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PhD thesis

Periodic Phenomena in the Theory of Large Atoms

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Abstract

Any sufficiently advanced mathematical model for atoms should in some way reflect the periodicity known from the periodic table of the elements appearing in nature. This thesis describes, in selected models, the periodicity of large atoms. In particular, we discuss periodic phenomena in a Thomas-Fermi mean-field model for the atom. In this model, the atom is described by a self-adjoint 1-particle Schrödinger operator, and electrons see each other only through a mean-field potential coming from the semi-classical Thomas-Fermi functional density theory. This defines an atom for each atomic number Z. It is proved that the operators of this model converge towards particular self-adjoint operators ("infinite atoms") in the strong resolvent sense, but only along certain subsequences $Z_n \to \infty$ describing the periodicity of the atoms to leading order. It is remarkable that this is a model sufficiently advanced to exhibit periodicity, while still simple enough so that one can completely describe the periodicity in the $Z \to \infty$ limit. We further treat some more abstract mathematical theory related to this main result: Firstly, strong resolvent convergence of general self-adjoint operators is related to convergence of symmetric operators which they extend via von Neumann's extension theory – and in particular to strong convergence of graphs of the latter. Secondly, the periodicity in the Thomas-Fermi mean-field model can be interpreted in terms of that of the scattering length (an object often studied in the physics literature) of the associated mean-field potentials. We develop a simple mathematical theory for the scattering length for a large class of real-valued potentials. As novel parts of this theory, the scattering length varies continuously as a function of the potentials, and we prove that differences in the number of negative eigenvalues of two one-dimensional Schrödinger operators can be measured by tracing the value of the scattering length along any choice of continuous curve connecting their respective potentials.

Resumé

Enhver tilstrækkeligt kompliceret matematisk atommodel burde afspejle den periodicitet, som kendes fra det periodiske system over naturligt fremkommende grundstoffer. Denne afhandling beskriver, i udvalgte modeller, periodiciteten af store atomer. Specielt diskuteres periodiske fænomener i en Thomas-Fermi middelfelt-model for atomet. I denne model beskrives atomet ved en selvadjungeret 1-partikel Schrödinger-operator, og elektroner ser hinanden alene gennem et middelfelt-potentiale, som kommer fra det semiklassiske Thomas-Fermi tæthedsfunktionale. Dette definerer et atom for hvert atomnummer Z. Det vises, at operatorene i denne model konvergerer imod specifikke selvadjungerede operatorer ("uendelige atomer") i stærk resolvent forstand, men at dette kun er tilfældet langs visse delfølger $Z_n \to \infty$, som beskriver atomernes periodicitet til ledende orden. Det er bemærkelsesværdigt, at denne model er tilstrækkeligt kompliceret til at udvise periodicitet, men stadig tilstrækkeligt simpel til at man kan beskrive periodiciteten fuldstændigt i grænsen $Z \to \infty$. Vi behandler videre mere abstrakt matematisk teori relateret til dette hovedresultat: For det første relateres stærk resolvent konvergens af generelle selvadjungerede operatorer til konvergens af symmetriske operatorer, som de udvider via von Neumanns udvidelsesteori – og specielt til stærk konvergens af sidstnævntes grafer. Desuden kan periodiciteten i Thomas-Fermi middelfelt-modellen fortolkes som periodicitet af spredningslængderne (et begreb ofte studeret i fysiklitteraturen) af de tilhørende middelfelt-potentialer. Vi udvikler en simpel matematisk teori for spredningslængden af en stor klasse af potentialer. Som originale bidrag fra denne teori vises, at spredningslængden varierer kontinuert som funktion af potentialerne, og at forskellen i antallet af negative egenværdier af to endimensionale Schrödinger-operatorer kan måles ved at følge spredningslængdens værdi langs ethvert valg af kontinuert kurve, der forbinder deres respektive potentialer.

Aknowledgements

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Vanløse, February 2024

Papers included in the thesis

In the thesis the paper draft "Periodicity of atomic structure in a Thomas-Fermi mean-field model" – to which both of its authors contributed equally – is included. Also, a version of [Bje23] by the author is included. For further details, see Chapters 2 and 3.

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Chapter 1

Introduction

1.1 Prologue: A mathematical story about large atoms

A very central motivation for studying the problems discussed in this thesis is the strive to understand the complex behaviour of large atoms. Being mathematicians, we of course consider the overly idealized situation where the atomic number Z of the atom actually tends towards infinity. While arbitrarily large atoms do not exist in the real world due to relativistic effects and the short range of the strong nuclear force, taking the $Z \to \infty$ limit provides a convenient framework in which we actually have a chance of presenting rigorous results. As will be explained below we wish in the ideal world to describe atoms by quantum mechanical Schrödinger theory where exact calculations can virtually never be carried out – but where semi-classical and related methods may often apply in the limiting situation to yield rigorous (and interesting) asymptotic results. The field of large atoms within mathematical physics is vast and contains many monumental conjectures (cf. [Sim00], Section 3), perhaps most prominently the ionization conjecture. See [Nam22] for a recommended review hereof. However, we now pursue another, although somewhat related, path of studying the leading order asymptotic behaviour of some physical quantities associated with the atom in the large Z limit.

Throughout this introduction (and thesis) we ignore relativistic effects. We use units in which $e = 2m_e = \hbar = 4\pi\varepsilon_0 = 1$. This is Hartree atomic units with the exception that we set the mass of an electron to $1/2$ instead of 1.

Many-body Schrödinger theory: Consider, as a general model for an atom having a nucleus with charge $Z > 0$ and $N \in \mathbb{N}$ electrons orbiting this nucleus, the operator

$$H_{N,Z} = \sum_{i=1}^{N} \left(-\Delta_i - \frac{Z}{|x_i|} + \frac{1}{2} \sum_{j \neq i} \frac{1}{|x_i - x_j|} \right) \tag{1.1}$$

acting on a suitable subspace of $L^2(\mathbb{R}^3;\mathbb{C}^2)^{\otimes N} \simeq L^2(\mathbb{R}^{3N};\mathbb{C}^{2^N})$. Here, the fact that functions are $\mathbb{C}^2$-valued is describing the spin of electrons, and $(x_1,\ldots,x_N)$ are the coordinates in $(\mathbb{R}^3)^N$. Equivalently, we may write functions in our Hilbert space as functions of $(x_1,\sigma_1),\ldots,(x_N,\sigma_N) =: \underline{x}_1,\ldots,\underline{x}_N$ with x_i as before and $\sigma_i \in \{\pm 1\}$. The i^{th} term in the outer sum in (1.1) more or less models the dynamics of the i^{th} electron: $-\Delta_i = -\partial_x^2 - \partial_y^2 - \partial_z^2$ is (minus) the Laplace operator acting on the i^{th} factor in the tensor product and takes care of the kinetic energy of the electron. Meanwhile, $-Z/|x_i|$ describes the electrostatic Coulomb interaction between the nucleus and the electron, and the last term describes half of this interaction between the i^{th} and the remaining electrons – the other half is naturally distributed over the other terms in the outer sum. It is a standard result that there exists a canonical self-adjoint realization of the expression (1.1) on $C_0^\infty(\mathbb{R}^{3N};\mathbb{C}^{2^N}) \subseteq L^2(\mathbb{R}^{3N};\mathbb{C}^{2^N})$. That is, we can consider $H_{N,Z}$ as a self-adjoint operator on $L^2(\mathbb{R}^3;\mathbb{C}^2)^{\otimes N}$. Moreover, this operator is bounded below. We do not treat the details of this construction here, but the interested reader can consult introductory textbooks on mathematical quantum mechanics as for example [Tes14], Chapter 11. Finally, we restrict this operator to the space of anti-symmetric functions on $(\mathbb{R}^3 \times \{\pm 1\})^N$, i.e. functions ψ satisfying $\psi(\underline{x}_{\pi(1)},\dots,\underline{x}_{\pi(N)}) = \operatorname{sgn}(\pi)\psi(\underline{x}_1,\dots,\underline{x}_N)$ for any permutation $\pi \in S_N$, yielding a self-adjoint and bounded below operator (still denoted $H_{N,Z}$) acting on the N-fold antisymmetric tensor-product of $L^2(\mathbb{R}^3;\mathbb{C}^2)$. Note that we can indeed consider the restriction since $H_{N,Z}$ commutes with the projection onto this subspace. The restricted operator is the tremendously successful ***many-body Schrödinger model for the atom***. It is widely taken as the standard for modelling atoms theoretically, but still many physical phenomena are far from understood within this theory – and most things even seem out of reach of something resembling anything like a mathematical proof.

Due to the fact that $H_{N,Z}$ is bounded below we can define the ground state energy

$$E(N,Z) := \inf \sigma(H_{N,Z}) = \inf_{\|\psi\|=1} \langle \psi, H_{N,Z}\psi\rangle > -\infty \tag{1.2}$$

of the atom. It is a landmark result of Zhislin, [Zhi60], that the last infimum in (1.2) is attained for some ψ whenever $N < Z+1$. This in particular proves the existence of stable neutral atoms in the Schrödinger model by taking $Z = N \in \mathbb{N}$. The interpretation of $|\psi|^2$ for a minimizer ψ in (1.2) is that it is the joint density of all electrons orbiting the atom in (one of) its ground state(s) ψ. We define from any possible state ψ the corresponding one-particle electron density ρ_ψ by

$$\rho_\psi(x) := N \sum_{\sigma_1,\dots,\sigma_N \in \{\pm 1\}} \int_{\mathbb{R}^{3(N-1)}} |\psi((x,\sigma_1),\underline{x}_2,\dots,\underline{x}_N)|^2 \, dx_2 \cdots dx_N.$$

Of particular interest is the behaviour of the one-particle densities ρ_ψ with ψ ground states of $H_{Z,Z}$ with integer Z's, i.e. for neutral atoms. For a fixed choice of such ground states $\{\psi_Z\}_{Z=1}^\infty$ we denote the corresponding densities by $\{\rho_Z\}_{Z=1}^\infty$ with the ground states implicit in the notation. Alternatively, one can instead, as it is done in for example [LS77] and [Lie81], consider the situation with a sequence $\{\psi_Z\}_{Z=1}^\infty$ of "approximate ground states" – that is, states for which $\langle \psi_Z, H_{Z,Z}\psi_Z\rangle$ in a certain sense approximate well $E(Z) := E(Z,Z)$ for large integer Z.

The periodic nature of the periodic table of the elements and the behaviour of physical quantities in simpler models treated below suggest that, for some choices of ground states, there may – along certain sequences $\{Z_n\}_{n=1}^\infty \subseteq \mathbb{N}$ satisfying $Z_n \to \infty$ – be some kind of convergence (cf.[1] [Nam22], Conjecture 16)

$$\rho_{Z_n} \longrightarrow \rho_{\infty,t} \tag{1.3(t)}$$

[1]The statements in [Nam22] is formulated in terms of $H_{N_c(Z),Z}$ where $N_c(Z)$ is the maximum number so that the last infimum in (1.2) is attained. However, it is believed that $N_c(Z) - Z$ is bounded as $Z \to \infty$ (the ionization conjecture), and thus the effects of replacing Z with $N_c(Z)$ should be negligible – at least for leading order asymptotics.

as $n \to \infty$. Here, $\{\rho_{\infty,t}\}_t$ is some parametrized family of "one-particle densities" in the infinite atom which might of course also depend on the choices of ground states for the finite atoms, and the convergence towards $\rho_{\infty,t}$ for different t's should hold for different sequences of Z_n's. It seems plausible that the families $\{\rho_{\infty,t}\}_t$ could be parametrized by the unit circle, i.e. that the infinite atoms themselves would be periodic of nature. Proving results like (1.3(t)) is way out of reach of any known methods, but, assuming it is true, it will be very interesting to study the sequences in the set

$$\mathscr{A}_t(\{\psi_Z\}_{Z=1}^{\infty}) := \Big\{ \text{Sequences } \{Z_n\}_{n=1}^{\infty} \subseteq \mathbb{N} \text{ satisfying } (1.3(t)) \Big\},$$

where $\{\psi_Z\}_{Z=1}^{\infty}$ is as usual choices of ground states. For example, determining leading order n asymptotics of $\{Z_n\}_{n=1}^{\infty} \in \mathscr{A}_t(\{\psi_Z\}_{Z=1}^{\infty})$ would be an interesting problem even on a heuristic level. A first result in this direction could be proving these asymptotics to be independent of $\{\psi_Z\}_{Z=1}^{\infty}$, yielding a "universal periodicity" in large atoms.

Also of interest is the large Z behaviour of the following quantities: The radius and the ionization energy of atoms. When defining the former, the story about the dependence of choices of ground states is the same as above. Therefore, we consider for now the situation in which all quantities are defined by a fixed sequence of ground states for $H_{Z,Z}$. Formally, we define then the Q-radius $R_Q(Z)$ of the neutral atom with atomic number $Z \in \mathbb{N}$ for some $Q < Z$ by

$$\int_{B^c_{R_Q(Z)}} \rho_Z(x)\, dx = Q$$

with $B_{R_Q(Z)}$ the ball of radius $R_Q(Z)$ and centre 0 in $\mathbb{R}^3$. This is to say that there are exactly Q electrons outside this ball. In the same set-up (assuming also $Q \in \mathbb{N}$), the Q-ionization energy is defined by $I_Q(Z) := E(Z-Q,Z) - E(Z)$. This is the energy required to excite the outermost Q electrons in the atom. It is conjectured (see [Sol16]) that for fixed Q both $R_Q(Z)$ and $I_Q(Z)$ are oscillating for $Z \to \infty$ but that they are bounded from above and below. None of this is currently known to be the case, but let us notice that if (1.3(t)) holds true then the convergence of the radii $R_Q(Z_n)$ towards some limit $R_Q(\infty,t)$ follows straightforwardly and implies the mentioned conjecture for the radii (assuming $\{\rho_{\infty,t}\}_t$ is continuously parametrized by, say, the unit circle). Conversely, if $\{\rho_{Z_n}\}_{n=1}^{\infty}$ is not convergent for any sequence $\{Z_n\}_{n=1}^{\infty} \subseteq \mathbb{N}$ then it might very well still be the case that $R_Q(Z_n) \to R_Q(\infty,t)$ along certain sequences satisfying $Z_n \to \infty$. In this case, one could redefine $\mathscr{A}_t(\{\psi_Z\}_{Z=1}^{\infty})$ above to be the sequences satisfying this convergence, and studying its structure will remain an interesting problem.

Thomas-Fermi theory – a simple model: Since not many large Z results are known in the many-body Schrödinger model, a natural first step is to consider more simple models for large atoms. While these might not model large atoms quite as accurately as the Schrödinger model, they do have the advantage of being more controllable in the $Z \to \infty$ limit. Moreover, both heuristic arguments and known results suggest that most reasonable models "agree" at least to leading order. The first and most important example of this kind of simple model is that of the Thomas-Fermi (TF) density functional theory for atoms dating back to [Tho27] and [Fer27].

This model is the result of imposing a Fermionic condition on a joint space-momentum density $\widetilde{\rho}(x,p)$ of the electrons in the atom. That is, $\widetilde{\rho}$ is an integrable function describing the assumption that for a fixed point $x \in \mathbb{R}^3$ in space the momentum space is filled uniformly with density $2h^{-3}$ (where h = Planck's constant = 2π in our units) up to a certain level $p_F(x) \geq 0$, the Fermi momentum at x. This is to say that there is "room for" exactly 2 electrons in each $h \times h \times h$ cube in momentum space due to the spin of the electrons. Concretely, this gives $\widetilde{\rho}(x,p) = 2h^{-3}\mathbb{1}_{\{|p|<p_F(x)\}}(x,p)$. Considering the marginal density ρ in the space-variable, we have

$$\rho(x) = \int_{\mathbb{R}^3} \widetilde{\rho}(x,p)\,dp = \frac{8\pi}{3h^3} p_F(x)^3. \tag{1.4}$$

Unlike Schrödinger theory, TF theory describes the one-particle density $\rho_{N,Z}$ in the atom by minimizing an energy functional $\mathcal{E}_Z^{\mathrm{TF}}[\rho]$ of the density directly. Here, the functional should somehow resemble the expression coming from (1.2) and (1.1), and in particular we need a closed expression for the kinetic energy corresponding to the integral of $|\nabla\psi|^2$ from Schrödinger theory. For this notice that by using (1.4) the kinetic energy is naturally modelled by

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |p|^2 \widetilde{\rho}(x,p)\,dp\,dx = 2h^{-3}\int_{\mathbb{R}^3}\int_{\{|p|<p_F(x)\}} |p|^2\,dp\,dx = \int_{\mathbb{R}^3} \frac{8\pi}{5h^3} p_F^5\,dx = c_{\mathrm{TF}}\int_{\mathbb{R}^3} \rho^{5/3}\,dx$$

with the constant $c_{\mathrm{TF}} = 3^{5/3}\cdot 20^{-1}\cdot \pi^{-2/3}\cdot h^2 = 3^{5/3}\cdot 5^{-1}\cdot \pi^{4/3}$ in our units. The other terms in the energy functional are given by more straightforward adaptations from the Schrödinger case, and we define

$$\mathcal{E}_Z^{\mathrm{TF}}[\rho] := c_{\mathrm{TF}}\int_{\mathbb{R}^3} \rho^{5/3}\,dx - Z\int_{\mathbb{R}^3} \frac{\rho(x)}{|x|}\,dx + \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}\,dx\,dy. \tag{1.5}$$

This is the ***Thomas-Fermi density functional for the atom***, and it has been studied extensively. Almost all fundamental results are presented and proved mathematically rigorously in [LS77]. For any $Z \geq N > 0$ the functional has a unique minimizer on the set $\mathcal{S}_N := \{\rho \in L^{5/3}(\mathbb{R}^3)\cap L^1(\mathbb{R}^3) \mid \rho \geq 0, \int \rho = N\}$, and setting

$$E^{\mathrm{TF}}(N,Z) = \inf_{\rho\in\mathcal{S}_N} \mathcal{E}_Z^{\mathrm{TF}}[\rho] = \mathcal{E}_Z^{\mathrm{TF}}[\rho_{N,Z}^{\mathrm{TF}}], \quad E^{\mathrm{TF}}(Z) = E^{\mathrm{TF}}(Z,Z) \quad \text{and} \quad \rho_Z^{\mathrm{TF}} = \rho_{Z,Z}^{\mathrm{TF}}$$

defines the TF ground state energies and one-particle densities. It is know that ρ_Z^{TF} is the unique minimizer of $\mathcal{E}_Z^{\mathrm{TF}}$ on the set of all non-negative densities in $L^{5/3}(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$.

An extremely convenient feature of the TF functional is the perfect scaling property $\mathcal{E}_Z^{\mathrm{TF}}[Z^2\rho(Z^{1/3}\cdot)] = Z^{7/3}\mathcal{E}_1^{\mathrm{TF}}[\rho]$ which can be readily verified from (1.5). As an immediate consequence,

$$E^{\mathrm{TF}}(N,Z) = Z^{7/3}E^{\mathrm{TF}}(N/Z,1) \quad \text{and} \quad \rho_{N,Z}^{\mathrm{TF}}(x) = Z^2\rho_{N/Z,1}^{\mathrm{TF}}(Z^{1/3}x). \tag{1.6}$$

Already before [LS77] it was proven (in [LS73]) that $E^{\mathrm{TF}}(Z)$ agrees asymptotically with $E(Z)$, i.e. that $E(Z) = Z^{7/3}E^{\mathrm{TF}}(1) + o_{Z\to\infty}(Z^{7/3})$. Later, $E(Z)$ has been expanded further in powers of $Z^{1/3}$: A Z^2-term was proven in [Hug86] and [SW87], and a remarkable

$Z^{5/3}$-term by Fefferman and Seco, cf. [FS90]. The fact that the TF energy describes $E(Z)$ to leading order is a strong justification of a more detailed study of its behaviour as $Z \to \infty$.

TF theory does, however, not describe the periodic structure that the many-body Schrödinger model is conjectured to exhibit. Indeed, the density ρ_1 is known (see [LS77] IV) to behave like $\rho_\infty^{\mathrm{TF}}(x) := (5c_{\mathrm{TF}}/\pi)^3|x|^{-6}$ as $|x| \to \infty$ which by (1.6) yields

$$|x|^6\rho_Z^{\mathrm{TF}}(x) = |Z^{1/3}x|^6\rho_1^{\mathrm{TF}}(Z^{1/3}x) \longrightarrow (5c_{\mathrm{TF}}/\pi)^3 = |x|^6\rho_\infty^{\mathrm{TF}}(x) \qquad \text{as} \quad Z \to \infty.$$

Defining the radius $R_Q^{\mathrm{TF}}(Z)$ in TF theory completely analogously as in the Schrödinger model we find from the convergence of the densities just described[2] that, as $Z \to \infty$,

$$R_Q^{\mathrm{TF}}(Z) \longrightarrow \left(\frac{3}{4\pi}\right)^{1/3} \frac{5c_{\mathrm{TF}}}{\pi}\, Q^{-1/3} =: R_\infty^{\mathrm{TF}} \cdot Q^{-1/3}.$$

Similarly, the ionization energy $I_Q^{\mathrm{TF}}(Z)$ in TF theory is defined as in Schrödinger theory, and – just as it was the case with the radius – also $I_Q^{\mathrm{TF}}(Z)$ is convergent as $Z \to \infty$: Benilan and Brezis managed to prove (cf. [Lie81] III.A – a proof can be found in Section 6 of [BB04]) that $(1-t)^{-4/3}dE^{\mathrm{TF}}(t,1)/dt \to -\alpha$ as $t \to 1$ for a universal constant $\alpha > 0$, and, using the scaling (1.6), one obtains from this

$$\begin{aligned} I_Q^{\mathrm{TF}}(Z) &= Z^{7/3}[E^{\mathrm{TF}}(1-Q/Z,1) - E^{\mathrm{TF}}(1)] = -Z^{7/3}\int_{1-\frac{Q}{Z}}^{1} \frac{d}{dt}E^{\mathrm{TF}}(t,1)\,dt \\ &= Z^{7/3}(\alpha + o_{Z\to\infty}(1))\int_{1-\frac{Q}{Z}}^{1}(1-t)^{4/3}\,dt = \frac{3\alpha}{7}Q^{7/3} + o_{Z\to\infty}(1), \end{aligned}$$

i.e. $I_Q^{\mathrm{TF}}(Z) \to (3\alpha/7)\cdot Q^{7/3} =: I_\infty^{\mathrm{TF}} \cdot Q^{7/3}$ in the large Z limit.

Intermediate theories: We now briefly present a few theories which are more advanced than TF theory while still easier to handle than the full many-body Schrödinger model.

Firstly we have some density functional theories that are obtained by adding correction terms to the TF functional (1.5): These are called Thomas-Fermi-Dirac (TFD), Thomas-Fermi-von Weizsäcker (TFW) and Thomas-Fermi-Dirac-von Weizsäcker (TFDW) respectively according to which selection of the correction terms

$$-c_D\int_{\mathbb{R}^3}\rho(x)^{4/3}\,dx \qquad \text{and} \qquad c_W\int_{\mathbb{R}^3}|\nabla\sqrt{\rho}(x)|^2\,dx$$

is added to $\mathcal{E}_Z^{\mathrm{TF}}$. These theories are treated in [Lie81].

Another model for the atom is obtained from the many-body Schrödinger model itself by restricting $H_{N,Z}$ to the space of Slater determinants. That is, to functions $\psi \in L^2(\mathbb{R}^3;\mathbb{C}^2)^{\otimes N}$ of the form

$$\psi(\underline{x}_1,\ldots,\underline{x}_N) = \det\{\psi_i(\underline{x}_j)\}_{i,j=1}^N$$

for some $\psi_1,\ldots,\psi_N \in L^2(\mathbb{R}^3;\mathbb{C}^2)$. This is the Hartree-Fock (HF) theory for atoms. It has some similarities to the density functional theories above in that it can be described at

[2] Strictly speaking we need here L^1-convergence of the densities away from the origin, but this is also easily checked by using the scaling properties and asymptotics of ρ_1^{TF} as above.

least by some energy (although not density-) functional – we refer to Section 3 of [Sol03] for the details.

We can define the one-particle densities, radius and ionization energy rigorously in these models more or less as in the TF model, and denote these by $\rho_Z^\star$, $R_Q^\star(Z)$ and $I_Q^\star(Z)$ where $\star \in \{\text{TFD, TFW, TFDW, HF}\}$. We record now a selection of known results and open problems concerning the large Z (and large Q) limits of these quantities.

- It was proven in [Sol90] that there exists a ρ_∞^{TFW} so that $\rho_Z^{\text{TFW}} \to \rho_\infty^{\text{TFW}}$ pointwise as $Z \to \infty$, and that it satisfies $\rho_\infty^{\text{TFW}}(x) = \rho_\infty^{\text{TF}}(x) + \mathcal{O}_{|x|\to 0}(|x|^{-4})$ near the origin. From this convergence it follows that $R_Q^{\text{TFW}}(Z)$ is convergent as $Z \to \infty$ just as in the TF case. It is further known for $\star \in \{\text{TFD, TFDW, HF}\}$ that $R_Q^\star(Z)$ is bounded as $Z \to \infty$ and moreover that

$$\lim_{Q\to\infty} Q^{1/3} \liminf_{Z\to\infty} R_Q^\star(Z) = R_\infty^{\text{TF}} = \lim_{Q\to\infty} Q^{1/3} \limsup_{Z\to\infty} R_Q^\star(Z)$$

  for all $\star \in \{\text{TFD, TFW, TFDW, HF}\}$. For $\star = \text{TFW}$ this follows from the asymptotics of ρ_∞^{TDW} near the origin stated above. For $\star = \text{TFDW}$ it is one of the main results of [FNV18], and the method of proof given here additionally applies to show also[3] the case $\star = \text{TFD}$. The case $\star = \text{HF}$ is shown in [Sol03].

- While the radius is generally rather well understood, much less is known about the ionization energy. In [Sol03] it was proven that $I_Q^{\text{HF}}(Z)$ is bounded as $Z \to \infty$ so that at least $\limsup_{Z\to\infty} I_Q^{\text{HF}}(Z)$ and $\liminf_{Z\to\infty} I_Q^{\text{HF}}(Z)$ is well defined for all Q. This is very likely to be the case also for the other theories treated in this paragraph. An educated guess is that further

$$\lim_{Q\to\infty} Q^{-7/3} \limsup_{Z\to\infty} I_Q^\star(Z) = I_\infty^{\text{TF}} = \lim_{Q\to\infty} Q^{-7/3} \liminf_{Z\to\infty} I_Q^\star(Z).$$

  for $\star \in \{\text{TFD, TFW, TFDW, HF}\}$. Efforts have been made, at least for $\star = \text{TFD}$, to prove this, but they have so far been unsuccessful. In [Sol16] it is conjectured that I_∞^{TF} describes in this way the asymptotic ionization energy even in the many-body Schrödinger model for the atom. In HF theory we also do not have a complete picture of the large Z asymptotics of the densities ρ_Z^{HF}. However, it seems likely that they would be oscillating implying also oscillation of the radii $R_Q^{\text{HF}}(Z)$ as $Z \to \infty$ for any fixed Q. This (potential) oscillation might also partly describe the structure of $\mathscr{A}_t(\{\psi_Z\}_{Z=1}^\infty)$ from the many-body Schrödinger model.

Summarizing, we see that in all cases where the large Q asymptotics are known, it agrees with the TF asymptotics to leading order. Loosely speaking, this is to say that TF theory describes large atoms in the same way as the more advanced models up to a number of electrons which is large – but still very small compared to the total number of electrons. This suggests that it should be the case also for the many-body Schrödinger model as it is directly conjectured in [Sol16].

[3] I was kindly made aware of this by Rupert Frank.

Mean-field models: We have so far discussed the asymptotic behaviour of most of the quantities introduced in the context of large atoms in the Schrödinger model above – except for the (conjectured) Z_n's in (1.3(t)), i.e. the structure of the $\mathscr{A}_t(\{\psi_Z\}_{Z=1}^{\infty})$'s. In the light of the discussion above our initial guess will be that these are described by TF theory to leading order. Meanwhile, we face the issue that there is no periodicity whatsoever in this theory: All quantities have a nice and clean $Z \to \infty$ limit.

In an attempt to fix this, we will introduce yet another model for neutral atoms which is closely related to TF theory. Firstly, we describe now a larger class of models. The biggest obstacle for fully understanding the operator in (1.1) is the electron-electron interactions $1/|x_i - x_j|$ since these act across different factors in the Hilbert space $L^2(\mathbb{R}^3;\mathbb{C}^2)^{\otimes N}$. The problems would be much more tractable if one was somehow able to approximate the operator $H_{Z,Z}$ by one acting only on $L^2(\mathbb{R}^3;\mathbb{C}^2)$, thus getting rid of this obstacle. This is a key motivation for introducing the theory of mean-field models for the atom in which the individual electron sees all other electrons (itself included) only through a mean-field. Letting $\widetilde{\rho}_Z$ be some description of the density of electrons in the atom with atomic number Z, the electrostatic forces that affect an electron are in this model naturally described by

$$-\frac{Z}{|x|} + \int_{\mathbb{R}^3} \frac{\widetilde{\rho}_Z(y)}{|x-y|} = -\frac{Z}{|x|} + \widetilde{\rho}_Z * \frac{1}{|x|} := -\Phi_Z^{\mathrm{MF}}(x), \tag{1.7}$$

where the convolution is called the electron mean-field. The object of primary interest is now the operator $H_Z^{\mathrm{MF}} := -\Delta - \Phi_Z^{\mathrm{MF}}$ acting on a suitable subspace of $L^2(\mathbb{R}^3)$. Note that letting the expression for H_Z^{MF} act on the Hilbert space $L^2(\mathbb{R}^3;\mathbb{C}^2)$ including spin would be unitarily equivalent to considering the direct sum $H_Z^{\mathrm{MF}} \oplus H_Z^{\mathrm{MF}}$ acting on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. Thus, for all practical purposes, we may consider the even simpler Hilbert space $L^2(\mathbb{R}^3)$. For reasonable choices of densities $\widetilde{\rho}_Z$ (as the ones we present below) the operator H_Z^{MF} is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, and the self-adjoint closure of this operator is a rigorous model for the atom. Taking $\widetilde{\rho}_Z = \rho_Z^{\mathrm{TF}}$ in (1.7) we arrive at the strictly positive TF mean-field potential denoted Φ_Z^{TFMF} and the operator $H_Z^{\mathrm{TFMF}} := -\Delta - \Phi_Z^{\mathrm{TFMF}}$. This is the ***Thomas-Fermi mean-field (TFMF) model for the neutral atom***. As it is described in [Won79], it has been used essentially already by Fermi as an approximate model for describing the structure of electrons in atoms (in particular the "Aufbau principle" or "Madelung's rule" in chemistry). In the same way one can define other mean-field potentials $\Phi_Z^{\star\mathrm{MF}}$ and -models $H_Z^{\star\mathrm{MF}}$ by taking $\widetilde{\rho}_Z = \rho_Z^{\star}$ in (1.7) for $\star \in \{\mathrm{TFD}, \mathrm{TFW}, \mathrm{TFDW}, \mathrm{HF}\}$.

Luckily, the large x asymptotics $\Phi_1^{\mathrm{TFMF}}(x) = (3/\pi)^2(5c_{\mathrm{TF}}/3)^3|x|^{-4} + o_{|x|\to\infty}(|x|^{-4})$ of the TF mean-field potential is well established (cf. [LS77] IV) and yields, when combining (1.7) with the scaling (1.6),

$$\Phi_Z^{\mathrm{TFMF}}(x) = Z^{4/3}\Phi_1^{\mathrm{TFMF}}(Z^{1/3}x) \longrightarrow \left(\frac{3}{\pi}\right)^2\left(\frac{5c_{\mathrm{TF}}}{3}\right)^3|x|^{-4} =: \Phi_\infty^{\mathrm{TFMF}}(x)$$

as $Z \to \infty$. Consequently, we have in this model at least a glimpse of hope of studying infinite atoms directly: If they exist they should definitely be some realizations of the operator $H_\infty^{\mathrm{TFMF}} := -\Delta - \Phi_\infty^{\mathrm{TFMF}}$ acting on a suitable subspace of $L^2(\mathbb{R}^3)$. What we prove in Chapter 2 below is that along certain subsequences $\{Z_n\}_{n=1}^{\infty} \subseteq \mathbb{N}$ satisfying $Z_n \to \infty$ we have a convergence

$$H_{Z_n}^{\mathrm{TFMF}} \longrightarrow H_{\infty,\theta}^{\mathrm{TFMF}} \tag{1.8(θ)}$$

as $n \to \infty$. Here, $\{H^{\mathrm{TFMF}}_{\infty,\theta}\}_{\theta\in[0,\pi)}$ is a family of self-adjoint realizations of $H^{\mathrm{TFMF}}_{\infty}$ on $C_0^\infty(\mathbb{R}^3\backslash\{0\})$, and the convergence is in the strong resolvent sense, i.e. we have strong convergence of the resolvent operators. Parametrizing infinite atoms with $t = (\cos 2\theta, \sin 2\theta)$ gives a continuous parametrization by the unit circle, and in this sense there is even a periodicity aspect to the family of infinite atoms in this model. We further prove that

$$\mathscr{A}^{\mathrm{TFMF}}_{\theta} := \Big\{ \text{Sequences } \{Z_n\}_{n=1}^\infty \subseteq \mathbb{N} \text{ satisfying } (1.8(\theta)) \Big\} = \left\{ \begin{matrix} \text{Sequences } \{Z_n\}_{n=1}^\infty \subseteq \mathbb{N} \text{ satisfying } Z_n \to \infty \\ \text{as well as } D_{\mathrm{cl}} Z_n^{1/3} \to \theta \bmod \pi \text{ as } n \to \infty \end{matrix} \right\} \tag{1.9}$$

where the constant

$$D_{\mathrm{cl}} := \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\Phi_1^{\mathrm{TFMF}}(x)^{1/2}}{|x|^2}\, dx$$

comes from a semi-classical approximation argument in the corresponding 1-dimensional problem. This settles completely the (strong resolvent) convergence question in this model. It is, on the other hand, a completely open question whether the large Z picture for $H^{\star\mathrm{MF}}_Z$ with $\star \in \{\mathrm{TFD}, \mathrm{TFW}, \mathrm{TFDW}, \mathrm{HF}\}$ is the same as it is for H^{TFMF}_Z. For studying this it would be a natural starting point to consider H^{TFWMF}_Z since here the existence of a reasonably well-understood limiting potential $\lim_{Z\to\infty} \Phi^{\mathrm{TFWMF}}_Z$ is already established (in [Sol90]) so that we have candidates for limiting operators.

Finally, we can ask the question what (1.9) might heuristically tell us about the structure of $\mathscr{A}_t(\{\psi_Z\}_{Z=1}^\infty)$ from above if we keep following the slogan "TF(MF) theory describes the large Z behaviour of $H_{Z,Z}$ to leading order". Note that here the asymptotics are more naturally formulated in a large n limit. A reformulation of (1.9) is that

$$\mathscr{A}^{\mathrm{TFMF}}_{\theta} \cap \{\text{Increasing sequences in } \mathbb{N}\} = \left\{ \begin{matrix} \text{Subsequences } \{Z_{n_k}\}_{k=1}^\infty \text{ of some increasing sequence} \\ \{Z_n\}_{n=1}^\infty \subseteq \mathbb{N} \text{ satisfying } Z_n = D_{\mathrm{cl}}^{-3}\pi^3 n^3 + 3D_{\mathrm{cl}}^{-3}\theta\pi^2 n^2 + o_{n\to\infty}(n^2) \end{matrix} \right\}, \tag{1.10}$$

and in light of this it would be natural to conjecture that

$$\mathscr{A}_t(\{\psi_Z\}_{Z=1}^\infty) \cap \{\text{Increasing sequences in } \mathbb{N}\} \subseteq \left\{ \begin{matrix} \text{Subsequences } \{Z_{n_k}\}_{k=1}^\infty \text{ of some sequence } \{Z_n\}_{n=1}^\infty \subseteq \mathbb{N} \\ \text{satisfying } Z_n = D_{\mathrm{cl}}^{-3}\pi^3 n^3 + o_{n\to\infty}(n^3) \end{matrix} \right\}$$

regardless of t and $\{\psi_Z\}_{Z=1}^\infty$. An interesting perspective on this is that it can be used as a description of the asymptotic length of the periods in the "infinite periodic table". To realize this we need the fact (discussed in Chapter 5 below) that if Z and $\widetilde{Z}$ are sufficiently large and satisfy $D_{\mathrm{cl}} Z^{1/3} \approx \pi n + \theta$ and $D_{\mathrm{cl}} \widetilde{Z}^{1/3} \approx \pi(n+1) + \theta$ then[4] $H^{\mathrm{TFMF}}_{\widetilde{Z}}$ has one more negative eigenvalue with radial eigenfunction than H^{TFMF}_Z does. It is an interpretation of this that the TFMF-atoms have passed through the first group in the periodic table somewhere between the atomic numbers Z and $\widetilde{Z}$. A similar argument might at the same time be made for finitely many of the "other groups". The conclusion will be that, in the TFMF model, the length of the n'th period behaves like $3D_{\mathrm{cl}}^{-3}\pi^3 n^2 + \mathcal{O}_{n\to\infty}(n)$ for large n. In other words, taking a trivial subsequence in (1.10) amounts to asymptotically choosing exactly one atom in each period while $H^{\mathrm{TFMF}}_{Z_n}$ converges towards $H^{\mathrm{TFMF}}_{\infty,\theta}$. This hints that, in the many-body Schrödinger model, the "length of the n'th period" – an object which is not as well defined here as in the mean-field models – morally behaves like $3D_{\mathrm{cl}}^{-3}\pi^3 n^2 + o_{n\to\infty}(n^2)$ for large n.

