Coulomb Green function $\mathcal{G}_z$, we have:

$$\begin{aligned}\mathcal{S}^{(0)}_{\lambda_{0,0}}(\varrho_1, \varrho_2) = \lim_{z \to -2} \Bigg[& \frac{1}{2\pi} \frac{\Gamma\left(\frac{1}{2} + \frac{i}{\sqrt{2z}}\right)}{i\sqrt{2z}\sqrt{\varrho_1 \varrho_2}} M\left(-\frac{i}{\sqrt{2z}}, 0, 2i\sqrt{2z}\varrho_<\right) \\ & \times W\left(-\frac{i}{\sqrt{2z}}, 0, 2i\sqrt{2z}\varrho_>\right) + \frac{1}{z+2}\psi_{0,0}(\varrho_1)\psi_{0,0}(\varrho_2) \Bigg] \\ = -\frac{\gamma}{8}\, & \psi_{0,0}(\varrho_1)\psi_{0,0}(\varrho_2),\end{aligned}$$

where we have used the expansion $\Gamma(x) = x^{-1} - \gamma + O(x)$ as $x \to 0$.

Now the scalar product of our interest is given by the following expression:

$$\begin{aligned}&(2\pi)^2 \int_0^\infty \int_0^\infty \psi_{0,0}(\varrho_1) W_a(\varrho_1) \mathcal{S}^{(0)}_{\lambda_{0,0}}(\varrho_1, \varrho_2) W_a(\varrho_2) \psi_{0,0}(\varrho_2) \varrho_1 \mathrm{d}\varrho_1 \varrho_2 \mathrm{d}\varrho_2 \\ &= -\frac{\gamma}{8} \left(2\pi \int_0^\infty \psi_{0,0}(\varrho)^2 W_a(\varrho) \varrho \mathrm{d}\varrho \right)^2 = -\frac{\gamma}{8} \langle \psi_{0,0},\ W_a \psi_{0,0} \rangle^2.\end{aligned}$$

The assertion of the proposition follows immediately from Proposition IV.19. □

Corollary IV.21 *With regard to the expansion (IV.31) and the estimate (IV.32), we have*

$$\begin{aligned}\lambda^{\mathrm{eff}}_{0,0}(a) = & E_1^a - 2 + 16 \left(\frac{1}{4} - \frac{1}{\pi^2} \right) a + 16 \left(\frac{1}{6} - \frac{1}{\pi^2} \right) a^2 \log a \\ & + 8 \left[(2\gamma - 1 + 2\log 2) \left(\frac{1}{6} - \frac{1}{\pi^2} \right) + 4\gamma \left(\frac{1}{4} - \frac{1}{\pi^2} \right)^2 + 16 C_{(IV.33)} \right] a^2 \\ & + O(a^3 \log^3 a).\end{aligned}$$

Let us introduce the following notation:

$$e_{m,n}(a) := \langle W_a \psi_{m,n},\ \psi_{m,n} \rangle,$$

where $\psi_{m,n} := \|\tilde{\psi}_{m,n}\|^{-1} \tilde{\psi}_{m,n}$ stands for the normalized eigenfunction of h_C with the eigenvalue $\lambda_{m,n}$ and the angular momentum m (see III.4). As $a \to 0+$, $e_{m,n} = c_{m,n}\, a + o(a)$. Indeed, we have:

Proposition IV.22 *For the coefficients* $c_{m,n} := \lim_{a\to 0+} a^{-1} e_{m,n}(a)$*, it holds*

$$c_{m,n} = 2\pi \left(\frac{1}{4} - \frac{1}{\pi^2}\right) \psi_{m,n}^2(0).$$

Namely,

$$c_{0,n} = \frac{2^4}{(2n+1)^3} \left(\frac{1}{4} - \frac{1}{\pi^2}\right)$$

and $c_{m,n} = 0$ *whenever* $|m| \geqslant 1$.

Proof. To expand $\langle W_a \psi_{m,n}, \psi_{m,n} \rangle$, it seems useful to work with Fourier images. For the Fourier transform of the eigenfunction $\psi_{m,n}$, we have:

$$\hat{\psi}_{m,n}(u) = \frac{1}{2\pi} \int_0^\infty \int_0^{2\pi} \mathrm{e}^{-iu\varrho\cos\varphi} \psi_{m,n}(\varrho) \varrho \mathrm{d}\varrho \mathrm{d}\varphi = \int_0^\infty J_0(u\varrho) \psi_{m,n}(\varrho) \varrho \mathrm{d}\varrho.$$

Since the functions $\psi_{m,n}$ are essentially of the form $\mathrm{e}^{-\alpha\varrho} \mathscr{P}(\varrho)$ with $\alpha > 0$ and $\mathscr{P}(\varrho)$ being a polynomial in ϱ, the latter integral may be evaluated using the so-called Lipshitz's integral $I(\alpha, \beta)$ (see [36]):

$$I(\alpha, \beta) := \int_0^\infty J_0(\beta x) \mathrm{e}^{-\alpha x} \, \mathrm{d}x = \frac{1}{\sqrt{\alpha^2 + \beta^2}} \quad \text{for } \alpha > 0$$

which implies

$$\int_0^\infty J_0(\beta x) x^n \mathrm{e}^{-\alpha x} \, \mathrm{d}x = (-)^n \frac{\partial^n}{\partial \alpha^n} \frac{1}{\sqrt{\alpha^2 + \beta^2}}. \tag{IV.34}$$

For example, we obtain

$$\hat{\psi}_{0,0}(u) = \sqrt{\frac{2}{\pi}} \frac{4}{(u^2 + 4)^{3/2}}.$$

Next we have

$$\begin{aligned} e_{m,n}(a) &= \frac{1}{2\pi} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \hat{\psi}_{m,n}(u) \left(\frac{1}{|\mathbf{u} - \mathbf{v}|} - \hat{V}_{\mathrm{eff}}^a(\mathbf{u} - \mathbf{v}) \right) \hat{\psi}_{m,n}(v) \mathrm{d}\mathbf{u} \mathrm{d}\mathbf{v} \\ &= \frac{a}{2\pi} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \hat{\psi}_{m,n}(u) \left(\frac{1}{a|\mathbf{u} - \mathbf{v}|} - \hat{V}_{\mathrm{eff}}^1(a(\mathbf{u} - \mathbf{v})) \right) \hat{\psi}_{m,n}(v) \mathrm{d}\mathbf{u} \mathrm{d}\mathbf{v}. \end{aligned}$$

By (IV.34), it follows that $\hat{\psi}_{m,n} \in L^1(\mathbb{R}^2)$, which together with Corollary IV.6 makes possible to use the Lebesgue theorem and interchange the limit $a \to 0+$ with the integration above. Hence, we have arrived at the following result:

$$\begin{aligned} \lim_{a\to 0+} a^{-1} e_{m,n}(a) &= \frac{1}{2\pi} \left(\frac{1}{4} - \frac{1}{\pi^2}\right) \left(\int_{\mathbb{R}^2} \hat{\psi}_{m,n}(u) \mathrm{d}\mathbf{u} \right)^2 \\ &= 2\pi \left(\frac{1}{4} - \frac{1}{\pi^2}\right) \left(\frac{1}{2\pi} \int_{\mathbb{R}^2} \mathrm{e}^{i\mathbf{0}\,\mathbf{u}} \hat{\psi}_{m,n}(u) \mathrm{d}\mathbf{u} \right)^2 = 2\pi \left(\frac{1}{4} - \frac{1}{\pi^2}\right) \psi_{m,n}^2(0). \end{aligned}$$

It may be directly verified that $\psi_{m,n}(0) = 0$ for $|m| \geqslant 1$, whereas

$$\psi_{0,n}^2(0) = \frac{\left(L_n^{(0)}(0)\right)^2}{\pi(n+\frac{1}{2})^3} = \frac{2^3}{\pi(2n+1)^3}.$$

$\square$

Corollary IV.23 *Since $\lambda_{m,n}$ is a single eigenvalue of h_C restricted to the eigenspace of the angular momentum with value m, the results of Section B.3 may be applied too. Thus, for the eigenvalues of H_{eff}^a, we get*

$$\lambda_{m,n}^{\text{eff}}(a) = E_1^a + \lambda_{m,n} + c_{m,n}a + o(a) \quad \textit{as } a \to 0+\,.$$