[4]We have so far no rigorous proof of this, but strongly believe it to be true – see Conjecture 5.5.

1.2 Structure of the thesis

This thesis consists of five chapters and two appendices. Large parts of it are structured around Chapter 2 which is a self-contained paper concerning large and infinite atoms in a Thomas-Fermi mean-field model with a particular focus on their asymptotic periodicity. In this context, the relation between the remaining chapters is as described below. The structure of the thesis might be illustrated as in Figure 1.1. Here, an arrow indicates a recommendation of reading one chapter before reading another. When lines are dotted this recommendation is solely for motivational reasons. Section 5.3 is omitted in the illustration since it covers open problems relevant to most parts of the thesis.

- Apart from what you are reading now, Chapter 1 contains an "appetizer" on large atoms in mathematical physics (Section 1.1) which reviews some known results and localizes the mean-field model used in Chapter 2 in this framework – hereby emphasizing its relevance. Additionally, we have included a review (Section 1.3) of the specific way in which we throughout the thesis realize Schrödinger operators on the positive half-axis as self-adjoint operators.

- Chapter 3 is a paper treating strong resolvent convergence of operators in an abstract setting. The questions answered here arise, from our perspective, from those treated in Chapter 2, but they are studied completely independently from the rest of the thesis.

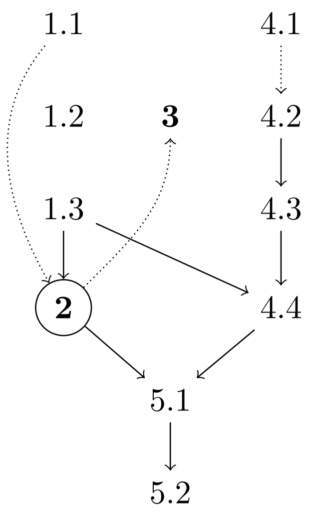

Figure 1.1

- Chapter 4 is an exposition on a particular approach to the concept of scattering lengths of potentials like those appearing in Chapter 2. It is written in monograph style introducing in detail the theory more or less from scratch. It is supposed to be largely independent from the remaining parts of the thesis. However, we will need in its last part (Section 4.4) specific results from Section 1.3. When these results are needed, we treat the details in the footnotes so that one can in principle read Chapter 4 without seeing the rest of the thesis (but then skipping some details).

- In Chapter 5 we explain the behaviour of the large atoms in Chapter 2 in terms of the theory of scattering lengths from Chapter 4, thus combining these chapters. The style in this chapter is less precise than in the remaining parts of the thesis, at times taking more the form of a discussion of the concepts treated. We close the thesis by presenting (in Section 5.3) a list of open problems which we find particularly interesting.

1.3 Self-adjoint realizations via generalized boundary conditions

In this section we review the fundamental theory of self-adjoint extensions – also called realizations – of certain Schrödinger operators on the positive half-axis $\mathbb{R}_+ = (0, \infty)$ through generalized boundary conditions at the origin. This theory will play a significant role in Chapter 2 as well as in Section 4.4. The proofs presented here are primarily adapted and extended versions of those from the more concise Appendix A in [BDG11]. Most results that rely on or treat only concepts from the theory of distributions on $\mathbb{R}_+$ are deferred to Appendix A below, and we focus for this presentation mostly on the results that are specific for Schrödinger operators. We use for this without specific references standard results about symmetric unbounded differential operators which can be found in for example [Gru09].

Consider a real-valued potential V lying in both of the spaces $L^2_{\mathrm{loc}}(\mathbb{R}_+)$ and $L^1((1,\infty))$. Throughout this section we will mean by V such potential[5]. The assumption $V \in L^2_{\mathrm{loc}}(\mathbb{R}_+)$ in particular opens the possibility of defining an unbounded differential operator H_0 on $L^2(\mathbb{R}_+)$ by setting

$$H_0 \colon C_0^\infty(\mathbb{R}_+) \ni u \longmapsto -u'' + Vu \in L^2(\mathbb{R}_+).$$

It is an easy check that this is a symmetric – and hence closable – operator. We introduce $H_{\min}$ as the operator closure of H_0 and denote its domain by $D(H_{\min})$. Recall that $H^*_{\min} = H^*_0$ and that this is a closed operator. We denote it by $H_{\max}$ and its domain by $D(H_{\max})$. Then $H^*_{\max} = H_{\min}$, and one can find that

$$D(H_{\max}) = \{\phi \in L^2(\mathbb{R}_+) \mid -\phi'' + V\phi \in L^2(\mathbb{R}_+)\},$$

where the last condition is in the distributional sense, and $H_{\max}\phi = -\phi'' + V\phi$ for $\phi \in D(H_{\max})$. Moreover, we have:

Lemma 1.1. Let $\phi \in D(H_{\max})$. Then $\phi \in C^1(\mathbb{R}_+)$ and $\phi(x), \phi'(x) \to 0$ as $x \to \infty$.

This result will be fundamental for developing the theory below (specifically it is essential in the proof of Proposition 1.5). To prove it we need a classical bound and another fundamental result[6].

[5] Although we will try to emphasize some places at which the assumption $V \in C(\mathbb{R}_+)$ makes proofs less technical.

[6] By $\|\cdot\|$ we mean always the L^2-norm on all of $\mathbb{R}_+$.

Lemma 1.2.

a) If $\phi \in H_0^1(\mathbb{R}_+)$ then $\mathbb{1}_{(1,\infty)} V^{1/2}\phi \in L^2(\mathbb{R}_+)$, and for each $\varepsilon > 0$ there exists $C_\varepsilon > 0$ so that

$$\|\mathbb{1}_{(1,\infty)} V^{1/2}\phi\|^2 \le \varepsilon\|\phi'\|^2 + C_\varepsilon\|\phi\|^2$$

for all $\phi \in H_0^1(\mathbb{R}_+)$.

b) Assume that $\phi \in L^p((2,\infty))$ for some $p \in \mathbb{R}_+$ and that ϕ is uniformly continuous on $(2,\infty)$. Then $\phi(x) \to 0$ as $x \to \infty$. This is a variant of what is sometimes called Barbalat's Lemma.

Proof. a) Let $\varepsilon > 0$ be arbitrary. Since $\mathbb{1}_{(1,\infty)} V^{1/2} \in L^2(\mathbb{R}_+)$ by assumption, this part of the lemma can be proved by showing the pointwise uniform bound $|\phi(x)|^2 \le \varepsilon\|\phi'\|^2 + \widetilde{C}_\varepsilon\|\phi\|^2$ for some $\widetilde{C}_\varepsilon > 0$ for all $\phi \in H_0^1(\mathbb{R}_+)$. As both sides of this inequality are continuous with respect to the H^1-norm, it suffices to argue in the case of $\phi \in C_0^\infty(\mathbb{R}_+)$. To this end note that for such ϕ we have

$$\phi(x)^2 = 2\int_0^x \phi\phi'\,dy = -2\int_x^\infty \phi\phi'\,dy$$

so that

$$|\phi(x)|^2 = \left|\int_0^x \phi\phi'\,dy - \int_x^\infty \phi\phi'\,dy\right| \le \int_0^\infty |\phi\phi'|\,dy \le \|\phi\|\,\|\phi'\|.$$

This is known as Agmon's inequality. Finally the fundamental inequality of numbers

$$\|\phi\|\,\|\phi'\| \le \varepsilon\|\phi'\|^2 + \frac{1}{4\varepsilon}\|\phi\|^2$$

yields the result with $\widetilde{C}_\varepsilon = 1/(4\varepsilon)$.

b) Consider a ϕ as in the lemma and assume that it is not the case that $\phi(x) \to 0$ as $x \to \infty$, i.e. that there is some $\varepsilon > 0$ and $2 < x_1 < x_2 < x_3 < \cdots$ so that $x_n \to \infty$ and $|\phi(x_n)| \ge \varepsilon$ for all n. Then we can use the uniform continuity assumption to find an $\widetilde{\varepsilon} > 0$ so that $|\phi(x)| \ge \varepsilon/2$ whenever $|x - x_n| \le \widetilde{\varepsilon}$. Now on the one hand

$$\int_{x_n-\widetilde{\varepsilon}}^{x_n+\widetilde{\varepsilon}} |\phi(x)|^p\,dx \ge 2\widetilde{\varepsilon}\frac{\varepsilon^p}{2^p} = 2^{1-p}\widetilde{\varepsilon}\varepsilon^p > 0$$

for all n, while, on the other hand, the integral on the left-hand side converges towards 0 as $n \to \infty$ by the L^p assumption on ϕ. This contradiction finishes the proof. □

Proof (of Lemma 1.1). Consider a $\phi \in D(H_{\max})$. Since we assume $V \in L^2_{\mathrm{loc}}(\mathbb{R}_+)$ it follows that

$$\phi'' = V\phi - (-\phi'' + V\phi) \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$$

so that the fundamental theorem of calculus for distributions[7] tells us that $\phi' \in C(\mathbb{R}_+)$ and consequently $\phi \in C^1(\mathbb{R}_+)$.

[7] An exact formulation and a proof is provided in Proposition A.2 in Appendix A below. It will be used extensively in the entire thesis. For differential functions one can, of course, replace this argument with the usual fundamental theorem of calculus.

A large part of the proof is to show that also $\phi \in H^1((2,\infty))$. For this we define χ_n for each $n = 3,4,\dots$ to be a real-valued function from $C_0^\infty(\mathbb{R}_+)$ which is 1 on $(2,n)$ and 0 on $(0,1)$ as well as on $(n+1,\infty)$. Moreover, we choose these so that $0 \le \chi_n(x) \le 1$ and $|\chi_n'(x)|, |\chi_n''(x)| \le c$ for all n and $x \in \mathbb{R}_+$ where $c > 0$ is some finite constant. It should not be difficult to realize that it is possible to construct such functions so that additionally χ_n and χ_m agree on $(0, \min(n,m))$. Observe that now $\chi_n\phi \in H_0^1(\mathbb{R}_+)$ and $\chi_n\phi' \in L^2(\mathbb{R}_+)$ for all n.

Since we know $\phi \in L^2(\mathbb{R}_+)$ it suffices to check that $\mathbb{1}_{(2,\infty)}\phi'$ is square integrable in order to conclude that $\phi \in H^1((2,\infty))$. As $\mathbb{1}_{(2,\infty)}|\phi'|^2 \le \chi_\infty^2|\phi'|^2$ pointwise, with χ_∞ the pointwise limit of the χ_n's as $n \to \infty$, we learn from the monotone convergence theorem that it is in turn sufficient to argue that the monotone sequence $\{\,\|\chi_n\phi'\|\,\}_{n=1}^\infty$ is bounded above. By the inequalities

$$\|\chi_n\phi'\| - c\|\phi\| \le \|\chi_n\phi'\| - \|\chi_n'\phi\| \le \|(\chi_n\phi)'\| \le \|\chi_n\phi'\| + \|\chi_n'\phi\| \le \|\chi_n\phi'\| + c\|\phi\|$$

this is equivalent to $\{\,\|(\chi_n\phi)'\|\,\}_{n=1}^\infty$ being bounded above which we will prove by showing that

$$\|(\chi_n\phi)'\|^2 \le C_1 + C_2\|(\chi_n\phi)'\| + \frac{1}{2}\|(\chi_n\phi)'\|^2 \tag{1.11}$$

for all n for some n-independent (but ϕ-dependent) constants C_1 and C_2.

For proving (1.11) we start by applying partial integration (cf. Proposition A.6 in Appendix A below – the assumptions here apart from $\chi_n\phi \in H_0^1(\mathbb{R}_+)$ will basically be verified in the subsequent estimation), yielding

$$\begin{aligned}\int_0^\infty |(\chi_n\phi)'|^2\,dx &= -\int_0^\infty \chi_n\overline{\phi}(\chi_n\phi)''\,dx = -\int_0^\infty \chi_n\chi_n''|\phi|^2 + 2\chi_n\chi_n'\overline{\phi}\phi' + \chi_n^2\overline{\phi}\phi''\,dx \\ &\le c\|\phi\|^2 + 2c\,\|\phi\|\,\|\chi_n\phi'\| + \int_0^\infty \chi_n^2|\phi|\,|\phi'' - V\phi| + \chi_n^2|V|\,|\phi|^2\,dx \\ &\le c\|\phi\|^2 + 2c^2\|\phi\|^2 + 2c\|\phi\|\,\|(\chi_n\phi)'\| + \|\phi\|\,\|\phi'' - V\phi\| + \int_1^\infty |V|\,|\phi|^2\,dx.\end{aligned}$$

Here, the last term is finite by Lemma 1.2(a), and moreover – by taking $\varepsilon = 1/2$ in this Lemma – it is bounded by $\|(\chi_n\phi)'\|^2/2 + C_{1/2}\|\phi\|^2$. Hence, we have verified (1.11) with

$$C_1 = c\|\phi\|^2 + 2c^2\|\phi\|^2 + \|\phi\|\,\|\phi'' - V\phi\| + C_{1/2}\|\phi\|^2 \quad \text{and} \quad C_2 = 2c\,\|\phi\|$$

thereby proving $\phi \in H^1((2,\infty))$.

Observe now that since $\phi'' \in L^1_{\text{loc}}(\mathbb{R}_+)$ (as noticed above) we have by the fundamental theorem of calculus for distributions

$$\phi'(x) = \phi'(2) + \int_2^x \phi''\,dy = \phi'(2) + \int_2^x V\phi\,dy + \int_2^x \phi'' - V\phi\,dy$$

for $x > 2$. Here, the second term on the right-hand side is uniformly continuous in x. Indeed, $\mathbb{1}_{(1,\infty)}V\phi \in L^1(\mathbb{R}_+)$ as both $\mathbb{1}_{(1,\infty)}V^{1/2}$ and $\mathbb{1}_{(1,\infty)}V^{1/2}\phi$ lie in $\in L^2(\mathbb{R}_+)$ (the latter by Lemma 1.2(a)), and definite integrals of integrable functions are uniformly continuous in the endpoint of the area of integration. Also, the last term on the right-hand side is uniformly continuous. To see this simply notice that

$$\left|\int_2^y \phi'' - V\phi\,dz - \int_2^x \phi'' - V\phi\,dz\right| \le \int_x^y |\phi'' - V\phi|\,dz \le |y-x|^{1/2}\,\|\phi'' - V\phi\|$$

for all $2 < x < y < \infty$. Thus, ϕ' is uniformly continuous on $(2,\infty)$ and lies in $L^2((2,\infty))$, and Lemma 1.2(b) tells us that $\phi'(x) \to 0$ as $x \to \infty$. To realize that also $\phi(x) \to 0$ as $x \to \infty$ one can proceed as the last part of the argument just presented. Using that $\phi' \in L^2((2,\infty))$ we can get the uniform continuity of ϕ, and since $\phi \in L^2(\mathbb{R}_+)$ Lemma 1.2(b) takes care of the rest. □

One more initial result is needed, before we move on to handling the main issues of the present section. Namely the fact that the space

$$\mathcal{N} := \{f \in L^1_{\text{loc}}(\mathbb{R}_+) \mid Vf \in L^1_{\text{loc}} \text{ and } f'' = Vf \text{ in the distributional sense}\}$$

is a two-dimensional subspace of $C^1(\mathbb{R}_+)$. This is Lemma A.3 in Appendix A below. Here the proof is also found as it relies mostly on distribution-theoretic results and the techniques from Section 4.2. Note, however, that for $V \in C(\mathbb{R}_+)$ this is a standard consequence of the existence and uniqueness of a solution to the initial value problem from the theory of ordinary differential equations.

Consider now and for the remaining part of the section a localizing function $\xi \in C^\infty(\mathbb{R}_+)$ so that $\xi(x) = 1$ for $x \in (0,1)$ and $\xi(x) = 0$ for $x \in (2,\infty)$. We make from this point onwards the ***important assumption*** that $\xi f \in L^2(\mathbb{R}_+)$ (or equivalently that $f \in L^2((0,1))$) for any $f \in \mathcal{N}$. In particular this means that $\xi f \in D(H_{\max})$ for any $f \in \mathcal{N}$. Indeed, it is easy to convince oneself[8] that $-(\xi f)'' + V\xi f$ is 0 on $(0,1)$, square integrable on $(1,2)$ and 0 again on $(2,\infty)$ making it surely $L^2(\mathbb{R}_+)$.

1.3.1 The Wronskian

The purpose of the present subsection is to introduce rigorously a function called the Wronskian on $C^1(\mathbb{R}_+)$ and to observe how it acts on the subspaces $D(H_{\min})$, $D(H_{\max})$ and $\mathcal{N}$ of $C^1(\mathbb{R}_+)$ introduced above. We begin with giving the definition of the Wronskian and then move on to the basic properties of its restriction to $\mathcal{N}$.

Definition 1.3. The Wronskian is the function defined by

$$\begin{aligned} W\colon \mathbb{R}_+ \times C^1(\mathbb{R}_+) \times C^1(\mathbb{R}_+) &\longrightarrow \mathbb{C} \\ (x,u,v) &\longmapsto u(x)v'(x) - u'(x)v(x). \end{aligned}$$

We use the notation $W_x(u,v)$ for $W(x,u,v)$.

Lemma 1.4. For functions $f, g \in \mathcal{N}$ the Wronskian of f and g is constant in x, i.e. $W_x(f,g) = C$ for some $C \in \mathbb{C}$ for all $x \in \mathbb{R}_+$. Moreover, $C \neq 0$ if and only if f and g are linearly independent.

[8] Strictly speaking the Leibniz formula in a general set-up is needed here. See Proposition A.4 in Appendix A below for the details.

Proof. Assuming $V \in C(\mathbb{R}_+)$ one has $\mathcal{N} \subseteq C^2(\mathbb{R}_+)$, and the first part of the result follows straightforwardly from differentiating the Wronskian with respect to x and observing that this gives 0. The general case (with essentially the same proof) is shown in Corollary A.5 in Appendix A below.

If f and g are linearly dependent, $f = \alpha g$, then

$$W_x(f,g) = f(x)\alpha f'(x) - f'(x)\alpha f(x) = 0.$$

On the other hand, suppose that $C = 0$. Either one of f and g is identically 0 so that f and g are indeed linearly dependent. Else, one of f and g, say f, is non-zero at some point $x_0 \in \mathbb{R}_+$ and by continuity this is also true on an open subinterval of $\mathbb{R}_+$ around x_0 – and the other function, say g, is not identically 0. Observing that

$$0 = \frac{W_x(f,g)}{f(x)^2} = \frac{d}{dx}\left(\frac{g}{f}\right)$$

we conclude that g/f is constant, or equivalently that f and g are linearly dependent, on an interval around x_0. If $V \in C(\mathbb{R}_+)$ then the last part of the lemma follows from the uniqueness of the solution to the initial value problem (which also rules out the possibility that both $g(x_0) = 0$ and $g'(x_0) = 0$ since $g \neq 0$ by assumption). But also in the case of a more general V we note that we can apply this: Showing that $f \in \mathcal{N}$ is completely determined by its value and derivative at a fixed point is part of the proof that $\dim \mathcal{N} = 2$ (Lemma A.3). □

Next, we examine how the Wronskian behaves when we consider the case where it is applied to $\phi, \psi \in D(H_{\max})$. Here it will be of significant importance how it looks for x's near the origin.

Proposition 1.5. The map

$$\begin{aligned} W_0\colon D(H_{\max}) \times D(H_{\max}) &\longrightarrow \mathbb{C} \\ (\phi,\psi) &\longmapsto \int_0^\infty \phi H_{\max}\psi - (H_{\max}\phi)\psi \, dx \end{aligned}$$

defines a bilinear form on $D(H_{\max})$. It is continuous with respect to the graph norm of $H_{\max}$, and for any $\phi, \psi \in D(H_{\max})$ it is given by

$$W_0(\phi,\psi) = \lim_{\varepsilon \to 0} W_\varepsilon(\phi,\psi).$$

Proof. The well-definedness of W_0 is a consequence of the fact that $\phi, \psi, H_{\max}\phi, H_{\max}\psi \in L^2(\mathbb{R}_+)$, and bilinearity is clear. In fact[9],

$$W_0(\phi,\psi) = \langle \overline{\phi}, H_{\max}\psi\rangle - \langle \overline{H_{\max}\phi}, \psi\rangle,$$

[9]We use the convention that the inner product $\langle \cdot, \cdot \rangle$ on $L^2(\mathbb{R}_+)$ is linear in the second coordinate.

which also shows that W_0 is continuous with respect to the graph norm. Now fix $\phi, \psi \in D(H_{\max})$ and $0 < \varepsilon < K < \infty$. We have (cf. Proposition A.4 in the case of a non-continuous potential) in the distributional sense

$$\phi H_{\max}\psi - (H_{\max}\phi)\psi = -\phi\psi'' + \phi''\psi = (\phi'\psi)' - (\phi\psi')'$$

so that, by the fundamental theorem of calculus for distributions,

$$\int_\varepsilon^K \phi H_{\max}\psi - (H_{\max}\phi)\psi\,dx = \int_\varepsilon^K (\phi'\psi)' - (\phi\psi')'\,dx = \phi'(K)\psi(K) - \phi(K)\psi'(K) + W_\varepsilon(\phi,\psi).$$

Notice finally that, by Lemma 1.1,

$$\begin{aligned} W_0(\phi,\psi) &= \lim_{\varepsilon\to 0}\lim_{K\to\infty}\int_\varepsilon^K \phi H_{\max}\psi - (H_{\max}\phi)\psi\,dx \\ &= \lim_{\varepsilon\to 0}\lim_{K\to\infty}\Big[\phi'(K)\psi(K) - \phi(K)\psi'(K) + W_\varepsilon(\phi,\psi)\Big] = \lim_{\varepsilon\to 0} W_\varepsilon(\phi,\psi) \end{aligned}$$

which shows also that the limit on the right hand actually exists. □

Corollary 1.6. If one of $\phi, \psi \in D(H_{\max})$ lies in $D(H_{\min})$ then $W_0(\phi,\psi) = 0$, and further

$$D(H_{\min}) = \{\phi \in D(H_{\max}) \mid W_0(\phi,\psi) = 0 \text{ for all } \psi \in D(H_{\max})\}.$$

Proof. The first statement is a consequence of the continuity of W_0 with respect to the graph norm and the fact that clearly $W_0(\phi,\psi) = \lim_{\varepsilon\to 0} W_\varepsilon(\phi,\psi) = 0$ whenever one of ϕ and ψ is in $C_0^\infty(\mathbb{R}_+)$. It proves also the one inclusion in the claimed equality of sets.

For the other inclusion assume that $W_0(\phi,\psi) = 0$ so that $\langle\overline{\phi}, H_{\max}\psi\rangle = \langle\overline{H_{\max}\phi},\psi\rangle$ for all $\psi \in D(H_{\max})$. Now the functional $D(H_{\max}) \ni \psi \mapsto \langle\overline{\phi}, H_{\max}\psi\rangle$ is clearly bounded with norm less than $\|H_{\max}\phi\|$ so that $\overline{\phi} \in D(H_{\max}^*) = D(H_{\min})$ and thus $\phi \in D(H_{\min})$ as needed. □

1.3.2 Description of the self-adjoint extensions of $H_{\min}$

Our main purpose is now to find all self-adjoint realizations of the differential operator $H := -d^2/dx^2 + V$ on $\mathbb{R}_+$. That is, all operators $H_{\min} \subseteq \widetilde{H} \subseteq H_{\max}$ with $\widetilde{H}$ self-adjoint. The starting point will be strengthening Corollary 1.6.

Lemma 1.7. Let $f_+, f_- \in \mathcal{N}$ be two linearly independent functions so that $W_x(f_+,f_-) = 1$ for all $x \in \mathbb{R}_+$ and let $h \in L^2_{\text{loc}}(\mathbb{R}_+)$ be given. If $Hh = \psi$ for some $\psi \in L^2(\mathbb{R}_+)$ then there exist unique numbers $a_+, a_- \in \mathbb{C}$ so that $h = (a_+ + \psi_-)f_+ + (a_- - \psi_+)f_-$ where

$$\psi_\pm(x) = \int_0^x f_\pm(y)\psi(y)\,dy,$$

and any h on this form satisfies $Hh = \psi$.

Proof. Let $\psi \in L^2(\mathbb{R}_+)$ be given. We start by proving that $h_0 = \psi_- f_+ - \psi_+ f_-$ solves $Hh_0 = \psi$. Note to this end that we have $f_\pm \in L^2((0,1))$. Thus, since also $\psi \in L^2((0,1))$, we obtain straightforwardly $f_\pm \psi \in L^1((0,1)) \cap L^1_{\text{loc}}(\mathbb{R}_+)$. Now using the fundamental theorem of calculus for distributions one sees that $\psi_\pm' = f_\pm \psi$. Consequently,

$$h_0' = f_- \psi f_+ + \psi_- f_+' - f_+ \psi f_- - \psi_+ f_-' = \psi_- f_+' - \psi_+ f_-',$$

and further

$$h_0'' = f_- \psi f_+' + \psi_- f_+'' - f_+ \psi f_-' - \psi_+ f_-'' = -\psi W_\cdot(f_+, f_-) + V[\psi_- f_+ - \psi_+ f_-] = -\psi + V h_0$$

yielding the desired $Hh_0 = \psi$.

Now if $Hh = \psi$ then obviously $h - h_0 \in \mathcal{N}$ implying that $h - h_0 = a_+ f_+ + a_- f_-$ for some unique constants $a_+, a_- \in \mathbb{C}$ as needed. Also, the last part of the lemma is an easy check when using this. □

Proposition 1.8. Let $f_+, f_- \in \mathcal{N}$ be two linearly independent functions so that $W_x(f_+, f_-) = 1$ for all $x \in \mathbb{R}_+$. We have the following equalities:

$$\begin{aligned} D(H_{\min}) &= \{\phi \in D(H_{\max}) \mid W_0(\phi, \xi f) = 0 \text{ for all } f \in \mathcal{N}\} \\ &= \{\phi \in D(H_{\max}) \mid W_0(\phi, \xi f_+) = W_0(\phi, \xi f_-) = 0\}. \end{aligned}$$

Proof. Note firstly that the last equality is simply a consequence of the fact that f_+ and f_- span $\mathcal{N}$. Corollary 1.6 tells us that $W_0(\phi, \xi f_+) = W_0(\phi, \xi f_-) = 0$ whenever $\phi \in D(H_{\min})$ so we need only to prove that for any $\phi \in D(H_{\max})$ the fact that $W_0(\phi, \xi f_+) = W_0(\phi, \xi f_-) = 0$ implies $\phi \in D(H_{\min})$.

For this fix a $\phi \in D(H_{\max})$ that satisfies $W_0(\phi, \xi f_+) = W_0(\phi, \xi f_-) = 0$. By Corollary 1.6 we need now simply to show that $W_0(\phi, h) = 0$ for all $h \in D(H_{\max})$ in order to prove the theorem, so we fix such h too. If we put $H_{\max} h = \psi \in L^2(\mathbb{R}_+)$ then we have, using the result and notation from Lemma 1.7, $h = a_+ f_+ + a_- f_- + h_0$. Using the expression for h_0' obtained in the proof of Lemma 1.7 we get now

$$\begin{aligned} W_0(\phi, h) &= \lim_{\varepsilon \to 0} \Big(\phi(\varepsilon) h'(\varepsilon) - \phi'(\varepsilon) h(\varepsilon) \Big) \\ &= \lim_{\varepsilon \to 0} \Big(\phi(\varepsilon)[a_+ f_+'(\varepsilon) + a_- f_-'(\varepsilon) + h_0'(\varepsilon)] - \phi'(\varepsilon)[a_+ f_+(\varepsilon) + a_- f_-(\varepsilon) + h_0(\varepsilon)] \Big) \\ &= a_+ W_0(\phi, \xi f_+) + a_- W_0(\phi, \xi f_-) + \lim_{\varepsilon \to 0} \Big(\phi(\varepsilon) h_0'(\varepsilon) - \phi'(\varepsilon) h_0(\varepsilon) \Big) \\ &= \lim_{\varepsilon \to 0} \Big(\phi(\varepsilon)[\psi_-(\varepsilon) f_+'(\varepsilon) - \psi_+(\varepsilon) f_-'(\varepsilon)] - \phi'(\varepsilon)[\psi_-(\varepsilon) f_+(\varepsilon) - \psi_+(\varepsilon) f_-(\varepsilon)] \Big) \\ &= \lim_{\varepsilon \to 0} \Big(\psi_-(\varepsilon)[\phi(\varepsilon) f_+'(\varepsilon) - \phi'(\varepsilon) f_+(\varepsilon)] - \psi_+(\varepsilon)[\phi(\varepsilon) f_-'(\varepsilon) - \phi'(\varepsilon) f_-(\varepsilon)] \Big) \\ &= \lim_{\varepsilon \to 0} \Big(\psi_-(\varepsilon) W_\varepsilon(\phi, \xi f_+) - \psi_+(\varepsilon) W_\varepsilon(\phi, \xi f_-) \Big) = 0 \end{aligned}$$

as we needed. This concludes the proof. □

Corollary 1.9. We have the following:

a) $\dim(D(H_{\max})/D(H_{\min})) = 2$.

b) If $f, g \in \mathcal{N}$ are linearly independent then $D(H_{\max}) = D(H_{\min}) \oplus \mathbb{C}\xi f \oplus \mathbb{C}\xi g$.

Proof. a): We need only to find an isomorphism from $D(H_{\max})/D(H_{\min})$ to $\mathbb{C}^2$. Letting f_+ and f_- be a basis for $\mathcal{N}$ satisfying $W_0(\xi f_+, \xi f_-) = 1$ we claim that we can use the linear map $\ell(\phi + D(H_{\min})) := (W_0(\phi, \xi f_+), W_0(\phi, \xi f_-))$. This is well-defined since if $\phi_1 - \phi_2 \in D(H_{\min})$ then $W_0(\phi_1, \xi f_\pm) - W_0(\phi_2, \xi f_\pm) = 0$ by Proposition 1.8. Conversely, if $W_0(\phi_1, \xi f_\pm) = W_0(\phi_2, \xi f_\pm)$ then $W_0(\phi_1 - \phi_2, \xi f_\pm) = 0$ and, by Proposition 1.8, $\phi_1 + D(H_{\min}) = \phi_2 + D(H_{\min})$. This proves injectivity of ℓ. For surjectivity simply note that $\ell(b\xi f_+ - a\xi f_- + D(H_{\min})) = (a, b)$ for any $a, b \in \mathbb{C}$.

b): Since clearly $\xi f \in D(H_{\max}) \setminus D(H_{\min})$ by Proposition 1.8 we know by (a) that $D(H_{\min}) + \mathbb{C}\xi f$ has co-dimension 1 in $D(H_{\max})$. If we prove that $\xi g \in D(H_{\max}) \setminus (D(H_{\min}) + \mathbb{C}\xi f)$ then we can conclude that $D(H_{\min}) + \mathbb{C}\xi f + \mathbb{C}\xi g$ has co-dimension 0 in $D(H_{\max})$, i.e. that it *equals* $D(H_{\max})$. To this end observe that if $\xi g = \phi + \alpha \xi f$ with $\phi \in D(H_{\min})$ and $\alpha \in \mathbb{C}$ then

$$0 = W_0(\xi g, \xi g) = W_0(\xi g, \phi) + \alpha W_0(\xi g, \xi f) = \alpha W_0(\xi g, \xi f)$$

meaning that $\alpha = 0$ since f and g are linearly independent and from $\mathcal{N}$, cf. Lemma 1.4. But this means that $\xi g \in D(H_{\min})$ which is clearly a contradiction by Proposition 1.8.

To prove the fact that the sum is direct assume that

$$\phi_1 + \alpha_1 \xi f + \beta_1 \xi g = \phi_2 + \alpha_2 \xi f + \beta_2 \xi g$$

where $\phi_1, \phi_2 \in D(H_{\min})$ and $\alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{C}$. Now

$$(\alpha_1 - \alpha_2)\xi f + (\beta_1 - \beta_2)\xi g = \phi_2 - \phi_1 \in D(H_{\min})$$

so that

$$\begin{aligned} 0 &= W_0(\phi_2 - \phi_1, (\overline{\alpha}_1 - \overline{\alpha}_2)\xi g - (\overline{\beta}_1 - \overline{\beta}_2)\xi f) \\ &= |\alpha_1 - \alpha_2|^2 W_0(\xi f, \xi g) - |\beta_1 - \beta_2|^2 W_0(\xi g, \xi f) = \left(|\alpha_1 - \alpha_2|^2 + |\beta_1 - \beta_2|^2\right) W_0(\xi f, \xi g). \end{aligned}$$

Hence, $\alpha_1 = \alpha_2$ and $\beta_1 = \beta_2$ which in turn yields $\phi_1 = \phi_2$. This proves the assertion. □

We are now in a position to prove the main result of this review: A characterization of all self-adjoint realizations of the differential operator H.

Theorem 1.10. Let $f \in \mathcal{N} \setminus \{0\}$ satisfy the following: $f = \gamma f_0$ where $\gamma \in \mathbb{C}$ and f_0 is real-valued. Then the restriction H_f of $H_{\max}$ to $D(H_f) := D(H_{\min}) \oplus \mathbb{C}\xi f$ is a self-adjoint realization of H. Conversely, if $\widetilde{H}$ is any self-adjoint realization of H then $\widetilde{H} = H_f$ for a $f \in \mathcal{N} \setminus \{0\}$ as above.

Proof. Firstly we prove that an operator H_f as described is indeed self-adjoint and start by arguing that it is symmetric: Observe that for any $\psi = \phi + \alpha\xi f \in D(H_f) \subsetneq D(H_{\max})$ we have

$$\begin{aligned}\langle H_f\psi,\psi\rangle - \langle\psi, H_f\psi\rangle = W_0(\overline{\psi},\psi) = W_0(\overline{\alpha}\xi\overline{f},\alpha\xi f) &= W_0(\overline{\alpha\gamma}\xi f_0,\alpha\gamma\xi f_0)\\ &= |\alpha\gamma|^2 W_0(\xi f_0,\xi f_0) = 0.\end{aligned}$$

Letting $g \in \mathcal{N}$ be linearly independent of f we can conclude by Corollary 1.9(b) that

$$D(H_f) \subseteq D(H_f^*) \subseteq D(H_{\min}^*) = D(H_{\max}) = (D(H_{\min}) \oplus \mathbb{C}\xi f) \oplus \mathbb{C}\xi g = D(H_f) \oplus \mathbb{C}\xi g, \quad (1.12)$$

from which we learn the following: If $\xi g \in D(H_f^*)$ then $H_f^* = H_{\max}$. But this would imply that

$$H_{\min} \subsetneq H_f \subseteq \overline{H_f} = H_f^{**} = H_{\max}^* = H_{\min}$$

– an obvious contradiction. Hence, $\xi g \notin D(H_f^*)$ and consequently $D(H_f^*) = D(H_f)$ by (1.12), i.e. H_f is self-adjoint since it is symmetric.

Assume now on the other hand that $\widetilde{H}$ is a self-adjoint realization of H. We must have $D(H_{\min}) \subsetneq D(\widetilde{H}) \subsetneq D(H_{\max})$ since we know for a fact that neither $H_{\min}$ nor $H_{\max}$ is self-adjoint (as these are unequal and each other's adjoints). From Corollary 1.9(b) it is now apparent that the domain $D(\widetilde{H})$ of $\widetilde{H}$ must contain a function on the form ξf with $f \in \mathcal{N}\setminus\{0\}$. Letting $g \in \mathcal{N}$ be linearly independent of f we see that

$$D(H_{\min}) \oplus \mathbb{C}\xi f \subseteq D(\widetilde{H}) \subsetneq D(H_{\max}) = D(H_{\min}) \oplus \mathbb{C}\xi f \oplus \mathbb{C}\xi g$$

from which we can conclude that $D(\widetilde{H}) = D(H_{\min}) \oplus \mathbb{C}\xi f$. We notice at this point that

$$0 = \langle \xi f, \widetilde{H}\xi f\rangle - \langle \widetilde{H}\xi f, \xi f\rangle = W_0(\xi\overline{f}, \xi f),$$

and as $\overline{f} \in \mathcal{N}$ this means by Lemma 1.4 that $f = \gamma_0\overline{f}$ for some $\gamma_0 \in \mathbb{C}$. Clearly, $|\gamma_0| = 1$ so that it has a square root γ with $\gamma^{-1} = \overline{\gamma}$. Consequently, $\overline{\gamma}f = \gamma^{-1}f = \gamma\overline{f}$ is a real-valued function from $\mathcal{N}$. This concludes the proof since $f = \gamma(\overline{\gamma}f)$. □

Chapter 2

Paper: Periodicity of atomic structure in a Thomas-Fermi mean-field model

This chapter contains a draft of a paper entitled "Periodicity of atomic structure in a Thomas-Fermi mean-field model", which is joint between the author and Jan Philip Solovej. The studies described here have been the backbone of the PhD project of which this thesis is the culmination. The paper draft is included in its entirety – including the title page, abstract and bibliography. To mark its independence from the rest of the thesis it has its own page numbering (at the bottom of pages), but it can be located within the thesis by the colour ■ at the top of pages. In the remaining parts of the thesis, references to the content of the paper draft are done by referring to its own theorem numbering etc. followed by "of/in Chapter 2".

The paper draft is self-contained with one important exception: It does not include a proof of its Proposition 2.3. For a proof we refer to Appendix B below.

Periodicity of atomic structure in a Thomas-Fermi mean-field model

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Abstract

We consider a Thomas-Fermi mean-field model for large neutral atoms. That is, Schrödinger operators $H_Z^{\mathrm{TF}} = -\Delta - \Phi_Z^{\mathrm{TF}}$ in three-dimensional space, where Z is the nuclear charge of the atom and Φ_Z^{TF} is a mean-field potential coming from the Thomas-Fermi density functional theory for atoms. For any sequence $Z_n \to \infty$ we prove that the corresponding sequence $H_{Z_n}^{\mathrm{TF}}$ is convergent in the strong resolvent sense if and only if $D_{\mathrm{cl}} Z_n^{1/3}$ is convergent modulo π for a universal constant D_{cl}. This can be interpreted in terms of periodicity of large atoms. We also characterize the possible limiting operators (infinite atoms) as a particular one-parameter family of self-adjoint extensions of $-\Delta - C_\infty |x|^{-4}$ for an explicit number C_∞.

1 Introduction

The motivation for the mathematical work in this paper is to understand the periodicity of the periodic table of the elements. More precisely, the question is why atoms in the groups of the periodic table, e.g., the noble gases or the alkali atoms, have very similar chemical properties.

Before we can properly ask this question we must first understand what even defines the different groups. Chemists tell us that this is related to filling electrons in atomic orbitals that span the subspaces with angular momentum quantum numbers $\ell = 0, 1, 2, \ldots$. The alkali atoms are those atoms where a new $\ell = 0$ orbital is being occupied by an electron (referred to as an s-electron in chemistry). The noble gases are those atoms where all[1] $2(2\ell+1) = 6$ electrons in an $\ell = 1$ subspace have been filled (p-electrons in the chemist's notation). A natural question is of course in which order the different ℓ subspaces are being filled. In chemistry this is described by the empirical Aufbau principle

[1]The factor 2 in $2(2\ell+1)$ is counting spin.

(or Madelung rule [12]). We shall not describe the rule in details here, but note that it gives us a general formula for the atomic number $Z_\ell(n)$, where we start filling an ℓ subspace for the n^{th} time. This general formula is

$$Z_\ell(n) = \frac{(n+2\ell-1)((n+2\ell)^2+4(n+2\ell)+9)}{6} - \frac{(1+(-1)^n)(n+2\ell+1)}{4} + 1 - 2\ell(\ell+2). \tag{1}$$

This formula is indeed reflected in the periodic table and is correct for the atoms

- $\ell = 0$: The alkali atoms in group 1 where we start filling a new s orbital, i.e., $Z = 1, 3, 11, 19, 37, 55, 87$
- $\ell = 1$: Where we fill a new p subspace, i.e., $Z = 5, 13, 31, 49, 81, 113$
- $\ell = 2$: Where we fill a new d subspace, i.e., $Z = 21, 39, 71$

It fails however for the case $(\ell, n) = (2, 4)$ and generally for $\ell = 3$. Here, the correct values are $Z_2(4) = 104$, $Z_3(1) = 58$ and $Z_3(2) = 91$ respectively, while the formula would give the numbers 103, 57 and 89. There are several other exceptions in the periodic table to the general Madelung rule.

Fermi [5] attempted to calculate $Z_\ell(n)$ in a model where electrons move independently in a mean-field potential describing the effect of the interaction of all the other electrons. Fermi used the mean-field potential derived from his own Thomas-Fermi model [6, 16]. The formula he derived, however, does not agree with the above expression. In particular it does not reproduce the 1/6 in the leading order term.

Other attempts [8, 17, 18], used a different mean-field potential suggested by Tietz in [17] which does reproduce the 1/6 asymptotically for large n. To the best of our knowledge there are no justifications for the use of the Tietz potential other than that it reproduces the Madelung rule (asymptotically).

In the full many-body quantum mechanical description of atoms the concept of electron orbitals is not well-defined. A possible approach is to consider the natural orbitals, i.e., the eigenfunctions of the 1-particle reduced density matrix γ of an atomic many-body ground state. These eigenfunctions are, however, unlikely to be labelled by angular momenta. We may of course always ask for the occupation number $n_\ell(Z) = \mathrm{Tr}[\gamma P_\ell]$ of the ground state in an angular momentum eigenspace given by the projection P_ℓ. In a forthcoming publication[2] we will show that $n_\ell(Z)$, as defined above, does not satisfy the Madelung rule asymptotically for large Z and almost all ℓ in a sense to be made precise in the publication. In fact, it turns out that Fermi's formula gives the correct answer here.

We will in the present paper consider exactly the same model as Fermi and will describe this model in more details in the next subsection. For each Z it gives a spherically symmetric mean-field potential and a corresponding mean-field Schrödinger operator. Fermi's idea was to ask whether the ordering of the energy levels — as a function of angular momenta — of this mean-field operator agrees with experimental data.

[2] In preparation. Joint with Søren Fournais and Peter Hearnshaw.

We will address the somewhat different issue of whether the model explains the similarity in chemical properties for certain sequences of atomic numbers, corresponding to the groups in the periodic table. To phrase this as a more mathematical question we ask whether the Thomas-Fermi mean-field operator converges in some appropriate sense as Z tends to infinity through certain sequences. The main result of this paper (Theorem 2.5) is that this is, indeed, the case in the sense of strong resolvent convergence of operators. Moreover, the sequences of Z agree with what Fermi found in his attempt to explain the structure of the periodic table. Note that strong resolvent convergence implies that the spectrum of the limiting operator is included in the limits of the spectra (spectral exclusion). Since spectra describe chemical properties such as, e.g., the ionization energies we may interpret our result as saying that these sequences represent atoms with similar chemical properties in this model.

1.1 Thomas-Fermi theory for atoms

Our mean-field model is based on the Thomas-Fermi density functional theory introduced in [16, 6]. We review now briefly some mathematical facts concerning this and refer to [10] or [11] for further details.

We consider 3-dimensional space. The energy of an atom with atomic number Z and electron density ρ is in Thomas-Fermi theory given by

$$\mathcal{E}_Z^{\mathrm{TF}}[\rho] = c_{\mathrm{TF}} \int \rho(x)^{5/3}\,dx - Z\int \frac{\rho(x)}{|x|}\,dx + \frac{1}{2}\int\int \frac{\rho(x)\rho(y)}{|x-y|}\,dx\,dy \tag{2}$$

where $c_{\mathrm{TF}} = \frac{3}{5}(3\pi^2)^{2/3}$. We have here[3] used the units that $\hbar = e = 2m = 1$, where m is the electron mass, and consider the case with spin 1/2, i.e. 2 spin degrees of freedom. Thomas-Fermi theory can be modified to include any spin degree of freedom by changing only the value of c_{TF}. It is known that the infimum

$$\inf_{\substack{\rho\in L^1\cap L^{5/3}\\ \rho\geq 0}} \mathcal{E}_Z^{\mathrm{TF}}[\rho] \tag{3}$$

is attained for some unique spherically symmetric ρ_Z^{TF} which is smooth on $\mathbb{R}^3\backslash\{0\}$ and has total mass Z. Of great importance to us will be the quantity

$$\Phi_Z^{\mathrm{TF}}(x) := \frac{Z}{|x|} - \int \frac{\rho_Z^{\mathrm{TF}}(y)}{|x-y|}\,dy \tag{4}$$

called the Thomas-Fermi potential. This clearly inherits spherical symmetry and smoothness from ρ_Z^{TF}, and it is moreover strictly positive. It describes the electrostatic interactions between a fixed electron and all electrons in the atom (itself included). From the minimization problem (3) one additionally finds that

$$\Phi_Z^{\mathrm{TF}} = \frac{5c_{\mathrm{TF}}}{3}(\rho_Z^{\mathrm{TF}})^{2/3}, \qquad \text{yielding} \qquad \Delta\Phi_Z^{\mathrm{TF}} = 4\pi\left(\frac{3\Phi_Z^{\mathrm{TF}}}{5c_{\mathrm{TF}}}\right)^{3/2}. \tag{5}$$

[3]These are the units used throughout the paper.

Here, the first equation is called the Thomas-Fermi equation, and the latter, valid on $\mathbb{R}^3\backslash\{0\}$, is obtained by combining this with the definition of Φ_Z^{TF}. The fact that Φ_Z^{TF} satisfies this differential equation together with some qualitative observations can be used to prove the asymptotics

$$\Phi_1^{\mathrm{TF}}(x) = \left(\frac{5c_{\mathrm{TF}}}{3}\right)^3 \frac{9}{\pi^2|x|^4} + o_{|x|\to\infty}(|x|^{-4}) \tag{6}$$

for the Thomas-Fermi potential near infinity. Moreover, it can be easily deduced from (4) that $|x|\Phi_Z^{\mathrm{TF}}(x) \to Z$ as $|x| \to 0$.

We notice further that it follows directly from the definition (2) of the energy functional that $\mathcal{E}_Z^{\mathrm{TF}}[Z^2\rho(Z^{1/3}\cdot)] = Z^{7/3}\mathcal{E}_1^{\mathrm{TF}}[\rho]$. From this we learn that $\rho_Z^{\mathrm{TF}}(x) = Z^2\rho_1^{\mathrm{TF}}(Z^{1/3}x)$ and in turn, by (4) or (5), $\Phi_Z^{\mathrm{TF}}(x) = Z^{4/3}\Phi_1^{\mathrm{TF}}(Z^{1/3}x)$. These perfect scaling properties will be essential for proving the results in this paper. However, they do at first sight seem to prove that Thomas-Fermi theory is useless for describing the periodicity of (large) atoms by implying

$$\Phi_Z^{\mathrm{TF}}(x) \longrightarrow \left(\frac{5c_{\mathrm{TF}}}{3}\right)^3 \frac{9}{\pi^2|x|^4} =: \Phi_\infty^{\mathrm{TF}}(x) \quad \text{and similarly} \quad \rho_Z^{\mathrm{TF}} \longrightarrow \rho_\infty^{\mathrm{TF}} \tag{7}$$

pointwise on $\mathbb{R}^3\backslash\{0\}$ as $Z \to \infty$. Crucially, the Z can converge towards ∞ in any possible way. The latter convergence can be interpreted as the exact opposite of periodicity of large atoms in this model: It says that the distribution of the electrons in the atom looks similar for large Z regardless of how these are chosen. To detect a periodicity we need thus to consider a slightly more advanced model.

1.2 The Thomas-Fermi mean-field model

Let us now define a mean-field model based on Thomas-Fermi theory. The asymptotics of Φ_Z^{TF} near the origin and infinity together with its continuity yield straightforwardly $\Phi_Z^{\mathrm{TF}} \in L^2$. Consequently, the Schrödinger operator

$$H_Z^{\mathrm{TF}} := -\Delta - \Phi_Z^{\mathrm{TF}}$$

acting on[4] $L^2(\mathbb{R}^3)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ by Kato's theorem. Its self-adjoint closure on this space is the ***Thomas-Fermi mean-field model for the atom***. We present below our findings concerning the convergence properties of these operators as $Z \to \infty$. The results use in their formulation the concepts of strong resolvent and norm resolvent convergence of self-adjoint operators. By definition, a sequence of self-adjoint operators $\{A_n\}_{n=1}^\infty$ on some fixed Hilbert space $\mathcal{H}$ converges towards another such operator A in the strong

[4]A more physical choice of Hilbert space would be $L^2(\mathbb{R}^3;\mathbb{C}^2)$ including spin degrees of freedom. Observe, however, that H_Z^{TF} acting on this Hilbert space is unitarily equivalent to $H_Z^{\mathrm{TF}} \oplus H_Z^{\mathrm{TF}}$ acting on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. Thus, nothing qualitative is gained by considering the larger Hilbert space.

resolvent sense or norm resolvent sense if the (bounded) resolvent operators $(A_n + i)^{-1}$ converge towards the corresponding $(A + i)^{-1}$ in the strong or norm sense respectively. This generalizes strong and norm convergence of bounded operators. For more details on these types of convergence, see [14] VIII.7.

Unlike the situation in (7) there is no general convergence of H_Z^{TF} as $Z \to \infty$. Rather, one must choose particular sequences $\{Z_n\}_{n=1}^{\infty}$ of atomic numbers and consider the corresponding sequences of atoms $\{H_{Z_n}^{\mathrm{TF}}\}_{n=1}^{\infty}$ in order to have strong resolvent convergence of the operators as $n \to \infty$. Concretely, we introduce the "classical constant"

$$D_{\mathrm{cl}} := \frac{1}{4\pi} \int \frac{\Phi_1^{\mathrm{TF}}(x)^{1/2}}{|x|^2}\, dx$$

and obtain the following result (Theorem 2.5): Suppose $Z_n \to \infty$. Then $\{H_{Z_n}^{\mathrm{TF}}\}_{n=1}^{\infty}$ is converging in the strong resolvent sense if and only if $Z_n^{1/3} D_{\mathrm{cl}} \to \theta$ modulo π for some number θ which can be taken to be in $[0, \pi)$. In the affirmative case,

$$H_{Z_n}^{\mathrm{TF}} \longrightarrow H_{\infty,\theta}^{\mathrm{TF}} \tag{8}$$

where $\{H_{\infty,\theta}^{\mathrm{TF}}\}_{\theta \in [0,\pi)}$ is a parametrized family of self-adjoint extensions of the operator $-\Delta - \Phi_\infty^{\mathrm{TF}}$ defined on $C_0^\infty(\mathbb{R}^3 \backslash \{0\})$. When rewriting the convergence condition imposed on $D_{\mathrm{cl}} Z_n^{1/3}$ we see that it is satisfied for sequences similar to $Z_\ell(n)$ in (1) but with the coefficient $D_{\mathrm{cl}}^{-3}\pi^3$ instead of 1/6 on the leading n^3-term (cf. the remark following Definition 2.6 below). In this sense we recover the periodicity lost in the Thomas-Fermi density functional theory – while our model, however, does not satisfy Madelung's rule asymptotically.

We show also, by providing a counterexample, that in the result in Theorem 2.5 described above one cannot generally replace "in the strong resolvent sense" with "in the norm resolvent sense". That is, there exists a sequence $\{Z_n\}_{n=1}^{\infty}$ so that $Z_n^{1/3} D_{\mathrm{cl}} \to \theta$ modulo π while $\{H_{Z_n}^{\mathrm{TF}}\}_{n=1}^{\infty}$ is not converging in the norm resolvent sense.

The $H_{\infty,\theta}^{\mathrm{TF}}$'s are distinct for different θ's, and they are naturally interpreted as the infinitely many different "kinds" of infinite atoms in the Thomas-Fermi mean-field model – corresponding to the groups in the periodic table of the (finite) atoms. Changing the parametrization to $t = (\cos 2\theta, \sin 2\theta)$ one obtains a continuous parametrization of the operators by the unit circle S^1, thus recovering a periodicity aspect even for infinite atoms in this model. We note that the possible limiting operators $\{H_{\infty,\theta}^{\mathrm{TF}}\}_{\theta \in [0,\pi)}$ in (8) is by no means an exhaustive list of possible self-adjoint realizations of $-\Delta - \Phi_\infty^{\mathrm{TF}}$. Even among realizations that commute with the orthogonal projections onto all different angular momentum eigenspaces of the Laplace operator there is a family of distinct realizations parametrized by $S^1 \times \mathbb{N}_0$. In this sense the nature of the finite Thomas-Fermi atoms singles out a specific 1-parameter family of "infinite Thomas-Fermi atoms" in a non-trivial way.

In Section 2 we present the results described above in a more general setup which in particular highlights the crucial properties of the Thomas-Fermi potential: Its asymptotic behaviour at the origin and infinity, and its perfect scaling in Z. The proofs of these results are found in Section 3. Finally, Section 4 presents the promised example of a sequence of finite atoms in the Thomas-Fermi mean-field model which converges in the strong resolvent sense but not in the norm resolvent sense.

2 Main results

We start now the description of our main result in a form which is slightly more general than the one presented in the introduction. As a first step, we introduce a class of potentials Φ that we allow to play the role corresponding to the Thomas-Fermi potential Φ_1^{TF} above.

Assumptions 2.1 *We consider a radially symmetric*[5] *potential* $\Phi\colon \mathbb{R}^3 \to \mathbb{R}$. *The assumptions on* Φ *(considered as a function of one variable; the radius* r*) will be*

1) Φ *is strictly positive,*

2) $\Phi(r) = C_0 r^\alpha + o(r^\alpha)$ *as* $r \to 0$ *for some* $\alpha > -2$ *and* $C_0 > 0$*,*

3) $\Phi(r) = C_\infty r^\beta + o(r^\beta)$ *as* $r \to \infty$ *for some* $\beta < -2$ *and* $C_\infty > 0$*,*

4) Φ *is twice continuously differentiable on* $\mathbb{R}_+$*,*

5) $r|\Phi'(r)|, r^2|\Phi''(r)| \lesssim r^\alpha$ *on* $(0,1)$ *and* $r|\Phi'(r)|, r^2|\Phi''(r)| \lesssim r^\beta$ *on* $(1,\infty)$*.*

For the remaining part of the present section we mean by Φ a potential which satisfies these assumptions. Notice that Φ_1^{TF} is an example of such with $\alpha = -1 > -2$ and $\beta = -4 < -2$ (here 5) can be verified for example by the help of 2), 3) and the differential equation in (5)). We define generally the potential Φ_κ for each $\kappa > 0$ – our choice of "large parameter" – by the rule $\Phi_\kappa(x) := \kappa^{-\beta}\Phi(\kappa x)$, and once again we can recover the situation from the introduction: In this notation the Thomas-Fermi potential Φ_Z^{TF} will due to its scaling properties simply be written as $(\Phi_1^{\mathrm{TF}})_{Z^{1/3}}$, i.e. $\Phi = \Phi_1^{\mathrm{TF}}$ and $\kappa = Z^{1/3}$. Finally, since $\Phi_\kappa \to C_\infty|x|^\beta$ as $\kappa \to \infty$ in a rather strong sense (except at the origin), we put $\Phi_\infty(x) := C_\infty|x|^\beta$.

The next task is now to define the operators on $L^2(\mathbb{R}^3)$ which will model finite and infinite atoms respectively. As it is explained in the introduction, these should act as $-\Delta - \Phi_\kappa$ and $-\Delta - \Phi_\infty$ respectively, but, as it is often the case, determining their domains of self-adjointness is a more delicate matter – especially in the infinite case. Even though we have other methods for the finite case, we present now a general construction through an angular momentum decomposition and apply this in all cases. The reason for doing so is twofold: Firstly, we really do need the construction for the infinite case, so we have to cover it anyway; secondly, the similar structure of operators describing finite and infinite atoms is crucial for the proof of the main results below.

[5] We will generally use the same notation for the 3-dimensional and the 1-dimensional radial part. It is the intent that the meaning is clear from the context throughout the material.

For the general discussion we consider an abstract potential V which we assume is continuous. The first key idea in the construction is to separate the radial and angular variables using the standard identification $L^2(\mathbb{R}^3) \simeq L^2(\mathbb{R}_+)\otimes L^2(S^2)$ via the map $U\psi(r,\omega) := r\psi(r\omega)$ (which is a multiple of a unitary map). Notice then that by writing the Laplace operator in polar coordinates, $\Delta = r^{-1}\partial_r^2 r + r^{-2}\Delta_{S^2}$ with Δ_{S^2} the Laplace-Beltrami operator on S^2, one gets

$$U(-\Delta - V)U^{-1}(\phi\otimes\psi) = \Big(-\frac{d^2}{dr^2} - V\Big)\phi\otimes\psi + r^{-2}\phi\otimes(-\Delta_{S^2}\psi) \tag{9}$$

for, say, $\phi \in C_0^\infty(\mathbb{R}_+)$ and $\psi \in C^\infty(S^2)$. Consequently, it is a very natural next step to further decompose the Hilbert space by using the spherical harmonics $Y_\ell^m \in \psi \in C^\infty(S^2)$, $\ell \in \mathbb{N}_0$, $m = -\ell,\dots,\ell$, which satisfy $-\Delta_{S^2} Y_\ell^m = \ell(\ell+1)Y_\ell^m$ and can be chosen so that they constitute an orthonormal basis of $L^2(S^2)$. For $\phi \in C_0^\infty(\mathbb{R}_+)$ and $\psi \in \operatorname{span}_{m=-\ell,\dots,\ell} Y_\ell^m$ we see that (9) reads $U(-\Delta - V)U^{-1}(\phi\otimes\psi) = L_\ell\phi\otimes\psi$ with

$$L_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} - V, \tag{10}$$

and it is using this structure we define our operators rigorously below in Definition 2.2. Before doing so, we do, however, also need to handle the problem of making the expression (10) into a self-adjoint operator on $L^2(\mathbb{R}_+)$.

To this end we define $H_{\kappa,\ell,\min}$ and $H_{\infty,\ell,\min}$ to be the closures of the symmetric operators acting as (10) on $C_0^\infty(\mathbb{R}_+)$ with $V = \Phi_\kappa$ and $V = \Phi_\infty$ respectively. By von Neumann's criterion all of these have self-adjoint extensions since they commute with complex conjugation. Moreover, the self-adjoint extensions are well understood by Weyl's limit point/limit circle criterion and the theory of generalized boundary conditions in 1-dimensional space. We now describe the results we need from these methods and refer for the details to for example the appendix to X.1 in [15] and Appendix A in [3].

A potential $W\colon \mathbb{R}_+ \to \mathbb{R}$ is said to be in the ***limit circle case*** at the origin and/or at infinity if all solutions to the equation $f'' = Wf$ are in $L^2((0,1))$ and/or $L^2((1,\infty))$ respectively. Otherwise, it is said to be in the ***limit point case*** at the origin/at infinity. It is a fundamental result by Weyl that the operator $-d^2/dr^2 + W$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}_+)$ if and only if W is in the limit point case at both the origin and infinity. If this is not the case, then the self-adjoint extensions are defined by restricting the adjoint of the operator on $C_0^\infty(\mathbb{R}_+)$ to a smaller domain by putting (generalized) boundary conditions at the places where the potential is in the limit circle case (i.e. at the origin and/or at infinity). In our situations with $W = \ell(\ell+1)/r^2 - \Phi_\kappa$ and $W = \ell(\ell+1)/r^2 - \Phi_\infty$ basic estimates using 2) and 3) in Assumptions 2.1 show that:

- All potentials are in the limit point case at infinity (cf. [15], Theorem X.8).

- For $\ell = 1,2,\dots$, the potentials $\ell(\ell+1)/r^2 - \Phi_\kappa$ are in the limit point case at the origin (cf. [15], Theorem X.10).

Thus, letting $H_{\kappa,\ell} := H_{\kappa,\ell,\min}$ for $\ell = 1,2,\ldots$, these are themselves the desired self-adjoint extensions. We have further:

- The potentials $\ell(\ell+1)/r^2 - \Phi_\infty$ for all ℓ are in the limit circle case at the origin (since they are decreasing as $r \to 0$ from the right). Also, $-\Phi_\kappa$ is in the limit circle case[6].

Consequently, we need in the remaining cases the notion of generalized boundary conditions. This gives, for a W that is limit point at infinity and limit circle at the origin, the following characterization of all self-adjoint extensions L_f of the closure of $-d^2/dr^2 + W$ on $C_0^\infty(\mathbb{R}_+)$ (briefly denoted $L_{\min}$): Take as domain the set $D(L_f) := D(L_{\min}) \oplus \mathbb{C}\xi f$ where f is a real-valued solution to $f'' = Wf$ and ξ is a smooth localizing function which is, say, 1 on $(0,1)$ and 0 on $(2,\infty)$[7], and let L_f act as $-d^2/dr^2 + W$ in the distributional sense. That is, self-adjoint extensions of $H_{\kappa,0,\min}$ and the $H_{\infty,\ell,\min}$'s are in one-to-one correspondence with real-valued solutions to $f'' = -\Phi_\kappa f$ and

$$f''(r) = \Big[\frac{\ell(\ell+1)}{r^2} - C_\infty r^\beta\Big] f(r) \tag{11}$$

respectively. For extending $H_{\kappa,0,\min}$ we use the fact that $r \mapsto r\Phi_\kappa(r)$ is in $L^1((0,1))$ so that there is a unique solution $f \in C^1([0,\infty))$ to $f'' = -\Phi_\kappa f$ satisfying $f(0) = 0$ and $f'(0) = 1$. See [4] Proposition 2.5 for a proof (this problem is a special case of "the Cauchy problem"). We define $H_{\kappa,0}$ to be the self-adjoint extension of $H_{\kappa,0,\min}$ obtained by choosing $D(H_{\kappa,0}) = D(H_{\kappa,0,\min}) \oplus \mathbb{C}\xi f$ with the distinguished f just described (which happens to be real-valued). In the light of Proposition 2.3 (a) below this turns out to be a very natural choice. The equation (11) can be solved explicitly with the space of solutions spanned by the real-valued[8] functions

$$F_{\beta,C_\infty,\ell}(r) := \sqrt{r}\cdot J_{\frac{2\ell+1}{2+\beta}}\left(\frac{-2C_\infty^{1/2}}{2+\beta} r^{\frac{2+\beta}{2}}\right) \quad \text{and} \quad G_{\beta,C_\infty,\ell}(r) := \sqrt{r}\cdot Y_{\frac{2\ell+1}{2+\beta}}\left(\frac{-2C_\infty^{1/2}}{2+\beta} r^{\frac{2+\beta}{2}}\right)$$

where J and Y are Bessel functions of the first and second kind respectively. A general reference to the properties of Bessel functions we need, including a treatment of some differential equations very similar to the ones just discussed, is [1]. An examination of the solution space described above shows that no distinguished solutions (near the origin) exist, and thus the best we can do is to come up with a convenient parametrization. Our choice is the following: For each $\ell \in \mathbb{N}_0$ and $\theta_\ell \in [0,\pi)$ we define $H_{\infty,\ell,\theta_\ell}$ to be the self-adjoint extension of $H_{\infty,\ell,\min}$ obtained by choosing

$$D(H_{\infty,\ell,\theta_\ell}) = D(H_{\infty,\ell,\min}) \oplus \mathbb{C}\xi(\cos\theta_\ell F_{\beta,C_\infty,\ell} + \sin\theta_\ell G_{\beta,C_\infty,\ell}).$$

[6] This is not entirely straightforward to realize. One way to do so is to check the definition of being in the limit circle case directly via refined knowledge about the Cauchy problem mentioned below combined with the fact that $r \mapsto r\Phi_\kappa(r)$ is integrable near the origin.

[7] For our entire presentation we mean by ξ a fixed choice of such localizing function.

[8] Recall that $2 + \beta < 0$.

This finishes the discussion concerning the needed self-adjoint extensions of the 1-dimensional operators. We are now in a position to define the Schrödinger operators which describe finite and infinite atoms. Recall that the motivation for the definition below is (9) together with the surrounding discussion – in particular the line just above (10).

Definition 2.2 *We define the Schrödinger operators describing finite atoms by setting $H_\kappa = U^{-1}\widetilde{H}_\kappa U$ where $\widetilde{H}_\kappa$ is the closure of the operator $\widetilde{H}_\kappa^0$ on $L^2(\mathbb{R}_+)\otimes L^2(S^2)$ given by*

$$D(\widetilde{H}_\kappa^0) = \Big\{\sum_{\ell=0}^{M}\sum_{m=-\ell}^{\ell} \phi_\ell^m \otimes Y_\ell^m \,\Big|\, M\in\mathbb{N}, \quad \phi_\ell^m \in D(H_{\kappa,\ell})\Big\},$$

$$\widetilde{H}_\kappa^0 \sum_{\ell=0}^{M}\sum_{m=-\ell}^{\ell} \phi_\ell^m \otimes Y_\ell^m = \sum_{\ell=0}^{M}\sum_{m=-\ell}^{\ell} H_{\kappa,\ell}\phi_\ell^m \otimes Y_\ell^m$$

with the self-adjoint operators $H_{\kappa,\ell}$ defined as above.

Similarly, we define Schrödinger operators by, for each sequence $\{\theta_\ell\}_{\ell=0}^\infty \subseteq [0,\pi)$, setting $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty} = U^{-1}\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}U$ where $\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ is the closure of the operator $\widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ on $L^2(\mathbb{R}_+)\otimes L^2(S^2)$ given by

$$D\Big(\widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}\Big) = \Big\{\sum_{\ell=0}^{M}\sum_{m=-\ell}^{\ell} \phi_\ell^m \otimes Y_\ell^m \,\Big|\, M\in\mathbb{N}, \quad \phi_\ell^m \in D(H_{\infty,\ell,\theta_\ell})\Big\},$$

$$\widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^\infty} \sum_{\ell=0}^{M}\sum_{m=-\ell}^{\ell} \phi_\ell^m \otimes Y_\ell^m = \sum_{\ell=0}^{M}\sum_{m=-\ell}^{\ell} H_{\infty,\ell,\theta_\ell}\phi_\ell^m \otimes Y_\ell^m$$

with the self-adjoint operators $H_{\infty,\ell,\theta_\ell}$ defined as above.

The operators just described have the following convenient properties:

Proposition 2.3

a) *For each $\kappa > 0$ the operator H_κ in Definition 2.2 is self-adjoint and coincides with the Friedrichs' extension of $-\Delta - \Phi_\kappa$ on $C_0^\infty(\mathbb{R}^3\backslash\{0\})$. If moreover $\alpha > -3/2$ this in turn coincides with the closure of $-\Delta-\Phi_\kappa$ on $C_0^\infty(\mathbb{R}^3)$.*

b) *For each sequence $\{\theta_\ell\}_{\ell=0}^\infty \subseteq [0,\pi)$ the operator $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ in Definition 2.2 is a self-adjoint extension of $-\Delta-\Phi_\infty$ on $C_0^\infty(\mathbb{R}^3\backslash\{0\})$. Additionally, $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty} \neq H_{\infty,\{\theta'_\ell\}_{\ell=0}^\infty}$ whenever $\{\theta_\ell\}_{\ell=0}^\infty \neq \{\theta'_\ell\}_{\ell=0}^\infty$.*

Now, having introduced rigorously the framework for our general model, the main results can be formulated. Recall that strong resolvent convergence of the H_{κ_n}'s means strong convergence of the resolvent operators $(H_{\kappa_n}+i)^{-1}$. We present firstly the general result and then specialize to the case of the Thomas-Fermi mean-field model discussed in the introduction above.

Theorem 2.4 *Consider a sequence $\{\kappa_n\}_{n=1}^{\infty}$ of positive real numbers such that $\kappa_n \to \infty$ as $n \to \infty$. The corresponding sequence of operators $\{H_{\kappa_n}\}_{n=1}^{\infty}$ is convergent in the strong resolvent sense if and only if*

$$\int_0^\infty \Phi_{\kappa_n}^{1/2}\,dr = \kappa_n^{-\frac{\beta}{2}-1}\int_0^\infty \Phi_1^{1/2}\,dr \longrightarrow \theta \pmod{\pi} \tag{12}$$

as $n \to \infty$ for some number $\theta \in [0,\pi)$. In the affirmative case the limiting operator is $H_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}$ from Definition 2.2 with

$$\theta_\ell = \theta - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{(2\ell+1)\pi}{4+2\beta} - \frac{\pi}{2} \pmod{\pi}.$$

Theorem 2.5 *Consider a sequence $\{Z_n\}_{n=1}^{\infty}$ of positive real numbers such that $Z_n \to \infty$ as $n \to \infty$. The corresponding sequence of operators $\{H_{Z_n}^{\mathrm{TF}}\}_{n=1}^{\infty}$ is convergent in the strong resolvent sense if and only if*

$$D_{\mathrm{cl}} Z_n^{1/3} = Z_n^{1/3}\int_0^\infty (\Phi_1^{\mathrm{TF}})^{1/2}\,dr \longrightarrow \theta \pmod{\pi} \tag{13}$$

as $n \to \infty$ for some number $\theta \in [0,\pi)$. In the affirmative case the limiting operator is $H_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}$ defined as in Definition 2.2 with $\Phi_\infty = \Phi_\infty^{\mathrm{TF}}$ and

$$\theta_\ell = \theta + \frac{\ell\pi}{2} + \frac{\pi}{4} \pmod{\pi}.$$

In particular, this act in the ℓ^{th} angular momentum sector as the self-adjoint operator

$$H_{\infty,\ell,\theta_\ell} = -\frac{d^2}{dx^2} + \frac{\ell(\ell+1)}{|x|^2} - C_\infty |x|^{-4}$$

with $C_\infty = (5c_{\mathrm{TF}}/3)^3 \cdot (9/\pi^2)$ and domain given by

$$D(H_{\infty,\ell,\min}) \oplus \mathbb{C}\xi\Big(\sin\Big(\theta + \frac{\ell\pi}{2} + \frac{\pi}{4}\Big) j_\ell(C_\infty^{1/2} r^{-1}) - \cos\Big(\theta + \frac{\ell\pi}{2} + \frac{\pi}{4}\Big) y_\ell(C_\infty^{1/2} r^{-1})\Big)$$

where j_ℓ and y_ℓ are the spherical Bessel functions of the first and second kind respectively. With our choice of units, $C_\infty = 81\pi^2$.

Definition 2.6 *We call the Schrödinger operators $H_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}$ that appear as limits of finite atoms in Theorem 2.4* ***infinite atoms****. Similarly, we define an* ***infinite Thomas-Fermi atom*** *to be one of the limiting operators in Theorem 2.5.*

Remark. In Theorem 2.5 it seems a natural question to ask if all infinite Thomas-Fermi atoms arise as strong resolvent limits of finite atoms with integer atomic numbers Z_n. This is indeed the case, and one can for example choose

$$Z_n = \left\lfloor D_{\mathrm{cl}}^{-3}(\pi n + \theta)^3 \right\rfloor \tag{14}$$

to obtain the convergence (13). More generally, taking these Z_n's and adding to them a term behaving like $Cn^2 + o_{n\to\infty}(n^2)$ for large n results in new sequence also satisfying (13) with $\theta + (CD_{\mathrm{cl}}^3)/(3\pi^2)$ instead of θ.

3 Proofs

3.1 First reductions

To reduce the problem of proving the "if"-part of Theorem 2.4 to a more concrete convergence problem, we introduce abstractly the notion of the ***strong limit of the graphs***, $\Gamma(A_n)$, of a sequence of operators $\{A_n\}_{n=1}^{\infty}$ on a fixed Hilbert space $\mathcal{H}$. That is, we let str.lim $\Gamma(A_n)$ be the set of $(\phi,\psi)\in\mathcal{H}\times\mathcal{H}$ satisfying that there exist $\phi_n\in D(A_n)$ so that $\phi_n\to\phi$ and $A_n\phi_n\to\psi$ in the Hilbert space as $n\to\infty$. This concept is closely related to strong graph convergence of operators which is discussed in for example [14] VIII.7. A diagonal argument shows that strong limits of graphs are closed subspaces of $\mathcal{H}\times\mathcal{H}$ – for the details of this and further results on strong limits of subspaces in general and of graphs in particular, we refer the reader to [2]. We do, however, in Lemma 3.1 and Proposition 3.3 provide proofs of the properties of these limits that are essential to our proof of Theorem 2.4. Firstly we have:

Lemma 3.1 *Consider sequences $\{\kappa_n\}_{n=1}^{\infty}\subseteq\mathbb{R}_+$ and $\{\theta_\ell\}_{\ell=0}^{\infty}\subseteq[0,\pi)$. If*

$$\Gamma\Big(\widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}\Big)\subseteq \text{str.lim}\,\Gamma(\widetilde{H}^0_{\kappa_n}) \tag{15}$$

then $H_{\kappa_n}\to H_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}$ in the strong resolvent sense as $n\to\infty$.