A. Figures

Figure A.1: Eigenvalues of the partial Hamiltonian H_0

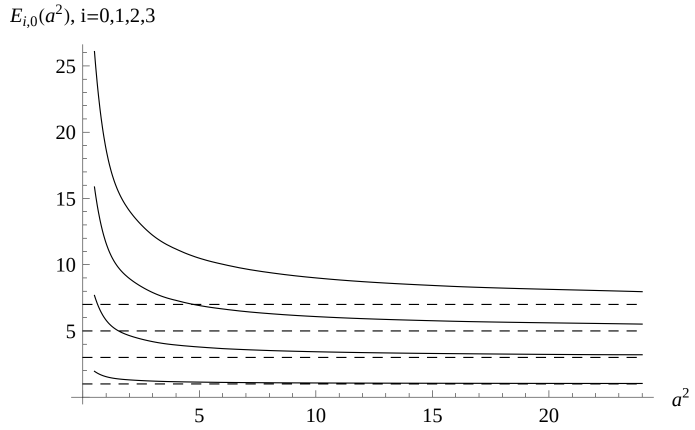


Figure A.2: Eigenvalues of the partial Hamiltonian H_1

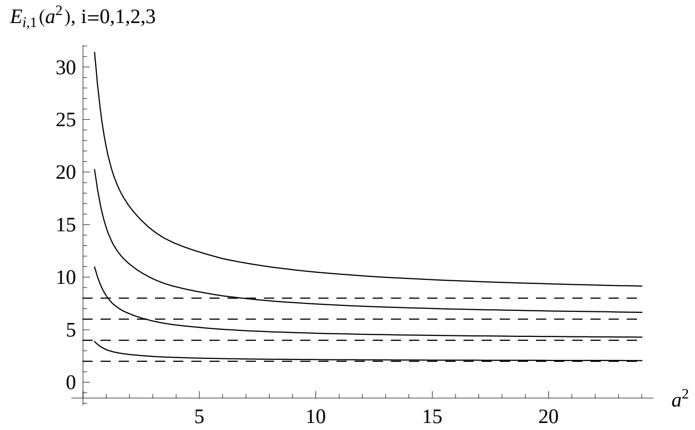


Figure A.3: The $1st$ eigenfunction of the partial Hamiltonian H_0

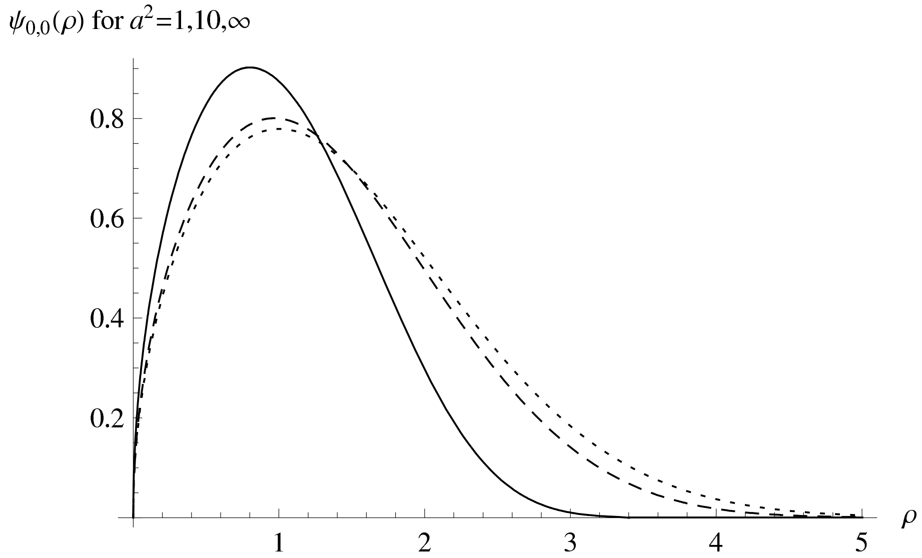


Figure A.4: The $2nd$ eigenfunction of the partial Hamiltonian H_0

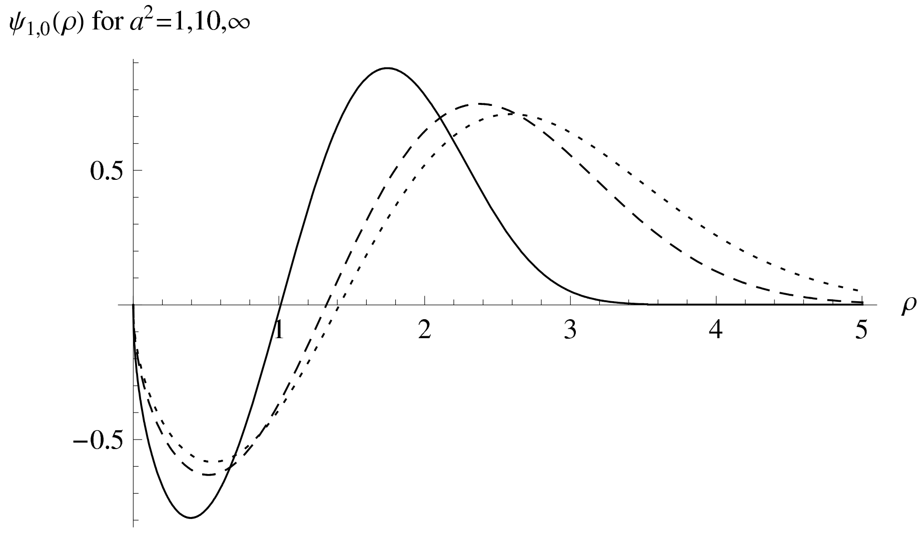


Figure A.5: The $3rd$ eigenfunction of the partial Hamiltonian H_0

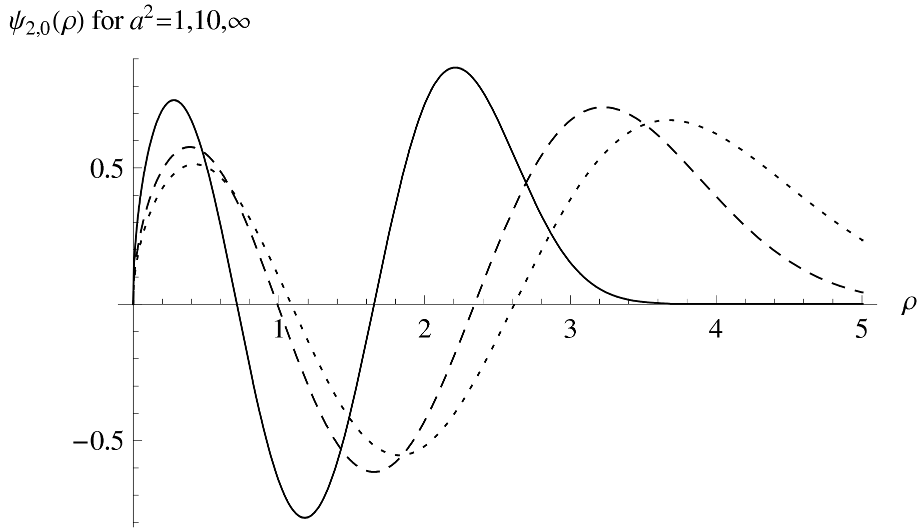


Figure A.6: The $1st$ eigenfunction of the partial Hamiltonian H_1

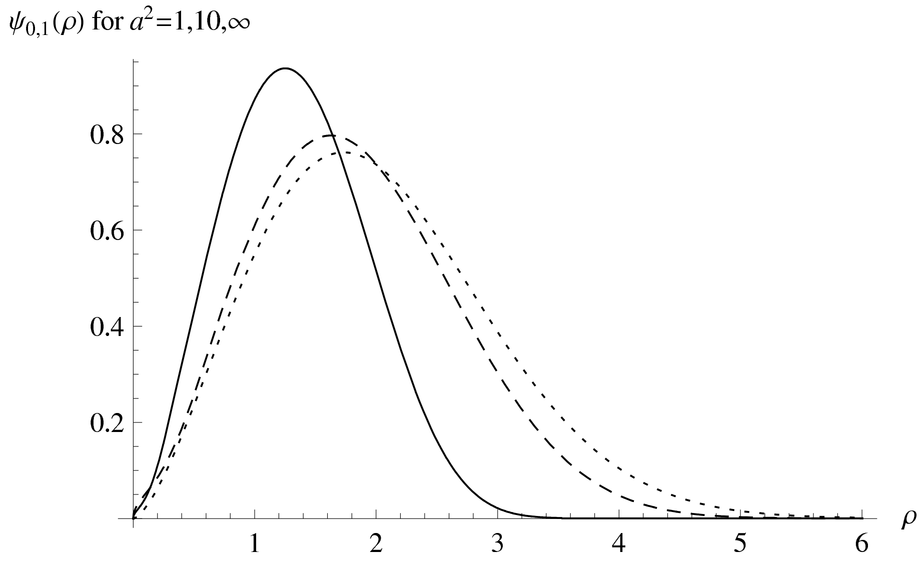


Figure A.7: The $2nd$ eigenfunction of the partial Hamiltonian H_1

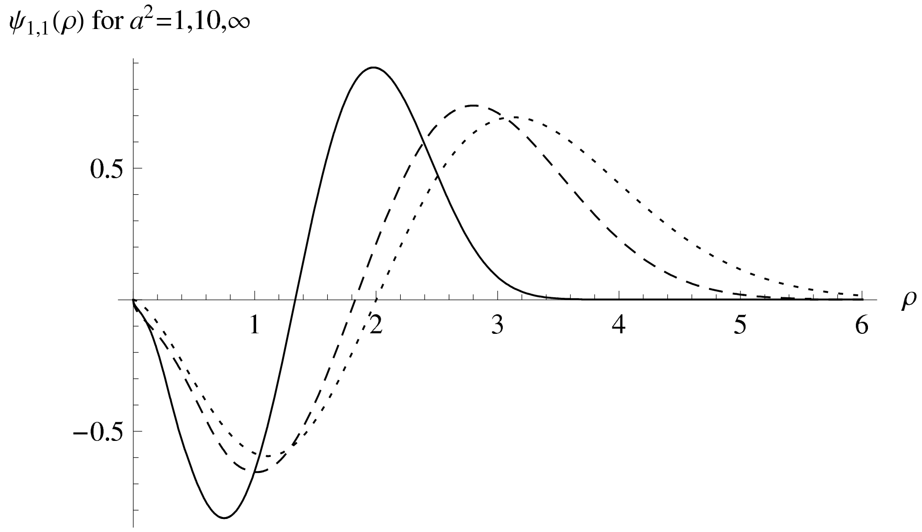


Figure A.8: The $3rd$ eigenfunction of the partial Hamiltonian H_1

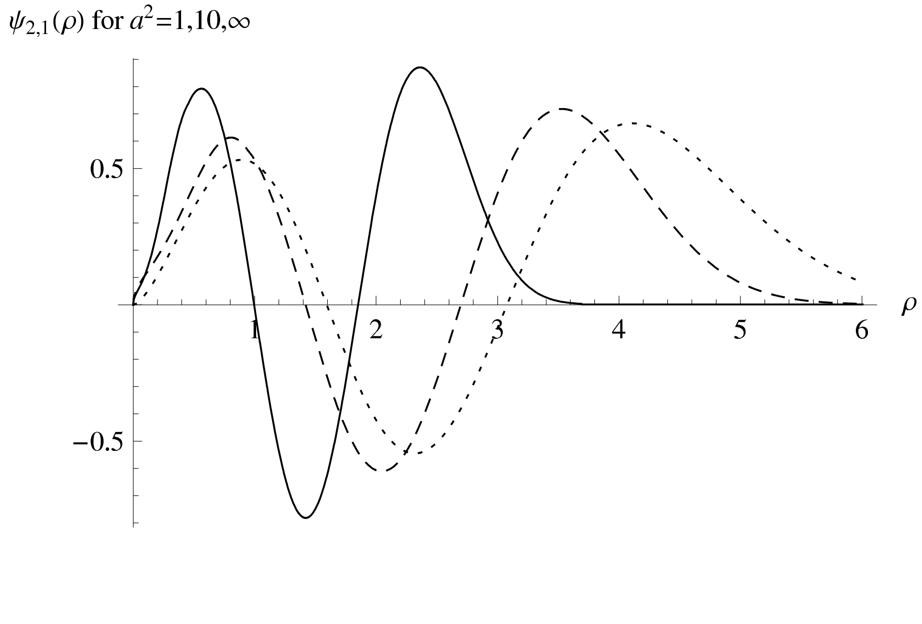


Figure A.9: Krein Q-function $Q^{H(\infty)}$ for $a^2 = 0.02$, 0.2, 1, and 5

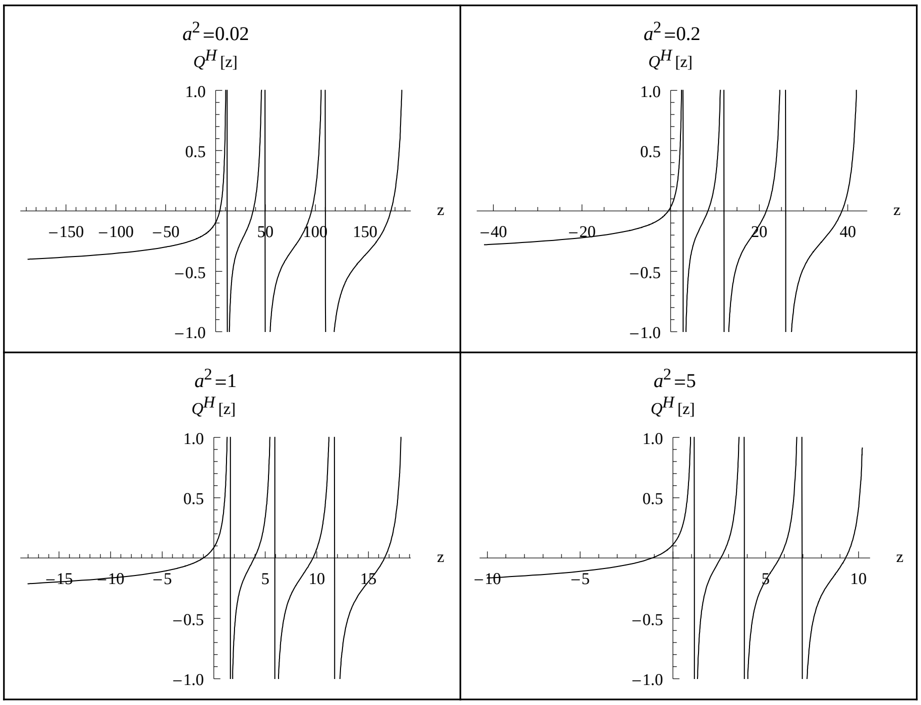


Figure A.10: Comparison of the Krein Q-functions for $a^2 = 24$ (the solid line) and $a^2 = \infty$
(the dashed line)

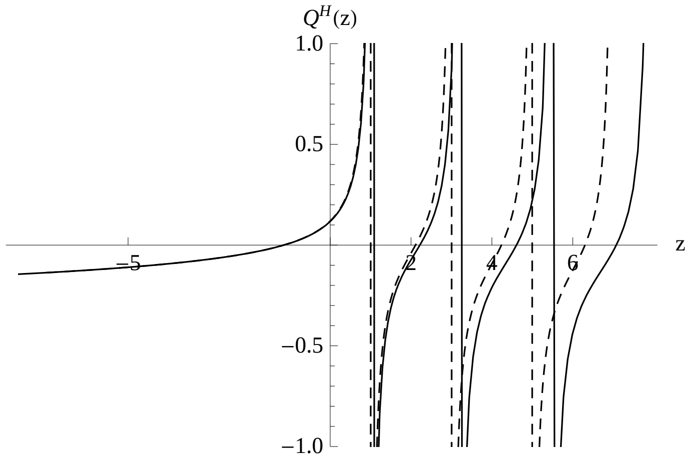


Figure A.11: Point levels of H(0)

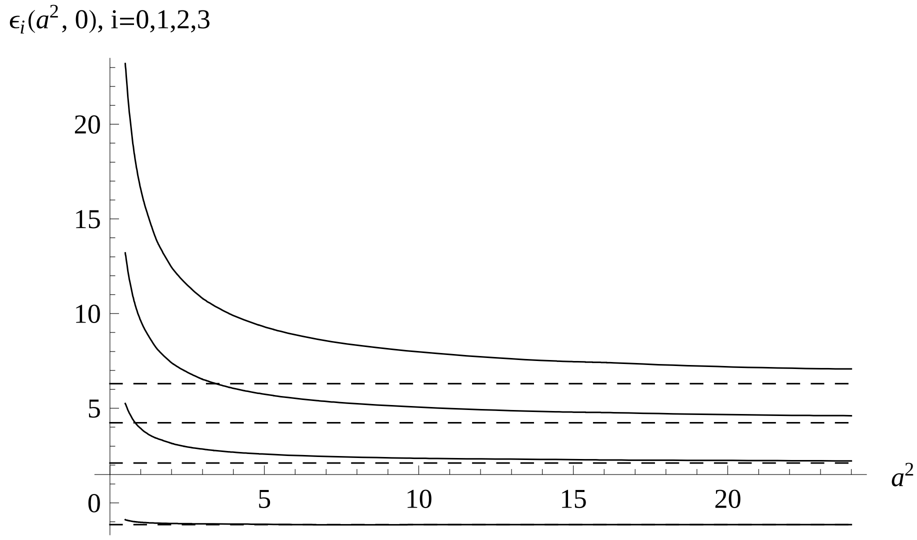


Figure A.12: Point levels of H(0.5)