Proof. We observe that strong resolvent convergence of H_{κ_n} towards $H_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}$ is clearly equivalent to that of $\widetilde{H}_{\kappa_n}$ towards $\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}$. Consider for the sake of proving the latter any function $\psi\in L^2(\mathbb{R}_+)\otimes L^2(S^2)=R(\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}+i)$ and write this as $\psi=(\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}+i)\phi$ for some $\phi\in D(\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}})$. Notice now that with the assumption (15) we have

$$\Gamma\Big(\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}\Big)=\overline{\Gamma\Big(\widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}\Big)}\subseteq\text{str.lim}\,\Gamma(\widetilde{H}^0_{\kappa_n})\subseteq\text{str.lim}\,\Gamma(\widetilde{H}_{\kappa_n}),$$

which means that there exist some $\phi_n\in D(\widetilde{H}_{\kappa_n})$ satisfying both $\phi_n\to\phi$ and $\widetilde{H}_{\kappa_n}\phi_n\to\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}\phi$. Consequently,

$$\begin{aligned}\Big[(\widetilde{H}_{\kappa_n}+i)^{-1}-(\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}+i)^{-1}\Big]\psi\\ =(\widetilde{H}_{\kappa_n}+i)^{-1}\Big[(\widetilde{H}_{\infty,\{\theta_\ell\}_{\ell=0}^{\infty}}+i)\phi-(\widetilde{H}_{\kappa_n}+i)\phi_n\Big]-\phi+\phi_n\longrightarrow 0,\end{aligned}$$

where we used the fact that $\|(\widetilde{H}_{\kappa_n}+i)^{-1}\|\leq 1$ for all n. This finishes the proof. □

We have also the following straightforward reduction of the proof:

Lemma 3.2 *In Theorem 2.4, the "only if"-part follows from all the remaining assertions.*

Proof. Suppose the remaining assertions of Theorem 2.4 hold true and consider a sequence $\{\kappa_n\}_{n=1}^{\infty}$ of positive real numbers so that $\kappa_n\to\infty$ but the integrals

$$\int_0^\infty \Phi_{\kappa_n}^{1/2}\,dr=:K_n$$

is not convergent modulo π. Since the latter (non-)convergence takes place in a compact space, it must be the case that $\{K_n\}_{n=1}^\infty$ has at least two accumulation points $\theta \neq \theta'$ in this space, i.e. modulo π. Now choosing subsequences along which $\{K_n\}_{n=1}^\infty$ converges towards θ and θ' respectively, the remaining assertions of the theorem tells us that along these subsequences the corresponding Schrödinger operators converge in the strong resolvent sense towards $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ and $H_{\infty,\{\theta'_\ell\}_{\ell=0}^\infty}$ respectively where $\{\theta_\ell\}_{\ell=0}^\infty \neq \{\theta'_\ell\}_{\ell=0}^\infty$. But by the last part of Proposition 2.3 (b) these operators are unequal, and hence this implies that $\{H_{\kappa_n}\}_{n=1}^\infty$ cannot converge towards any single operator in the strong resolvent sense. □

Concluding this subsection, the promised reduction of the question concerning strong resolvent convergence in Theorem 2.4 to a more concrete convergence question is presented below.

Proposition 3.3 *In order to prove Theorem 2.4 it suffices to verify the following statement:*

Consider a sequence $\{\kappa_n\}_{n=1}^\infty$ such that $\kappa_n \to \infty$ and (12) as $n \to \infty$. Then there exist functions $\phi_{n,\ell} \in D(H_{\kappa_n,\ell})$ so that

- $\phi_{n,\ell} \longrightarrow \xi(\cos\theta_\ell F_{\beta,C_\infty,\ell} + \sin\theta_\ell G_{\beta,C_\infty,\ell})$
- $H_{\kappa_n,\ell}\phi_{n,\ell} \longrightarrow H_{\infty,\ell,\theta_\ell}(\xi(\cos\theta_\ell F_{\beta,C_\infty,\ell} + \sin\theta_\ell G_{\beta,C_\infty,\ell}))$

in $L^2(\mathbb{R}_+)$ as $n \to \infty$ for all $\ell \in \mathbb{N}_0$ with the θ_ℓ's given in the theorem and $F_{\beta,C_\infty,\ell}$ and $G_{\beta,C_\infty,\ell}$ the solutions to (11) defined in Section 2.

Proof. From Lemmas 3.1 and 3.2 we learn that in order to prove Theorem 2.4 it suffices to argue that $\kappa_n \to \infty$ and (12) as $n \to \infty$ implies the inclusion (15). Hence, we need to show that the existence of the $\phi_{n,\ell}$'s above implies (15) in order to prove the present proposition.

To this end we suppose from this point onwards that such $\phi_{n,\ell}$'s exist and show firstly that the inclusion $\Gamma(H_{\infty,\ell,\theta_\ell}) \subseteq \text{str.lim}\,\Gamma(H_{\kappa_n,\ell})$ holds for all $\ell \in \mathbb{N}_0$. This relies on the fact that

$$\Gamma(H_{\infty,\ell,\theta_\ell}) = \Gamma(H_{\infty,\ell,\min}) \oplus \mathbb{C}(\lim_{n\to\infty}\phi_{n,\ell}, \lim_{n\to\infty} H_{\kappa_n,\ell}\phi_{n,\ell}),$$

where the direct sum is in $L^2(\mathbb{R}_+) \times L^2(\mathbb{R}_+)$ and the last term clearly is a subset of $\text{str.lim}\,\Gamma(H_{\kappa_n,\ell})$. Moreover, we have for any $h \in C_0^\infty(\mathbb{R}_+)$ the convergence

$$\int_0^\infty |H_{\infty,\ell,\min}h - H_{\kappa_n,\ell}h|^2\,dr = \int_0^\infty |h|\cdot|\Phi_{\kappa_n} - \Phi_\infty|^2\,dr \longrightarrow 0$$

so that also

$$\Gamma(H_{\infty,\ell,\min}) = \overline{\Gamma(H_{\infty,\ell,\min}|_{C_0^\infty(\mathbb{R}_+)})} \subseteq \overline{\text{str.lim}\,\Gamma(H_{\kappa_n,\ell})} = \text{str.lim}\,\Gamma(H_{\kappa_n,\ell})$$

as claimed.

Next, we show that the inclusions $\Gamma(H_{\infty,\ell,\theta_\ell}) \subseteq \text{str.lim}\,\Gamma(H_{\kappa_n,\ell})$ imply (15) and consider thus an arbitrary element

$$\sigma := \sum_{\ell=0}^{M} \sum_{m=-\ell}^{\ell} \phi_\ell^m \otimes Y_\ell^m \in D\Big(\widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}\Big).$$

Taking $\psi_{\ell,n}^m \in D(H_{\kappa_n,\ell})$ so that $\psi_{\ell,n}^m \to \phi_\ell^m$ and $H_{\kappa_n,\ell}\psi_{\ell,n}^m \to H_{\infty,\ell,\theta_\ell}\phi_\ell^m$ as $n \to \infty$ and defining

$$\sigma_n := \sum_{\ell=0}^{M} \sum_{m=-\ell}^{\ell} \psi_{\ell,n}^m \otimes Y_\ell^m \in D(\widetilde{H}^0_{\kappa_n}),$$

it is an easy check that similarly $\sigma_n \to \sigma$ and $\widetilde{H}^0_{\kappa_n}\sigma_n \to \widetilde{H}^0_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}\sigma$. This proves exactly that (15) is satisfied. □

3.2 Approximation of zero energy solutions (strategy)

We should now begin the process of verifying the statement in Proposition 3.3 and discuss at this point briefly the strategy that we follow to do so, in addition to fixing some notation. While the line of thought explained here is not strictly speaking the one we will follow for the technical verification of the statement in Proposition 3.3, we do believe that it provides sufficient intuition about the problem for us to begin tackling the details hereof. For the remaining part of the present section we mean by Φ a potential that satisfies the Assumptions 2.1 and by Φ_κ, Φ_∞, H_κ and $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ the quantities introduced in Section 2.

Since we will be in a 1-dimensional setting, we change the space variable from the radial r to the more standard choice of x. Adapting to the nature of the statement in Proposition 3.3, we also allow ourselves to treat ℓ simply as a constant from this point onwards. We use the notation "$\lesssim$" to indicate "less than up to a constant". Here the constant might depend on ℓ and on the potential Φ, but it may not depend on x, κ or λ (see below). In the same spirit, "$\propto$" always indicates "proportional to" as a function *only* of x.

The overall idea of the proof is from this point to examine the behaviour of some particular solutions $f_{\kappa,\ell}$ to the equations $f''_{\kappa,\ell} = [\ell(\ell+1)x^{-2} - \Phi_\kappa]f_{\kappa,\ell}$ for large κ in order to conclude that $\kappa_n \to \infty$ and (12) implies

$$f_{\kappa_n,\ell} \longrightarrow \cos\theta_\ell F_{\beta,C_\infty,\ell} + \sin\theta_\ell G_{\beta,C_\infty,\ell}$$

up to an overall sign and in an appropriate sense near the origin. This should more or less yield the first bullet point in Proposition 3.3 – at least if we manage to obtain $\xi f_{\kappa,\ell} \in D(H_{\kappa,\ell})$ – and, ignoring the localizing function ξ, the second point must hold regardless of (12) since both sides are 0 from the $f_{\kappa_n,\ell}$'s solving the above equations.

The entire analysis will be carried out after a ***Langer transformation*** – a change of variable $x \to \kappa^{-1}e^x$ – which was first suggested in [9] for studying the JWKB approximation in the context of the Schrödinger equation for the hydrogen atom. The fact that this problem is very similar to ours already hints that the Langer transformation might help us. Its usefulness will be more apparent below, but let us observe for the moment that if we put $\lambda = \kappa^{-(2+\beta)/2}$ and $g_{\lambda,\ell}(x) = e^{-x/2} f_{\kappa,\ell}(\kappa^{-1}e^x)$ with $f_{\kappa,\ell}$ solving the equation from above then, with $L = \ell + 1/2$,

$$\begin{aligned} g''_{\lambda,\ell}(x) &= \Big[\Big(\ell + \frac{1}{2}\Big)^2 - \kappa^{-2-\beta} e^{2x}\Phi(e^x)\Big] g_{\lambda,\ell}(x) \\ &= \lambda^2 \Big[L^2\lambda^{-2} - e^{2x}\Phi(e^x)\Big] g_{\lambda,\ell}(x) =: -\lambda^2 V_{\lambda,\ell}(x) g_{\lambda,\ell}(x) \end{aligned} \tag{16}$$

on $\mathbb{R}$. Now it is actually possible to determine the asymptotic behaviour of the solutions of interest to this equation if we look at some regions separately: Near plus and minus infinity we can use 2) and 3) from Assumptions 2.1 to control solutions directly. On the remaining part of the real axis, $V_{\lambda,\ell}$ will be strictly positive for large λ by 1), and 4) and 5) from Assumptions 2.1 allow us to use the ***Liouville-Green approximation*** to describe solutions here as well. Lastly, we can put an appropriate boundary condition at minus infinity and from there "glue together" the descriptions that we have of the solutions on the different regions. A sufficiently detailed examination of these solutions will virtually finish the verification of the statement in Proposition 3.3.

We note here that a very similar approach (although using the method of exact WKB analysis on the entire real axis) reaching many of the same conclusions, but for a much smaller class of potentials Φ (not including Φ_1^{TF}), is discussed in [7]. The results from this paper have been an inspiration to us when carrying out the approximation of the solutions to (16).

3.3 The regular zero energy solutions

From this point onwards we use the notation from subsection 3.2, i.e. Φ, Φ_κ, $H_{\kappa,\ell}$, $H_{\infty,\ell,\theta_\ell}$, λ and $V_{\lambda,\ell}$ are as described above. As a first step in the analysis of the "zero energy solutions", i.e. the solutions to $f''_{\kappa,\ell} = [\ell(\ell+1)x^{-2} - \Phi_\kappa] f_{\kappa,\ell}$ and (16), we prove the existence of these with certain boundary conditions. For the former this means that $\xi f_{\kappa,\ell} \in D(H_{\kappa,\ell})$ and for the latter that the solution is exponentially small at minus infinity. As mentioned above, the finer analysis takes place after the Langer transformation.

Proposition 3.4 *Let $W : \mathbb{R} \to \mathbb{R}$ be any continuous potential satisfying*

$$\int_{-\infty}^{x} |W(y)|\, dy =: Q(x) < \infty \tag{17}$$

for all $x \in \mathbb{R}$ and let $L > 0$ be any number. Then there exists a real-valued solution $g \in C^2(\mathbb{R})$ to the equation $g'' = [L^2 + W]g$ satisfying $e^{-Lx}g(x) \to 1$ and $e^{-Lx}g'(x) \to L$ as $x \to -\infty$.

Proof. The proof is constructive with the following construction of the solution g: Define $h_0(x) = e^{Lx}$ and then

$$h_i(x) = \frac{1}{L}\int_{-\infty}^{x} \sinh\Big(L(x-y)\Big) W(y) h_{i-1}(y)\, dy$$

for each $i = 1, 2, 3, \ldots$. We notice that $|h_i(x)| \le e^{Lx} Q(x)^i/(L^i i!)$ for all $i \in \mathbb{N}_0$ so that this is well-defined. Indeed, this can be seen by the induction step

$$|h_i(x)| \le \frac{e^{Lx}}{L} \int_{-\infty}^{x} |W(y)| \frac{Q(y)^{i-1}}{L^{i-1}(i-1)!}\, dy = e^{Lx} \frac{Q(x)^i}{L^i i!}, \tag{18}$$

where we estimated $\sinh z \le e^z$ for $z > 0$, and this bound implies that the integral defining each h_i is convergent. Also, we get from the estimate, on any interval of the form $(-\infty, x_0]$, uniform convergence of the series

$$\sum_{i=0}^{\infty} h_i(x)$$

towards some real-valued continuous function g that satisfies $|g(x)| \le e^{Lx+Q(x)/L}$ and similarly of

$$\sum_{i=0}^{\infty} e^{-Lx} h_i(x)$$

towards $e^{-Lx} g(x)$. In turn this tells us that

$$\begin{aligned} e^{Lx} &+ \int_{-\infty}^{x} \frac{\sinh\big(L(x-y)\big)}{L} W(y) g(y)\, dy \\ &= h_0(x) + \sum_{i=0}^{\infty} \int_{-\infty}^{x} \frac{\sinh\big(L(x-y)\big)}{L} W(y) h_i(y)\, dy = g(x) \end{aligned}$$

so that g is differentiable with

$$g'(x) = L e^{Lx} + \int_{-\infty}^{x} \cosh\big(L(x-y)\big) W(y) g(y)\, dy \tag{19}$$

and further

$$g''(x) = L^2 e^{Lx} + W(x) g(x) + L \int_{-\infty}^{x} \sinh\big(L(x-y)\big) W(y) g(y)\, dy = [L^2 + W(x)] g(x)$$

as needed. The C^2-property of g follows from this equation and the fact that g is continuous.

For the first assertion about the limit as $x \to -\infty$ simply notice that in this limit

$$|e^{-Lx} g(x) - 1| = \left| e^{-Lx} \sum_{i=1}^{\infty} h_i(x) \right| \le \sum_{i=1}^{\infty} \frac{Q(x)^i}{L^i i!} = e^{Q(x)/L} - 1 \longrightarrow 0,$$

where we used once again the estimate (18). For the second one observe that further

$$\left| e^{-Lx} \int_{-\infty}^{x} \cosh\big(L(x-y)\big) W(y) g(y)\, dy \right| \le e^{Q(x)/L} \int_{-\infty}^{x} |W(y)|\, dy \longrightarrow 0,$$

where we estimated $\cosh(z) \le e^z$ for $z > 0$ and $e^{-Ly}|g(y)| \le e^{Q(y)/L}$, so that (19) yields the desired conclusion. □

Definition 3.5 *For W and L as in Proposition 3.4 we call the g constructed in the proof hereof the* **regular solution** *of $g'' = [L^2 + W]g$. Moreover, we define for each $\lambda > 0$ and $\ell \in \mathbb{N}_0$ the function $g_{\lambda,\ell}$ as the regular solution to (16) (which is of the form $g'' = [L^2 + W]g$ with $L = \ell + 1/2$ and $W(x) = -\lambda^2 e^{2x}\Phi(e^x)$) and for each $\kappa = \lambda^{-(2+\beta)/2} > 0$ and $\ell \in \mathbb{N}_0$ the function $f_{\kappa,\ell}(x) = \sqrt{x}\, g_{\lambda,\ell}(\ln\kappa + \ln x)$.*

Lemma 3.6 *For each $\kappa > 0$ and $\ell \in \mathbb{N}_0$ the function $f_{\kappa,\ell}$ satisfies the equation $f''_{\kappa,\ell} = [\ell(\ell+1)x^{-2} - \Phi_\kappa]f_{\kappa,\ell}$, and $\xi f_{\kappa,\ell} \in D(H_{\kappa,\ell})$ where ξ is as described in Section 2.*

Proof. The fact that $f_{\kappa,\ell}$ satisfies the equation is a straightforward calculation using the equation for $g_{\lambda,\ell}$. For the other assertion we recall that

$$D(H_{\kappa,\ell}) = D(H^*_{\kappa,\ell,\min}) = \Big\{\psi \in L^2(\mathbb{R}_+) \,\Big|\, -\psi'' + [\ell(\ell+1)x^{-2} - \Phi_\kappa]\psi \in L^2(\mathbb{R}_+)\Big\}$$

for $\ell = 1, 2, 3, \ldots$. It is easy to verify that $\psi = \xi f_{\kappa,\ell}$ is in this set: It is continuous, tends towards 0 as near the origin, as is easily verified, and has support in $(0,2)$, and is thus in $L^2(\mathbb{R}_+)$. The other condition holds true since the expression that is required to be in $L^2(\mathbb{R}_+)$ is continuous in addition to being 0 on $(0,1)$ (by the equation that $f_{\kappa,\ell}$ solves) and on $(2,\infty)$ (since $\psi \equiv 0$ here).

In order to show $\xi f_{\kappa,0} \in D(H_{\kappa,0})$ it suffices by the definition of this domain to argue that $f_{\kappa,0} \in C^1([0,\infty))$ with $f_{\kappa,0}(0) = 0$ (notice that since $f_{\kappa,0}$ is not identically 0, we then cannot have $f'_{\kappa,0}(0) = 0$). As mentioned above, it is easy to check that $f_{\kappa,0} \in C([0,\infty))$ with $f_{\kappa,0}(0) = 0$. For the remaining part of the statement simply observe that

$$\begin{aligned}
f'_{\kappa,0}(x) &= \frac{1}{2}x^{-1/2} g_{\lambda,0}(\ln\kappa + \ln x) + x^{-1/2} g'_{\lambda,0}(\ln\kappa + \ln x)\\
&= \frac{\sqrt{\kappa}}{2} e^{-\frac{1}{2}(\ln\kappa + \ln x)} g_{\lambda,0}(\ln\kappa + \ln x) + \sqrt{\kappa} e^{-\frac{1}{2}(\ln\kappa + \ln x)} g'_{\lambda,0}(\ln\kappa + \ln x)\\
&\longrightarrow \frac{\sqrt{\kappa}}{2} + \frac{\sqrt{\kappa}}{2} = \kappa
\end{aligned}$$

as $x \to 0$ since $g_{\lambda,0}$ is the regular solution to an equation of the form $g'' = [L^2 + W]g$ with $L = 0 + 1/2 = 1/2$. □

For later use we need some continuity properties of the regular solution as a function of the potential W in order to control $g_{\lambda,\ell}$ near minus infinity. These will be the last abstract results on regular solutions in the sense of Definition 3.5 presented here, and we do so now to keep the treatment hereof somewhat concise.

Lemma 3.7 *Let W and $\widetilde{W}$ be two real-valued continuous potentials satisfying (17) for all $x \in \mathbb{R}$ and denote by $\widetilde{Q}(x)$ the number corresponding to the one defined in (17) with W replaced by $\widetilde{W}$. If, for some fixed $L > 0$, g and $\widetilde{g}$ are the regular solutions to $g'' = [L^2 + W]g$ and $\widetilde{g}'' = [L^2 + \widetilde{W}]\widetilde{g}$ respectively then*

$$|g(x) - \widetilde{g}(x)| \le e^{Lx} L^{-1} D(x) e^{(Q(x)+\widetilde{Q}(x))/L}$$

for all $x \in \mathbb{R}$ *where*

$$D(x) := \int_{-\infty}^{x} |W(y) - \widetilde{W}(y)|\,dy.$$

Proof. Denoting by h_i the functions from the proof of Proposition 3.4 and by $\widetilde{h}_i$ the similar quantities for $\widetilde{W}$ readily see that the bounds

$$|h_i(x) - \widetilde{h}_i(x)| \le e^{Lx} L^{-i} D(x) \frac{(Q(x) + \widetilde{Q}(x))^{i-1}}{(i-1)!}$$

for $i = 1, 2, \ldots$ imply the bound in the lemma. The proof of these is by induction, starting with

$$|h_1(x) - \widetilde{h}_1(x)| \le \frac{1}{L} \int_{-\infty}^{x} \sinh\big(L(x-y)\big) |W(y) - \widetilde{W}(y)| e^{Ly}\,dy \le e^{Lx} L^{-1} D(x).$$

Then, for $i = 1, 2, \ldots,$

$$\begin{aligned}
&|h_{i+1}(x) - \widetilde{h}_{i+1}(x)| \\
&\quad \le \frac{1}{L} \int_{-\infty}^{x} \sinh\big(L(x-y)\big) |W(y) h_i(y) - \widetilde{W}(y) \widetilde{h}_i(y)|\,dy \\
&\quad \le \frac{1}{L} \int_{-\infty}^{x} \sinh\big(L(x-y)\big) \Big[|W(y) - \widetilde{W}(y)| \cdot |h_i(y)| + |\widetilde{W}(y)| \cdot |h_i(y) - \widetilde{h}_i(y)| \Big]\,dy \\
&\quad \le \frac{e^{Lx}}{L} \int_{-\infty}^{x} |W(y) - \widetilde{W}(y)| \frac{Q(y)^i}{L^i i!} + |\widetilde{W}(y)| \cdot D(y) \frac{(Q(y) + \widetilde{Q}(y))^{i-1}}{L^i (i-1)!}\,dy \\
&\quad \le \frac{e^{Lx}}{L^{i+1}} D(x) \Big[\frac{Q(x)^i}{i!} + \int_{-\infty}^{x} |\widetilde{W}(y)| \frac{(Q(y) + \widetilde{Q}(y))^{i-1}}{(i-1)!}\,dy \Big],
\end{aligned}$$

where we used (18) and the induction hypothesis in the third inequality. Furthermore,

$$\begin{aligned}
&\int_{-\infty}^{x} |\widetilde{W}(y)| \frac{(Q(y) + \widetilde{Q}(y))^{i-1}}{(i-1)!}\,dy \\
&\qquad = \frac{1}{(i-1)!} \sum_{j=0}^{i-1} \binom{i-1}{j} \int_{-\infty}^{x} |\widetilde{W}(y)| Q(y)^j \widetilde{Q}(y)^{i-1-j}\,dy \\
&\qquad \le \frac{1}{(i-1)!} \sum_{j=0}^{i-1} \binom{i-1}{j} Q(x)^j \int_{-\infty}^{x} |\widetilde{W}(y)| \widetilde{Q}(y)^{i-1-j}\,dy \\
&\qquad = \frac{1}{(i-1)!} \sum_{j=0}^{i-1} \binom{i-1}{j} Q(x)^j \frac{\widetilde{Q}(x)^{i-j}}{i-j} = \frac{1}{i!} \sum_{j=0}^{i-1} \binom{i}{j} Q(x)^j \widetilde{Q}(y)^{i-j} \\
&\qquad = \frac{(Q(x) + \widetilde{Q}(x))^i}{i!} - \frac{Q(x)^i}{i!},
\end{aligned}$$

finishing the induction. $\square$

3.4 Application of the Liouville-Green approximation

We now aim for determining parts of the asymptotic behaviour of $g_{\lambda,\ell}$ from Definition 3.5 for fixed ℓ in the $\lambda \to \infty$ limit away from $x = \pm\infty$, i.e. on the part of the real axis where we cannot take advantage of our knowledge of the asymptotics of Φ. For this we use the Liouville-Green (LG) approximation and in particular the very precise pointwise estimates for this given in Theorem 4 in [13]. Slightly reformulating this result to adapt it to our set-up, it reads as presented in Proposition 3.8 below. We remind the reader that our conventions for "$\propto$" and "$\lesssim$" are as stated in Subsection 3.2.

Proposition 3.8 *For $\lambda > 0$, let W_λ be a C^2 and strictly positive potential defined on some finite interval $(x_1(\lambda), x_2(\lambda))$ that might depend on the value of λ. Now, if g_λ is real-valued and solves the equation $g_\lambda'' = -\lambda^2 W_\lambda g_\lambda$ then*

$$g_\lambda(x) \propto W_\lambda(x)^{-1/4}\Big[\cos\Big(\lambda \int_{x_1(\lambda)}^{x} W_\lambda^{1/2}\, dy + \theta(\lambda)\Big) + \varepsilon_\lambda(x)\Big]$$

for some number $\theta(\lambda)$ with the error estimate

$$\frac{|\varepsilon_\lambda(x)|}{2} \leq \exp\Big(\lambda^{-1}\int_{x_1(\lambda)}^{x_2(\lambda)} W_\lambda^{-1/4}\Big|\frac{d^2}{dx^2}\Big(W_\lambda^{-1/4}\Big)\Big|\, dx\Big) - 1$$

for all $x \in (x_1(\lambda), x_2(\lambda))$.

In order to apply Proposition 3.8 we should first of all find an appropriate interval $(x_1(\lambda), x_2(\lambda))$ on which $V_{\lambda,\ell}$ is positive – and then we can hope to be able to control the error estimate in Proposition 3.8 on this interval. As a first step towards this notice that due to 2) and 3) in Assumptions 2.1 we have

$$b_0 e^{(2+\alpha)x} - \lambda^{-2}\Big(\ell + \frac{1}{2}\Big)^2 \leq V_{\lambda,\ell}(x) \leq B_0 e^{(2+\alpha)x} - \lambda^{-2}\Big(\ell + \frac{1}{2}\Big)^2 \tag{20}$$

for $x \in (-\infty, 0)$ and

$$b_\infty e^{(2+\beta)x} - \lambda^{-2}\Big(\ell + \frac{1}{2}\Big)^2 \leq V_{\lambda,\ell}(x) \leq B_\infty e^{(2+\beta)x} - \lambda^{-2}\Big(\ell + \frac{1}{2}\Big)^2 \tag{21}$$

for $x \in (0, \infty)$ for some positive constants b_0, B_0, b_∞ and B_∞. In particular this implies that

$$V_{\lambda,\ell} \text{ is positive on } \Big(\frac{2\ln(\ell+1/2) - \ln b_0 - 2\ln\lambda}{2+\alpha}, \frac{2\ln(\ell+1/2) - \ln b_\infty - 2\ln\lambda}{2+\beta}\Big),$$

and initially this could be our guess for where to apply the LG approximation for large λ. However, we need to be a tiny bit more restrictive than this. To formalize this, we introduce a technical tool, η, with the properties that

η is a real-valued function on $\mathbb{R}_+$ satisfying $\eta(\lambda) \to \infty$ as $\lambda \to \infty$,
but so that this convergence might be arbitrarily slow.

We will take as the interval for our LG approximation $(x_1(\lambda), x_2(\lambda)) = (-\frac{\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{\ln\lambda}{2+\beta} - \eta(\lambda))$ on which $V_{\lambda,\ell}$ is clearly positive for sufficiently large λ if $\eta(\lambda)$ tends towards ∞ sufficiently slowly as $\lambda \to \infty$. As a first result we have:

Lemma 3.9 *For any $\ell \in \mathbb{N}_0$ there exists a family $\{\widetilde{\theta}(\lambda,\ell)\}_{\lambda>0}$ of constants so that*

$$g_{\lambda,\ell}(x) \propto V_{\lambda,\ell}(x)^{-1/4}\left[\cos\left(\lambda\int_{-\infty}^{x}[V_{\lambda,\ell}]_+^{1/2}\,dy + \widetilde{\theta}(\lambda,\ell)\right) + o_{\lambda\to\infty}(1)\right] \qquad (22)$$

for $x \in (-\frac{\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{\ln\lambda}{2+\beta} - \eta(\lambda))$. Here, $o_{\lambda\to\infty}(1)$ is uniform in x on this interval.

Proof. Note firstly that

$$V_{\lambda,\ell}(x) < 0 \quad \text{for} \quad x < \frac{2\ln(\ell+1/2) - \ln B_0 - 2\ln\lambda}{2+\alpha}$$

by (20) so that the integral in (22) is well-defined. Since, moreover, this integral differs from

$$\int_{-\frac{\ln\lambda}{2+\alpha}+\eta(\lambda)}^{x} V_{\lambda,\ell}(y)^{1/2}\,dy$$

only by a constant (in x), the result (22) follows from Proposition 3.8 if we manage to show that

$$\lambda^{-1}\int_{-\frac{\ln\lambda}{2+\alpha}+\eta(\lambda)}^{-\frac{\ln\lambda}{2+\beta}-\eta(\lambda)} V_{\lambda,\ell}^{-1/4}\left|\frac{d^2}{dx^2}\left(V_{\lambda,\ell}^{-1/4}\right)\right|dx$$

$$\lesssim \lambda^{-1}\int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{\frac{-2\ln\lambda}{2+\beta}-\eta(\lambda)} \frac{|V_{\lambda,\ell}'(x)|^2}{V_{\lambda,\ell}(x)^{5/2}} + \frac{|V_{\lambda,\ell}''(x)|}{V_{\lambda,\ell}(x)^{3/2}}\,dx$$

tends towards 0 as $\lambda \to \infty$. By 5) in Assumptions 2.1 we obtain straightforwardly

$$|V_{\lambda,\ell}'(x)|, |V_{\lambda,\ell}''(x)| \lesssim \begin{cases} e^{(2+\alpha)x} & \text{on } (-\infty,0) \\ e^{(2+\beta)x} & \text{on } (0,\infty) \end{cases}$$

which we can use to verify the described convergence. In particular, we see that

$$\lambda^{-1}\int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \frac{|V_{\lambda,\ell}'(x)|^2}{V_{\lambda,\ell}(x)^{5/2}}\,dx \lesssim \lambda^{-1}\int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \frac{e^{(4+2\alpha)x}}{\left[b_0 e^{(2+\alpha)x} - \lambda^{-2}\left(\ell+\frac{1}{2}\right)^2\right]^{5/2}}\,dx$$

$$= \lambda^{-1}\int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \left[b_0 e^{\frac{1}{5}(2+\alpha)x} - \lambda^{-2}\left(\ell+\frac{1}{2}\right)^2 e^{-\frac{4}{5}(2+\alpha)x}\right]^{-5/2}dx$$

$$= \left[\lambda^{-1}\frac{4\lambda^{-2}\left(\ell+\frac{1}{2}\right)^2 - 6b_0 e^{(2+\alpha)x}}{3(2+\alpha)b_0^2\left[b_0 e^{(2+\alpha)x} - \lambda^{-2}\left(\ell+\frac{1}{2}\right)^2\right]^{3/2}}\right]_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0}$$

$$= \left[\frac{4\left(\ell+\frac{1}{2}\right)^2 - 6b_0\lambda^2 e^{(2+\alpha)x}}{3(2+\alpha)b_0^2\left[b_0\lambda^2 e^{(2+\alpha)x} - \left(\ell+\frac{1}{2}\right)^2\right]^{3/2}}\right]_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \longrightarrow 0$$

as $\lambda \longrightarrow \infty$ by insertion of the limits, as well as

$$\lambda^{-1} \int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \frac{|V''_{\lambda,\ell}(x)|}{V_{\lambda,\ell}(x)^{3/2}}\,dx \lesssim \lambda^{-1} \int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \frac{e^{(2+\alpha)x}}{\left[b_0 e^{(2+\alpha)x} - \lambda^{-2}\left(\ell+\frac{1}{2}\right)^2\right]^{3/2}}\,dx$$
$$= \lambda^{-1} \int_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \left[b_0 e^{\frac{1}{3}(2+\alpha)x} - \lambda^{-2}\left(\ell+\frac{1}{2}\right)^2 e^{-\frac{2}{3}(2+\alpha)x}\right]^{-3/2} dx$$
$$= \left[-2\lambda^{-1} b_0^{-1}(2+\alpha)^{-1}\left[b_0 e^{(2+\alpha)x} - \lambda^{-2}\left(\ell+\frac{1}{2}\right)^2\right]^{-1/2}\right]_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0}$$
$$= \left[-2b_0^{-1}(2+\alpha)^{-1}\left[b_0\lambda^2 e^{(2+\alpha)x} - \left(\ell+\frac{1}{2}\right)^2\right]^{-1/2}\right]_{\frac{-2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{0} \longrightarrow 0.$$

Completely analogously we have

$$\lambda^{-1} \int_0^{\frac{-2\ln\lambda}{2+\beta}-\eta(\lambda)} \frac{|V'_{\lambda,\ell}(x)|^2}{V_{\lambda,\ell}(x)^{5/2}}\,dx \lesssim \left[\frac{4\left(\ell+\frac{1}{2}\right)^2 - 6b_\infty\lambda^2 e^{(2+\beta)x}}{3(2+\beta)b_\infty^2\left[b_\infty\lambda^2 e^{(2+\beta)x} - \left(\ell+\frac{1}{2}\right)^2\right]^{3/2}}\right]_0^{\frac{-2\ln\lambda}{2+\beta}-\eta(\lambda)}$$

and

$$\lambda^{-1} \int_0^{\frac{-2\ln\lambda}{2+\beta}-\eta(\lambda)} \frac{|V''_{\lambda,\ell}(x)|}{V_{\lambda,\ell}(x)^{3/2}}\,dx$$
$$\lesssim \left[-2b_\infty^{-1}(2+\beta)^{-1}\left[b_\infty\lambda^2 e^{(2+\beta)x} - \left(\ell+\frac{1}{2}\right)^2\right]^{-1/2}\right]_0^{\frac{-2\ln\lambda}{2+\beta}-\eta(\lambda)},$$

both of which tend towards 0 as $\lambda \longrightarrow \infty$. This finishes the proof. □

As a next step we wish to replace the potentials $V_{\lambda,\ell}$ with some λ-independent potentials in the expression (22). The factor $V_{\lambda,\ell}(x)^{-1/4}$ is rather easy to rewrite, and hence we focus for the moment our energy on replacing the integrand with some λ-independent expression. When doing so we naturally end up changing both the constant term inside the cosine and the error term, but this is not important. Knowledge about the result below in particular cases goes back to the early days of quantum mechanics (at least in the non-Langer-transformed set-up). In the very specific case of meromorphic potentials with $\alpha = 0$ or $\alpha = -1$ it is essentially Proposition 12 in [7] up to a change of variable.

Lemma 3.10 *The $\lambda \longrightarrow \infty$ asymptotics*

$$\lambda \int_{-\infty}^{x} e^y \Phi(e^y)^{1/2}\,dy - \lambda \int_{-\infty}^{x} [V_{\lambda,\ell}(y)]_+^{1/2}\,dy = \frac{(2\ell+1)\pi}{4+2\alpha} + o_{\lambda\to\infty}(1)$$

holds uniformly for $x \in (\frac{-2\ln\lambda}{2+\alpha} + \eta(\lambda), \frac{-2\ln\lambda}{2+\beta} - \eta(\lambda))$.