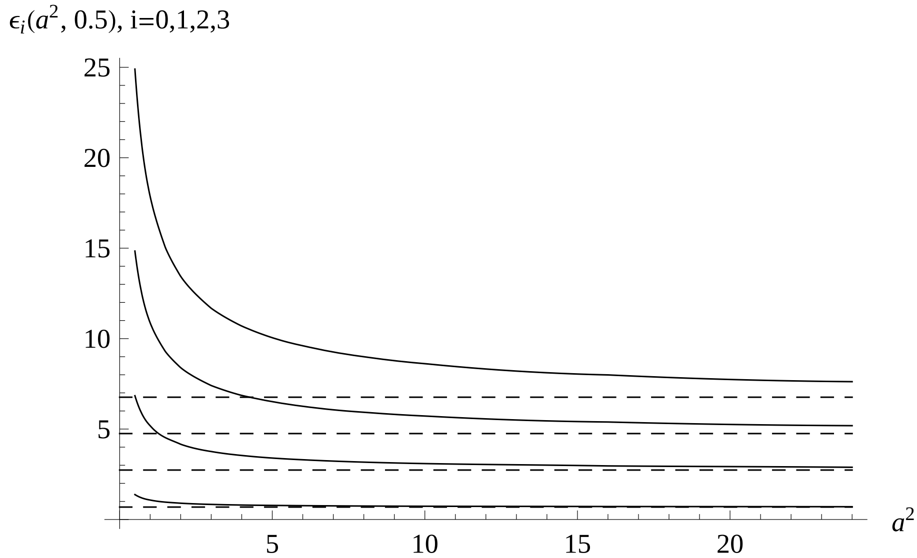


Figure A.13: The $4th$ point level of $H(\kappa)$

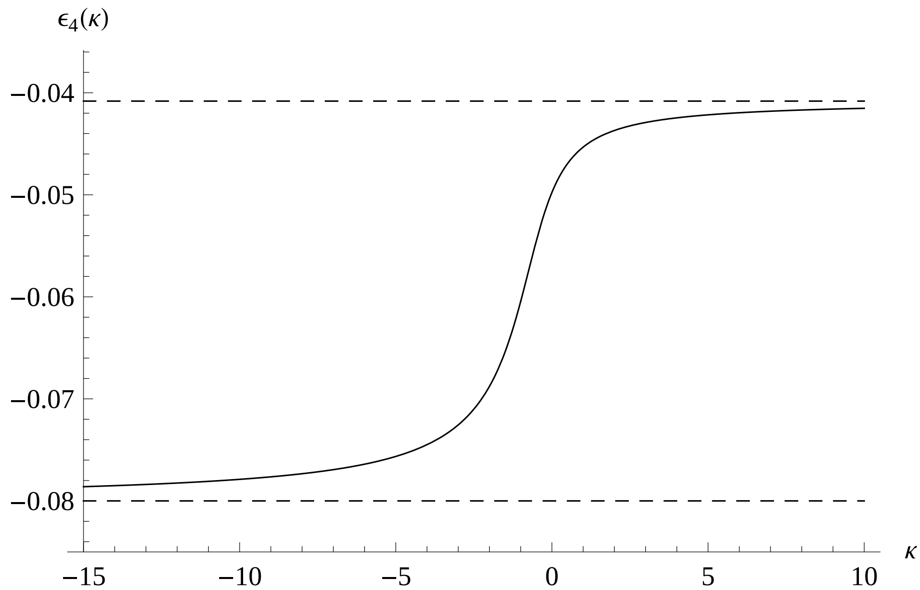


Figure A.14: The $3rd$ point level of $H(\kappa)$

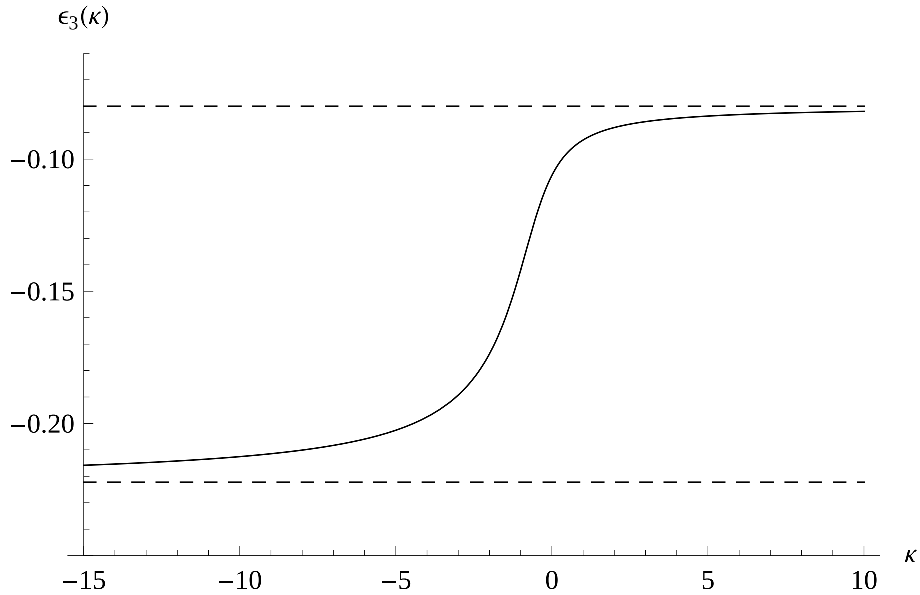


Figure A.15: The $2nd$ point level of $H(\kappa)$

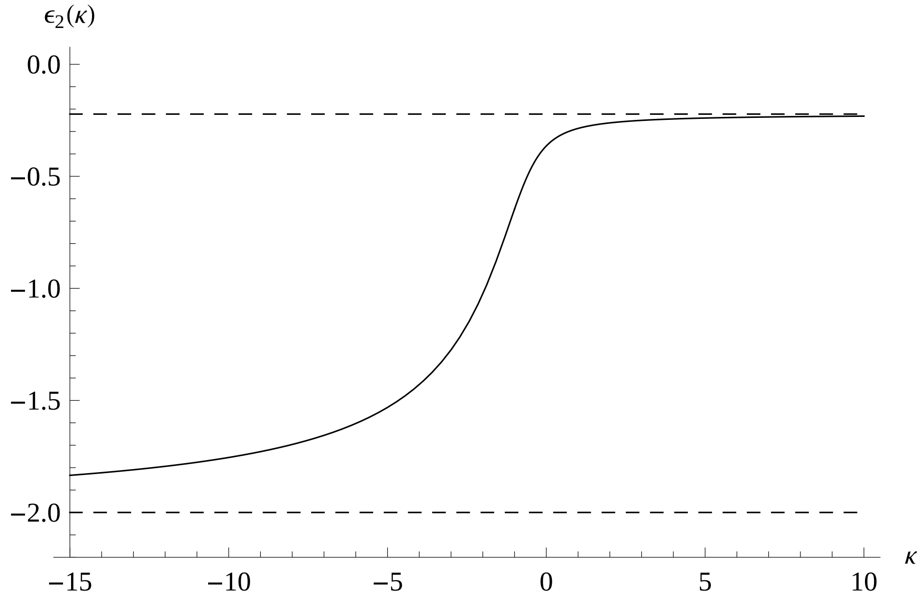
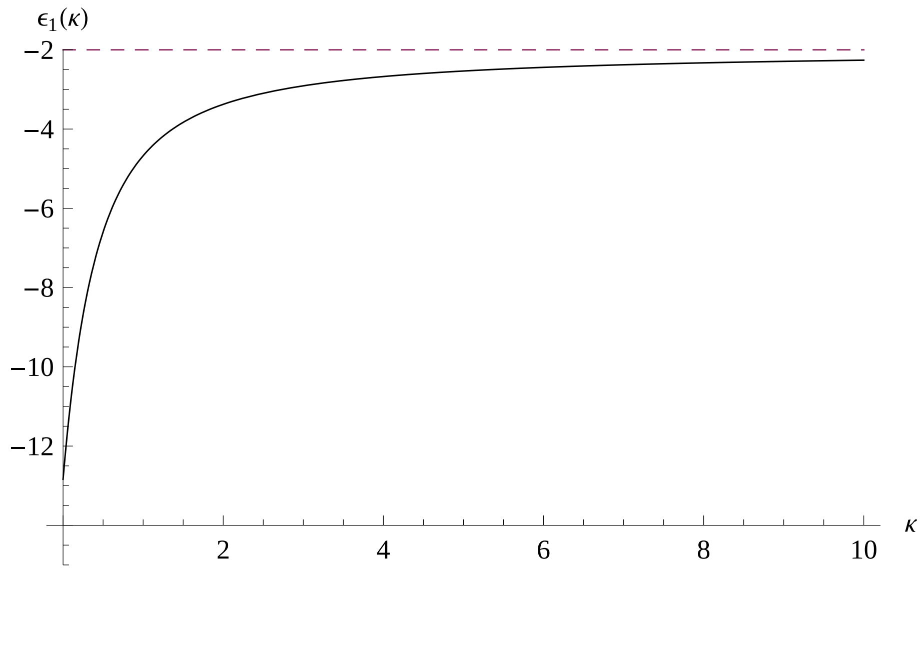


Figure A.16: The $1st$ point level of $H(\kappa)$



B. Auxiliary Results

The following auxiliary computation is needed for the evaluation of scalar products of eigenfunctions.

Proposition B.1 *Let* ${}_1F_1(a,b,t)$ *stands for the Kummer confluent hypergeometric function, and* $n, m, l \in \mathbb{N}_0$. *Then*

$$\int_0^\infty t^{m+l} \mathrm{e}^{-t} {}_1F_1(-n, 1+m, t)^2 \,\mathrm{d}t = (m!)^2 \sum_{k=\max\{0,n-l\}}^{n} (-1)^{n+k} \binom{n}{k} \frac{(k+l)!}{(k+m)!} \binom{k+m+l}{n+m}. \tag{B.1}$$

Proof. By definition,

$${}_1F_1(-n, 1+m, t) := \sum_{k=0}^{n} \frac{(-n)_k \, t^k}{(1+m)_k \, k!} = m! \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{t^k}{(m+k)!}\,.$$

Let us denote the LHS of (B.1) by I. Then the integral representation of the gamma function implies

$$I = (m!)^2 \sum_{j,k=0}^{n} (-1)^{j+k} \binom{n}{j} \binom{n}{k} \frac{(j+k+m+l)!}{(m+j)!(m+k)!}\,. \tag{B.2}$$

Partial summation in (B.2) can be carried out,

$$\sum_{j=0}^{n} (-1)^j \binom{n}{j} \frac{(j+k+m+l)!}{(m+j)!} = \frac{\mathrm{d}^{k+l}}{\mathrm{d}x^{k+l}} \left(x^{k+m+l}(1-x)^n \right) \Big|_{x=1}. \tag{B.3}$$

Expression (B.3) vanishes for $k < n - l$ and equals

$$(-1)^n (k+l)! \binom{k+m+l}{n+m}$$

for $k \geqslant n - l$. The proposition follows immediately. □

Corollary B.2 *In the case* $l = 0$, *(B.1) takes a particularly simple form:*

$$\int_0^\infty t^m \mathrm{e}^{-t} {}_1F_1(-n, 1+m, t)^2 \,\mathrm{d}t = \frac{n!}{(m+n)!}\,.$$

When dealing with a direct sum of Hilbert spaces, likewise in Section IV.3, the following result may be of use.

Proposition B.3 *Let $A: \mathscr{H}_2 \to \mathscr{H}_1$ and $B = B^\dagger : \mathscr{H}_2 \to \mathscr{H}_2$ be bounded operators. Then*

$$\left\| \begin{pmatrix} 0 & A \\ A^\dagger & B \end{pmatrix} \right\| \leqslant \|A\| + \|B\|.$$

Proof. Let $x \in \mathscr{H}_1$ and $y \in \mathscr{H}_2$. Then, since we deal with a s.a. operator,

$$\left\| \begin{pmatrix} 0 & A \\ A^\dagger & B \end{pmatrix} \right\| = \sup_{\|x\oplus y\|=1} \left| \left\langle \begin{pmatrix} 0 & A \\ A^\dagger & B \end{pmatrix} x \oplus y,\, x \oplus y \right\rangle \right| = \sup_{\|x\oplus y\|=1} |2\Re\langle Ay,\, x\rangle + \langle By,\, y\rangle|$$

$$\leqslant \sup_{\|x\oplus y\|=1} 2\|A\|\|y\|\|x\| + \|B\|\|y\|^2 \leqslant \sup_{\|x\oplus y\|=1} (\|A\| + \|B\|)(\|x\|^2 + \|y\|^2) = \|A\| + \|B\|,$$

where the appropriate scalar products and norms are involved. □

The following auxiliary result was needed for comparing dimensions of eigenprojections.

Lemma B.4 *Let P_1 and P_2 be projections. Denote $\dim P_i$ the dimension of $\mathrm{Ran} P_i$ and let $0 < \dim P_2 < \infty$. Then $\|P_1 - P_2\| < 1$ implies $\dim P_1 = \dim P_2$.*

Proof. Let $\dim P_1 > \dim P_2$ and $\{\psi_i\}$ be an orthonormal basis of $\mathrm{Ran} P_1$. Now, two cases may occur:

i. There exists an index i such that $P_2\psi_i = 0$. In this case set $\psi = \psi_i$.

ii. For all basis vectors, $P_2\psi_i \neq 0$. Then there must exist a finite linear combination, ψ, of basis vectors such that $P_2\psi = 0$. Contrary would imply $\dim P_2 \in \{\dim P_1,\ \infty\}$.

In both cases $\psi \in \mathrm{Ran} P_1 \cap (\mathrm{Ran} P_2)^\perp$. Consequently, $(P_1 - P_2)\psi = \psi$ and so $\|P_1 - P_2\| \geqslant 1$ which proves the statement. □

When comparing eigenvalues of two s.a. operators, the following lemma may be of interest.

Lemma B.5 *Let H_1 and H_2 be s.a. positive operators on a Hilbert space $\mathscr{H}$. If we define*

$$\lambda_n^{(i)} := \sup_{\mathscr{L}_{n-1}} \inf_{\substack{\psi \neq 0 \\ \psi \in \mathscr{L}_{n-1}^\perp \cap Q(H_i)}} \frac{\|H_i^{1/2}\psi\|^2}{\|\psi\|^2},$$

where $n \in \mathbb{N}$ and $\mathscr{L}_{n-1}$ is a $n-1$ dimensional subspace of $\mathscr{H}$, then it holds

$$|(\lambda_n^{(1)})^{-1} - (\lambda_n^{(2)})^{-1}| \leqslant \|H_1^{-1} - H_2^{-1}\|.$$

Let us recall that according to the min-max principle, $\lambda_n^{(i)}$ is either the n-th eigenvalue (counting the multiplicity) of H_i bellow the bottom of the essential spectrum or $\lambda_n^{(i)}$ is the bottom of the essential spectrum and in that case $\lambda_n^{(i)} = \lambda_{n+1}^{(i)} = \lambda_{n+2}^{(i)} = \dots$

Proof. One immediately obtains:

$$
\begin{aligned}
(\lambda_n^{(i)})^{-1} &= \inf_{\mathscr{L}_{n-1}} \sup_{\substack{\psi\neq 0\\ \psi\in\mathscr{L}_{n-1}^{\perp}\cap Q(H_i)}} \frac{\|\psi\|^2}{\|H_i^{1/2}\psi\|^2} = \inf_{\mathscr{L}_{n-1}} \sup_{\substack{\phi\neq 0\\ \phi\in\mathscr{L}_{n-1}^{\perp}}} \frac{\|H_i^{-1/2}\phi\|^2}{\|\phi\|^2} \\
&= \inf_{\mathscr{L}_{n-1}} \sup_{\substack{\phi\neq 0\\ \phi\in\mathscr{L}_{n-1}^{\perp}}} \frac{\langle\phi,\ H_i^{-1}\phi\rangle}{\|\phi\|^2}.
\end{aligned}
$$

Consequently, we have

$$
(\lambda_n^{(1)})^{-1} = \inf_{\mathscr{L}_{n-1}} \sup_{\substack{\phi\neq 0\\ \phi\in\mathscr{L}_{n-1}^{\perp}}} \left(\frac{\langle\phi,\ (H_1^{-1}-H_2^{-1})\phi\rangle}{\|\phi\|^2} + \frac{\langle\phi,\ H_2^{-1}\phi\rangle}{\|\phi\|^2}\right) \leqslant \|H_1^{-1}-H_2^{-1}\| + (\lambda_n^{(2)})^{-1}
$$

and similarly $(\lambda_n^{(2)})^{-1} \leqslant \|H_1^{-1}-H_2^{-1}\| + (\lambda_n^{(1)})^{-1}$. □

B.1 Kato inequality

Furthermore, the so-called two-dimensional Kato inequality is the most needed in Chapter IV. Here it is reproduced as stated and proven in [37]. It is worth of mentioning that this inequality is a special case of a more general one treated in even older paper [38].

Theorem B.1 (Kato inequality) *Let $-\Delta_{x,y} \equiv \Delta$ stands for the two-dimensional Laplacian. Then the following inequality holds*

$$
\frac{1}{\sqrt{x^2+y^2}} \leqslant \frac{\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\sqrt{-\Delta}. \tag{B.4}
$$

An approximate value of the constant involved in (B.4) is 4.379.

Corollary B.6 *Set $\varrho := \sqrt{x^2+y^2}$. Then ϱ^{-1} is $-\Delta$ infinitesimally form bounded.*

Proof. Let $\psi \in \mathcal{H}^1(\mathbb{R}^2) = Q(-\Delta)$, then by (B.4):

$$
\begin{aligned}
&\int_{\mathbb{R}^2} \varrho^{-1}|\psi(x,y)|^2 \mathrm{d}x\mathrm{d}y \leqslant \frac{\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\|(-\Delta)^{1/4}\psi\|^2 = \frac{\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\||\lambda|^{1/2}\hat{\psi}\|^2 = \frac{\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\langle|\lambda|\hat{\psi},\ \hat{\psi}\rangle \\
&\leqslant \frac{\Gamma\left(\frac{1}{4}\right)^4}{4\pi^2}\left(\frac{1}{2a}\langle|\lambda|\hat{\psi},\ |\lambda|\hat{\psi}\rangle + \frac{a}{2}\langle\hat{\psi},\ \hat{\psi}\rangle\right) = \frac{\Gamma\left(\frac{1}{4}\right)^4}{8\pi^2}\left(\frac{1}{a}\|\nabla\psi\|^2 + a\|\psi\|^2\right),
\end{aligned}
$$

where the parameter $a > 0$ may be chosen arbitrarily large. Note that the first inequality holds even for $\psi \in \mathcal{H}^{1/2}(\mathbb{R}^2)$. □

B.2 Dirichlet Schrödinger operators

Properties of the Dirichlet Laplacian Δ_D on a bounded region are widely discussed in [39]. When a bounded region Ω is considered, the Dirichlet Laplacian is defined as a unique s.a. operator associated with the closed positive form $q(f,g) = -\langle \nabla f,\ \nabla g\rangle$ defined on $\mathcal{H}_0^1(\Omega)$. Note that by the definition of $\mathcal{H}_0^1(\Omega)$, the space $C_C^\infty(\Omega)$ is a core of the form q. Let us introduce a linear space $C_0^\infty(\bar{\Omega})$ of smooth functions on Ω with $f|_{\partial\Omega} = 0$ and $f|_{\mathrm{ext}\,\Omega} = 0$ whose partial derivatives can be continuously extended to $\bar{\Omega}$. Then by Lemma 6.1.3 in [39], $C_0^\infty(\Omega)$ is also a core of the form q.

In the case of an unbounded region Ω (e.g., the slab Ω_a considered in Chapter IV), the Dirichlet Laplacian may be introduced in the same manner but $C_0^\infty(\bar{\Omega})$ is no longer a form core. However, $C_0^\infty(\bar{\Omega}) \cap \mathcal{H}^1(\Omega)$ is already a core. To prove it, we will follow the proof of the respective lemma in [39] only with some little modifications.

Proposition B.7 *$C_0^\infty(\bar{\Omega}) \cap \mathcal{H}^1(\Omega)$ is a form core of the Dirichlet Laplacian.*

Proof. Essentially, one has to prove that the closures of $C_0^\infty(\bar{\Omega}) \cap \mathcal{H}^1(\Omega)$ and $C_C^\infty(\Omega)$ with respect to the norm of $\mathcal{H}^1(\Omega)$:

$$|||f||| = \left(\|f\|^2 + \|\nabla f\|^2\right)^{1/2}$$

are the same.

Since obviously, $C_C^\infty(\Omega) \subset C_0^\infty(\bar{\Omega}) \cap \mathcal{H}^1(\Omega)$, it suffices to show that $C_C^\infty(\Omega)$ is dense in $C_0^\infty(\bar{\Omega}) \cap \mathcal{H}^1(\Omega)$ with respect to $|||.|||$ norm. Taking real and imaginary part separately, we will consider functions bellow to be real-valued. At first let us define a smooth function $F_\epsilon : \mathbb{R} \to \mathbb{R}$ such that

a) $F_\epsilon(x) = x$ if $|x| \geqslant 2\epsilon$
b) $F_\epsilon(x) = 0$ if $|x| \leqslant \epsilon$
c) $|F_\epsilon(x)| \leqslant |x|\ \forall x \in \mathbb{R}$
d) $0 \leqslant F_\epsilon'(x) \leqslant 3\ \forall x \in \mathbb{R}$

and for any $f \in C_0^\infty(\bar{\Omega}) \cap \mathcal{H}^1(\Omega)$ set $f_\epsilon(\mathbf{x}) := F_\epsilon(f(\mathbf{x}))$. Then f_ϵ is smooth and $f_\epsilon(\mathbf{x}) = 0$ on some neighborhood of $\partial\Omega$. Moreover, since f is smooth and lies in $L^2(\Omega)$, $K > 0$ exists such that $|\mathbf{x}| > K$ implies $|f(\mathbf{x})| < \epsilon$. Consequently, $f_\epsilon \in C_C^\infty(\Omega)$.

As $\lim_{\epsilon\to 0+} f_\epsilon(\mathbf{x}) = f(\mathbf{x})$ and $|f_\epsilon(\mathbf{x})| \leqslant |f(\mathbf{x})|$ for all $\mathbf{x} \in \Omega$, we have $\lim_{\epsilon\to 0+} \|f - f_\epsilon\| = 0$ by the dominated convergence theorem. Furthermore,

$$\lim_{\epsilon\to 0+} \nabla f_\epsilon(\mathbf{x}) = \begin{cases} \nabla f(\mathbf{x}) & \text{if } f(\mathbf{x}) \neq 0 \\ 0\ (\neq \nabla f(\mathbf{x}) \text{ in general}) & \text{if } f(\mathbf{x}) = 0. \end{cases}$$

Let us define a set $B := \{\mathbf{x} :\ f(\mathbf{x}) = 0 \wedge \nabla f(\mathbf{x}) \neq 0\}$. By the implicit function theorem, B is a hypersurface of codimension 1 and so $\mu(B) = 0$. Hence, ∇f_ϵ converges to ∇f a.e., and since by the assumption d), $|\nabla f_\epsilon(\mathbf{x})| \leqslant 3|\nabla f(\mathbf{x})|$, it follows that

$\lim_{\epsilon\to 0+} \|\nabla f - \nabla f_\epsilon\| = 0$ by the dominated convergence theorem too. All in all, $\lim_{\epsilon\to 0+} |||f - f_\epsilon||| = 0$ which proves the proposition. □

Next we may ask how to define a 'Dirichlet Schrödinger' operator. It seems natural to consider the following form sum $-\frac{1}{2}\Delta_D \dot{+} V$, where V stands for a potential part. Bellow we will look for a class of potentials which this form sum is well defined for. Notice that in the present moment, we are not looking for the most general class of such operators, rather we want the Coulomb potential to be included. At first, let us reproduce an useful inequality as stated in [40]:

Lemma B.8 (Hardy inequality) *For any $u \in \mathcal{D}^{1,2}(\mathbb{R}^3)$ which is the completion of $C_C^\infty(\mathbb{R}^3)$ with respect to the norm*

$$\|u\|^2 = \int_{\mathbb{R}^3} |\nabla u(\mathbf{x})|^2 \mathrm{d}\mathbf{x}$$

it holds

$$\frac{1}{4}\int_{\mathbb{R}^3} \frac{|u(\mathbf{x})|^2}{r^2}\mathrm{d}\mathbf{x} \leqslant \int_{\mathbb{R}^3} |\nabla u(\mathbf{x})|^2 \mathrm{d}\mathbf{x}, \tag{B.5}$$

where $r = |\mathbf{x}| = \sqrt{x^2 + y^2 + y^2}$ as usual.

Since any function $u \in \mathcal{H}_0^1(\Omega) = Q(-\Delta_D)$ may be uniquely extended to a function in $\mathcal{H}^1(\mathbb{R}^3) \subset \mathcal{D}^{1,2}(\mathbb{R}^3)$ which vanishes outside Ω, the inequality (B.5) holds for any $u \in \mathcal{H}_0^1(\Omega)$ too.

Proposition B.9 *Let $0 < \alpha < 2$. Then $r^{-\alpha} << -\Delta_D$.*

Proof. We will focus on the nontrivial case $0 \in \operatorname{int}\Omega$. Let $A > 0$, then $\epsilon > 0$ exists such that $\frac{A}{4r^2} \geqslant \frac{1}{r^\alpha}$ for all $r \leqslant \epsilon$. For any $\psi \in \mathcal{H}_0^1(\Omega)$, one can make the following estimates:

$$\int_\Omega \frac{|\psi(\mathbf{x})|^2}{r^\alpha}\mathrm{d}\mathbf{x} = \int_{\Omega, r\leqslant\epsilon} \frac{|\psi(\mathbf{x})|^2}{r^\alpha}\mathrm{d}\mathbf{x} + \int_{\Omega, r>\epsilon} \frac{|\psi(\mathbf{x})|^2}{r^\alpha}\mathrm{d}\mathbf{x} \leqslant A\int_{\Omega, r\leqslant\epsilon} \frac{|\psi(\mathbf{x})|^2}{4r^2}\mathrm{d}\mathbf{x}$$
$$+ \int_{\Omega, r>\epsilon} \frac{|\psi(\mathbf{x})|^2}{r^\alpha}\mathrm{d}\mathbf{x} \leqslant \{(\mathrm{B.5})\} \leqslant A\int_\Omega |\nabla\psi|^2 \mathrm{d}\mathbf{x} + \frac{1}{\epsilon^\alpha}\|\psi\|^2$$

that prove the statement. □

Hence $-\frac{1}{2}\Delta_D \dot{+} V$ is a s.a. operator with the form domain $\mathcal{H}_0^1(\Omega)$ for potentials that are bounded in infinity and on the boundary $\partial\Omega$, and that have at worst singularities of $r^{-2+\epsilon}$ type. Now let us turn to the case of Chapter IV, i.e., $V = -\frac{C}{r}$.

Proposition B.10 *Let Ω be an open set with a boundary that is Lipschitz continuous on each component (so the integration by parts may be used) and let $H = -\frac{1}{2}\Delta_D \dot{+} (-\frac{C}{r})$. Then* Dom $H = \mathcal{H}_0^1(\Omega) \cap \mathcal{H}^2(\Omega)$.