Proof. First off we observe that

$$
\begin{aligned}
|\lambda e^y \Phi(e^y)^{1/2} - \lambda V_{\lambda,\ell}(y)^{1/2}| &\leq \lambda^{-1}\Big(\ell + \frac{1}{2}\Big)^2 e^{-y}\Phi(e^y)^{-1/2} \\
&\lesssim \begin{cases} \lambda^{-1}\Big(\ell + \frac{1}{2}\Big)^2 e^{-\frac{2+\alpha}{2}y} & \text{on } (-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), 0) \\ \lambda^{-1}\Big(\ell + \frac{1}{2}\Big)^2 e^{-\frac{2+\beta}{2}y} & \text{on } (0, -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda)) \end{cases}
\end{aligned}
$$

and that a simple insertion of this in the integral yields

$$
\int_{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)}^{-\frac{2\ln\lambda}{2+\beta}-\eta(\lambda)} |\lambda e^y \Phi(e^y)^{1/2} - \lambda V_{\lambda,\ell}(y)^{1/2}|\, dy \longrightarrow 0
$$

as $\lambda \to \infty$ as long as $\eta(\lambda) \to \infty$ as $\lambda \to \infty$. Hence, we only need to prove

$$
\begin{aligned}
\lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} e^y \Phi(e^y)^{1/2}\, dy - \lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} [V_{\lambda,\ell}(y)]_+^{1/2}\, dy \\
= \frac{(2\ell+1)\pi}{4+2\alpha} + o_{\lambda\to\infty}(1)
\end{aligned} \tag{23}
$$

to have shown the full statement of the lemma. The idea is from this point to approximate $\Phi(e^y)$ by $C_0 e^{\alpha y}$ everywhere. For the first term in (23) this gives the error

$$
\begin{aligned}
&\lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} e^y |\Phi(e^y)^{1/2} - C_0^{1/2} e^{\frac{\alpha}{2}y}|\, dy \\
&\qquad = \lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} e^{(1+\frac{\alpha}{2})y} |e^{-\frac{\alpha}{2}y}\Phi(e^y)^{1/2} - C_0^{1/2}|\, dy \\
&\qquad \lesssim e^{(1+\frac{\alpha}{2})\eta(\lambda)} \sup_{y \leq -\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} |e^{-\frac{\alpha}{2}y}\Phi(e^y)^{1/2} - C_0^{1/2}| \longrightarrow 0
\end{aligned}
$$

if η tends towards ∞ sufficiently slowly. Next step is to try to replace $V_{\lambda,\ell}(y)$ by $C_0 e^{(2+\alpha)x} - \lambda^{-2}(\ell + 1/2)^2$ in the second term of (23). For this we use the general inequality

$$
\Big|[u]_+^{1/2} - [v]_+^{1/2}\Big| \leq |u - v|^{1/2}
$$

for real numbers u and v together with

$$
\Big|V_{\lambda,\ell}(y) + \lambda^{-2}\Big(\ell + \frac{1}{2}\Big)^2 - C_0 e^{(2+\alpha)y}\Big| = e^{(2+\alpha)y}|e^{-\alpha y}\Phi(e^y) - C_0|
$$

to conclude that

$$\int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} \Big|\lambda[V_{\lambda,\ell}(y)]_+^{1/2} - \lambda\Big[C_0 e^{(2+\alpha)y} - \lambda^{-2}\Big(\ell+\frac{1}{2}\Big)^2\Big]_+^{1/2}\Big|\,dy$$
$$\leq \lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} e^{(1+\frac{\alpha}{2})y} |e^{-\alpha y}\Phi(e^y) - C_0|^{1/2}\,dy$$
$$\lesssim e^{(1+\frac{\alpha}{2})\eta(\lambda)} \sup_{y \leq -\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} |e^{-\alpha y}\Phi(e^y) - C_0|^{1/2} \longrightarrow 0$$

as before. This means that we obtain

$$\lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} e^y \Phi(e^y)^{1/2}\,dy - \lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} [V_{\lambda,\ell}(y)]_+^{1/2}\,dy$$
$$= \lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} C_0^{1/2} e^{(1+\frac{\alpha}{2})y}\,dy - \lambda \int_{-\infty}^{-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda)} \Big[C_0 e^{(2+\alpha)y} - \lambda^{-2}\Big(\ell+\frac{1}{2}\Big)^2\Big]_+^{1/2}\,dy$$
$$+ o_{\lambda\to\infty}(1),$$

and an explicit calculation of the right hand side here is all there is left to do in order to prove the lemma. Here, the first term clearly equals

$$C_0^{1/2}\Big(1+\frac{\alpha}{2}\Big)^{-1} e^{(1+\frac{\alpha}{2})\eta(\lambda)} =: T_\lambda$$

which tends towards $+\infty$ as $\lambda \to \infty$, and the second term equals

$$\Big(T_\lambda^2 - \Big(1+\frac{\alpha}{2}\Big)^{-2}\Big(\ell+\frac{1}{2}\Big)^2\Big)^{1/2} - \frac{2\ell+1}{2+\alpha}\tan^{-1}\Big(\Big(\ell+\frac{1}{2}\Big)^{-1}\Big(\Big(1+\frac{\alpha}{2}\Big)^2 T_\lambda^2 - \Big(\ell+\frac{1}{2}\Big)^2\Big)^{1/2}\Big)$$
$$= \Big(T_\lambda + o_{\lambda\to\infty}(1)\Big) - \frac{2\ell+1}{2+\alpha}\Big(\frac{\pi}{2} + o_{\lambda\to\infty}(1)\Big).$$

Finally, subtracting these yields the claimed result. □

Collecting the pieces in the present subsection, we can now obtain the desired relation between $g_{\lambda,\ell}$ and the LG approximation.

Proposition 3.11 *For any $\ell \in \mathbb{N}_0$ there exists a family $\{\theta(\lambda,\ell)\}_{\lambda>0}$ of constants so that*

$$e^{x/2}\Phi(e^x)^{1/4} g_{\lambda,\ell}(x) \propto \cos\Big(\lambda \int_{-\infty}^{x} e^y \Phi(e^y)^{1/2}\,dy + \theta(\lambda,\ell)\Big) + o_{\lambda\to\infty}(1) \tag{24}$$

for $x \in (-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$. Here, $o_{\lambda\to\infty}(1)$ is uniform in x on this interval. In particular,

$$e^{\frac{2+\alpha}{4}x} g_{\lambda,\ell}(x) \propto \cos\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha} e^{(1+\frac{\alpha}{2})x} + \theta(\lambda,\ell)\Big) + o_{\lambda\to\infty}(1) \tag{25}$$

for $x \in (-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\alpha} + 2\eta(\lambda))$ *and*

$$e^{\frac{2+\beta}{4}x} g_{\lambda,\ell}(x) \propto \cos\Big(\int_0^\infty \Phi_\kappa(y)^{1/2}\,dy + \frac{2C_\infty^{1/2}\lambda}{2+\beta} e^{(1+\frac{\beta}{2})x} + \theta(\lambda,\ell)\Big) + o_{\lambda\to\infty}(1) \quad (26)$$

for $x \in (-\frac{2\ln\lambda}{2+\beta} - 2\eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$.

Proof. The asymptotics in (24) is basically a consequence of Lemmas 3.9 and 3.10 as soon as one realizes that

$$V_{\lambda,\ell}(x)^{-1/4} = e^{-x/2}\Phi(e^x)^{-1/4}\big(1 + o_{\lambda\to\infty}(1)\big)$$

uniformly on the interval. This can be seen for example by examining the last term in

$$\frac{V_{\lambda,\ell}(x)}{e^{2x}\Phi(e^x)} = 1 - \lambda^{-2}e^{-2x}\Phi(e^x)^{-1}\Big(\ell + \frac{1}{2}\Big)^2$$

for $x \in (-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$.

Similarly, we find that

$$V_{\lambda,\ell}(x)^{-1/4} = e^{-\frac{2+\alpha}{4}x}\big(C_0^{-1/4} + o_{\lambda\to\infty}(1)\big) \text{ and } V_{\lambda,\ell}(x)^{-1/4} = e^{-\frac{2+\beta}{4}x}\big(C_\infty^{-1/4} + o_{\lambda\to\infty}(1)\big)$$

uniformly on $(-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\alpha} + 2\eta(\lambda))$ and $(-\frac{2\ln\lambda}{2+\beta} - 2\eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$ respectively. For proving (25) and (26) it thus remains only to argue that

$$\lambda\int_{-\infty}^x e^y\Phi(e^y)^{1/2}\,dy = \frac{2C_0^{1/2}\lambda}{2+\alpha}e^{(1+\frac{\alpha}{2})x} + o_{\lambda\to\infty}(1) \quad (27)$$

and

$$\lambda\int_{-\infty}^x e^y\Phi(e^y)^{1/2}\,dy = \int_0^\infty \Phi_\kappa(y)^{1/2}\,dy + \frac{2C_\infty^{1/2}\lambda}{2+\beta}e^{(1+\frac{\beta}{2})x} + o_{\lambda\to\infty}(1) \quad (28)$$

uniformly for $x < 2\eta(\lambda) - 2\ln\lambda/(2+\alpha)$ and $x > -2\eta(\lambda) - 2\ln\lambda/(2+\beta)$ respectively. Since (27) was more or less proved during the proof of Lemma 3.10, we focus our attention on (28). On the interval of interest we have by the change of variables $y \to e^y$ the following estimates:

$$\begin{aligned}
&\Big|\int_0^\infty \Phi_\kappa(y)^{1/2}\,dy - \lambda\int_{-\infty}^x e^y\Phi(e^y)^{1/2}\,dy + \frac{2C_\infty^{1/2}\lambda}{2+\beta}e^{(1+\frac{\beta}{2})x}\Big| \\
&\quad = \Big|\lambda\int_x^\infty e^y\Phi(e^y)^{1/2}\,dy - \lambda\int_x^\infty C_\infty^{1/2}e^{(1+\frac{\beta}{2})y}\,dy\Big| \\
&\quad \le \lambda\int_x^\infty e^{(1+\frac{\beta}{2})y}|e^{-\frac{\beta}{2}y}\Phi(e^y)^{1/2} - C_\infty^{1/2}|\,dy \lesssim \lambda e^{(1+\frac{\beta}{2})x}\sup_{y\ge x}|e^{-\frac{\beta}{2}y}\Phi(e^y)^{1/2} - C_\infty^{1/2}| \\
&\quad \le e^{-(2+\beta)\eta(\lambda)} \sup_{y\ge -\frac{2\ln\lambda}{2+\beta} - 2\eta(\lambda)} |e^{-\frac{\beta}{2}y}\Phi(e^y)^{1/2} - C_\infty^{1/2}| \longrightarrow 0,
\end{aligned}$$

where the convergence holds as long as $\eta(\lambda)$ tends towards ∞ sufficiently slowly as $\lambda \to \infty$. This finishes the proof. □

3.5 Gluing together the solutions

From Proposition 3.11 we need to control the constants $\theta(\lambda,\ell)$ and continue $g_{\lambda,\ell}$ in an appropriate way further to the right where the LG-approximation no longer works. For both these tasks we use the asymptotic behaviour of Φ, firstly combined with Lemma 3.7.

Lemma 3.12 *Let $\{\theta(\lambda,\ell)\}_{\lambda>0}$ be families of constants so that (24), (25) and (26) hold true as in Proposition 3.11. Then these constants satisfy*

$$\theta(\lambda,\ell) \to -\frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4} \pmod{\pi}$$

as $\lambda \to \infty$.

Remark. Observe that combining (24) (+ its proof) with Lemmas 3.12 and 3.10 we learn, after a simple change of variables $x \to e^x$, the following: If U_λ is a solution to $U_\lambda'' = -\lambda^2 \Phi U_\lambda$ on $\mathbb{R}_+$, $U_\lambda(0) = 0$, then the large λ asymptotics

$$U_\lambda(x) \propto \Phi_\lambda^{\mathrm{LM}}(x)^{-1/4}\left[\cos\left(\lambda \int_0^x [\Phi_\lambda^{\mathrm{LM}}]_+^{1/2}\, dy - \frac{\pi}{4}\right) + o_{\lambda\to\infty}(1)\right]$$

holds for the *Langer modified potential* $\Phi_\lambda^{\mathrm{LM}}(x) = \Phi(x) - 4^{-1}\lambda^{-2}x^{-2}$ uniformly on $(\lambda^{\frac{-2}{2+\alpha}} e^{\eta(\lambda)}, \lambda^{\frac{-2}{2+\beta}} e^{-\eta(\lambda)})$. In particular, this approximation applies on any fixed interval (a,b). This is more or less what Langer suggested in [9] – but where Langer presents only a heuristic argument, we have here a rigorous statement and a full proof in the $\lambda \to \infty$ limit. While we here use the theory for $\ell = 0$, the corresponding statements for $\ell = 1, 2, \ldots$ are completely similar, replacing $\ell(\ell+1)$ by $(\ell+1/2)^2$ to produce a Langer modification of the potentials $\Phi - \ell(\ell+1)x^{-2}$. We can summarize these results in the slogan: After a Langer transformation of the equation, the constant term $-\pi/4$ in the cosine part of the LG approximation is universal.

Proof (of Lemma 3.12). The idea of the proof is to consider the regular solutions $h_{\lambda,\ell}$ to the equations $h_{\lambda,\ell}'' = [L^2 + W_\lambda] h_{\lambda,\ell}$ with $L = \ell + 1/2$ and $W_\lambda(x) = -\lambda^2 C_0 e^{(2+\alpha)x}$ and compare this to $g_{\lambda,\ell}$ on $(-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\alpha} + 2\eta(\lambda))$. By the help of Lemma 3.7 it will be possible to infer the needed asymptotics of $\theta(\lambda,\ell)$ from this comparison.

In the spirit of Lemma 3.7 we define thus the quantities

$$Q_\lambda(x) = \lambda^2 \int_{-\infty}^x e^{2y}\Phi(e^y)\, dy \quad \text{and} \quad \widetilde{Q}_\lambda(x) = C_0 \lambda^2 \int_{-\infty}^x e^{(2+\alpha)y}\, dy,$$

noticing that $Q_\lambda(x) \lesssim \widetilde{Q}_\lambda(x) \lesssim \lambda^2 e^{(2+\alpha)x}$ for $x < 0$, and

$$D_\lambda(x) = \lambda^2 \int_{-\infty}^x |e^{2y}\Phi(e^y) - C_0 e^{(2+\alpha)y}|\, dy.$$

Now the space of solutions to the equation that $h_{\lambda,\ell}$ solves is spanned by the real-valued functions

$$J_{\frac{2\ell+1}{2+\alpha}}\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha}e^{\frac{2+\alpha}{2}x}\Big) \qquad \text{and} \qquad Y_{\frac{2\ell+1}{2+\alpha}}\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha}e^{\frac{2+\alpha}{2}x}\Big),$$

and from the characterization of the regular solution from Proposition 3.4 together with the asymptotic behaviour of the Bessel function at the origin (cf. [1] p.360) one can conclude that

$$h_{\lambda,\ell}(x) = c(\ell,\alpha,C_0)\lambda^{-\frac{2\ell+1}{2+\alpha}} J_{\frac{2\ell+1}{2+\alpha}}\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha}e^{\frac{2+\alpha}{2}x}\Big). \tag{29}$$

with $c(\ell,\alpha,C_0)$ a constant independent of λ. Hence, when looking at $x \in (-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda), -\frac{2\ln\lambda}{2+\alpha}+2\eta(\lambda))$, we can use the asymptotics of the Bessel function at infinity (cf. [1] p.364) to see that

$$\lambda^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{\frac{2+\alpha}{4}x}h_{\lambda,\ell}(x) = \cos\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha}e^{\frac{2+\alpha}{2}x} - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}\Big) + o_{\lambda\to\infty}(1) \tag{30}$$

uniformly on this interval up to an overall constant independent of λ. Applying Lemma 3.7 we obtain also, for all $x < -\frac{2\ln\lambda}{2+\alpha}+2\eta(\lambda)$, the key inequalities

$$\begin{aligned}
\lambda^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{\frac{2+\alpha}{4}x}|g_{\lambda,\ell}(x)-h_{\lambda,\ell}(x)| &\lesssim \lambda^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{\frac{2+\alpha}{4}x}e^{(\ell+\frac{1}{2})x}D_\lambda(x)e^{c'(Q_\lambda(x)+\widetilde{Q}_\lambda(x))}\\
&\leq \exp\Big(\frac{4\ell+4+\alpha}{4+2\alpha}\ln\lambda + \frac{4\ell+4+\alpha}{4}x\Big)D_\lambda(x)e^{c''\widetilde{Q}_\lambda(x)}\\
&\leq e^{(2\ell+2+\frac{\alpha}{2})\eta(\lambda)}D_\lambda\Big(\frac{-2\ln\lambda}{2+\alpha}+2\eta(\lambda)\Big)e^{c''\widetilde{Q}_\lambda\left(\frac{-2\ln\lambda}{2+\alpha}+2\eta(\lambda)\right)}\\
&\leq e^{(2\ell+2+\frac{\alpha}{2})\eta(\lambda)}e^{c'''e^{2(2+\alpha)\eta(\lambda)}}D_\lambda\Big(\frac{-2\ln\lambda}{2+\alpha}+2\eta(\lambda)\Big)
\end{aligned}$$

for some ℓ-depending constants c', c'' and c''' where

$$\begin{aligned}
D_\lambda\Big(\frac{-2\ln\lambda}{2+\alpha}+2\eta(\lambda)\Big) &= \lambda^2\int_{-\infty}^{\frac{-2\ln\lambda}{2+\alpha}+2\eta(\lambda)} e^{(2+\alpha)y}|e^{-\alpha y}\Phi(e^y)-C_0|\,dy\\
&\lesssim e^{2(2+\alpha)\eta(\lambda)} \sup_{y\leq -\frac{2\ln\lambda}{2+\alpha}+2\eta(\lambda)} |e^{-\alpha y}\Phi(e^y)-C_0|.
\end{aligned}$$

If $\eta(\lambda)\to\infty$ sufficiently slowly for $\lambda\to\infty$ then this shows that

$$\lambda^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{\frac{2+\alpha}{4}x}|g_{\lambda,\ell}(x)-h_{\lambda,\ell}(x)| \longrightarrow 0 \tag{31}$$

uniformly on this interval. We conclude from this and the expression (30) for $h_{\lambda,\ell}$ that, up to an overall constant, (30) remains true when replacing $h_{\lambda,\ell}$ by $g_{\lambda,\ell}$. Comparing with (25),

$$\begin{aligned}
&\cos\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha}e^{(1+\frac{\alpha}{2})x}+\theta(\lambda,\ell)\Big)+o_{\lambda\to\infty}(1)\\
&\qquad\qquad \propto\ \cos\Big(\frac{2C_0^{1/2}\lambda}{2+\alpha}e^{(1+\frac{\alpha}{2})x} - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}\Big) + o_{\lambda\to\infty}(1)
\end{aligned}$$

for $x \in (-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\alpha} + 2\eta(\lambda))$ with uniform errors. Since $\lambda e^{(1+\frac{\alpha}{2})x}$ ranges over arbitrarily large values for x varying in this interval, it must be the case that the constant terms inside the cosines agree asymptotically modulo π, proving exactly the lemma. □

Combining the last part of Proposition 3.11, i.e. (26), and Lemma 3.12 we obtain directly:

Corollary 3.13 *For any $\ell \in \mathbb{N}_0$,*

$$e^{\frac{2+\beta}{4}x} g_{\lambda,\ell}(x) \propto \cos\left(\int_0^\infty \Phi_\kappa(y)^{1/2}\,dy + \frac{2C_\infty^{1/2}\lambda}{2+\beta} e^{(1+\frac{\beta}{2})x} - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}\right) + o_{\lambda\to\infty}(1)$$

for $x \in (-\frac{2\ln\lambda}{2+\beta} - 2\eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$. Here, $o_{\lambda\to\infty}(1)$ is uniform in x on this interval.

While the function $g_{\lambda,\ell}$ should approximately continue like a solution to the "asymptotic equations" $g''(x) = [(\ell+1/2)^2 - \lambda^2 C_\infty e^{(2+\beta)x}]g(x)$ after the LG approximation stops telling us anything useful, we cannot really apply techniques similar to those from Lemma 3.7 on this part of the real axis. This is because we do not control the boundary condition of $g_{\lambda,\ell}$ at plus infinity the way we did at minus infinity – there is no reason to believe that it should be "regular" near plus infinity in that sense. Instead, we will modify the potential Φ itself slightly to obtain modified $V_{\lambda,\ell}$'s for which we have complete knowledge about their behaviour on the interval in Corollary 3.13 and further to the right of this. The tricky part is to modify the potentials only so slightly so that the asymptotics in Corollary 3.13 remain valid even for the solutions to the corresponding modified equations (and so that other important features of the potentials do not change too much). The reward, on the other hand, is complete knowledge also about the solutions space to these modified equations from a certain point onwards since these will be the asymptotic equations described above, which are completely solvable.

More precisely, for each $\lambda > 0$ we let ζ_λ be a smooth function with values in $[0,1]$ and which is 1 on $(0, \kappa e^{-3\eta(\lambda)})$ and 0 on $(\kappa e^{-2\eta(\lambda)}, \infty)$ and additionally satisfies

$$\sup_{\mathbb{R}_+}|\zeta_\lambda'| \lesssim (\kappa e^{-2\eta(\lambda)} - \kappa e^{-3\eta(\lambda)})^{-1} \quad \text{and} \quad \sup_{\mathbb{R}_+}|\zeta_\lambda''| \lesssim (\kappa e^{-2\eta(\lambda)} - \kappa e^{-3\eta(\lambda)})^{-2}.$$

It is an easy check that such functions exist by scaling appropriately a fixed smooth function. Since $\zeta_\lambda' = \zeta_\lambda'' \equiv 0$ on $(\kappa e^{-2\eta(\lambda)}, \infty)$, the above uniform bounds on the derivatives imply

$$|\zeta_\lambda'(x)| \lesssim \frac{1}{x} \qquad \text{and} \qquad |\zeta_\lambda''(x)| \lesssim \frac{1}{x^2}. \tag{32}$$

We then use the ζ_λ's to define the modified potentials

$$\Psi_\lambda := \zeta_\lambda \Phi + (1-\zeta_\lambda)\Phi_\infty$$

for each $\lambda > 0$. Correspondingly, we put

$$\widetilde{V}_{\lambda,\ell}(x) := e^{2x}\Psi_\lambda(e^x) - \lambda^{-2}\Big(\ell + \frac{1}{2}\Big)^2$$

and let $\widetilde{g}_{\lambda,\ell}$ be the regular solutions to $\widetilde{g}_{\lambda,\ell} = -\lambda^2 \widetilde{V}_{\lambda,\ell}\widetilde{g}_{\lambda,\ell}$. Notice that we have $g_{\lambda,\ell}(x) = \widetilde{g}_{\lambda,\ell}(x)$ for $x < \ln\kappa - 3\eta(\lambda) = -\frac{2\ln\lambda}{2+\beta} - 3\eta(\lambda)$ by construction. A key feature of the $\widetilde{g}_{\lambda,\ell}$'s is that they behave almost as the $g_{\lambda,\ell}$'s even for slightly larger x-values.

Lemma 3.14 *The entire content of Corollary 3.13 remains true when $g_{\lambda,\ell}$ is replaced with $\widetilde{g}_{\lambda,\ell}$.*

Proof. We simply need to argue that we can carry out all the intermediate steps in the approximation leading to Corollary 3.13 when replacing Φ (for all $\lambda > 0$) with Ψ_λ and letting $\lambda \to \infty$.

The bounds (20) and (21) clearly hold also when replacing $V_{\lambda,\ell}$ by $\widetilde{V}_{\lambda,\ell}$, and thus the entire discussion preceding Lemma 3.9 remains valid in the modified case. Looking at the proof of Lemma 3.9 we see that the crucial part for having existence of a family $\{\widetilde{\theta}(\lambda,\ell)\}_{\lambda>0}$ of constants so that

$$\widetilde{g}_{\lambda,\ell}(x) \propto \widetilde{V}_{\lambda,\ell}(x)^{-1/4}\Big[\cos\Big(\lambda\int_{-\infty}^{x}[\widetilde{V}_{\lambda,\ell}]_+^{1/2}\,dy + \widetilde{\theta}(\lambda,\ell)\Big) + o_{\lambda\to\infty}(1)\Big] \tag{33}$$

for $x \in (-\frac{\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{\ln\lambda}{2+\beta} - \eta(\lambda))$ are the bounds

$$|\widetilde{V}'_{\lambda,\ell}(x)|, |\widetilde{V}''_{\lambda,\ell}(x)| \lesssim \begin{cases} e^{(2+\alpha)x} & \text{on } (-\infty,0) \\ e^{(2+\beta)x} & \text{on } (0,\infty). \end{cases}$$

Here the bound on $(-\infty,0)$ is as before. The bound on $(0,\infty)$ will follow from proving the equivalent of the second part of 5) in Assumptions 2.1 for the modified potentials Ψ_λ independently of $\lambda > 0$. Using (32) we get this from the simple computation

$$\begin{aligned}|\Psi'_\lambda| = |\zeta'_\lambda(\Phi - \Phi_\infty) + \zeta_\lambda\Phi' + (1-\zeta_\lambda)\Phi'_\infty| &\le \zeta'_\lambda(|\Phi| + |\Phi_\infty|) + \zeta_\lambda|\Phi'| + (1-\zeta_\lambda)|\Phi'_\infty| \\ &\lesssim x^{\beta-1},\end{aligned}$$

and completely similarly $|\Psi''_\lambda| = \cdots \lesssim x^{\beta-2}$ as needed. Hence, we have (33).

From here the proofs of Lemma 3.10 and Proposition 3.11 with only very slight modifications show that

$$e^{x/2}\Psi_\lambda(e^x)^{1/4}\widetilde{g}_{\lambda,\ell}(x) \propto \cos\Big(\lambda\int_{-\infty}^{x} e^y\Psi_\lambda(e^y)^{1/2}\,dy + \theta(\lambda,\ell)\Big) + o_{\lambda\to\infty}(1) \tag{34}$$

uniformly for $x \in (-\frac{2\ln\lambda}{2+\alpha} + \eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$ for some family of constants $\{\theta(\lambda,\ell)\}_{\lambda>0}$ (which is a priori not the same as in Proposition 3.11). To realize this simply recall that $g_{\lambda,\ell} = \widetilde{g}_{\lambda,\ell}$ on $(-\infty, -\frac{2\ln\lambda}{2+\beta} - 3\eta(\lambda))$ and every time one approximates $\Phi(x)$ with $\Phi_\infty(x)$ for large x, the approximation only gets better when replacing Φ by Ψ_λ for any $\lambda > 0$. In (34), the constants $\{\theta(\lambda,\ell)\}_{\lambda>0}$ must satisfy the convergence in Proposition 3.12 since essentially only (24) for $x \in (-\frac{2\ln\lambda}{2+\alpha}+\eta(\lambda), -\frac{2\ln\lambda}{2+\alpha}+2\eta(\lambda))$ is required in the proof hereof, and (24) reads exactly like (34) on this interval. Therefore, we get directly

$$e^{\frac{2+\beta}{4}x}\widetilde{g}_{\lambda,\ell}(x) \propto \cos\Big(\lambda\int_{-\infty}^{x} e^y \Psi_\lambda(e^y)^{1/2}\,dy - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}\Big) + o_{\lambda\to\infty}(1) \tag{35}$$

uniformly for $x \in (-\frac{2\ln\lambda}{2+\beta} - 2\eta(\lambda), -\frac{2\ln\lambda}{2+\beta} - \eta(\lambda))$. Finally, to arrive at the desired result, we need only to observe that, on this interval,

$$\begin{aligned}
\Big|\int_0^\infty \Phi_\kappa(y)^{1/2}\,dy - \lambda\int_{-\infty}^{x} e^y\Psi_\lambda(e^y)^{1/2}\,dy + \frac{2C_\infty^{1/2}\lambda}{2+\beta}e^{(1+\frac{\beta}{2})x}\Big|& \\
= \Big|\lambda\int_{-\infty}^{\infty} e^y\Phi(e^y)^{1/2}\,dy - \lambda\int_{-\infty}^{\infty} e^y\Psi_\lambda(e^y)^{1/2}\,dy\Big|& \\
\le \lambda\int_{-\infty}^{\infty} e^{(1+\frac{\beta}{2})y}|e^{-\frac{\beta}{2}x}\Phi(e^y)^{1/2} - e^{-\frac{\beta}{2}x}\Psi_\lambda(e^y)^{1/2}|\,dy& \\
\le \lambda\int_{-\frac{2\ln\lambda}{2+\beta}-3\eta(\lambda)}^{\infty} e^{(1+\frac{\beta}{2})y}|e^{-\frac{\beta}{2}x}\Phi(e^y)^{1/2} - C_\infty^{1/2}|\,dy& \\
\lesssim e^{-(3+\frac{3\beta}{2})\eta(\lambda)} \sup_{y\ge -\frac{2\ln\lambda}{2+\beta}-3\eta(\lambda)} |e^{-\frac{\beta}{2}y}\Phi(e^y)^{1/2} - C_\infty^{1/2}| \longrightarrow 0&
\end{aligned}$$

when $\eta(\lambda)\to\infty$ sufficiently slowly as $\lambda\to\infty$. □

We are now with the result from Lemma 3.14 in a position to prove our main result. The proof is split into two parts: Part 1 which formalizes more or less the discussion in Subsection 3.2, and Part 2 which takes care of a technical issue of bounding certain normalized regular solutions near the origin.

Proof of Theorem 2.4.
Part 1: Assume that $\kappa_n\to\infty$ and (12) as $n\to\infty$ and consider also the numbers $\lambda_n = \kappa_n^{-(2+\beta)/2}\to\infty$. We know from Proposition 3.3 that constructing $\phi_{n,\ell}$'s with the properties described here is all we need to do in order to prove the theorem. We take as our candidates for these functions $\phi_{n,\ell} := c_n\xi\widetilde{f}_{\kappa_n,\ell}$ where $\widetilde{f}_{\kappa,\ell}(x) := \sqrt{x}\,\widetilde{g}_{\lambda,\ell}(\ln\kappa + \ln x)$ and $c_n \neq 0$ are constants to be determined below. It is not difficult to realize that $\phi_{n,\ell} - c_n\xi f_{\kappa_n,\ell} \in D(H_{\kappa_n,\ell,\min}) \subseteq D(H_{\kappa_n,\ell})$ since these functions are in $C^2(\mathbb{R}_+)$ and have compact support in $\mathbb{R}_+$. Consequently, Lemma 3.6 tells us that $\phi_{n,\ell}\in D(H_{\kappa_n,\ell})$, and moreover that

$$H_{\kappa_n,\ell}\phi_{n,\ell}(x) = 0 \qquad \text{for} \quad x < e^{-3\eta(\lambda_n)} \tag{36}$$

since $\phi_{n,\ell} = c_n f_{\kappa_n,\ell}$ on this interval. We now proceed to verify the two convergences in the statement in Proposition 3.3 for our choice of $\phi_{n,\ell}$'s.

For the first convergence we take a closer look at the $\widetilde{g}_{\lambda_n,\ell}$'s on the intervals $(-\frac{2\ln\lambda_n}{2+\beta} - 2\eta(\lambda_n), \infty)$. As they solve the equations $\widetilde{g}''_{\lambda_n,\ell}(x) = [(\ell+1/2)^2 - \lambda_n^2 C_\infty e^{(2+\beta)x}]\widetilde{g}_{\lambda_n,\ell}(x)$ here and are real-valued, they must be on the form

$$\widetilde{g}_{\lambda_n,\ell}(x) = \frac{1}{c_n}\left[\cos\theta_{n,\ell}\cdot J_{\frac{2\ell+1}{2+\beta}}\left(\frac{-2C_\infty^{1/2}\lambda_n}{2+\beta}e^{\frac{2+\beta}{2}x}\right) + \sin\theta_{n,\ell}\cdot Y_{\frac{2\ell+1}{2+\beta}}\left(\frac{-2C_\infty^{1/2}\lambda_n}{2+\beta}e^{\frac{2+\beta}{2}x}\right)\right]$$

for some numbers $\theta_{n,\ell}$ which are fixed modulo 2π and some real $c_n \neq 0$. These are the c_n's we use to define our $\phi_{n,\ell}$'s. In particular this means that

$$\phi_{n,\ell} = \xi(\cos\theta_{n,\ell} F_{\beta,C_\infty,\ell} + \sin\theta_{n,\ell} G_{\beta,C_\infty,\ell}) \tag{37}$$

on $(e^{-2\eta(\lambda_n)}, \infty)$. Thus, it will prove the first convergence in the statement[9] of Proposition 3.3 if we manage to show that

$$\theta_{n,\ell} \longrightarrow \theta - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{(2\ell+1)\pi}{4+2\beta} - \frac{\pi}{2} =: \theta_\ell \pmod{\pi} \quad \textit{as} \quad n\to\infty \tag{38}$$

and

$$\textit{for each } \ell\in\mathbb{N}_0,\ \phi_{n,\ell} \textit{ tends uniformly towards } 0 \textit{ on } (0, e^{-2\eta(\lambda_n)}). \tag{39}$$

For the former we notice that on $(e^{-2\eta(\lambda_n)}, e^{-\eta(\lambda_n)})$ we have on the one hand, by (37) and the asymptotics of the Bessel-functions (cf. [1] p.364),

$$x^{\beta/4}\phi_{n,\ell}(x) \propto \cos\left(\theta_{n,\ell} + \frac{2C_\infty^{1/2}}{2+\beta}x^{\frac{2+\beta}{2}} + \frac{(2\ell+1)\pi}{4+2\beta} + \frac{\pi}{4}\right) + o_{n\to\infty}(1)$$

uniformly on the interval. On the other hand, by the definition of $\phi_{n,\ell}$ and Lemma 3.14 we have, also uniformly,

$$\begin{aligned} x^{\beta/4}\phi_{n,\ell}(x) &\propto \cos\left(\int_0^\infty \Phi_{\kappa_n}^{1/2}\,dy + \frac{2C_\infty^{1/2}}{2+\beta}x^{\frac{2+\beta}{2}} - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}\right) + o_{n\to\infty}(1) \\ &\propto \cos\left(\theta + \frac{2C_\infty^{1/2}}{2+\beta}x^{\frac{2+\beta}{2}} - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}\right) + o_{n\to\infty}(1), \end{aligned}$$

and, as $x^{\frac{2+\beta}{2}}$ ranges over arbitrarily large values for $x\in(e^{-2\eta(\lambda_n)}, e^{-\eta(\lambda_n)})$, we conclude that

$$\theta_{n,\ell} + \frac{(2\ell+1)\pi}{4+2\beta} + \frac{\pi}{4} \longrightarrow \theta - \frac{(2\ell+1)\pi}{4+2\alpha} - \frac{\pi}{4}$$

modulo π from which (38) follows. The property (39) is proved below in Part 2 of the proof.

In order to verify the second convergence in the statement of Proposition 3.3 notice that this amounts to proving

$$\int_0^\infty |H_{\kappa_n,\ell}\phi_{n,\ell} - H_{\infty,\ell,\theta_\ell}(\xi(\cos\theta_\ell F_{\beta,C_\infty,\ell} + \sin\theta_\ell G_{\beta,C_\infty,\ell}))|^2\,dx \longrightarrow 0$$

[9] By possibly multiplying some of the $\phi_{n,\ell}$'s by -1. This does not affect the remaining part of the proof.

as $n \to \infty$. On $(0, e^{-3\eta(\lambda_n)})$ and $(2,\infty)$ the integrand is 0 by (36) and the definition of ξ so we need not worry about these parts of $\mathbb{R}_+$. Further, on $(1,2)$ we get by (38) uniform convergence of $(\cos\theta_{n,\ell}F_{\beta,C_\infty,\ell} - \sin\theta_{n,\ell}G_{\beta,C_\infty,\ell})^{(p)}$ towards $(\cos\theta_\ell F_{\beta,C_\infty,\ell} - \sin\theta_\ell G_{\beta,C_\infty,\ell})^{(p)}$ for $p = 0,1,2$, and – together with the uniform convergence of Φ_{κ_n} towards Φ_∞ on this interval – this rather straightforwardly takes care of the L^2-convergence here. We are thus left with the task of estimating

$$\begin{aligned}
&\int_{e^{-3\eta(\lambda_n)}}^1 |H_{\kappa_n,\ell}\phi_{n,\ell} - H_{\infty,\ell,\theta_\ell}(\xi(\cos\theta_\ell F_{\beta,C_\infty,\ell} + \sin\theta_\ell G_{\beta,C_\infty,\ell}))|^2\,dx \\
&\qquad = \int_{e^{-3\eta(\lambda_n)}}^1 |H_{\kappa_n,\ell}\phi_{n,\ell}|^2\,dx \le \int_{e^{-3\eta(\lambda_n)}}^1 |\phi_{n,\ell}|^2 \cdot |\Phi_{\kappa_n} - \Phi_\infty|^2\,dx \\
&\qquad \lesssim \int_{e^{-3\eta(\lambda_n)}}^\infty |\Phi_{\kappa_n} - \Phi_\infty|^2\,dx = \kappa_n^{-2\beta}\int_{e^{-3\eta(\lambda_n)}}^\infty |\Phi(\kappa_n x) - C_\infty(\kappa_n x)^\beta|^2\,dx \\
&\qquad = \kappa_n^{-2\beta-1}\int_{\kappa_n e^{-3\eta(\lambda_n)}}^\infty |\Phi(x) - C_\infty x^\beta|^2\,dx \\
&\qquad = \kappa_n^{-2\beta-1}\int_{\kappa_n e^{-3\eta(\lambda_n)}}^\infty x^{2\beta}|x^{-\beta}\Phi(x) - C_\infty|^2\,dx \\
&\qquad \le e^{-3(2\beta+1)\eta(\lambda_n)} \sup_{x \ge \kappa_n e^{-3\eta(\lambda_n)}} |x^{-\beta}\Phi(x) - C_\infty|^2 \longrightarrow 0
\end{aligned}$$

as long as $\eta(\lambda_n) \to \infty$ sufficiently slowly as $n \to \infty$, where we have used (39) along the way. This proves the second convergence in the statement in Proposition 3.3 and thus proves the main theorem – up to proving the property (39).

<u>Part 2:</u> We now focus on proving (39). Firstly note that for $x < e^{-2\eta(\lambda_n)}$ we have

$$\phi_{n,\ell}(x) = c_n\widetilde{f}_{\kappa_n,\ell}(x) = c_n\sqrt{x}\widetilde{g}_{\lambda_n,\ell}(\ln\kappa_n + \ln x) = c_n\kappa_n^{-1/2}e^{\frac{\ln\kappa_n + \ln x}{2}}\widetilde{g}_{\lambda_n,\ell}(\ln\kappa_n + \ln x)$$

so that proving (39) actually amounts to arguing that $c_n\kappa_n^{-1/2}e^{x/2}\widetilde{g}_{\lambda_n,\ell}(x)$ converges uniformly towards 0 on $(-\infty, \ln\kappa_n - 2\eta(\lambda_n)) = (-\infty, \frac{-2\ln\lambda_n}{2+\beta} - 2\eta(\lambda_n))$. We denote this property by (39)'.