Proof. By the form representation theorem, $f \in \mathrm{Dom}\, H$ iff $f \in Q(H) = H_0^1(\Omega)$ and $g \in L^2(\Omega)$ exists such that

$$q(f,\psi) := \frac{1}{2}\langle \nabla f, \nabla \psi\rangle - C\int_\Omega \frac{1}{r} f(\mathbf{x})\overline{\psi(\mathbf{x})}\mathrm{d}\mathbf{x} = \langle g, \psi\rangle, \quad \forall \psi \in Q(H).$$

Since, by the Hardy inequality, $r^{-1}f \in L^2(\Omega)$; the equation above implies that

$$\frac{1}{2}\langle \nabla f, \nabla \psi\rangle = \Big\langle g + \frac{C}{r} f, \psi \Big\rangle$$

for all $\psi \in Q(H)$ and so for all $\psi \in C_C^\infty(\Omega)$ too. This means that the weak derivative $-\Delta f$ exists and $-\Delta f = 2g + 2Cr^{-1}f \in L^2(\Omega)$ which gives $\mathrm{Dom}\, H \subset \mathcal{H}_0^1(\Omega) \cap \mathcal{H}^2(\Omega)$. To prove the opposite inclusion, consider $f \in \mathcal{H}_0^1(\Omega) \cap \mathcal{H}^2(\Omega)$ and $\psi \in Q(H)$. Let $\{\psi_n\} \subset C_C^\infty(\Omega)$ be a sequence such that $\lim_{n\to\infty} |||\psi - \psi_n||| = 0$. Then we may integrate by parts:

$$q(f,\psi_n) = -\frac{1}{2}\langle \Delta f, \psi_n\rangle + \frac{1}{2}\int_{\partial\Omega} \nabla f(\mathbf{x})\overline{\psi_n(\mathbf{x})}\mathrm{d}\mathbf{S} - \Big\langle \frac{C}{r} f, \psi_n\Big\rangle = \Big\langle -\frac{1}{2}\Delta f - \frac{C}{r} f, \psi_n \Big\rangle.$$

The integration over the boundary $\partial\Omega$ is well defined since $\nabla f \in \mathcal{H}^1(\Omega)$ implies $\nabla f|_{\partial\Omega} \in \mathcal{H}^{1/2,2}(\partial\Omega) \subset L^2(\partial\Omega)$ (see Paragraph 7.56 in [41]), and is zero since $\psi_n|_{\partial\Omega} = 0$. Passing to the limit $n \to \infty$, we conclude that

$$q(f,\psi) = \Big\langle -\frac{1}{2}\Delta f - \frac{C}{r} f, \psi \Big\rangle.$$

So setting $g = -\frac{1}{2}\Delta f - \frac{C}{r} f \in L^2(\Omega)$ completes the proof. □

Remark B.11 *Following the same line of reasoning as above, one can prove that*

$$\mathrm{Dom}\,(-\Delta_D) = \mathcal{H}_0^1(\Omega) \cap \mathcal{H}^2(\Omega)$$

too. Actually, such proof is even more effortless. The selfadjointness of the Coulomb Hamiltonian may be then deduced using the Kato-Rellich theorem since, by the Hardy inequality (B.5), it holds

$$\begin{aligned}\|Cr^{-1}\psi\|^2 &\leqslant 4C^2\|\nabla\psi\|^2 = 4C^2\langle \psi, -\Delta_D\psi\rangle \leqslant 4C^2\frac{1}{\epsilon}\|\psi\|\,\epsilon\| - \Delta_D\psi\| \\ &\leqslant 2C^2\left(\epsilon^2\| - \Delta_D\psi\|^2 + \frac{1}{\epsilon^2}\|\psi\|^2\right),\end{aligned}$$

for all $\psi \in \mathrm{Dom}\,(-\Delta_D)$ *and* $\epsilon > 0$.

B.3 Error estimate for a perturbation expansion

In the famous book of Kato [35], one can find several error estimates for a perturbation expansion. Here we provide one more. Let $H_a := H \dotplus V_a$, where V_a stands for a scalar potential, be 'a perturbation' of the Hamiltonian H. For our purposes, it means that a positive decreasing function $\mathcal{W}$ exists such that $\lim_{a\to 0+} \mathcal{W}(a) = 0$ and, for every $\xi \in \operatorname{Res} H \cap \mathbb{R}$, $\|K_a(\xi)\| \leqslant \max\left\{1, \operatorname{dist}(\xi, \sigma(H))^{-1}\right\} \mathcal{W}(a)$ where $K_a(\xi) := |R(\xi)|^{1/2} V_a R(\xi)^{1/2}$ with $R(\xi)$ being the resolvent of H. Generalizing the results of Section IV.5.1, this implies that for $\delta > 0$ small enough, there is exactly one single eigenvalue $\lambda_a \in \sigma(H_a)$ in the δ-neighborhood of an isolated single eigenvalue $\lambda \in \sigma(H)$ if a is smaller then some a_δ. Practically, it is useful to consider $\delta \leqslant \operatorname{dist}(\lambda, \sigma(H) \setminus \{\lambda\})/2$, i.e., smaller then a half of the so-called isolation distance.

Let Γ be an anti-clockwise oriented circle of the radius δ and with the center λ. Then, by the recursive application of the resolvent formula:

$$(H_a - \xi)^{-1} =: R_a(\xi) = R(\xi) - R_a(\xi) V_a R(\xi), \tag{B.6}$$

we have (see [35] for details)

$$\lambda_a - \lambda = \frac{1}{2\pi i} \sum_{p=1}^{N} \frac{(-1)^p}{p} \operatorname{Tr} \int_\Gamma (V_a R(\xi))^p \,\mathrm{d}\xi + \mathscr{R}_{N+1}(a) \tag{B.7}$$

with

$$\mathscr{R}_{N+1}(a) := \frac{(-1)^N}{2\pi i} \operatorname{Tr} \int_\Gamma (\xi - \lambda) R_a(\xi) (V_a R(\xi))^{N+1} \,\mathrm{d}\xi. \tag{B.8}$$

The integral in (B.8) is a finite rank operator and hence its trace may be estimated by the norm. Indeed, using the following expansion:

$$R_{(a)}(\xi) = -\frac{P_{(a)}}{\xi - \lambda_{(a)}} + S_{(a)}(\xi) = \sum_{n=-1}^{\infty} (\xi - \lambda_{(a)})^n S_{(a)}^{(n+1)},$$

where $S(\xi)$ and $S_a(\xi)$ are reduced resolvents of H and H_a, respectively, $S_{(a)}^{(n)} := -P_{(a)}$ for $n = 0$ and $S_{(a)}(\lambda_{(a)})^n$ otherwise; we have

$$\begin{aligned}
&\frac{1}{2\pi i} \int_\Gamma (\xi - \lambda) R_a(\xi) (V_a R(\xi))^{N+1} \,\mathrm{d}\xi \\
=&\frac{1}{2\pi i} \int_\Gamma \frac{-P_a}{\xi - \lambda_a} \sum_{\substack{i_j \geqslant -1 \\ i_1 + i_2 + \ldots + i_{N+1} \neq -2}} (\xi - \lambda)^{i_1 + i_2 + \ldots + i_{N+1} + 1} \prod_{j=1}^{N+1} V_a S^{(i_j+1)} \,\mathrm{d}\xi \\
&+ \frac{1}{2\pi i} \int_\Gamma \frac{-P_a}{(\xi - \lambda_a)(\xi - \lambda)} \sum_{\substack{i_j \geqslant -1 \\ i_1 + i_2 + \ldots + i_{N+1} = -2}} \prod_{j=1}^{N+1} V_a S^{(i_j+1)} \,\mathrm{d}\xi \\
&+ \frac{1}{2\pi i} \int_\Gamma S_a(\xi) \frac{1}{\xi - \lambda} \sum_{\substack{i_j \geqslant -1 \\ i_1 + i_2 + \ldots + i_{N+1} = -2}} \prod_{j=1}^{N+1} V_a S^{(i_j+1)} \,\mathrm{d}\xi
\end{aligned}$$

$$= -P_a \sum_{\substack{i_j \geqslant -1 \\ i_1+i_2+\ldots+i_{N+1} \neq -2}} (\lambda_a - \lambda)^{i_1+i_2+\ldots+i_{N+1}+1} \prod_{j=1}^{N+1} V_a S^{(i_j+1)}$$

$$+ S_a(\lambda) \sum_{\substack{i_j \geqslant -1 \\ i_1+i_2+\ldots+i_{N+1} = -2}} \prod_{j=1}^{N+1} V_a S^{(i_j+1)}.$$

The rank of the first term is one since P_a is a projection. Each term of the second sum is also a rank one operator because it contains at least two projections P. As the number of terms in this sum is one for $N = 1$ and $\binom{N+1}{2}\binom{2N-3}{N-2}$ otherwise, it follows that

$$\text{Rank(integral on RHS of (B.8))} \leqslant 1 + \binom{N+1}{2}\binom{2N-3}{N-2}.$$

Notice that the estimate is valid even if $\lambda_a = \lambda$.

Due to the cyclic property of the trace, it holds

$$\begin{aligned} &\operatorname{Tr}(\xi - \lambda) R_a(\xi)(V_a R(\xi))^{N+1} \\ &= \operatorname{Tr} |R(\xi)|^{1/2} (\xi - \lambda) R(\xi)^{1/2} (H - \xi)^{1/2} R_a(\xi) (H - \xi)^{1/2} \operatorname{sgn} R(\xi) K_a(\xi)^{N+1}. \end{aligned}$$

The latter expression is ready to be estimated by the norm. Consider $\delta < 1$ and $\xi \in \Gamma$. Furthermore, define $\xi_+ := \lambda + \delta$. Then using the functional calculus, we obtain:

$$\|K_a(\xi)\| \leqslant \||R(\xi)|^{1/2} |H - \xi_+|^{1/2}\| \|K_a(\xi_+)\| \|(H - \xi_+)^{1/2} R(\xi)^{1/2}\| \leqslant 3\delta^{-1} \mathcal{W}(a).$$

Since $\operatorname{sgn} R(\xi)$ is an isometry, it is of unit norm. Next we have

$$\||R(\xi)|^{1/2} (\xi - \lambda) R(\xi)^{1/2}\| \leqslant \||R(\xi)|^{1/2}\|^2 \delta = 1.$$

Finally, for a small enough (namely, such that $\delta^{-1}\mathcal{W}(a) \leqslant 1/6$), it holds

$$\begin{aligned} &\|(H - \xi)^{1/2} R_a(\xi)(H - \xi)^{1/2}\| = \|(R(\xi)^{1/2}(H + V_a - \xi) R(\xi)^{1/2})^{-1}\| \\ &= \|(Id + R(\xi)^{1/2} V_a R(\xi)^{1/2})^{-1}\| \leqslant \frac{1}{1 - \|K_a(\xi)\|} \leqslant 2. \end{aligned}$$

Altogether, we have arrived at the following estimate

$$|\mathscr{R}_{N+1}(a)| \leqslant 2\left[1 + \binom{N+1}{2}\binom{2N-3}{N-2}\right] \delta^{-N} 3^{N+1} \mathcal{W}(a)^{N+1}. \qquad \text{(B.9)}$$

Using the Stirling formula, it may be deduced that

$$\binom{N+1}{2}\binom{2N-3}{N-2} = 4^N \frac{N^{3/2}}{16\sqrt{\pi}}(1 + o(1)) \quad \text{as } N \to \infty$$

from which it follows that if we consider $a \leqslant \min\{a_\delta, a_0\}$, where a_0 is defined by the equation $\delta^{-1}\mathcal{W}(a_0) = 1/13$, then $\lim_{N\to\infty} \mathscr{R}_N(a) = 0$, i.e., the perturbation expansion converges.

C. Spheroidal Functions

The spheroidal functions are solutions to the equation

$$(1-\xi^2)\frac{\partial^2\psi}{\partial\xi^2} - 2\xi\frac{\partial\psi}{\partial\xi} + \left[\lambda + 4\theta(1-\xi^2) - \mu^2(1-\xi^2)^{-1}\right]\psi = 0, \tag{C.1}$$

where all parameters are in general complex numbers. Let us briefly summarize basic definitions and notions related to the spheroidal functions following the notation of the source [6]. Then let us make several observations on these functions.

There are two solutions to (C.1) that behave like ξ^ν times a single-valued function and $\xi^{-\nu-1}$ times a single-valued function at ∞. The exponent ν is a function of λ, θ, μ, and is called the characteristic exponent. Usually, it is more convenient to regard λ as a function of ν, μ and θ. We shall write $\lambda = \lambda_\nu^\mu(\theta)$. If ν or μ is an integer we denote it by n or m, respectively. The functions $\lambda_\nu^\mu(\theta)$ obey the symmetry relations

$$\lambda_\nu^\mu(\theta) = \lambda_\nu^{-\mu}(\theta) = \lambda_{-\nu-1}^\mu(\theta) = \lambda_{-\nu-1}^{-\mu}(\theta). \tag{C.2}$$

A first group of solutions (the radial spheroidal functions) is obtained as expansions in series of the Bessel functions,

$$S_\nu^{\mu(j)}(\xi,\theta) = (1-\xi^{-2})^{-\mu/2} s_\nu^\mu(\theta) \sum_{r=-\infty}^{\infty} a_{\nu,r}^\mu(\theta)\psi_{\nu+2r}^{(j)}(2\theta^{1/2}\xi), \tag{C.3}$$

$j = 1,2,3,4$, where the factor $s_\nu^\mu(\theta)$ is determined below and where

$$\psi_\nu^{(1)}(\zeta) = \sqrt{\frac{\pi}{2\zeta}}\, J_{\nu+1/2}(\zeta), \quad \psi_\nu^{(2)}(\zeta) = \sqrt{\frac{\pi}{2\zeta}}\, Y_{\nu+1/2}(\zeta),$$
$$\psi_\nu^{(3)}(\zeta) = \sqrt{\frac{\pi}{2\zeta}}\, H_{\nu+1/2}^{(1)}(\zeta), \quad \psi_\nu^{(4)}(\zeta) = \sqrt{\frac{\pi}{2\zeta}}\, H_{\nu+1/2}^{(2)}(\zeta).$$

The coefficients $a_{\nu,r}^\mu(\theta)$ (sometimes denoted only by a_r for the sake of simplicity) satisfy a three term recurrence relation

$$\gamma_{\nu,r}^\mu(\theta)a_{\nu,r-1}^\mu(\theta) + \beta_{\nu,r}^\mu(\theta)a_{\nu,r}^\mu(\theta) + \alpha_{\nu,r}^\mu(\theta)a_{\nu,r+1}^\mu(\theta) = -\lambda_\nu^\mu(\theta)a_{\nu,r}^\mu(\theta), \tag{C.4}$$

where

$$\alpha^{\mu}_{\nu,r}(\theta) = \frac{(\nu+2r+\mu+2)(\nu+2r+\mu+1)}{(\nu+2r+3/2)(\nu+2r+5/2)}\,\theta,$$

$$\beta^{\mu}_{\nu,r}(\theta) = -(\nu+2r)(\nu+2r+1) + \frac{(\nu+2r)(\nu+2r+1)+\mu^2-1}{(\nu+2r-1/2)(\nu+2r+3/2)}\,2\theta,$$

$$\gamma^{\mu}_{\nu,r}(\theta) = \frac{(\nu+2r-\mu)(\nu+2r-\mu-1)}{(\nu+2r-3/2)(\nu+2r-1/2)}\,\theta.$$

Here and in what follows we assume that $\nu+1/2$ is not an integer (to our knowledge, the omitted case is not yet fully investigated).

The coefficients $a^{\mu}_{\nu,r}(\theta)$ may be chosen such that

$$a^{\mu}_{\nu,0}(\theta) = a^{\mu}_{-\nu-1,0}(\theta) = a^{-\mu}_{\nu,0}(\theta),$$

and so (see (C.2))

$$a^{\mu}_{\nu,r}(\theta) = a^{\mu}_{-\nu-1,-r}(\theta) = \frac{(\nu-\mu+1)_{2r}}{(\nu+\mu+1)_{2r}}\,a^{-\mu}_{\nu,r}(\theta) \tag{C.5}$$

where $(a)_r := a(a+1)(a+2)\dots(a+r-1) = \Gamma(a+r)/\Gamma(a)$, $(a)_0 := 1$. Equation (C.4) leads to a convergent infinite continued fraction and this way one can prove that

$$\lim_{r\to\infty}\frac{r^2 a_r}{a_{r-1}} = \lim_{r\to-\infty}\frac{r^2 a_r}{a_{r+1}} = \frac{\theta}{4}. \tag{C.6}$$

From (C.6) and the asymptotic formulae for Bessel functions, it follows that (C.3) converges if $|\xi|>1$.

If we set in (C.3)

$$s^{\mu}_{\nu}(\theta) = \left[\sum_{r=-\infty}^{\infty}(-1)^r a^{\mu}_{\nu,r}(\theta)\right]^{-1} \tag{C.7}$$

then $S^{\mu(j)}_{\nu}(\xi,\theta) \sim \psi^{(j)}_{\nu}(2\theta^{1/2}\xi)$, for $|\arg(\theta^{1/2}\xi)|<\pi$, as $\xi\to\infty$. So we have the asymptotic forms, valid as $\xi\to\infty$,

$$S^{\mu(3)}_{\nu}(\xi,\theta) = \frac{1}{2}\,\theta^{-1/2}\xi^{-1}\mathrm{e}^{i(2\theta^{1/2}\xi-\nu\pi/2-\pi/2)}[1+O(|\xi|^{-1})] \quad \text{for } -\pi<\arg(\theta^{1/2}\xi)<2\pi, \tag{C.8}$$

and

$$S^{\mu(4)}_{\nu}(\xi,\theta) = \frac{1}{2}\,\theta^{-1/2}\xi^{-1}\mathrm{e}^{-i(2\theta^{1/2}\xi-\nu\pi/2-\pi/2)}[1+O(|\xi|^{-1})] \quad \text{for } -2\pi<\arg(\theta^{1/2}\xi)<\pi. \tag{C.9}$$

The radial spheroidal functions satisfy the relation

$$S^{\mu(3)}_{\nu} = \frac{1}{i\cos(\nu\pi)}\left(S^{\mu(1)}_{-\nu-1} + i\,\mathrm{e}^{-i\pi\nu}S^{\mu(1)}_{\nu}\right). \tag{C.10}$$

They are especially useful for a large values of ξ; the larger is ξ the better is the convergence of the expansion. To obtain solutions useful near ± 1, and even on the segment $(-1,1)$, it is convenient to turn to expansions in series of the Legendre functions,

$$\begin{aligned} Ps^{\mu}_{\nu}(\xi,\theta) &= \sum_{r=-\infty}^{\infty} (-1)^r a^{\mu}_{\nu,r}(\theta) P^{\mu}_{\nu+2r}(\xi), \\ Qs^{\mu}_{\nu}(\xi,\theta) &= \sum_{r=-\infty}^{\infty} (-1)^r a^{\mu}_{\nu,r}(\theta) Q^{\mu}_{\nu+2r}(\xi). \end{aligned} \tag{C.11}$$

These solutions are called the angular spheroidal functions and are related to the radial spheroidal functions by the following formulae:

$$\begin{aligned} S^{\mu(1)}_{\nu}(\xi,\theta) &= \pi^{-1}\sin[(\nu-\mu)\pi]\mathrm{e}^{-i\pi(\nu+\mu+1)} K^{\mu}_{\nu}(\theta) Qs^{\mu}_{-\nu-1}(\xi,\theta), \\ S^{m(1)}_{n}(\xi,\theta) &= K^{m}_{n}(\theta) Ps^{m}_{n}(\xi,\theta), \end{aligned} \tag{C.12}$$

where $K^{\mu}_{\nu}(\theta)$ may be expressed in the coefficients $a^{\mu}_{\nu,r}(\theta)$, and sometimes it is called the joining factor. In more detail, for any $k \in \mathbb{Z}$ it holds true that

$$K^{\mu}_{\nu}(\theta) = \frac{1}{2}\left(\frac{\theta}{4}\right)^{\nu/2+k} \Gamma(1+\nu-\mu+2k)\,\mathrm{e}^{(\nu+k)\pi i} s^{\mu}_{\nu}(\theta)\, \frac{\displaystyle\sum_{r=-\infty}^{k} \frac{(-1)^r a^{\mu}_{\nu,r}(\theta)}{(k-r)!\,\Gamma(\nu+k+r+3/2)}}{\displaystyle\sum_{r=k}^{\infty} \frac{(-1)^r a^{\mu}_{\nu,r}(\theta)}{(r-k)!\,\Gamma(1/2-\nu-k-r)}}.$$

The following auxiliary result concerns the asymptotic expansion of the radial spheroidal function of the third kind.

Proposition C.1 *Let $m \in \mathbb{N}$, $\nu \notin \mathbb{Z}$. Then*

$$\begin{aligned} S^{m(3)}_{\nu}(\xi,\theta) =& \frac{\mathrm{e}^{i(\nu+3/2)\pi}\tan(\nu\pi)}{2\pi}\left(K^{m}_{-\nu-1}(\theta) + \frac{K^{m}_{\nu}(\theta)}{\mathrm{e}^{i(3\nu+1/2)\pi}}\right)\left(\frac{1+\xi}{1-\xi}\right)^{m/2} \\ &\times \sum_{k=0}^{m-1} \frac{(-1)^{m-k}(m-k-1)!(-\nu)_k(\nu+1)_k}{k!}\left(\frac{1-\xi}{2}\right)^{k} \\ &+ O\left((1-\xi)^{m/2}\log(1-\xi)\right) \end{aligned}$$

as $\xi \to 1+$.