Now in order to prove (39)' we observe that on $(-\frac{2\ln\lambda_n}{2+\beta} - 2\eta(\lambda_n), -\frac{2\ln\lambda_n}{2+\beta} - \eta(\lambda_n))$, by the definition of c_n and the asymptotics of the Bessel functions,

$$c_n\lambda_n^{1/2}e^{\frac{2+\beta}{4}x}\widetilde{g}_{\lambda_n,\ell}(x) = \cos\left(\theta_{n,\ell} + \frac{2C_\infty^{1/2}\lambda_n}{2+\beta}e^{\frac{2+\beta}{2}x} + \frac{(2\ell+1)\pi}{4+2\beta} + \frac{\pi}{4}\right) + o_{n\to\infty}(1)$$

up to a constant independent of n. Since $e^{\frac{2+\beta}{4}x} = e^{x/2}\Psi_\lambda(e^x)^{1/4}$ on this interval (where, as usual, $\lambda_n e^{\frac{2+\beta}{2}x}$ ranges over arbitrarily large values), (34) tells us that

$$c_n\lambda_n^{1/2}e^{x/2}\Psi_{\lambda_n}(e^x)^{1/4}\widetilde{g}_{\lambda_n,\ell}(x) = \cos\left(\lambda\int_{-\infty}^x e^y\Psi_{\lambda_n}(e^y)^{1/2}\,dy + \theta(n,\ell)\right) + o_{n\to\infty}(1)$$

up to a constant independent of n for some sequence $\{\theta(n,\ell)\}_{n=0}^{\infty}$ of constants everything uniformly on the (larger) interval $(\frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n), \frac{-2\ln\lambda_n}{2+\beta}-\eta(\lambda_n))$. In particular, on this larger interval,

$$|c_n|\kappa_n^{-1/2}e^{x/2}|\widetilde{g}_{\lambda_n,\ell}(x)| \lesssim \kappa_n^{-1/2}\lambda_n^{-1/2}\Psi_{\lambda_n}(e^x)^{-1/4} \lesssim \kappa_n^{\beta/4}\cdot\max\{e^{-\frac{\alpha}{4}x}, e^{-\frac{\beta}{4}x}\}$$
$$\leq \max\{\lambda_n^{\gamma}, e^{\frac{\beta}{4}\eta(\lambda_n)}\} \longrightarrow 0,$$

where "$\lesssim$" means less than up to a constant independent of n, and

$$\gamma := \frac{\alpha}{2\alpha+4} - \frac{\beta}{2\beta+4} < 0.$$

Thus, we need now only to prove (39)' on the remaining part of the interval, i.e. on $(-\infty, \frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n))$.

For this we need some refined knowledge about the constant c_n. To obtain this we note that on this interval $\widetilde{g}_{\lambda_n,\ell} = g_{\lambda_n,\ell}$ and focus our attention on the interval $(\frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n), \frac{-2\ln\lambda_n}{2+\alpha}+2\eta(\lambda_n))$ for the moment. Here, we have basically just argued that

$$|c_n|\kappa_n^{-1/2}e^{\frac{2+\alpha}{4}x}|g_{\lambda_n,\ell}(x)| \lesssim |c_n|\kappa_n^{-1/2}e^{x/2}\Phi(e^x)^{1/4}|\widetilde{g}_{\lambda_n,\ell}(x)| \lesssim \kappa_n^{-1/2}\lambda_n^{-1/2} = \kappa_n^{\beta/4},$$

but on the other hand (30) and (31) show that the function $\lambda_n^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{\frac{2+\alpha}{4}x}|g_{\lambda_n,\ell}(x)|$ does not converge towards 0 on this interval. We can thus conclude that we have $|c_n|\kappa_n^{-1/2} \lesssim \kappa_n^{\beta/4}\lambda_n^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}$, and consequently that

$$\begin{aligned}|c_n|\kappa_n^{-1/2}&e^{x/2}|g_{\lambda_n,\ell}(x)| \\ &\lesssim \kappa_n^{\beta/4}\lambda_n^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{x/2}|h_{\lambda_n,\ell}(x)| + \kappa_n^{\beta/4}\lambda_n^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{x/2}|g_{\lambda_n,\ell}(x)-h_{\lambda_n,\ell}(x)|\end{aligned} \tag{40}$$

uniformly on all of $(-\infty, \frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n))$ where $h_{\lambda_n,\ell}$ is as in the proof of Lemma 3.12. Here, the first term on the right hand side is (cf. (29))

$$\kappa^{\beta/4}e^{-\frac{\alpha}{4}x}c(\ell,\alpha,C_0)\lambda_n^{1/2}e^{\frac{2+\alpha}{4}x}\left|J_{\frac{2\ell+1}{2+\alpha}}\left(\frac{2C_0^{1/2}\lambda_n}{2+\alpha}e^{\frac{2+\alpha}{2}x}\right)\right| \tag{41}$$

which we claim tends uniformly towards 0 on $(-\infty, \frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n))$. Indeed, to realize that this is the case on $(\frac{-2\ln\lambda_n}{2+\alpha}, \frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n))$ we can use the facts that $\kappa_n^{\beta/4}e^{-\frac{\alpha}{4}x} \leq \max\{\lambda_n^{\gamma}, \kappa_n^{\beta/4}\} \to 0$ here and that $y \mapsto \sqrt{y}J_\nu(y)$ is uniformly bounded on $\mathbb{R}_+$ for $\nu > 0$. On $(-\infty, \frac{-2\ln\lambda_n}{2+\alpha})$ we see that the expression inside the Bessel function is bounded and hence so is the Bessel function part of (41). Noticing that $\kappa^{\beta/4}\lambda_n^{1/2} = \kappa_n^{-1/2} \to 0$ it follows easily that all of (41) tends towards 0 uniformly here as well. Finally, we claim that also the last term on the right hand side in (40) tends uniformly towards 0 on $(-\infty, \frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n))$.

On $(\frac{-2\ln\lambda_n}{2+\alpha}, \frac{-2\ln\lambda_n}{2+\alpha}+\eta(\lambda_n))$ we can as before use the fact that $\kappa^{\beta/4}e^{-\frac{\alpha}{4}x}\to 0$ uniformly and (31) to realize that this is the case here. On $(-\infty, \frac{-2\ln\lambda_n}{2+\alpha})$ we need some calculations using the notation from the proof of Lemma 3.12: It is an easy check that here Q_{λ_n} and $\widetilde{Q}_{\lambda_n}$ (and hence D_{λ_n}) are uniformly bounded as functions of x and n. Thus, we get – similarly to in the proof of Lemma 3.12 – the inequalities

$$\begin{aligned}\kappa_n^{\beta/4}\lambda_n^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{x/2}|g_{\lambda_n,\ell}(x)-h_{\lambda_n,\ell}(x)| &\lesssim \kappa_n^{\beta/4}\lambda_n^{\frac{2\ell+1}{2+\alpha}+\frac{1}{2}}e^{(\ell+1)x}\\ &\le \lambda_n^{-\frac{\beta}{2\beta+4}+\frac{2\ell+1}{2+\alpha}+\frac{1}{2}-\frac{2\ell+2}{2+\alpha}} = \lambda_n^{\gamma}\longrightarrow 0\end{aligned}$$

here. Combining these uniform convergences with the bound (40) we have managed to prove (39)', finishing the proof. □

4 A negative result

We argue in this section that one cannot generally strengthen the convergence of the operators in the "if"-part of the result in Theorem 2.5 to be in the norm resolvent sense. Recall that norm resolvent convergence of a sequence $\{A_n\}_{n=1}^{\infty}$ of self-adjoint operators towards A simply means norm convergence of the resolvent operators $(A_n-i)^{-1}\to(A-i)^{-1}$ or, equivalently, that $h(A_n)\to h(A)$ in norm for any continuous function h on $\mathbb{R}$ that tends towards 0 at $\pm\infty$.

More precisely, we will prove that the conditions $Z_n\to\infty$ and (13) are not sufficient to conclude that $H_{Z_n}^{\mathrm{TF}}$ is convergent in this stronger sense. For this we use the natural notational convention of adding "TF" to any of the operators in Section 2 to indicate that it is defined by the Thomas-Fermi potential Φ_1^{TF} (or $\Phi_\infty^{\mathrm{TF}}$). Firstly, we need some intermediate results.

Lemma 4.1 *Consider the set-up from Section 2. Then the following is true:*

a) For each $\mu<0$ and $\ell\in\mathbb{N}_0$ there exists a $\theta(\ell,\mu)\in[0,\pi)$ so that μ is an eigenvalue for $H_{\infty,\ell,\theta(\ell,\mu)}^{\mathrm{TF}}$,

b) If $H_{Z_n}^{\mathrm{TF}}\to H_{\infty,\{\theta_\ell\}_{\ell=1}^{\infty}}^{\mathrm{TF}}$ in the strong resolvent sense as $n\to\infty$ for some sequences $\{Z_n\}_{n=1}^{\infty}\subseteq\mathbb{R}_+$ and $\{\theta_\ell\}_{\ell=0}^{\infty}\subseteq[0,\pi)$ then also $H_{Z_n,\ell}^{\mathrm{TF}}\to H_{\infty,\ell,\theta_\ell}^{\mathrm{TF}}$ in the strong resolvent sense as $n\to\infty$ for all $\ell\in\mathbb{N}_0$,

c) There exist sequences $\{Z_\ell\}_{\ell=1}^{\infty}\subseteq\mathbb{N}$ and $\{\mu_\ell\}_{\ell=1}^{\infty}\subseteq(-\infty,0)$ so that $\mu_\ell\in\sigma(H_{Z_\ell,\ell}^{\mathrm{TF}})$ for each $\ell=1,2,3,\ldots$ and so that $Z_\ell\to\infty$ and $\mu_\ell\to-1$ as $\ell\to\infty$.

Proof. *a*) For this part we claim that it suffices to find a real-valued solution $f\in L^2(\mathbb{R}_+)$ to the equation

$$-f''(x)+\Big[\frac{\ell(\ell+1)}{x^2}-\Phi_\infty^{\mathrm{TF}}(x)\Big]f(x)=\mu f(x). \tag{42}$$

To see this we recall the fundamental structure of the extensions of $H^{\mathrm{TF}}_{\infty,\ell,\min}$ which relies on the fact that we are (cf. Section 2) in the limit circle case. For the details see Appendix A in [3]. One has

$$\begin{aligned}\{\phi \in L^2(\mathbb{R}_+) | -\phi'' + [\ell(\ell+1)x^{-2} - \Phi^{\mathrm{TF}}_\infty]\phi \in L^2(\mathbb{R}_+)\} &= D((H^{\mathrm{TF}}_{\infty,\ell,\min})^*) \\ &= D(H^{\mathrm{TF}}_{\infty,\ell,\min}) \oplus \mathbb{C}\xi f_1 \oplus \mathbb{C}\xi f_2\end{aligned} \tag{43}$$

with f_1 and f_2 two linearly independent solutions to the equation $f'' = [\ell(\ell+1)x^{-2} - \Phi^{\mathrm{TF}}_\infty]f$. We observe that clearly a solution $f \in L^2(\mathbb{R}_+)$ to (42) will be in the domain (43), and consequently it must be in $D(H^{\mathrm{TF}}_{\infty,\ell,\min}) \oplus \mathbb{C}\xi\widetilde{f}$ for some real-valued[10] solution $\widetilde{f}$ to $\widetilde{f}'' = [\ell(\ell+1)x^{-2} - \Phi^{\mathrm{TF}}_\infty]\widetilde{f}$. But any domain on this form is the domain of one of the self-adjoint extensions $H^{\mathrm{TF}}_{\infty,\ell,\theta_\ell}$ of $H^{\mathrm{TF}}_{\infty,\ell,\min}$ from Section 2. Thus, the assertion follows from (42).

Now to find a real-valued $f \in L^2(\mathbb{R}_+)$ solving (42) we apply Proposition 3.4 with $L = \sqrt{-\mu}$ and $W(x) = \ell(\ell+1)x^{-2} - \Phi^{\mathrm{TF}}_\infty(-x)$ to get a solution g to

$$g''(x) = \Big[-\mu + \frac{\ell(\ell+1)}{x^2} - \Phi^{\mathrm{TF}}_\infty(-x)\Big]g(x)$$

with $e^{-\sqrt{-\mu}x}g(x) \to 1$ as $x \to -\infty$. Considering $f(x) := g(-x)$ we get in this way a real-valued solution to (42) satisfying $f \in L^2((1,\infty))$. Moreover, it is a general consequence (cf. [15] Theorem X.6) of being in the limit circle case that all solutions f to (42) for ***any*** $\mu \in \mathbb{C}$ are L^2 near the origin, say on $(0,1)$. Hence, we have found the desired f.

b) This is simply an exercise in digesting the definitions of the operators in Section 2. It is easily verified that

$$(H^{\mathrm{TF}}_{Z_n,\ell} + i)^{-1}\phi \otimes Y^0_\ell = (\widetilde{H}^{\mathrm{TF}}_{Z_n} + i)^{-1}(\phi \otimes Y^0_\ell)$$

for any $\phi \in L^2(\mathbb{R}_+)$, and similarly for the operators defining infinite atoms. Consequently, if $H^{\mathrm{TF}}_{Z_n} \to H^{\mathrm{TF}}_{\infty,\{\theta_\ell\}^\infty_{\ell=1}}$ in the strong resolvent sense (and since we have chosen the spherical harmonics to be normalized in $L^2(S^2)$),

$$\begin{aligned}&\|(H^{\mathrm{TF}}_{Z_n,\ell} + i)^{-1}\phi - (H^{\mathrm{TF}}_{\infty,\ell,\theta_\ell} + i)^{-1}\phi\| \\ &\qquad = \|(\widetilde{H}^{\mathrm{TF}}_{Z_n} + i)^{-1}(\phi \otimes Y^0_\ell) - (\widetilde{H}^{\mathrm{TF}}_{\infty,\{\theta_\ell\}^\infty_{\ell=0}} + i)^{-1}(\phi \otimes Y^0_\ell)\| \longrightarrow 0\end{aligned}$$

as $n \to \infty$ for any $\phi \in L^2(\mathbb{R}_+)$. This proves the claimed strong resolvent convergence.

c) We will now combine the results from (*a*) and (*b*), and will prove by induction that there exist natural numbers $Z_1 < Z_2 < Z_3 < \cdots$ so that

$$\text{there exists } \mu_\ell \in \sigma(H^{\mathrm{TF}}_{Z_\ell,\ell}) \text{ so that } |\mu_\ell + 1| < \ell^{-1} \tag{44}$$

[10] The fact that $\widetilde{f}$ must be real-valued relies crucially on the facts that f itself is real-valued and that the operator commutes with complex conjugation.

for all ℓ. To this end we fix ℓ and show that we can have (44) for arbitrarily large Z_ℓ's.

Choose θ'_ℓ so that

$$\theta'_\ell + \frac{\ell\pi}{2} + \frac{\pi}{4} = \theta(\ell,-1) \tag{45}$$

modulo π where $\theta(\ell,-1)$ is the number from (a). Then choose $Z_{\ell,n}$ to be the number from the right-hand side of (14) with $\theta = \theta'_\ell$ for each $n = 1,2,\ldots$ so that in particular $Z_{\ell,n} \to \infty$ as $n \to \infty$. From Theorem 2.5 we learn that then $H^{\mathrm{TF}}_{Z_{\ell,n}} \to H^{\mathrm{TF}}_{\infty,\{\theta_m\}_{m=0}^\infty}$ in the strong resolvent sense as $n \to \infty$ with $\{\theta_m\}_{m=0}^\infty$ defined by

$$\theta_m = \theta'_\ell + \frac{m\pi}{2} + \frac{\pi}{4}.$$

Thus, by (b) and (45), $H^{\mathrm{TF}}_{Z_{\ell,n},\ell} \to H^{\mathrm{TF}}_{\infty,\ell,\theta(\ell,-1)}$ in the strong resolvent sense as $n \to \infty$. Moreover, since $-1 \in \sigma(H^{\mathrm{TF}}_{\infty,\ell,\theta(\ell,-1)})$, we find by the general concept of spectral exclusion under strong resolvent convergence (cf. [14] Theorem VIII.24) that there are numbers $\mu_{\ell,n} \in \sigma(H^{\mathrm{TF}}_{Z_{\ell,n},\ell}) \subseteq \mathbb{R}$ so that $\mu_{\ell,n} \to -1$ as $n \to \infty$. Now choosing n_0 sufficiently large we can achieve both $Z_{\ell,n_0} > Z_{\ell-1}$ and $|\mu_{\ell,n_0} + 1| < \ell^{-1}$, and by setting $Z_\ell := Z_{\ell,n_0}$ and $\mu_\ell := \mu_{\ell,n_0}$ we complete the proof. □

Lemma 4.2 *Let $\{Z_\ell\}_{\ell=1}^\infty$ and $\{\mu_\ell\}_{\ell=1}^\infty$ be sequences as in Lemma 4.1(c). For each $\ell = 1,2,3,\ldots$ the number μ_ℓ is an eigenvalue of $\widetilde{H}^{\mathrm{TF}}_{Z_\ell}$, and there exists a non-zero eigenvector*

$$\phi_\ell \in D(\widetilde{H}^{\mathrm{TF}}_{Z_\ell}) \cap [L^2(\mathbb{R}_+) \otimes \operatorname{span} Y^0_\ell] =: D(\widetilde{H}^{\mathrm{TF}}_{Z_\ell}) \cap \mathcal{V}_\ell$$

so that $\widetilde{H}^{\mathrm{TF}}_{Z_\ell}\phi_\ell = \mu_\ell\phi_\ell$.

Proof. We recall firstly that since $H^{\mathrm{TF}}_{Z_\ell}$ is the closure of $-\Delta - \Phi^{\mathrm{TF}}_{Z_\ell}$ on $C_0^\infty(\mathbb{R}^3)$ by Proposition 2.3(a) and $\Phi^{\mathrm{TF}}_{Z_\ell} \in L^2(\mathbb{R}^3)$ it is a standard consequence of Weyl's Theorem that $\sigma_{\mathrm{ess}}(\widetilde{H}^{\mathrm{TF}}_{Z_\ell}) = \sigma_{\mathrm{ess}}(H^{\mathrm{TF}}_{Z_\ell}) = [0,\infty)$.

Fix ℓ. As $\mu_\ell \in \sigma(H^{\mathrm{TF}}_{Z_\ell,\ell})$ there exists a sequence $\{\psi_{\ell,n}\}_{n=1}^\infty \subseteq D(H^{\mathrm{TF}}_{Z_\ell,\ell})$ so that $\|\psi_{\ell,n}\| = 1$ and $\|H^{\mathrm{TF}}_{Z_\ell,\ell}\psi_{\ell,n} - \mu_\ell\psi_{\ell,n}\| \longrightarrow 0$ as $n \to \infty$. Letting

$$\{\phi_{\ell,n}\}_{n=1}^\infty := \left\{\psi_{\ell,n} \otimes Y^0_\ell\right\}_{n=1}^\infty \subseteq D(H^{\mathrm{TF}}_{Z_\ell,\ell}) \otimes \operatorname{span} Y^0_\ell \subseteq D(\widetilde{H}^{\mathrm{TF}}_{Z_\ell}) \cap \mathcal{V}_\ell,$$

we find straightforwardly that $\|\phi_{\ell,n}\| = 1$ (since we take $\|Y^0_\ell\| = 1$) and

$$\|\widetilde{H}^{\mathrm{TF}}_{Z_\ell}\phi_{\ell,n} - \mu_\ell\phi_{\ell,n}\| = \|H^{\mathrm{TF}}_{Z_\ell,\ell}\psi_{\ell,n} - \mu_\ell\psi_{\ell,n}\| \longrightarrow 0 \tag{46}$$

as $n \to \infty$. By taking a subsequence (still denoted $\{\phi_{\ell,n}\}_{n=1}^\infty$) we can assume that the $\phi_{\ell,n}$'s converge towards some ϕ_ℓ weakly in $L^2(\mathbb{R}_+) \otimes \operatorname{span} Y^0_\ell$ as $n \to \infty$.

Now this ϕ_ℓ cannot be 0 as then we would have $\mu_\ell \in \sigma_{\text{ess}}(\widetilde{H}_{Z_\ell}^{\text{TF}}) \cap (-\infty, 0) = \emptyset$. Moreover, this weak convergence together with (46) yields

$$\langle \phi_\ell, \widetilde{H}_{Z_\ell}^{\text{TF}} \phi \rangle = \lim_{n\to\infty} \langle \phi_{\ell,n}, \widetilde{H}_{Z_\ell}^{\text{TF}} \phi \rangle = \lim_{n\to\infty} \langle \widetilde{H}_{Z_\ell}^{\text{TF}} \phi_{\ell,n}, \phi \rangle = \langle \mu_\ell \phi_\ell, \phi \rangle$$

for any $\phi \in D(\widetilde{H}_{Z_\ell}^{\text{TF}})$ proving $\phi_\ell \in D((\widetilde{H}_{Z_\ell}^{\text{TF}})^*) = D(\widetilde{H}_{Z_\ell}^{\text{TF}})$ and $\widetilde{H}_{Z_\ell}^{\text{TF}} \phi_\ell = \mu_\ell \phi_\ell$. This finishes the proof. □

Consider now the sequences $\{Z_\ell\}_{\ell=1}^\infty$ and $\{\phi_\ell\}_{\ell=1}^\infty$ from Lemmas 4.1(c) and 4.2 respectively. As in the proof of Lemma 3.2 we take a subsequence $\{Z_{\ell_k}\}_{k=1}^\infty$ of $\{Z_\ell\}_{\ell=1}^\infty$ so that $Z_{\ell_k} \to \infty$ and (13) as $k \to \infty$ for some θ. We claim that $\{H_{Z_{\ell_k}}^{\text{TF}}\}_{k=1}^\infty$ is an example of a sequence of Thomas-Fermi atoms which converges in the strong resolvent sense – this follows directly from Theorem 2.5 – but ***not*** in the norm resolvent sense.

To prove the last part of this statement we choose natural numbers $p_1 < p_2 < p_3 < \cdots$ so that

$$\frac{\ell_{p_k}(\ell_{p_k}+1)}{x^2} - \Phi_{Z_{\ell_k}}^{\text{TF}}(x) \geq 0, \qquad \text{implying} \qquad \widetilde{H}_{Z_{\ell_k}}^{\text{TF}}\Big|_{D(\widetilde{H}_{Z_{\ell_k}}^{\text{TF}}) \cap \mathcal{V}_{\ell_{p_k}}} \geq 0, \tag{47}$$

where the $\mathcal{V}_{\ell_{p_k}}$'s are as in Lemma 4.2. By the construction we have of course $p_k \geq k$. If we let h be a smooth function with compact support in $(-\infty, 0)$ we claim that $h(\widetilde{H}_{Z_{\ell_k}}^{\text{TF}})\phi_{\ell_{p_k}} = 0$. Indeed, $\mathcal{V}_{\ell_{p_k}}$ is an invariant subspace for $\widetilde{H}_{Z_{\ell_k}}^{0,\text{TF}}$ and hence also for $\widetilde{H}_{Z_{\ell_k}}^{\text{TF}}$, and since $\phi_{\ell_{p_k}} \in \mathcal{V}_{\ell_{p_k}}$ this assertion follows from (47) and the abstract functional calculus. As additionally $h(\widetilde{H}_{Z_{\ell_{p_k}}}^{\text{TF}})\phi_{\ell_{p_k}} = h(\mu_{\ell_{p_k}})\phi_{\ell_{p_k}}$ we can choose h to be 1 on a neighbourhood around -1 and obtain

$$\left\|\phi_{\ell_{p_k}}\right\| = \left\|h(\widetilde{H}_{Z_{\ell_{p_k}}}^{\text{TF}})\phi_{\ell_{p_k}} - h(\widetilde{H}_{Z_{\ell_k}}^{\text{TF}})\phi_{\ell_{p_k}}\right\| \leq \left\|\phi_{\ell_{p_k}}\right\| \cdot \left\|h(\widetilde{H}_{Z_{\ell_{p_k}}}^{\text{TF}}) - h(\widetilde{H}_{Z_{\ell_k}}^{\text{TF}})\right\|$$

for sufficiently large k where the last norm is the usual operator norm. This proves that $\{H_{Z_{\ell_k}}^{\text{TF}}\}_{k=1}^\infty$ simply cannot be convergent in the norm resolvent sense.

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References

[1] Milton Abramowitz and Irene A. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. Tenth Printing.* (As it appears on the public web page https://personal.math.ubc.ca/~cbm/aands/abramowitz_and_stegun.pdf). National Bureau of Standards, 1972.

[2] August Bjerg. "Convergence of operators with deficiency indices (k, k) and of their self-adjoint extensions". In: *Annales Henri Poincaré* (2023). URL: https://doi.org/10.1007/s00023-023-01397-9.

[3] Laurent Bruneau, Jan Dereziński, and Vladimir Georgescu. "Homogeneous Schrödinger operators on half-line". In: *Annales Henri Poincaré* 12 (2011), pp. 547–590.

[4] Jan Dereziński and Vladimir Georgescu. "One-Dimensional Schrödinger Operators with Complex Potentials". In: *Annales Henri Poincaré* 21.6 (2020), pp. 1947–2008.

[5] Enrico Fermi. "Sulla deduzione statistica di alcune proprietá dell'atomo. Applicazione alla teoria del sistema periodico degli elementi". In: *Rend. Lincei* 7 (1928), p. 342.

[6] Enrico Fermi. "Un metodo statistico per la determinazione di alcune priorieta dell'atome". In: *Rend. Accad. Naz. Lincei* 6 (1927), pp. 602–607.

[7] Setsuro Fujiié and Thierry Ramond. "Exact WKB analysis and the Langer modification with application to barrier top resonances". In: *Toward the exact WKB analysis of differential equations, linear or non-linear*. Kyoto Univ. Press, Kyoto, 2000, pp. 15–31.

[8] V.M. Klechkovskii. "Justification of the rule for successive filling of $(n+\ell)$ groups". In: *Soviet Physics-JETP* 14 (1962), pp. 334–335.

[9] Rudolph E. Langer. "On the Connection Formulas and the Solutions of the Wave Equation". In: *Physical Review* 51.8 (1937), pp. 669–676.

[10] Elliott Lieb and Barry Simon. "The Thomas-Fermi theory of atoms, molecules and solids". In: *Advances in mathematics* 23.1 (1977), pp. 22–116.

[11] Elliott H. Lieb. "Thomas-fermi and related theories of atoms and molecules". In: *Review of Modern Physics* 53.4 (1981), pp. 603–641.

[12] Erwin Madelung. *Die mathematischen hilfsmittel des physikers*. Vol. 4. Springer-Verlag, 1950.

[13] F. W. J. Olver. "Error bounds for the Liouville–Green (or WKB) approximation". In: *Mathematical Proceedings of the Cambridge Philosophical Society* 57.4 (1961), pp. 790–810.

[14] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics. I Functional Analysis*. 2nd ed. Academic Press, 1980.

[15] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics. II Fourier Analysis, Self-adjointness*. Academic Press, 1975.

[16] Llewellyn H. Thomas. "The calculation of atomic fields". In: *Mathematical proceedings of the Cambridge philosophical society*. Vol. 23. 5. Cambridge University Press. 1927, pp. 542–548.

[17] T. Tietz. "Elektronengruppen im periodischen System der Elemente in der statistischen Theorie des Atoms". In: *Annalen der Physik* 460.3-4 (1960), pp. 237–240.

[18] D. Pan Wong. "Theoretical justification of madelung's rule". In: *Journal of Chemical Education* 56.11 (1979), pp. 714–717.

Chapter 3

Paper: Convergence of operators with deficiency indices (k,k) and of their self-adjoint extensions

This chapter contains the paper [Bje23] by the author. It is a result of asking some natural abstract questions concerning conditions for strong resolvent convergence that arose during the study of large atoms presented in Chapter 2. The paper is included in its entirety in the form publicly available at[a] https://arxiv.org/abs/2306.02745v2 – that is, including title page, abstract and bibliography. It is not the published version (Version of Record) which can be found at https://doi.org/10.1007/s00023-023-01397-9. To mark its independence from the rest of the thesis it has its own page numbering (at the bottom of pages), but it can be located within the thesis by the colour ■ at the top of pages.

[a] Any deviations from the version on arXiv.org is solely due to using different compiling tools.

Convergence of operators with deficiency indices (k,k) and of their self-adjoint extensions

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Abstract: We consider an abstract sequence $\{A_n\}_{n=1}^{\infty}$ of closed symmetric operators on a separable Hilbert space $\mathcal{H}$. It is assumed that all A_n's have equal deficiency indices (k,k) and thus self-adjoint extensions $\{B_n\}_{n=1}^{\infty}$ exist and are parametrized by partial isometries $\{U_n\}_{n=1}^{\infty}$ on $\mathcal{H}$ according to von Neumann's extension theory. Under two different convergence assumptions on the A_n's we give the precise connection between strong resolvent convergence of the B_n's and strong convergence of the U_n's.

1 Introduction

We investigate in the following the notion of strong resolvent convergence of sequences of self-adjoint extensions of already specified (unbounded) closed symmetric operators on a Hilbert space. For the general theory on these topics we refer to [2] VIII and [1] X and introduce now the framework in which we will be working for the present section as well as for Section 3 where our main results are found. In Section 2 we treat also more general operators than considered here.

Consider a symmetric and closed operator A on an infinite dimensional separable Hilbert space $\mathcal{H}$[1] defined on a dense subspace $D(A)$. The kernels $\mathcal{H}_{\mp} := Z(A^* \pm i)$ are the *deficiency subspaces* and the pair $(\dim\mathcal{H}_+, \dim\mathcal{H}_-)$ is the *deficiency indices*. We assume that the latter are equal and finite, i.e. $(\dim\mathcal{H}_+, \dim\mathcal{H}_-) = (k,k)$ for some $k = 1,2,\ldots$ (however, see Remark 11). This implies, cf. [1] Theorem X.2, that A has self-adjoint extensions, and moreover any self-adjoint extension B of A is given by the rule

$$D(B) = \{\phi_0 + \phi_+ + U\phi_+ \mid \phi_0 \in D(A),\ \phi_+ \in \mathcal{H}_+\},$$

$$B(\phi_0 + \phi_+ + U\phi_+) = A\phi_0 + i\phi_+ - iU\phi_+$$

where $U\colon \mathcal{H}_+ \to \mathcal{H}_-$ is a unitary map which can be extended to a partial isometry on all of $\mathcal{H}$ by letting $U\phi = 0$ for $\phi \in [\mathcal{H}_+]^{\perp}$. Conversely, all extensions of A of this form are self-adjoint.

We introduce now sequences $\{A_n\}_{n=1}^{\infty}$ and $\{B_n\}_{n=1}^{\infty}$ of such operators. That is, the A_n's are densely defined, symmetric and closed operators on $\mathcal{H}$ with deficiency subspaces $\mathcal{H}_{\pm}^n$ and deficiency indices (k,k) independent of n, and B_n is a self-adjoint extension of A_n defined by a unitary map $U_n\colon \mathcal{H}_+^n \to \mathcal{H}_-^n$ (which can all, once again, be considered as partial isometries on $\mathcal{H}$) as described above for each n. In this set-up we think of A, B and U as limiting operators of the sequences of A_n's, B_n's and U_n's respectively, and our

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[1] We adopt the convention that the inner product on $\mathcal{H}$ is linear in the second entry

main goal will be to examine the interplay between the convergence of these sequences. A very natural question is for example whether we can obtain results along the lines of

$$\text{"Suppose } A_n \to A. \text{ Then } B_n \to B \text{ if and only if } U_n \to U.\text{"} \tag{1}$$

Of course one needs here to specify which notions of convergences we involve in this statement for it to be mathematically interesting. For the purposes of this note we focus on strong convergence of operators on Hilbert spaces. Hence, $U_n \to U$ should be understood as usual strong convergence of bounded operators and $B_n \to B$ as strong resolvent convergence of self-adjoint unbounded operators, i.e. as strong convergence of $(B_n + i)^{-1}$ towards $(B + i)^{-1}$ – for an introduction to the topic and an explanation why this is in some sense the only "right" way of extending the concept of strong convergence to self-adjoint unbounded operators, see [2] VIII.7. For the A_n's, however, we cannot use this generalized version of strong convergence since these are not self-adjoint.

This issue will be addressed in Section 2. Once this theoretical framework is in place, we will gradually progress towards presenting statements of the form (1) in Corollaries 14 and 15. Finally, an exposition on the optimality of these results – in particular of the latter – is included for completeness.

Example 1. As a final note before diving into technical details we mention the structure of a class of motivational examples that illuminates why we even care to search for results like (1).

Consider a sequence $\{\widetilde{A}_n\}_{n=1}^{\infty}$ of explicitly given symmetric differential operators on an open subset Ω of $\mathbb{R}^d$ defined on $D(\widetilde{A}_n) = C_c^{\infty}(\Omega)$. Now the usual way to realize $\widetilde{A}_n$ as a self-adjoint operator on $L^2(\Omega) = \mathcal{H}$ is the following: Let A_n be the closure of $\widetilde{A}_n$ for each n and if this is not already self-adjoint extend it by the above procedure to some self-adjoint operator B_n. Here we have an example where the sequence $\{A_n\}_{n=1}^{\infty}$ is concretely described and not often subject to change. It describes not only how the A_n's but also (through the A_n^*'s) how the B_n's act on their domain, and often it will not be to difficult to prove that $A_n \to A$ for some A in an appropriate sense. We suppose that this convergence has been established. Moreover, natural examples of sequences of this form will in most cases satisfy the crucial property that all the operators have the same deficiency indices. The deficiency subspaces will be parts of solutions spaces of differential equations and usually the U_n's will be simple maps between such spaces. Hence, in this case, strong convergence of the U_n's is a property which is a lot easier to handle than the full strong resolvent convergence of the B_n's.

Now one can envision a couple of situations: If a sequence of B_n's is known, (1) could help us determine a self-adjoint extension B of A so that $B_n \to B$ in the strong resolvent sense. One needs only to find the strong limit of the U_n's (if this exists) and use this to extend A. If the strong limit of the U_n's does not exists then the result will conversely tell us that the B_n's do not converge towards any self-adjoint extension of A. On the other hand it could be that B was a fixed self-adjoint extension of A and the result could in the same manner be used to find a sequence of B_n's which extends the A_n's and converge towards B in the strong resolvent sense – or whether such sequence exists at all. ▲

2 Strong graph convergence and convergence of graph projections

Now some candidates for types of convergences for the A_n's in (1) are treated. Along the way we introduce the machinery needed for both formulating and proving our main results. Firstly we need to introduce a particular notion of convergence of subspaces of a Hilbert space.

Definition 2. Let $\{V_n\}_{n=1}^{\infty}$ be a sequence of subspaces of a Hilbert space $\mathcal{H}$. The subspace

$$V_\infty := \left\{ x \in \mathcal{H} \,\middle|\, \begin{array}{c}\text{There exists a sequence } \{x_n\}_{n=1}^{\infty} \subseteq \mathcal{H} \text{ with} \\ x_n \in V_n \text{ for each } n \text{ so that } x_n \to x \text{ as } n \to \infty \end{array} \right\}$$

is called the *strong limit* of $\{V_n\}_{n=1}^{\infty}$ and we write $V_n \to V_\infty$ strongly.

One should not be misled by the fact that we call this type of convergence "strong". We note that *any* sequence of subspaces has a limit in the above sense (although it might be the trivial 0-subspace), and hence this way of converging cannot be a particularly strong one. The word "strong" merely refers to the fact that $\{x_n\}_{n=1}^{\infty}$ should converge towards x strongly, i.e. with respect to the Hilbert space norm.

Another notion of convergence of sequences of closed subspaces of a Hilbert space is that of the orthogonal projections onto these converging strongly towards the orthogonal projection onto a limiting subspace. In fact, this is generally a stronger notion of convergence of subspaces than the above "strong" convergence.

Lemma 3. Let $\{V_n\}_{n=1}^{\infty}$ be a sequence of closed subspaces of a Hilbert space $\mathcal{H}$ and denote the orthogonal projections onto these by $\{P_n\}_{n=1}^{\infty}$. Denote similarly by P the orthogonal projection onto another subspace $V \subseteq \mathcal{H}$.

(a) V is contained in the strong limit of $\{V_n\}_{n=1}^{\infty}$ if and only if $P_n x \to x = Px$ for all $x \in V$.

(b) If $P_n \to P$ strongly then V is the strong limit of $\{V_n\}_{n=1}^{\infty}$.

Proof. (a): Assume on the one hand that V is contained in the strong limit of $\{V_n\}_{n=1}^{\infty}$. Then, for any $x \in V$, there exists a sequence $\{x_n\}_{n=1}^{\infty} \subseteq \mathcal{H}$ with $x_n \in V_n$ for all n so that $x_n \to x$. Hence, $\|P_n x - x\| \leq \|x_n - x\| \longrightarrow 0$ as needed. The other implication is clear if one considers the sequence $\{P_n x\}_{n=1}^{\infty}$ for each $x \in V$.

(b): Assume $P_n \to P$ strongly and denote by V_∞ the strong limit of $\{V_n\}_{n=1}^{\infty}$. By (a) we need only to argue that $V_\infty \subseteq V$ or equivalently $V^\perp \subseteq V_\infty^\perp$. However, if $y \in V^\perp$ then for any $x \in V_\infty$ we can choose a sequence $\{x_n\}_{n=1}^{\infty} \subseteq \mathcal{H}$ as for the x in (a) and obtain

$$\langle y, x \rangle = \lim_{n\to\infty} \langle (1 - P_n) y, x_n \rangle = 0$$

proving $y \in V_\infty^\perp$ as needed. $\square$

Remark 4. While Lemma 3(b) shows that convergence of projections is a stronger type of convergence than "strong" convergence in the sense of Definition 2, the following example shows that it is actually *strictly* stronger – a fact which will be important later on.

Consider a sequence $\{V_n\}_{n=1}^{\infty}$ of subspaces of a Hilbert space $\mathcal{H}$ of the form $V_n = [\mathbb{C}x_n]^{\perp}$ where $x_n \in \mathcal{H}$ is of unit length and denote by V_∞ the strong limit of this sequence. Suppose that $x_n = x_0$ is fixed for n odd and $x_n = y_n$ for n even where $\{y_n\}_{n=1}^{\infty}$ is a sequence which is weekly convergent towards 0. Now $x_0 \notin V_\infty$ since for n odd we have $\operatorname{dist}(V_n, x_0) = 1$. If, however, $x \in [\mathbb{C}x_0]^{\perp}$ then we can consider the sequence z_n which is $x \in V_n$ for n odd and $x - \langle y_n, x\rangle y_n \in V_n$ for n even. As $\langle y_n, x\rangle \to 0$ we see that $z_n \to x$ proving $x \in V_\infty$. We conclude that $V_\infty = [\mathbb{C}x_0]^{\perp}$.

On the the other hand the orthogonal projections P_n onto the V_n's do not converge strongly at all. In particular $P_n x_0$ is 0 for n odd and $x_0 - \langle y_n, x_0\rangle y_n \to x_0$ for n even. ■

Letting operators once again enter the picture we can now easily define a notion of convergence of any sequence of operators on a Hilbert space: The strong graph convergence which is also treated in [2] VIII.7.

Definition 5. Let $\{A_n\}_{n=1}^{\infty}$ be any sequence of operators on a fixed Hilbert space $\mathcal{H}$. If the graphs $\operatorname{Gr}(A_n)$ converge strongly towards the graph $\operatorname{Gr}(A)$ of some operator A on $\mathcal{H}$ as subspaces of $\mathcal{H} \oplus \mathcal{H}$ then we say that A is the *strong graph limit* of the A_n's and write $A = \operatorname{str.gr.lim} A_n$.

Let us return to the case of a sequence of densely defined and closed operators $\{A_n\}_{n=1}^{\infty}$ for the remaining part of the section and fix once and for all the following convenient notation: By Γ_∞ we mean the strong limit of $\{\operatorname{Gr}(A_n)\}_{n=1}^{\infty}$ and by Γ_∞^* the strong limit of $\{\operatorname{Gr}(A_n^*)\}_{n=1}^{\infty}$. Note that $(\phi, \psi) \in \Gamma_\infty$ if and only if there exists a sequence $\{\phi_n\}_{n=1}^{\infty} \subseteq \mathcal{H}$ such that both $\phi_n \to \phi$ and $A_n\phi_n \to \psi$, and we have the similar characterization of Γ_∞^*. We can now present some basic properties of these subspaces.

Lemma 6. Let $\{A_n\}_{n=1}^{\infty}$ be a sequence of densely defined and closed operators and let A be an operator with the same properties as the A_n's.

(a) If $\operatorname{Gr}(A) \subseteq \Gamma_\infty$ then $\Gamma_\infty^* \subseteq \operatorname{Gr}(A^*)$.

(b) If $\operatorname{Gr}(A) \subseteq \Gamma_\infty$ and $\operatorname{Gr}(A^*) \subseteq \Gamma_\infty^*$ then $\operatorname{Gr}(A) = \Gamma_\infty$ and $\operatorname{Gr}(A^*) = \Gamma_\infty^*$

(c) If moreover the A_n's are symmetric and A is self-adjoint then $A = \operatorname{str.gr.lim} A_n$ if and only if $\operatorname{Gr}(A) \subseteq \Gamma_\infty$.

Proof. (a): Take $(\phi, \psi) \in \Gamma_\infty^*$ arbitrary and a corresponding sequence $\{\phi_n\}_{n=1}^{\infty}$ with $\phi_n \in D(A_n^*)$ so that $\phi_n \to \phi$ and $A_n^*\phi_n \to \psi$. Now for any $\eta \in D(A)$ there exists a sequence $\{\eta_n\}_{n=1}^{\infty}$ with $\eta_n \in D(A_n)$ so that $\eta_n \to \eta$ and $A_n\eta_n \to A\eta$. Using these sequences we see that

$$\langle \phi, A\eta\rangle = \lim_{n\to\infty} \langle \phi_n, A_n\eta_n\rangle = \lim_{n\to\infty} \langle A_n^*\phi_n, \eta_n\rangle = \langle \psi, \eta\rangle$$

proving that $\phi \in D(A^*)$ and $A^*\phi = \psi$ as needed.

(b): This is a simple application of (a) and the fact that $T^{**} = T$ for any closed operator T.

(c): We need only to prove that $\mathrm{Gr}(A) \subseteq \Gamma_\infty$ implies $\Gamma_\infty \subseteq \mathrm{Gr}(A)$. This is seen by the inclusions $\Gamma_\infty \subseteq \Gamma_\infty^*$ (by symmetry of the A_n's) and $\Gamma_\infty^* \subseteq \mathrm{Gr}(A^*) = \mathrm{Gr}(A)$ (by (a) and self-adjointness of A). □

The connection to convergence of the projections onto the graphs of the A_n's is now given in the below proposition. It tells us that the difference between strong graph convergence and strong convergence of the sequence of graph projections is measured by the absence of strong graph convergence of the sequence of adjoint operators.

Proposition 7. Let $\{A_n\}_{n=1}^\infty$ be a sequence of densely defined and closed operators and let A be an operator with the same properties as the A_n's. Denote by P_n and P the orthogonal projections in $\mathcal{H} \oplus \mathcal{H}$ onto $\mathrm{Gr}(A_n)$ and $\mathrm{Gr}(A)$ respectively. Then $P_n \to P$ strongly if and only if both $\mathrm{Gr}(A) = \Gamma_\infty$ and $\mathrm{Gr}(A^*) = \Gamma_\infty^*$ (or equivalently if and only if both $\mathrm{Gr}(A) \subseteq \Gamma_\infty$ and $\mathrm{Gr}(A^*) \subseteq \Gamma_\infty^*$, cf. Lemma 6(b)).

Proof. We will use the standard fact, see for example [4] Theorem 12.5, that

$$\mathcal{H} \oplus \mathcal{H} = \mathrm{Gr}(T) \oplus W\,\mathrm{Gr}(T^*) \tag{2}$$

for any densely defined and closed operator T on $\mathcal{H}$ where the sum is orthogonal and W is the unitary map $(\phi, \psi) \mapsto (-\psi, \phi)$.

Now if $P_n \to P$ strongly then $\mathrm{Gr}(A) = \Gamma_\infty$ by Lemma 3(b). Also, $1 - P_n \to 1 - P$ strongly so that similarly $W\,\mathrm{Gr}(A_n^*) \to W\,\mathrm{Gr}(A^*)$ strongly by the decomposition (2). It is an easy exercise to check that this is equivalent to $\mathrm{Gr}(A^*) = \Gamma_\infty^*$.

If, on the other hand, $\mathrm{Gr}(A) = \Gamma_\infty$ and $\mathrm{Gr}(A^*) = \Gamma_\infty^*$ then also $W\,\mathrm{Gr}(A_n^*) \to W\,\mathrm{Gr}(A^*)$ strongly. Using this we get by Lemma 3(a) that $P_n x \to Px$ for any $x \in \mathrm{Gr}(A)$ and, by using additionally (2), $(1 - P_n)y \to (1 - P)y$ for any $y \in W\,\mathrm{Gr}(A^*)$. Combining these convergences and (2) we conclude that $P_n z \to Pz$ for any $z \in \mathcal{H} \oplus \mathcal{H}$. □

To conclude this technical section we include a result on strong resolvent convergence of self-adjoint operators together with some observations. This result is well established, cf. [5] Lemma 28 (and [2] Theorem VIII.26 for a partial result). In the formulation below [5] states and proves the equivalence of (i), (ii) and (iv) and [2] that of (i) and (ii). Meanwhile, both proofs are sufficient to include also (iii) to these lists.

Theorem 8. Let $\{B_n\}_{n=1}^{\infty}$ be a sequence of self-adjoint operators on a Hilbert space $\mathcal{H}$ and B another self-adjoint operator on $\mathcal{H}$. Let further Q_n and Q be the orthogonal projections onto $\mathrm{Gr}(B_n)$ and $\mathrm{Gr}(B)$ respectively and denote by Γ_{∞}^{B} the strong limit of $\{\mathrm{Gr}(B_n)\}_{n=1}^{\infty}$. The following statements are equivalent:

(i) $B_n \to B$ in the strong resolvent sense,

(ii) $B = \mathrm{str.gr.lim}\, B_n$ (i.e. $\mathrm{Gr}(B) = \Gamma_{\infty}^{B}$),

(iii) $\mathrm{Gr}(B) \subseteq \Gamma_{\infty}^{B}$,

(iv) $Q_n \to Q$ strongly.

Proof. When using the self-adjointness of the operators, the equivalence between (ii) and (iii) is Lemma 6(c) and the equivalence between (ii) and (iv) is Proposition 7.

Suppose $B_n \to B$ in the strong resolvent sense and let $\phi \in D(B)$ be arbitrary. By self-adjointness the relation $\psi = (B_n + i)\phi_n = (B+i)\phi$ defines besides the $\psi \in \mathcal{H}$ also for each n a $\phi_n \in D(B_n)$. Moreover,

$$\begin{aligned}\|(\phi_n, B_n\phi_n) - (\phi, B\phi)\|^2 &= \|\phi_n - \phi\|^2 + \|B_n\phi_n - B\phi\|^2 = \|\phi_n - \phi\|^2 + \|i\phi - i\phi_n\|^2 \\ &= 2\|(B_n + i)^{-1}\psi - (B+i)^{-1}\psi\|^2 \longrightarrow 0\end{aligned}$$

which proves that (i) implies (iii).

Suppose finally that $\mathrm{Gr}(B) \subseteq \Gamma_{\infty}^{B}$ and let $\psi \in \mathcal{H}$ be arbitrary. Since $\mathcal{H} = R(B+i)$ we have $\psi = (B+i)\phi$ for some $\phi \in D(B)$ and by the assumption there exists a sequence $\{\phi_n\}_{n=1}^{\infty} \subseteq \mathcal{H}$ so that $(\phi_n, B_n\phi_n) \to (\phi, B\phi)$. Hence,

$$[(B_n + i)^{-1} - (B+i)^{-1}]\psi = (B_n + i)^{-1}[(B+i)\phi - (B_n + i)\phi_n] - \phi + \phi_n \longrightarrow 0$$

where we use the fact that $\|(B_n + i)^{-1}\| \leq 1$ for all n. This proves that (iii) implies (i) and thus the full theorem. □

We observe that though (ii)-(iv) in Theorem 8 are equivalent for sequences of self-adjoint operators, Proposition 7 tells us that (iii) follows from (ii) and (iv) respectively even when assuming only that the B_n's and B are densely defined and closed. Moreover, (iii) is a consequence of pointwise convergence on a common core of the sequence and is thus easy to verify for for example differential operators, see Proposition 17 and Example 18. Thus, the first question we examine in Section 3 below will be the following: If we in the set-up from Section 1 impose the condition (iii) on the sequence $\{A_n\}_{n=1}^{\infty}$ what more do we need in order for it to hold for the sequence $\{B_n\}_{n=1}^{\infty}$ of extensions (thus yielding strong resolvent convergence)?

3 Main results

From the previous section we obtain two candidates for convergence type to impose on the A_n's in (1): Strong graph convergence and strong convergence of graph projections.

That these are actually both natural choices is illuminated by Theorem 8 which states that for sequences of self-adjoint operators each of them is equivalent to strong resolvent convergence – exactly the convergence type we seek! Throughout this section we use the following conventions: Let $\{A_n\}_{n=1}^\infty$, $\{B_n\}_{n=1}^\infty$, $\{U_n\}_{n=1}^\infty$, A, B and U be as in the beginning of Section 1. Let Γ_∞ be the strong limit of $\{\mathrm{Gr}(A_n)\}_{n=1}^\infty$ and Γ_∞^* the strong limit of $\{\mathrm{Gr}(A_n^*)\}_{n=1}^\infty$. Denote by P_n and P the orthogonal projections in $\mathcal{H}\oplus\mathcal{H}$ onto $\mathrm{Gr}(A_n)$ and $\mathrm{Gr}(A)$ respectively.

The answer to the question closing Section 2 is straightforward and given below in Corollary 9, and in applications it can be useful even in this raw form.

Corollary 9 (to Theorem 8). Consider operators A_n, A, B_n and B as described in Section 1 and suppose $\mathrm{Gr}(A) \subseteq \Gamma_\infty$. If moreover for every pair (or, equivalently, for k linearly independent pairs) $(\phi, B\phi)$ from the orthogonal complement of $\mathrm{Gr}(A)$ inside the Hilbert space $\mathrm{Gr}(B)$ there exists a sequence $\{\phi_n\}_{n=1}^\infty \subseteq \mathcal{H}$ so that $\phi_n \in D(B_n)$ for all n and $(\phi_n, B_n\phi_n) \to (\phi, B\phi)$ then $B_n \to B$ in the strong resolvent sense.

Proof. Denoting the strong limit of $\{\mathrm{Gr}(B_n)\}_{n=1}^\infty$ by Γ_∞^B it is basically the assumption above that the orthogonal complement of $\mathrm{Gr}(A)$ inside $\mathrm{Gr}(B)$ is contained in Γ_∞^B. Moreover, $\mathrm{Gr}(A) \subseteq \Gamma_\infty \subseteq \Gamma_\infty^B$ since all the B_n's are extensions of the A_n's. This concludes the proof. For the fact that it suffices to consider k linearly independent pairs, see the first couple of lines of the proof of Theorem 12. □

For the remaining part of this section we formulate and prove results like (1) with the different notions of convergence of the A_n's introduced above. For this it will be essential to have at our disposal the following characterization of strong convergence of the U_n's defining the self-adjoint extensions of the A_n's.

Lemma 10. Consider the U_n's and the U described in Section 1. We have $U_n \to U$ strongly if and only if the following statement is true:

$$\begin{gathered}\text{For each } \phi_+ \in \mathcal{H}_+ \text{there exists a sequence } \{\phi_+^n\}_{n=1}^\infty \subseteq \mathcal{H} \text{ so that}\\ \phi_+^n \in \mathcal{H}_+^n \text{ for all } n \text{ and } (\phi_+^n, U_n\phi_+^n) \to (\phi_+, U\phi_+).\end{gathered} \tag{3}$$

Note that the condition (3) actually says that the strong limit of the graphs of the U_n's considered as operators only on $\mathcal{H}_+^n$ contains the corresponding graph of U.

Proof (of Lemma 10). Observe firstly that if $\psi_n \to \psi$ then the inequalities

$$\|U_n\psi_n - U\psi\| \le \|\psi_n - \psi\| + \|U_n\psi - U\psi\| \le 2\|\psi_n - \psi\| + \|U_n\psi_n - U\psi\|$$

show that

$$U_n\psi_n \to U\psi \quad \text{if and only if} \quad U_n\psi \to U\psi. \tag{4}$$

For each n denote by P_n the orthogonal projection onto $\mathcal{H}_+^n$ and by P the orthogonal projection onto $\mathcal{H}_+$. Assume $U_n \to U$ strongly. Then, for any $\phi_+ \in \mathcal{H}_+$ and $\psi \in \mathcal{H}$, we have

$$\langle P_n\phi_+, \psi\rangle = \langle U_n^* U_n\phi_+, \psi\rangle = \langle U_n\phi_+, U_n\psi\rangle \longrightarrow \langle U\phi_+, U\psi\rangle = \langle P\phi_+, \psi\rangle = \langle \phi_+, \psi\rangle$$

so that $P_n\phi_+ \to \phi_+$ weakly in $\mathcal{H}$. As further

$$\|\phi_+\| \le \liminf_{n\to\infty} \|P_n\phi_+\| \le \limsup_{n\to\infty} \|P_n\phi_+\| \le \|\phi_+\|$$

by lower semi-continuity of the norm it is apparent that additionally $\|P_n\phi_+\| \to \|\phi_+\|$ and consequently $P_n\phi_+ \to \phi_+$ with respect to the Hilbert space norm. We claim that letting $\{\phi_+^n\}_{n=1}^\infty := \{P_n\phi_+\}_{n=1}^\infty$ for each $\phi_+ \in \mathcal{H}_+$ verifies (3). Indeed, since then $\phi_+^n \to \phi_+$, the strong convergence $U_n \to U$ and (4) yield the desired conclusion.

Suppose now that (3) is satisfied. For any $\phi_+ \in \mathcal{H}_+$ we can choose the sequence from this condition and (4) implies that $U_n\phi_+ \to U\phi_+$. For proving convergence of $U_n\psi$ for $\psi \in [\mathcal{H}_+]^\perp$ fix such ψ and consider an orthonormal basis $\{\phi_{+,1},\ldots,\phi_{+,k}\}$ of $\mathcal{H}_+$. By (3) there exist sequences $\{\phi_{+,1}^n\}_{n=1}^\infty,\ldots,\{\phi_{+,k}^n\}_{n=1}^\infty \subseteq \mathcal{H}$ with $\phi_{+,\ell}^n \in \mathcal{H}_+^n$ for all n and $\ell = 1,\ldots,k$ and $\phi_{+,\ell}^n \to \phi_{+,\ell}$ for all ℓ. Now by applying the Gram-Schmidt process to $\{\phi_{+,1}^n,\ldots,\phi_{+,k}^n\}$ for each n we obtain new sequences $\{\widetilde{\phi}_{+,1}^n\}_{n=1}^\infty,\ldots,\{\widetilde{\phi}_{+,k}^n\}_{n=1}^\infty \subseteq \mathcal{H}$ with $\{\widetilde{\phi}_{+,1}^n,\ldots,\widetilde{\phi}_{+,k}^n\}$ an orthonormal basis of $\mathcal{H}_+^n$ for sufficiently large n. Induction in ℓ shows that also $\widetilde{\phi}_{+,\ell}^n \to \phi_{+,\ell}$ for all ℓ. Consequently,

$$[\mathcal{H}_+^n]^\perp \ni \psi_n := \psi - \sum_{\ell=1}^{k} \langle \widetilde{\phi}_{+,\ell}^n, \psi\rangle \widetilde{\phi}_{+,\ell}^n \longrightarrow \psi$$

and, since $U_n\psi_n = 0 = U\psi$ for large n, a final application of (4) proves that $U_n\psi \to U\psi$. □

Remark 11. Lemma 10 is actually the main reason why we assume that the deficiency indices of the A_n's are finite, since then we can simply restate the condition (3) as strong convergence of the U_n's – which is exactly the kind of formulation we seek. If one, in the case of infinite deficiency indices, replaces "$U_n \to U$ strongly" with (3) then the remaining results of this note in Theorem 12 and Corollaries 14 and 15 indeed remain valid. One can realize that these conditions are truly different in the infinite case by taking the U_n's and the U to be projections and recalling the content of Remark 4. ■

While this description of strong convergence of the U_n's not at first sight simplifies things, the fact that it is so closely related to the definition of strong graph convergence will help us apply our theory from Section 2 via Theorem 8. With this, we are now in a position to state and prove the main theoretical statement of this note.

Theorem 12. Let $\{A_n\}_{n=1}^\infty$, $\{B_n\}_{n=1}^\infty$, $\{U_n\}_{n=1}^\infty$, A, B and U be as in the beginning of Section 1. Let Γ_∞ be the strong limit of $\{\mathrm{Gr}(A_n)\}_{n=1}^\infty$, and denote by P_n and P the orthogonal projections in $\mathcal{H}\oplus\mathcal{H}$ onto $\mathrm{Gr}(A_n)$ and $\mathrm{Gr}(A)$ respectively. Then the following holds:

(a) If $\mathrm{Gr}(A) \subseteq \Gamma_\infty$ and $U_n \to U$ strongly then $B_n \to B$ in the strong resolvent sense and $P_n \to P$ strongly.

(b) If $B_n \to B$ in the strong resolvent sense and $P_n \to P$ strongly then $U_n \to U$ strongly.

Proof. (a): Recall that, cf. [1] X.1,

$$\mathrm{Gr}(B) = \mathrm{Gr}(A) \oplus \{(\phi_+ + U\phi_+, i\phi_+ - iU\phi_+) \mid \phi_+ \in \mathcal{H}_+\},$$

where the sum is orthogonal, from which the k-dimensional orthogonal complement of $\mathrm{Gr}(A)$ in $\mathrm{Gr}(B)$ is apparent. Applying Lemma 10 we can for any $\phi_+ \in \mathcal{H}_+$ find $\{\phi_+^n\}_{n=1}^\infty \subseteq \mathcal{H}$ so that $\phi_+^n \in \mathcal{H}_+^n$ for all n and

$$(\phi_+^n + U_n\phi_+^n, i\phi_+^n - iU_n\phi_+^n) \longrightarrow (\phi_+ + U\phi_+, i\phi_+ - iU\phi_+).$$

Hence, Corollary 9 implies $B_n \to B$ in the strong resolvent sense. Likewise we have also (cf. [1] X.1)

$$\mathrm{Gr}(A^*) = \mathrm{Gr}(A) \oplus \{(\phi_+, i\phi_+) \mid \phi_+ \in \mathcal{H}_+\} \oplus \{(U\phi_+, -iU\phi_+) \mid \phi_+ \in \mathcal{H}_+\}$$

and a similar application of Lemma 10 tells us that $\mathrm{Gr}(A^*) \subseteq \Gamma_\infty^*$ (the strong limit of $\{\mathrm{Gr}(A_n^*)\}_{n=1}^\infty$). By invoking Proposition 7 we get thus additionally $P_n \to P$ strongly.

(b): We note that by Theorem 8 (and using the notation herein) we have $Q_n \to Q$ strongly, and consequently $Q_n - P_n \to Q - P$ strongly. Now $Q_n - P_n$ is the orthogonal projection onto the orthogonal complement of $\mathrm{Gr}(A_n)$ inside $\mathrm{Gr}(B_n)$ and similarly for $Q - P$. But we have just seen in the proof of (a) that these are exactly

$$\{(\phi_+^n + U_n\phi_+^n, i\phi_+^n - iU_n\phi_+^n) \mid \phi_+^n \in \mathcal{H}_+^n\} \quad \text{and} \quad \{(\phi_+ + U\phi_+, i\phi_+ - iU\phi_+) \mid \phi_+ \in \mathcal{H}_+\}$$

respectively. Hence, Lemma 3(b) tells us that for each $\phi_+ \in \mathcal{H}_+$ there exists a sequence $\{\phi_+^n\}_{n=1}^\infty \subseteq \mathcal{H}$ so that $\phi_+^n \in \mathcal{H}_+^n$ for all n and

$$(\phi_+^n + U_n\phi_+^n, i\phi_+^n - iU_n\phi_+^n) \longrightarrow (\phi_+ + U\phi_+, i\phi_+ - iU\phi_+).$$

By taking linear combinations of the entries we see that for this sequence $\phi_+^n \to \phi_+$ and $U_n\phi_+^n \to U\phi_+$, and to wrap things up Lemma 10 yields the claimed strong convergence of the U_n's towards U as needed. □

Remark 13. We present here a more transparent way of proving $B_n \to B$ in the strong resolvent sense in Theorem 12(a) than the one presented above which in particular avoids the use of Corollary 9 and hence of Theorem 8.

Define the subspace $V := \{\phi_+ + U\phi_+ \mid \phi_+ \in \mathcal{H}_+\}$ in $\mathcal{H}$ and write

$$\mathcal{H} = R(B+i) = R(A+i) + R(B|_V + i).$$

Now since we assume $\mathrm{Gr}(A) \subseteq \Gamma_\infty$ the convergence of $(B_n+i)^{-1}$ towards $(B+i)^{-1}$ on $R(A+i)$ is proved as in (iii)⇒(i) in Theorem 8. Notice then that

$$(B+i)(\phi_+ + U\phi_+) = 2i\phi_+ \qquad \text{and} \qquad (B_n+i)(\phi_+^n + U_n\phi_+^n) = 2i\phi_+^n$$

for any $\phi_+ \in \mathcal{H}_+$ and $\phi_+^n \in \mathcal{H}_+^n$. This proves that $R(B|_V + i) = \mathcal{H}_+$, and for each $\phi_+ \in \mathcal{H}_+$ we can use Lemma 10 to find a sequence $\{\phi_+^n\}_{n=1}^\infty \subseteq \mathcal{H}$ so that $\phi_+^n \in \mathcal{H}_+^n$ for each n and

$$\begin{aligned}
&\|(B_n+i)^{-1}\phi_+ - (B+i)^{-1}\phi_+\| \\
&\qquad \le \|(B_n+i)^{-1}\phi_+ - (B_n+i)^{-1}\phi_+^n\| + \|(B_n+i)^{-1}\phi_+^n - (B+i)^{-1}\phi_+\| \\
&\qquad \le \|\phi_+ - \phi_+^n\| + \frac{1}{2}\|(\phi_+^n + U_n\phi_+^n) - (\phi_+ + U\phi_+)\| \longrightarrow 0.
\end{aligned}$$

■

We can now use Theorem 12 to prove various statements of the form (1). Taking $A_n \to A$ to be in terms of strong convergence of the orthogonal projections onto the graphs, i.e. $P_n \to P$ strongly, we have also $\mathrm{Gr}(A) \subseteq \Gamma_\infty$ due to Proposition 7, and thus we get a particularly clean statement.

Corollary 14. Consider the set-up in Theorem 12 and suppose $P_n \to P$ strongly. Then $B_n \to B$ in the strong resolvent sense if and only if $U_n \to U$ strongly. □

The downside of Corollary 14 is, however, that the condition $P_n \to P$ strongly is often not easy to verify in concrete cases. Another approach is to assume the convergence of the A_n's only in the sense that $\mathrm{Gr}(A) \subseteq \Gamma_\infty$. We note that this is a strictly weaker notion of convergence than strong convergence of the graph projections, so one cannot expect the implications of this assumption to be as strong as the equivalence between strong convergence of the B_n's and of the U_n's in Corollary 14. Another application of Proposition 7 yields:

Corollary 15. Consider the set-up in Theorem 12 and suppose $\mathrm{Gr}(A) \subseteq \Gamma_\infty$. Then $U_n \to U$ strongly if and only if both $B_n \to B$ in the strong resolvent sense and $\mathrm{Gr}(A^*) \subseteq \Gamma_\infty^*$. □

An obvious question now arises: Is this the best we can do? In particular we can in the light of Corollary 14 ask whether the condition $\mathrm{Gr}(A^*) \subseteq \Gamma_\infty^*$ in Corollary 15 is actually needed. As a matter of fact it is by the following observations.

Remark 16. We do not in general have the result "Suppose $\mathrm{Gr}(A) \subseteq \Gamma_\infty$. Then $U_n \to U$ strongly if and only if $B_n \to B$ in the strong resolvent sense." as the example below shows. Even changing $\mathrm{Gr}(A) \subseteq \Gamma_\infty$ to $A = \mathrm{str.gr.lim}\, A_n$ does not make the statement true. The backbone of the example is the extension theory for a well-studied class of operators on $L^2(\mathbb{R}^3) = \mathcal{H}$. This is treated in for example [3] I.1.1 to which we refer for the details.

Let $\{y_n\}_{n=1}^\infty \subseteq \mathbb{R}^3$ be a sequence yet to be specified and define for each n the operator A_n to be the closure of $-\Delta$ on $C_c^\infty(\mathbb{R}^3 \setminus \{y_n\})$. One can now find the deficiency subspaces

$$\mathcal{H}_\pm^n = \mathbb{C}\phi_\pm^n, \qquad \phi_\pm^n(x) = \frac{e^{i\sqrt{\pm i}|x-y_n|}}{4\pi|x-y_n|}$$

where $\mathrm{Im}\sqrt{\pm i} > 0$. Moreover, if one defines a self-adjoint extension B_n of A_n by the unitary map $U_n : \mathcal{H}_+^n \ni \phi_+^n \mapsto -\phi_-^n \in \mathcal{H}_-^n$ as in Section 1 then $B_n = B$ is actually the free Laplacian $-\Delta$ defined on the Sobolev space $H^2(\mathbb{R}^3)$ *independently* of n. Now we have the orthogonal decomposition

$$\mathrm{Gr}(B) = \mathrm{Gr}(A_n) \oplus \mathbb{C}(\phi_+^n - \phi_-^n, i\phi_+^n + i\phi_-^n) =: \mathrm{Gr}(A_n) \oplus \mathbb{C}v_n,$$

and consequently $\mathrm{Gr}(A_n)$ is the orthogonal complement of $\mathbb{C}v_n$ in $\mathrm{Gr}(B)$ for each n. Notice now that the v_n's depend only on the y_n's. Choosing y_n so that $|y_n| \to \infty$ it is not difficult to realize that the sequences $\{\phi_\pm^n\}_{n=1}^\infty$ converge weakly towards 0 in $L^2(\mathbb{R}^3)$: This follows from the fact that they are translations of a fixed L^2-function. With such sequence of y_n's we get thus

$$\langle(\phi,\psi),v_n\rangle = \langle\phi,\phi_+^n\rangle - \langle\phi,\phi_-^n\rangle + i\langle\psi,\phi_+^n\rangle + i\langle\psi,\phi_-^n\rangle \longrightarrow 0$$

for all $(\phi,\psi)\in\mathcal{H}\oplus\mathcal{H}$, i.e. $v_n\to 0$ weakly in $\mathcal{H}\oplus\mathcal{H}$ and hence in $\mathrm{Gr}(B)$.

We observe from the above facts that by choosing a sequence of y_n's which is a fixed $y_n = y_0$ for n odd and with $\{y_{2n}\}_{n=1}^{\infty}$ unbounded we can make the sequence $\{\mathrm{Gr}(A_n)\}_{n=1}^{\infty}$ of subspaces of the Hilbert space $\mathrm{Gr}(B)$ into a sequence like $\{V_n\}_{n=1}^{\infty}$ in Remark 4. Consequently, the operator $A = A_1$ is the strong graph limit of the A_n's (and of course $B_n \to B$), but the orthogonal projections onto the graphs $\mathrm{Gr}(A_n)$ do not converge strongly towards the orthogonal projection onto $\mathrm{Gr}(A)$, and hence Theorem 12(a) tells us that we cannot have $U_n \to U$ strongly. Alternatively this can be checked more directly by using Lemma 10. ■

We conclude by proving a simple requirement for having $\mathrm{Gr}(A)\subseteq\Gamma_\infty$, thus providing a procedure for checking the assumptions in Corollary 15. Recall that a core for a closed operator A is a subspace of $D(A)$ satisfying that the restriction of A to this has closure A. We obtain now:

Proposition 17. Assume that $\mathcal{D}$ is a common core for A and all A_n's. If $A_n\phi\to A\phi$ for all $\phi\in\mathcal{D}$ then $\mathrm{Gr}(A)\subseteq\Gamma_\infty$.

Proof. The assumption tells us that $\Gamma_{\mathcal{D}} := \{(\phi,A\phi)\mid \phi\in\mathcal{D}\}\subseteq\Gamma_\infty$. Thus, if we argue that Γ_∞ is closed, we have also $\mathrm{Gr}(A) = \overline{\Gamma_{\mathcal{D}}}\subseteq\Gamma_\infty$. But closedness is a general property of any strong limit of subspaces by the following argument:

Let $\{V_n\}_{n=1}^{\infty}$ be any sequence of subspaces of a Hilbert space $\mathcal{H}$ and denote as usual its strong limit by V_∞. If we consider an arbitrary convergent sequence $\{x_k\}_{k=1}^{\infty}\subseteq V_\infty$ with limit x_0 then we need only to find a sequence $\{\widetilde{x}_n\}_{n=1}^{\infty}\subseteq\mathcal{H}$ with $\widetilde{x}_n\in V_n$ for all n such that $\widetilde{x}_n\to x_0$ in order to obtain $x_0\in V_\infty$ and hence prove that V_∞ is closed. We now construct such sequence. Firstly we choose for each k a sequence $\{x_n^k\}_{n=1}^{\infty}$ with $x_n^k\in V_n$ for all n and $x_n^k\to x_k$, and then we take natural numbers $N_1<N_2<N_3<\cdots$ so that $\|x_n^k - x_k\| < 1/k$ for all $n\geq N_k$. Defining $\widetilde{x}_n := x_n^1$ for $n = 1,2,\dots,N_2-1$; $\widetilde{x}_n := x_n^2$ for $n = N_2,\dots,N_3-1$ and generally $\widetilde{x}_n := x_n^k$ for $n = N_k,\dots,N_{k+1}-1$ one can check using the triangular inequality that this is indeed a sequence with the properties we seek. □

Example 18. To make things even more concrete than requiring pointwise convergence of the A_n's on a common core, we can ask what this means for differential operators like those in Example 1. To simplify things let us consider a sequence of Schrödinger operators – that is, the A_n's are the closures of $-\Delta+\Phi_n$ defined on $C_c^\infty(\Omega)\subseteq L^2(\Omega)$ for some open set $\Omega\subseteq\mathbb{R}^d$ and some potentials Φ_n (say, real-valued and continuous) on this set. Hence, $C_c^\infty(\Omega)$ is a common core for the A_n's and also for $A = -\Delta+\Phi$ if we define this in the same manner. Now, for any $\phi\in C_c^\infty(\Omega)$,

$$\|A_n\phi - A\phi\|^2 = \|\Phi_n\phi - \Phi\phi\|^2 = \int_\Omega |\phi|^2|\Phi_n-\Phi|^2\,dx \leq \|\phi\|_\infty^2\int_{\mathrm{supp}\,\phi}|\Phi_n-\Phi|^2\,dx$$

where $\|\cdot\|_\infty$ is the supremum norm. Now if $\Phi_n \to \Phi$ in $L^2_{\mathrm{loc}}(\Omega)$ then we conclude that $A_n\phi \to A\phi$ for all $\phi \in C_c^\infty(\Omega)$. If, on the other hand, we assume the latter, then we see that $\Phi_n \to \Phi$ in $L^2(K)$ for any compact subset $K \subseteq \Omega$ by choosing $\phi \equiv 1$ on K, i.e. we get $\Phi_n \to \Phi$ in $L^2_{\mathrm{loc}}(\Omega)$. Being able to consider only local L^2-convergence is often desirable if one deals for example with potentials with singularities. ▲

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Comments

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Bibliography

[1] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics. II Fourier Analysis, Self-adjointness*. Academic Press, 1975.

[2] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics. I Functional Analysis*. Academic Press, 2 edition, 1980.

[3] Sergio Albeverio, Friedrich Gesztesy, Raphael Høegh-Krohn, and Helge Holden. *Solvable Models in Quantum Mechanics*. Springer-Verlag, 1988.

[4] Gerd Grubb. *Distributions and Operators*. Springer, 2009.

[5] Fabian Portmann, Jérémy Sok, and Jan Philip Solovej. Self-adjointness and spectral properties of dirac operators with magnetic links. *Journal de Mathématiques Pures et Appliquées*, 119:114–157, 2018. DOI: 10.1016/j.matpur.2017.10.010.

Chapter 4

An elementary mathematical approach to the scattering length

4.1 Introduction

In this chapter we consider the concept of scattering lengths of a relatively large class of potentials. In the literature on both the physical and mathematical aspects of quantum theory it appears in many forms depending heavily on the context. Prominently, it arises in the theory of 3-dimensional dilute Bose gases where the celebrated Lee-Huang-Yang formula (see [LHY57][1]) expresses the asymptotic ground state energy of the gas at small densities to leading orders only in terms of the scattering length and the density – even though the gas itself is described by the full behaviour of the potential. The standard interpretation of the scattering length in this context is as an *effective range* of the potential. It also appears in the context of scattering theory on both the mathematical and physical side of things – but in both cases mainly due to its physical interpretation as the *natural scattering parameter*, cf. [RS79] p136.

The purpose of this chapter is twofold: On the one hand, as it is explained below in subsection 4.1.3, there are very appealing technical reasons to take a slightly different approach to introducing the concept of scattering lengths than the two mentioned above. This is what we do in this chapter. On the other hand, we believe that we present the theory in a sufficiently detailed way so that a relatively deep understanding of many of the key properties of the scattering length and its relation to other important concepts can be motivated and obtained almost only on a mathematical basis. In other words, we wish to detach ourselves from the physical motivation for introducing the scattering length and instead make it an object of significant mathematical interest on its own! As a positive side-effect, this also means that our presentation of many interesting and important concepts of the general theory is quite self-contained.