Proof. By the definition (C.10) and by (C.12) one has

$$S^{m(3)}_{\nu}(\xi,\theta) = \frac{\mathrm{e}^{i(\nu+3/2)\pi}\tan(\nu\pi)}{\pi}\left(K^{m}_{-\nu-1}(\theta) Qs^{m}_{\nu}(\xi,\theta) + \frac{K^{m}_{\nu}(\theta) Qs^{m}_{-\nu-1}(\xi,\theta)}{\mathrm{e}^{i(3\nu+1/2)\pi}}\right).$$

The asymptotic expansion for the Legendre functions reads (the best reference here is [42], the standard work of interest is [43]),

$$Q_\nu^m(\xi) = \frac{1}{2}\left(\frac{1+\xi}{1-\xi}\right)^{m/2}\sum_{k=0}^{m-1}\frac{(-1)^{m-k}(m-k-1)!(-\nu)_k(\nu+1)_k}{k!}\left(\frac{1-\xi}{2}\right)^k$$
$$+\,O\left((1-\xi)^{m/2}\log(1-\xi)\right) \quad \text{as } \xi\to 1+,$$

from which it follows

$$Q_{-\nu-1}^m(\xi) = Q_\nu^m(\xi) + O\left((1-\xi)^{m/2}\log(1-\xi)\right) \quad \text{as } \xi\to 1+\,.$$

This together with (C.11) and (C.5) implies that

$$Qs_{-\nu-1}^m(\xi,\theta) = Qs_\nu^m(\xi,\theta) + O\left((1-\xi)^{m/2}\log(1-\xi)\right) \quad \text{as } \xi\to 1+$$

which completes the proof. □

Two following propositions answer the question when a spheroidal eigenvalue is real.

Proposition C.2 *Let $\nu = -1/2 + it$ where $t\in\mathbb{R}$, and μ, $\theta\in\mathbb{R}$. Then $\lambda_\nu^\mu(\theta)\in\mathbb{R}$.*

Proof. One may view the set of equations (C.4), with $r\in\mathbb{Z}$, as an eigenvalue equation for $\lambda_\nu^\mu(\theta)$ that is an analytic function of θ. A particular solution is fixed by the condition $\lambda_\nu^\mu(0) = \nu(\nu+1)$. Consider the set of complex conjugated equations. Since $\overline{\beta_{\nu,r}^\mu} = \beta_{\overline{\nu},r}^\mu(\theta) = \beta_{-\nu-1,r}^\mu(\theta)$, and the similar is true for $\alpha_{\nu,r}^\mu(\theta)$ and $\gamma_{\nu,r}^\mu(\theta)$,

$$\beta_{-\nu-1,r}^\mu(\theta)\overline{a_{\nu,r-1}^\mu(\theta)} + \alpha_{-\nu-1,r}^\mu\overline{a_{\nu,r}^\mu(\theta)} + \gamma_{-\nu-1,r}^\mu(\theta)\overline{a_{\nu,r+1}^\mu(\theta)} = \overline{\lambda_\nu^\mu(\theta)}\,\overline{a_{\nu,r}^\mu(\theta)}.$$

Furthermore, since for each ν of the form considered,

$$\lambda_{-\nu-1}^\mu(0) = (-\nu-1)(-\nu) = \nu(\nu+1) = \overline{\nu(\nu+1)} = \overline{\lambda_\nu^\mu(0)},$$

one has $\lambda_{-\nu-1}^\mu(\theta) = \overline{\lambda_\nu^\mu(\theta)}$. Moreover, by (C.2), $\lambda_{-\nu-1}^\mu(\theta) = \lambda_\nu^\mu(\theta)$ in general. We conclude that $\lambda_\nu^\mu(\theta)\in\mathbb{R}$. □

Proposition C.3 *Let μ, ν, $\theta\in\mathbb{R}$ and $\nu+1/2\notin\mathbb{Z}$. Then $\lambda_\nu^\mu(\theta)\in\mathbb{R}$.*

Proof. Following the same line of reasoning as in the proof of Proposition C.2, we conclude that $\lambda_\nu^\mu(\theta)$ and $\overline{\lambda_\nu^\mu(\theta)}$ are the eigenvalues of the same matrix and simultaneously $\lambda_\nu^\mu(0) = \nu(\nu+1) = \overline{\lambda_\nu^\mu(0)}$ which means that $\lambda_\nu^\mu(\theta) = \overline{\lambda_\nu^\mu(\theta)}$ for all $\theta\in\mathbb{R}$. □

Acknowledgments

First of all, I would like to thank my supervisor professor Pavel Šťovíček for numerous fruitful discussions, encouragement, and other help during the whole PhD study. I also wish to express my thanks to professor Pierre Duclos for suggesting the problem of Chapter IV, stimulating conversations, and his hospitality during my stays in Marseille; and to David Krejčiřík for pointing out the usefulness of Lemma B.5. Next, I would like to acknowledge partial support from the grant No. 202/08/H072 of the Czech Science Foundation. Last but not least, I thank my family, friends, and Eva for their support during my studies.

Bibliography

[1] M. Reed and B. Simon. *Methods of Modern Mathematical Physics I.* Academic Press, 1980.

[2] M. Reed and B. Simon. *Methods of Modern Mathematical Physics II.* Academic Press, 1975.

[3] M. Reed and B. Simon. *Methods of Modern Mathematical Physics III.* Academic Press, 1979.

[4] M. Reed and B. Simon. *Methods of Modern Mathematical Physics IV.* Academic Press, 1978.

[5] M. Abramowitz and I.A. Stegun. *Handbook of Mathematical Functions.* National Bureau of Standards, 1964.

[6] H. Bateman and A. Erdélyi. *Higher Transcendental Functions III.* McGraw-Hill Book Company, 1955.

[7] B. Simon. *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms.* Princeton University Press, 1971.

[8] J. Brüning, V. Geyler, and I. Lobanov. Spectral properties of a short-range impurity in a quantum dot. *J. Math. Phys.*, 46:1267–1290, 2004.

[9] B. A. Joyce, P.C. Kelires, A.G. Naumovets, and D.D. Vvedensky. *Quantum Dots: Fundamentals, Applications, and Frontiers.* Springer, 2005.

[10] A. Comtet. On the Landau levels on the hyperbolic plane. *Ann. Physics*, 173:185–209, 1987.

[11] M. Antoine, A. Comtet, and S. Ouvry. Scattering on a hyperbolic torus in a constant magnetic field. *J. Phys. A: Math. Gen.*, 23:3699–3710, 1990.

[12] Yu. A. Kuperin, R. V. Romanov, and H. E. Rudin. Scattering on the hyperbolic plane in the Aharonov-Bohm gauge field. *Lett. Math. Phys.*, 31:271–278, 1994.

[13] O. Lisovyy. Aharonov-Bohm effect on the Poincaré disk. *J. Math. Phys.*, 48, 2007.

[14] D. V. Bulaev, V. A. Geyler, and V. A. Margulis. Effect of surface curvature on magnetic moment and persistent currents in the two-dimensional quantum rings and dots. *Phys. Rev. B*, 69, 2004.

[15] J. F. Cariñena, M. F. Rañada, and M. Santander. The quantum harmonic oscillator on the sphere and the hyperbolic plane. *Ann. Physics*, 322:2249–2278, 2007.

[16] J. Meixner and F.V. Schäfke. *Mathieusche Funktionen und Sphäroidfunktionen.* Springer-Verlag, 1954.

[17] X.L. Yang, S.H. Guo, and F.T. Chan. Analytic solution of a two-dimensional hydrogen atom. I. Nonrelativistic theory. *Phys. Rev. A*, 43(3):1186–1196, 1991.

[18] L.C. Hostler. Coulomb Green's function in f-dimensional space. *J. Math. Phys.*, 11(10):2966–2970, 1970.

[19] L. Chaos-Cador and E. Ley-Koo. Common generating function for two-dimensional hydrogen atom complete wave functions. *International Journal of Quantum Chemistry*, 107(1):12–22, 2007.

[20] L. Chaos-Cador and E. Ley-Koo. Two-dimensional hydrogen atom confined in circles, angles, and circular sectors. *International Journal of Quantum Chemistry*, 103(4):368–87, 2005.

[21] M. Robnik and V.G. Romanovski. Two-dimensional hydrogen atom in a strong magnetic field. *J. Phys. A: Math. Gen.*, 36(29), 2003.

[22] C. Grimaldi. Energy levels of a two-dimensional hydrogen atom with spin-orbit Rashba interaction. *Phys. Rev. B*, 77(11), 2008.

[23] D.G.W. Parfitt and M.E. Portnoi. The two-dimensional hydrogen atom revisited. *J. Math. Phys.*, 43, 2002.

[24] O. Atabek, C. Deutsh, and M. Lavaud. Schrödinger equation for two-dimensional Coulomb potential. *Phys. Rev. A*, 9(6):2617–2624, 1974.

[25] M. F. Rañada and M. Santader. On harmonic oscillators on the two-dimensional sphere S^2 and the hyperbolic plane H^2. *J. Math. Phys.*, 43, 2002.

[26] N. Dunford and J.T. Schwartz. *Linear Operators Part II: Spectral theory. Self Adjoint Operators in Hilbert Space.* Wiley-Interscience Publication, 1988.

[27] J. Weidmann. *Linear Operators in Hilbert Spaces.* Springer-Verlag, 1980.

[28] S. Albeverio, F. Gesztesy, R. Høegh-Krohn, and H. Holden. *Solvable Models in Quantum Mechanics.* Springer-Verlag, 1988.

[29] J. Brüning, V. Geyler, and K. Pankrashkin. On-diagonal singularities of the Green functions for Schrödinger operators. *J. Math. Phys.*, 46, 2005.

[30] F. A. Berezin and M. A. Shubin. *The Schrödinger Equation.* Kluwer Academic Publishers, 1991.

[31] V. Geyler and I. Popov. Eigenvalues imbedded in the band spectrum for a periodic array of quantum dots. *Rep. Math. Phys.*, 39:275–281, 1997.

[32] Matěj Tušek. Masters thesis: Analysis of two-dimensional quantum models with singular potentials. `http://kmlinux.fjfi.cvut.cz/~tusekmat/download/tusek_thesis.pdf`, 2006.

[33] J. Brüning, V. Geyler, and K. Pankrashkin. Spectra of self-adjoint extensions and applications to solvable Schrödinger operators. *Rev. Math. Phys.*, 20:1–70, 2008.

[34] R. Brumellhuis and P. Duclos. Effective Hamiltonians for atoms in very strong magnetic fields. *J. Math. Phys.*, 47, 2006.

[35] T. Kato. *Perturbation theory for linear operators.* Springer-Verlag, 1966.

[36] Frank Bowman. *Introduction to Bessel Functions.* Dover Publications, 1958.

[37] A. Bouzouina. Stability of the two-dimensional Brown-Ravenhall operator. *Proc. Roy. Soc. Edinburgh Sect. A*, 132.

[38] I.W. Herbst. Spectral theory of the operator $(p^2 + m^2)^{1/2} - Ze^2/r$. *Commun. Math. Phys.*, 53:285–294, 1977.

[39] E.B. Davies. *Spectral Theory and Differential Operators.* Press Syndicate of the University of Cambridge, 1995.

[40] Zhi-Qiang Wang and Meijun Zhu. Hardy inequalities with boundary terms. *Electronic Journal of Differential Equations*, 43, 2003.

[41] R.A. Adams. *Sobolev Spaces.* Academic Press, 1975.

[42] functions.wolfram.com. `http://functions.wolfram.com/07.11.06.0009.01`.

[43] H. Bateman. *Higher Transcendental Functions I.* McGraw-Hill Book Company, 1953.