4.1.1 First examples and intuition

Let us for a moment use the simplest possible examples to explain how we would like to think about the scattering length of a potential $V\colon \mathbb{R}_+ \to \mathbb{R}$. Consider to this end $V := \mathbb{1}_{(0,1)}$ and the associated equation $f'' = Vf$ which we from this point call the *scattering equation*. Solving this (in the distributional sense) subject to the boundary

[1] For the current status of the mathematical treatment we refer the reader to [FS23] and [BCS21] and the references herein.

condition $f(0) = 0$ we obtain

$$f(x) = \begin{cases} c \cdot \sinh(x) & \text{for } x \in (0,1] \\ c \cdot (\sinh(1) - \cosh(1) + \cosh(1)x) & \text{for } x \in (1,\infty) \end{cases}$$

for some constant c and notice that in particular f is linear on $(1,\infty)$. It is clear that this will generally be the case as long as the support of V lies in $(0,1]$ and, more generally, f will be linear from a point onwards whenever V has compact support[2]. That is, $f(x) = \alpha(V) + \beta(V)x$ for some V-dependent constants $\alpha(V)$ and $\beta(V)$ up to an overall constant near infinity for such potentials. In this set-up we call the fraction $a(V) := \alpha(V)/\beta(V)$ the *scattering length* of V. For the concrete potential above we get thus

$$a(V) = a(\mathbb{1}_{(0,1)}) = \frac{\sinh(1) - \cosh(1)}{\cosh(1)} = -\frac{2}{1+e^2}.$$

Now, for some purposes this number will be interesting by itself, but we will additionally pay a great amount of attention to what happens to $a(V)$ when one varies the potential V. A nice illustration of this can be obtained by considering $a(CV)$ where $V := \mathbb{1}_{(0,1)}$ as before and $C \in \mathbb{R}$ is a constant that we can vary freely. Solving the scattering equation $f_C'' = CVf_C$ as above we see that, up to an overall constant,

$$f_C(x) = \begin{cases} \sinh(\sqrt{C}x) & \text{for } x \in (0,1] \\ \sinh(\sqrt{C}) - \sqrt{C}\cosh(\sqrt{C}) + \sqrt{C}\cosh(\sqrt{C})x & \text{for } x \in (1,\infty) \end{cases}$$

if $C > 0$ and

$$f_C(x) = \begin{cases} \sin(\sqrt{-C}x) & \text{for } x \in (0,1] \\ \sin(\sqrt{-C}) - \sqrt{-C}\cos\sqrt{-C}) + \sqrt{-C}\cos(\sqrt{-C})x & \text{for } x \in (1,\infty) \end{cases}$$

if $C < 0$. Of course we have $f(x) = x$ for $C = 0$. We are now interested in tracking the behaviour of $a(CV)$ when letting C tend towards ∞ and $-\infty$ respectively. A straightforward calculation yields

$$a(CV) = \begin{cases} C^{-1/2}\tanh(\sqrt{C}) - 1 & \text{for } C > 0 \\ 0 & \text{for } C = 0 \\ (-C)^{-1/2}\tan(\sqrt{-C}) - 1 & \text{for } C < 0 \end{cases}$$

from which we make the following observations:

1) When ignoring the (perhaps at this point a bit disturbing) values of $C < 0$ where $\tan(\sqrt{-C})$ is not well-defined, the quantity $a(CV)$ is a differentiable function of C, and a simple calculation shows that the derivative $da(CV)/dC$ is everywhere negative. Hence, at least locally, the scattering length is decreasing in C. These are examples of the fundamental fact that the scattering length of a potential is a

[2]Let us remark at this point also that this is true in an even wider sense: If the potential has "almost compact support" then f will be "almost linear" near infinity both things in a sense to be made much more precise below.

both continuous and monotone function of the potential. This continuity should of course be understood in an appropriate topology, and the monotonicity of the scattering length is a consequence of pointwise monotonicity of the potentials. These properties of the scattering length will be stated properly and proved for a very natural and quite large class of potentials in Section 4.3 below.

2) If $C \to \infty$ we find that $a(CV)$ converges towards -1 monotonely from above. Looking at $-a(CV)$ instead – the need for doing this is just a consequence of our sign convention when defining $a(CV)$ – this completely supports the Bose gas interpretation of the scattering length as the effective range of the potential briefly mentioned above. Indeed, looking at the scattering solution f_C from a point far from the origin one first of all sees a solution that depends only on $-a(CV)$ and not on the complete structure of CV. Secondly, it is an easy check that the solution gets closer and closer to what one obtains when solving the free scattering equation $f'' = 0$ with the condition $f(1) = 0$. An interpretation of this is that the potential CV for large C almost prohibits particles from being closer than a distance of 1 to the origin (or, for the Bose gas, to each other) since the boundary condition is virtually moved to 1 instead of 0. Another way of visualizing this is to imagine solving the scattering equation $f'' = V_{\text{h.c.}}f$ with a so-called "hard core potential" with radius 1, i.e. $V_{\text{h.c.}}(x) = +\infty$ for $x \leq 1$ and $V_{\text{h.c.}}(x) = 0$ for $x > 1$ that forces the solution f to be constantly 0 on $(0,1)$ until it is "released" at $x = 1$.

   In the simple case just explained the conclusion seems very natural since CV actually converges pointwise monotonely towards exactly the hard core potential. However, many of the observations are also relevant more generally: Looking at the solution of a scattering equation with virtually any in some sense "short-range" potential W from a point far from the origin, what one sees will almost be a linear solution depending only on the scattering length of the potential. Moreover, this solution will be the same as one gets when solving the free scattering equation $f'' = 0$ with the condition $f(-a(W)) = 0$ or, equivalently, when one solves the scattering equation with the hard core potential with range $-a(W)$ (whenever this is non-negative) which can thus be considered the effective range of the potential.

3) If $C \to -\infty$ there is no simple convergence of $a(CV)$ as there is when $C \to \infty$. On the other hand some interesting phenomena that will never be seen for non-negative potentials occur. Especially when looking at the scattering solution f_C things are looking different for $C < 0$ than for $C > 0$. Simply considering the expression $f_C(x) = \sin(\sqrt{-C}x)$ which is valid up to an overall constant on $(0,1]$ for negative C we observe that the scattering solution in this case oscillates between positive and negative values on this interval. Moreover, the more negative the C the more oscillations take place. This should be compared to the situation with $C > 0$. In fact, a solution to $f'' = Wf$ with any non-negative potential W – for example $W = CV$ for a positive C – cannot possibly change sign: If it starts out positive it will stay so forever since it is then forced to be convex, and if it starts out negative it will stay so forever since it is then forced to be concave.

A way of understanding this different behaviour of the scattering solutions in terms of Schrödinger operators is beautifully captured by the Sturm-Liouville oscillation theorem. When looking at the one-dimensional differential operator $H = -d^2/dx^2 + W$ on $L^2(\mathbb{R}_+)$ with a Dirichlet boundary condition at the origin for some potential W it says that: The number of negative eigenvalues of H is exactly the number of zeroes of the solution to the equation $f'' = Wf$ with $f(0) = 0$ which is in this context often called the 0 energy solution since morally $Hf = 0$. As observed above taking W to be non-negative means that f has no zeroes, and hence H has no negative eigenvalues matching perfectly the fact that then $H \geq -d^2/dx^2 \geq 0$. The general oscillation theory is explained in detail and adapted to our set-up in Section 4.4.

We conclude that as $C \to -\infty$ the Schrödinger operator $H = -d^2/dx^2 + CV$ gets more and more negative eigenvalues. Additionally, one can check from the expression above that the "new" zeroes and hence the new eigenvalues enter exactly the moment after $\tan(\sqrt{-C})$ is not well defined. Just before this point (when we *decrease* C), $a(CV)$ increases towards $+\infty$ and just after it comes up from $-\infty$ and the operator has obtained one more negative eigenvalue. Between the "points of new eigenvalues" the scattering length simply increases from $-\infty$ to ∞. This in some sense periodic behaviour of the scattering length and its implications will be of central interest to us later on in Section 4.4, and as it will only appear as the varying potentials get more and more negative, this interest also partly motivates our sign convention for the scattering length: If the Shchrödinger operators H_t associated to some parametrized family of potentials V_t, $t \geq 0$, gets more and more negative eigenvalues as $t \to \infty$ then it might be convenient to let the scattering length of these potentials (which describe the appearance of the eigenvalues) be increasing as well.

4.1.2 Relation between the 3- and 1-dimensional scattering problem

Let us now briefly discuss how the examples in Subsection 4.1.1 and, more generally, the theory that we will introduce throughout the present chapter actually arise from the physically more relevant 3-dimensional scattering equation.

In short, determining the scattering length $a(V_0)$ of some "short range" potential $V_0 : \mathbb{R}_+ \to \mathbb{R}$ amounts to finding the asymptotic behaviour of a function $g : \mathbb{R}^3 \to \mathbb{R}$ that solves the following problem: Define the 3-dimensional radially symmetric potential $V : \mathbb{R}^3 \to \mathbb{R}$ by $V(x) = V_0(|x|)$ and let g be the solution to the 3-dimensional scattering equation,

$$\Delta g = Vg, \qquad g \text{ is radially symmetric and regular, say } g \in C(\mathbb{R}^3).$$

To see this write $g(x) = g_0(|x|)$ for some $g_0 \in C([0,\infty))$ and define the function $f(r) := rg_0(r)$ for $r \in \mathbb{R}_+$. Then writing the Laplace operator in spherical coordinates yields

$$\frac{1}{|x|}V_0(|x|)f(|x|) = V_0(|x|)g_0(|x|) = V(x)g(x) = \Delta g(x) = \frac{1}{|x|} \cdot \frac{d^2}{dr^2}\Big(rg_0(r)\Big)\Big|_{r=|x|} = \frac{1}{|x|}f''(|x|),$$

and consequently $f'' = V_0 f$. Moreover, f extends continuously to $r = 0$ with $f(0) = \lim_{r\to 0} r g_0(r) = 0$. Now, cf. the discussion above,

$$f(r) \approx \alpha(V_0) + \beta(V_0) r \;\propto\; a(V_0) + r$$

up to an overall constant for large r, and correspondingly $g(x) \approx 1 + a(V_0)/|x|$ is described only in terms of the scattering length for large (norms of) x. It is in other words evident that there is a close connection between the 3- and 1-dimensional scattering problem.

In a more physical language the condition that g should be radial is phrased as solving the problem of s-wave scattering, and in that sense what we call simply the scattering length (of a 1-dimensional potential) can be seen also as the s-wave scattering length of a radially symmetric 3-dimensional potential. This viewpoint additionally explains our perhaps at first sight arbitrary boundary condition $f(0) = 0$ as this arises simply from the very natural regularity condition on g in the 3-dimensional problem.

4.1.3 Our approach in context

Focusing on the fully rigorous treatments of the scattering length there exist at least two rather different approaches to the topic which are both relatively widely used and have some mathematical depth:

1) In the following all concepts and quantities are set in 3-dimensional space. Assume that V is radially symmetric and non-negative (or at least that the associated Schrödinger operator $-\Delta + V$ has no bound states). Then the scattering length a of V can be defined through a variational principle – by considering the radial minimizer ϕ_0 of the quadratic form associated to $-\Delta + V$,

$$\mathcal{E}[\phi] = \int |\nabla\phi|^2 + V|\phi|^2 \, dx, \tag{4.1}$$

with suitable boundary conditions, and observing its asymptotic behaviour[3] for large x, i.e. $\phi_0 \approx 1 - a/|x|$ as the sign convention here is typically the opposite of ours. This definition morally agrees with the observations in Subsection 4.1.2 above since ϕ_0 satisfies the Euler-Lagrange equation for the functional (4.1) which happens to be exactly the scattering equation $\Delta\phi_0 = V\phi_0$. For the details we refer to [LY01] and [Lie+05], but sadly no comprehensive treatment of this approach is collected in any single reference. Instead, the theory is scattered around research papers where relevant properties are proven when they are needed for showing more physically interesting results.

Though it is often assumed that V has compact support in this approach, it is not strictly needed, and actually very general potentials are allowed. Assuming non-negativity and compact support any measurable and radial $V\colon \mathbb{R}^3 \to [0,\infty]$ can be assigned a scattering length, and we can additionally allow adding a positive radial measure. This includes many potentials that will not be treated in our approach,

[3]Concretely, the scattering length is defined as a function of the minimal energy $\mathcal{E}[\phi_0]$ which by a partial integration in (4.1) has this interpretation.

but, on the other hand, the hard assumption on the Schrödinger operator having no bound states is truly restrictive from many different viewpoints, and it would be very desirable not to be limited by this for a general theory for the scattering length. Therefore, we seek an alternative to this approach.

2) A second way of introducing the scattering length rigorously is through the "spectral shift function" in the less elementary mathematical (quantum) scattering theory. We provide below a concise review of this, assuming at all times that the potential V satisfies suitable conditions. For details we refer to for example [RS79] XI.3, XI.4 and XI.8 on which we also base our presentation.

The fundamental objects of scattering theory are the wave operators

$$\Omega^{\pm} := \operatorname*{s-lim}_{t\to\mp\infty} e^{itH}e^{it\Delta}$$

with s-lim the strong limit and $H = -\Delta + V$ the usual Schrödinger operator. We wish to determine how different potentials affect particles that over time evolve according to Schrödinger's equation. As a reference one uses here a so-called free particle $\psi_t^{\text{Free}} = e^{it\Delta}\psi$ which is in some fixed state ψ at time $t = 0$. This should be compared to the particle which as $t \to -\infty$ looks like $e^{it\Delta}\phi$ for some other fixed state ϕ but which then evolves according to the Schrödinger equation including the potential V. At time $t = 0$ this is described by $\Omega^+\phi$ and thus its general form at time t is $\phi_t = e^{-itH}\Omega^+\phi$. Now, observe that

$$\langle \psi_t^{\text{Free}}, \phi_t\rangle = \langle e^{itH}e^{it\Delta}\psi, \Omega^+\phi\rangle \longrightarrow \langle \Omega^-\psi, \Omega^+\phi\rangle = \langle \psi, (\Omega^-)^*\Omega^+\phi\rangle$$

as $t \to \infty$ for any states ϕ and ψ, i.e. the operator $S := (\Omega^-)^*\Omega^+$ – the S-matrix – describes exactly how introducing a potential changes the long-term behaviour of particles compared to free particles. It turns out the S-matrix is unitary – at least on a suitable subspace. Furthermore, since it commutes with the Laplace operator, it is (unitarily equivalent to) a decomposable operator

$$S = \int_{\mathbb{R}_+} S(E)\,dE, \qquad S(E)\colon L^2(S^2) \longrightarrow L^2(S^2),$$

where S^2 is the unit sphere, and each of the unitary operators $S(E)$ leaves the constant function $\mathbb{1}_{S^2}$ invariant. This yields for each energy level $E \in \mathbb{R}_+$ a complex number $s(E)$ with unit norm by the relation $S(E)\mathbb{1}_{S^2} = s(E)\mathbb{1}_{S^2}$, and the spectral shift function $\delta\colon \mathbb{R}_+ \to \mathbb{R}$ is then finally defined by putting $s(E) = e^{2i\delta(E)}$. This morally describes in a convenient way the effect of the potential in the radial part of wave functions (in other words, as mentioned above, it describes s-wave scattering).

From the spectral shift function one can then define the scattering length as

$$a := \lim_{E\to 0} \frac{\delta(E) - \delta(0)}{\sqrt{E}} = \lim_{x\to\infty} \frac{f(x) - xf'(x)}{f'(x)} \tag{4.2}$$

where f is as in Subsection 4.1.1, and the last equality is in many cases not too difficult to verify once the heavy machinery described above is fully established.

The usual next step in this approach is then to apply a wide range of complicated concepts from scattering theory (relying heavily on rather abstract spectral-theoretic results) to motivate a as a natural "scattering parameter". But here the story more or less ends in the sense that further development of the theory is phrased in terms of quantities which might be closely related to – but which is not – the scattering length. An example of such quantity is the spectral shift function on which there exists a wide variety of detailed and rigorous results, also to some extent aligning with what we achieve in this chapter[4]. This leaving the scattering length behind might be a consequence of the fact that proving the existence of the first limit in (4.2) is a non-trivial task; it requires strictly more than just the spectral shift function to be defined which is in itself a topic that one can spend dozens of pages understanding properly. Altogether, the “scattering theory approach” to the scattering length is a very general and deep one, but it uses a lot of energy for achieving largely only the justification of the underlying physical intuition[5]. Therefore, we also seek an alternative to this approach.

As just described in our above review of two examples of already existing approaches to the theory of the scattering length at least these both have significant shortcomings and/or inconveniences. What we suggest in this chapter is a third approach explaining the mechanisms of the examples in Subsection 4.1.1 for a large class of potentials without using unnecessarily heavy machinery:

3) Instead of taking the long route of defining the scattering length through the spectral shift function we simply define it to be the last limit in (4.2). This turns out to be rather convenient since determining many potentials for which this limit exists is a manageable task. For example: As long as a potential is dominated by $x^{-2+\varepsilon}$ near the origin and by $x^{-3-\varepsilon}$ at infinity, it has a well-defined scattering length. Moreover, the space of allowed potentials can be described more or less as a weighted L^1-space, and the scattering length itself turns out to be a continuous function of potentials varying in this space! This truly opens the door to a simple theory for the scattering length that can include as a key element also a controlled continuous variation of the potentials – so that there is a chance of describing the phenomena in the example from Subsection 4.1.1 for very general potentials.

   Additionally, this approach does in no way need the assumption of a non-negative potential V (in particular, the associated Schrödinger operator can have bound states) since it apart from very weak regularity assumptions only puts conditions on the asymptotic behaviour of potentials. On the other hand it still has the feature that the scattering length explains how the asymptotically linear scattering solution is looking near infinity. In fact, inserting a linear function $f(x) = x + a$ – corresponding to a potential V with compact support – into our definition, we see

[4] Levinson's theorem is a nice instance of this, cf. [RS79] XI.8.E and Theorem 4.29

[5] We should remark at this point that the treatment of scattering theory presented Chapter 4 of [Yaf10] is a noteworthy exception to many of our complaints discussed here. To some extent this presentation is carried out with the same mindset, we intend to have for parts of Sections 4.2 and 4.3 below.

that $f(x) - xf'(x) \equiv a$ and $f'(x) \equiv 1$ so that scattering length is indeed the expected one.

Altogether we believe that this is a relatively simple approach that is still capable of rigorously describing most fundamental properties of the scattering length as a function defined on a large class of potentials.

We begin now the systematic and rigorous treatment of the scattering length following this third approach. In Section 4.2 we set the scene by solving the general scattering equation as explicitly as possible and hereby controlling the scattering solutions. Then, in Section 4.3, the scattering length itself is introduced, and all of its fundamental (although most of them are rather non-trivial) properties are proven. As a final topic Section 4.4 explains in detail how the picture of new eigenvalues of the associated Schrödinger operator appearing from the example in Subsection 4.1.1 is explained satisfactorily by our approach in a very general set-up.

4.2 Scattering solutions

This section lays the foundation for further studies of the scattering length by providing a very general theory for solutions of scattering equations. The assumptions put on the potentials are exactly the ones that allow the methods used to apply, yielding a wide class of admissible potentials.

Firstly we prove the existence (and later on uniqueness) of certain solutions to the scattering equation. These are very well-known results sometimes treated under the name of "the Cauchy problem", see for example [DG20] 2.5 and [RS75] XI.8E – our presentation of this part is basically a modification of the latter. Secondly, we combine the technique from the existence proof with the binomial formula to obtain bounds on the variation of scattering solutions in terms of the variation of the potentials in the relevant scattering equations. This part is definitely non-standard in textbooks, and the bounds yield very natural and powerful continuity properties of the scattering solutions which we will soon be using to control the scattering length. The main results are collected in Proposition 4.10 for convenience.

4.2.1 The regular solution to the scattering equation

We consider in this subsection a measurable potential V on the positive real axis $\mathbb{R}_+$ which satisfies the crucial assumption

$$Q(x) := \int_0^x y|V(y)|\,dy < \infty \tag{4.3}$$

for all $x \in \mathbb{R}_+$. Firstly, we construct a regular solution f to the scattering equation $f'' = Vf$. Here, regular means that $f \in C^1([0,1))$ with $f(0) = 0$ and $f'(0) = 1$, and the equation is in the distributional sense. To this end we consider the integral kernel

$$K(x,y) = y\left(1 - \frac{y}{x}\right)V(y) \tag{4.4}$$

and define the "building blocks" $\{r_n\}_{n=0}^{\infty}$ of our regular solution by $r_0 \equiv 1$ and

$$r_{n+1}(x) = \int_0^x K(x,y) r_n(y)\, dy \tag{4.5}$$

for all other n. It is not difficult to see that each r_n is well-defined and continuous by the assumption (4.3) and induction. A key estimate for the construction is the following:

Lemma 4.1. For all $n \in \mathbb{N}_0$ and $x \in \mathbb{R}_+$ we have $|r_n(x)| \le Q(x)^n/n!$.

Proof. For $n = 0$ the inequality is clear. Now, if we suppose that it holds for some n then

$$|r_{n+1}(x)| \le \int_0^x |K(x,y) r_n(y)|\, dy \le \int_0^x y|V(y)| \frac{Q(y)^n}{n!}\, dy = \frac{Q(x)^{n+1}}{(n+1)!}$$

by the substitution $z = Q(y)$, $dz = y|V(y)|\, dy$. This completes the proof. □

The lemma leads towards the result of primary interest.

Proposition 4.2. The series

$$\sum_{n=0}^{\infty} r_n$$

converges uniformly on compact subsets of $[0,\infty)$ towards a function r. Putting $f(x) := xr(x)$ this f is a regular solution to the scattering equation.

Proof. The first part is a simple application of Lemma 4.1 and Weierstrass' M-test. The resulting r satisfies

$$1 + \int_0^x K(x,y) r(y)\, dy = 1 + \sum_{n=0}^{\infty} \int_0^x K(x,y) r_n(y)\, dy = 1 + \sum_{n=0}^{\infty} r_{n+1}(x) = r(x)$$

and thus

$$f(x) = x + \int_0^x K(x,y) x r(y)\, dy = x + \int_0^x K(x,y) \frac{x}{y} f(y)\, dy = x + \int_0^x (x-y) V(y) f(y)\, dy.$$

Consequently,

$$f'(x) = 1 + \int_0^x V(y) f(y)\, dy \tag{4.6}$$

and $f'' = Vf$, i.e. f satisfies the scattering equation as claimed (the reader might want to consult Appendix A below[6] for the details in the case of a non-continuous V). From the two last lines of equations it is also clear by taking $x \to 0$ that f is a regular solution. □

[6] Here we use in particular the fundamental theorem of calculus for distributions, Proposition A.2, and the Leibniz formula in a general set-up, Proposition A.4. Moving forward we will refer to these results simply by these names.

Now, Lemma 4.1 tells us not only how to construct the regular solution. It can also be used to estimate the difference between regular solutions of two scattering equations in terms of a certain distance between the corresponding potentials. Consider for this another potential $\widetilde{V}$ and denote by $\widetilde{r}_n$, $\widetilde{r}$, $\widetilde{f}$ and $\widetilde{Q}$ the quantities analogous to r_n, r, f and Q respectively, and by D the "distance"

$$D(x) := \int_0^x y|V(y) - \widetilde{V}(y)|\,dy.$$

In terms of this we have the following estimates:

Proposition 4.3. Let $x \in \mathbb{R}_+$. Then:

a) $|f(x) - \widetilde{f}(x)| \leq xD(x)\exp\big(Q(x) + \widetilde{Q}(x)\big)$,

b) $|f'(x) - \widetilde{f}'(x)| \leq D(x)\exp\big(Q(x) + \widetilde{Q}(x)\big)\min\{Q(x)+1, \widetilde{Q}(x)+1\}$.

The proof of Proposition 4.3 goes through a lemma in the proof of which the binomial formula plays a key role.

Lemma 4.4. For all $n \geq 1$ and $x \in \mathbb{R}_+$ we have $|r_n(x) - \widetilde{r}_n(x)| \leq D(x)(Q(x)+\widetilde{Q}(x))^{n-1}/(n-1)!$.

Proof. For $n = 1$ one observes that

$$|r_1(x) - \widetilde{r}_1(x)| \leq \int_0^x y|V(y)r_0(y) - \widetilde{V}(y)\widetilde{r}_0(y)|\,dy = \int_0^x y|V(y) - \widetilde{V}(y)|\,dy = D(x),$$

and for $n \geq 1$, by induction,

$$\begin{aligned}
|r_{n+1}(x) - \widetilde{r}_{n+1}(x)| &\leq \int_0^x y|V(y)r_n(y) - \widetilde{V}(y)\widetilde{r}_n(y)|\,dy \\
&\leq \int_0^x y|V(y) - \widetilde{V}(y)| \cdot |r_n(y)| + y|\widetilde{V}(y)| \cdot |r_n(y) - \widetilde{r}_n(y)|\,dy \\
&\leq \int_0^x y|V(y) - \widetilde{V}(y)| \cdot \frac{Q(y)^n}{n!} + y|\widetilde{V}(y)| \cdot \frac{D(y)(Q(y)+\widetilde{Q}(y))^{n-1}}{(n-1)!}\,dy \\
&\leq D(x)\Big(\frac{Q(x)^n}{n!} + \int_0^x y|\widetilde{V}(y)| \cdot \frac{(Q(y)+\widetilde{Q}(y))^{n-1}}{(n-1)!}\,dy\Big).
\end{aligned}$$

Since

$$\begin{aligned}
\int_0^x y|\widetilde{V}(y)| \cdot \frac{(Q(y)+\widetilde{Q}(y))^{n-1}}{(n-1)!}\,dy &= \frac{1}{(n-1)!}\sum_{k=0}^{n-1}\binom{n-1}{k}\int_0^x y|\widetilde{V}(y)|Q(y)^k\widetilde{Q}(y)^{n-1-k}\,dy \\
&\leq \frac{1}{(n-1)!}\sum_{k=0}^{n-1}\binom{n-1}{k}Q(x)^k\int_0^x y|\widetilde{V}(y)|\widetilde{Q}(y)^{n-1-k}\,dy \\
&= \frac{1}{(n-1)!}\sum_{k=0}^{n-1}\binom{n-1}{k}Q(x)^k\frac{\widetilde{Q}(x)^{n-k}}{n-k} \\
&= \frac{1}{n!}\sum_{k=0}^{n-1}\binom{n}{k}Q(x)^k\widetilde{Q}(x)^{n-k} = \frac{(Q(x)+\widetilde{Q}(x))^n}{n!} - \frac{Q(x)^n}{n!},
\end{aligned}$$

the lemma follows. □

Proof (of Proposition 4.3). a) This is a straightforward application of the Lemma 4.4 using the power series for the exponential function.

b) Very similarly to in the proof of Lemma 4.4 – and using again the power series for the exponential function – we observe by (4.6) that for example

$$
\begin{aligned}
|f'(x) - \widetilde{f}'(x)| &\le \int_0^x y|V(y)| \cdot |r(y) - \widetilde{r}(y)| + y|V(y) - \widetilde{V}(y)| \cdot |\widetilde{r}(y)|\, dy \\
&\le Q(x)D(x)\exp\Big(Q(x) + \widetilde{Q}(x)\Big) + D(x)\exp\Big(\widetilde{Q}(x)\Big).
\end{aligned}
$$

Since we can do this also with Q and $\widetilde{Q}$ interchanged, we obtain the result by estimating $\exp(-Q(x))$ and $\exp(-\widetilde{Q}(x))$ from above by 1. □

Finally, we observe that we can actually talk about *the* regular solution since it is unique.

Proposition 4.5. There is at most one regular solution f to the equation $f'' = Vf$.

Proof. Suppose f and g are two such solutions. Then $h := f - g \in C^1([0,\infty))$ solves $h'' = Vh$ and $h(0) = h'(0) = 0$. Hence, by the fundamental theorem of calculus for distributions,

$$|h'(x)| \le \int_0^x |h''(y)|\, dy = \int_0^x y|V(y)| \frac{|h(y)|}{y}\, dy$$

for all $x \in \mathbb{R}_+$. By induction this implies that $|h'(x)| \le c_b Q(x)^n/n!$ for all $x \in (0,b)$ and $n \in \mathbb{N}_0$ where $b > 0$ is arbitrary and $c_b > 0$ is a constant depending on b. Indeed, this assertion is clearly true for $n = 0$ by choosing $c_b = \sup_{x\in(0,b]}|h'(x)|$, and further we obtain with this choice from the above, and by induction,

$$|h'(x)| \le \int_0^x y|V(y)| \cdot |h'(\xi_y)|\, dy \le \int_0^x y|V(y)| c_b \frac{Q(y)^n}{n!}\, dy \le \frac{c_b Q(x)^{n+1}}{(n+1)!}$$

for each $n = 1,2,3,\ldots$ and $x \in (0,b)$ where $\xi_y \in (0,y) \subseteq (0,b)$. By taking $n \to \infty$ we see that $h'(x) = 0$ for all $x \in \mathbb{R}_+$, and consequently $h \equiv 0$, i.e. $f = g$ as claimed. □

4.2.2 The other solution to the scattering equation

In this subsection we discuss a solution, whenever such exists, f to the scattering equation $f'' = Vf$ on $\mathbb{R}_+$ which lies in $C^1([0,\infty))$ with $f(0) = 1$ and $f'(0) = 0$. Morally we simply need to replace the norm from $L^1(x\,dx)$ with that from[7] $L^1((1 \vee x)\,dx)$ in all assumptions and results in Subsection 4.2.1 for them to give results for this solution. Thus, we assume in this subsection

$$Q(x) := \int_0^x ys(y)|V(y)|\, dy < \infty$$

[7] We use throughout this chapter the symbols $\vee$ and $\wedge$ for maximum and minimum respectively.

where here and throughout the present subsection $s(y) := y^{-1} \vee 1$. If we define the integral kernel $K(x,y)$ as in (4.4) and put $r_0(x) = 1/x$ then we observe that the iterative definition of the functions $\{r_n\}_{n=1}^{\infty}$ as in (4.5) yields a sequence of well-defined continuous functions on $\mathbb{R}_+$ by our updated assumption. Now one has

Lemma 4.6. For all $n \in \mathbb{N}_0$ and $x \in \mathbb{R}_+$ we have $|r_n(x)| \le (Q(x)^n s(x))/n!$.

Proof. For $n = 0$ the inequality is clear. Now, if we suppose that it holds for some n then

$$|r_{n+1}(x)| \le \int_0^x |K(x,y) r_n(y)|\, dy \le \int_0^x ys(y)|V(y)| \frac{Q(y)^n}{n!}\, dy = \frac{Q(x)^{n+1}}{(n+1)!} \le \frac{Q(x)^{n+1} s(x)}{(n+1)!}$$

by the substitution $z = Q(y)$, $dz = ys(y)|V(y)|\, dy$. This completes the proof. □

Proposition 4.7. The series

$$\sum_{n=0}^{\infty} x r_n(x)$$

converges uniformly on compact subsets of $[0,\infty)$ towards a function $f \in C^1([0,\infty))$ which satisfies $f'' = Vf$, $f(0) = 1$ and $f'(0) = 0$.

Proof. Again, using Lemma 4.6, the first part is a simple application of Weierstrass' M-test. For the limit f we get

$$\begin{aligned} 1 + \int_0^x (x-y)V(y)f(y)\, dy &= 1 + \sum_{n=0}^{\infty} \int_0^x y(x-y)V(y) r_n(y)\, dy \\ &= 1 + \sum_{n=0}^{\infty} x \int_0^x K(x,y) r_n(y)\, dy = 1 + \sum_{n=0}^{\infty} x r_{n+1}(x) = f(x). \end{aligned}$$

From this it follows that

$$f'(x) = \int_0^x V(y) f(y)\, dy$$

and hence $f'' = Vf$ as well as $f(0) = 1$ and $f'(0) = 0$. □

Next, we state and prove the estimates of the difference of these solutions to the scattering equations for two different potentials. These are, also, completely analogous to the corresponding results for the regular solutions in Subsection 4.2.1. For this let $\widetilde{V}$, $\widetilde{r}_n$, $\widetilde{f}$ and $\widetilde{Q}$ as here (with the updated assumption on $\widetilde{V}$) and further

$$D(x) := \int_0^x ys(y)|V(y) - \widetilde{V}(y)|\, dy.$$

Then:

Lemma 4.8. For all $n \geq 1$ and $x \in \mathbb{R}_+$ we have $|r_n(x) - \widetilde{r}_n(x)| \leq D(x)(Q(x) + \widetilde{Q}(x))^{n-1}/(n-1)!$.

Proof. For $n = 1$ one observes that

$$|r_1(x) - \widetilde{r}_1(x)| \leq \int_0^x y|V(y)r_0(y) - \widetilde{V}(y)\widetilde{r}_0(y)|\,dy = \int_0^x |V(y) - \widetilde{V}(y)|\,dy \leq D(x).$$

For $n \geq 1$ we have

$$\begin{aligned}
|r_{n+1}(x) - \widetilde{r}_{n+1}(x)| &\leq \int_0^x y|V(y)r_n(y) - \widetilde{V}(y)\widetilde{r}_n(y)|\,dy \\
&\leq \int_0^x y|V(y) - \widetilde{V}(y)| \cdot |r_n(y)| + y|\widetilde{V}(y)| \cdot |r_n(y) - \widetilde{r}_n(y)|\,dy \\
&\leq \int_0^x ys(y)|V(y) - \widetilde{V}(y)| \cdot \frac{Q(y)^n}{n!} + y|\widetilde{V}(y)| \cdot \frac{D(y)(Q(y) + \widetilde{Q}(y))^{n-1}}{(n-1)!}\,dy \\
&\leq D(x)\Big(\frac{Q(x)^n}{n!} + \int_0^x ys(y)|\widetilde{V}(y)| \cdot \frac{(Q(y) + \widetilde{Q}(y))^{n-1}}{(n-1)!}\,dy\Big).
\end{aligned}$$

Now, by almost the exact same calculation as in the proof of Lemma 4.4,

$$\int_0^x ys(y)|\widetilde{V}(y)| \cdot \frac{(Q(y) + \widetilde{Q}(y))^{n-1}}{(n-1)!}\,dy \leq \frac{(Q(x) + \widetilde{Q}(x))^n}{n!} - \frac{Q(x)^n}{n!}$$

so that indeed

$$|r_{n+1}(x) - \widetilde{r}_{n+1}(x)| \leq D(x)\frac{(Q(x) + \widetilde{Q}(x))^n}{n!}$$

as claimed. □

These bounds gives easily

Proposition 4.9. The result from Proposition 4.3 holds word for word in the set-up of the present subsection. □

4.2.3 Overview of the scattering solutions

We collect here the results from the two preceding subsections together with some of their almost direct implications.

Proposition 4.10. Consider a measurable potential V defined in $\mathbb{R}_+$.

a) If

$$\int_0^x y|V(y)|\,dy < \infty$$

for all $x \in \mathbb{R}_+$ then there exists a unique solution $f \in C^1([0,\infty))$ to the equation $f'' = Vf$ with $f(0) = 0$ and $f'(0) = 1$.

b) The result in a) in particular defines a map

$$\mathscr{S}: L^1(\mathbb{R}_+, x\,dx) \ni V \longmapsto f \in C^1([0,\infty))$$

which has the following continuity properties: If $V_n \to V$ in $L^1(\mathbb{R}_+, x\,dx)$ then $x^{-1}\mathscr{S}(V_n) \to x^{-1}\mathscr{S}(V)$ and $\mathscr{S}(V_n)' \to \mathscr{S}(V)'$ uniformly on $\mathbb{R}_+$. In particular $\mathscr{S}(V_n)(x) \to \mathscr{S}(V)(x)$ for any fixed $x \in \mathbb{R}_+$.

c) If
$$\int_0^x |V(y)|\,dy < \infty \qquad \text{or, equivalently,} \qquad \int_0^x (1 \vee y)|V(y)|\,dy < \infty$$
for all $x \in \mathbb{R}_+$ then there exists a unique solution $f \in C^1([0,\infty))$ to the equation $f'' = Vf$ with $f(0) = 1$ and $f'(0) = 0$.

d) The result in c) in particular defines a map
$$\mathscr{T} : L^1(\mathbb{R}_+, (1 \vee x)\,dx) \ni V \longmapsto f \in C^1([0,\infty))$$
which has the following continuity properties: If $V_n \to V$ in $L^1(\mathbb{R}_+, (1 \vee x)\,dx)$ then $x^{-1}\mathscr{T}(V_n) \to x^{-1}\mathscr{T}(V)$ and $\mathscr{T}(V_n)' \to \mathscr{T}(V)'$ uniformly on $\mathbb{R}_+$. In particular $\mathscr{T}(V_n)(x) \to \mathscr{T}(V)(x)$ for any fixed $x \in \mathbb{R}_+$.

Proof. a) is treated in Subsection 4.2.1. To verify b) notice that if $V, \widetilde{V} \in L^1(\mathbb{R}_+, x\,dx)$ then Proposition 4.3(a) yields
$$\begin{aligned}\Big|\frac{f(x)}{x} - \frac{\widetilde{f}(x)}{x}\Big| &\le D(x)\exp\big(Q(x) + \widetilde{Q}(x)\big) \\ &\le \int_0^\infty x|V(x) - \widetilde{V}(x)|\,dx \cdot \exp\Big(\int_0^\infty x\big(|V(x)| + |\widetilde{V}(x)|\big)\,dx\Big) \longrightarrow 0\end{aligned}$$
whenever V approaches $\widetilde{V}$ in $L^1(\mathbb{R}_+, x\,dx)$. By a similar argument Proposition 4.3(b) gives the uniform convergence $\mathscr{S}(V_n)' \to \mathscr{S}(V)'$. For the uniqueness of f in c) we can use the fact that the space of solutions to the scattering equation $f'' = Vf$ is two dimensional (Lemma A.3). Hence, if $f_1(0) = 1 = f_2(0)$ and $f_1'(0) = 0 = f_2'(0)$ for some functions $f_1 \neq f_2$ from this space then these will span the entire space (since they must clearly be linearly independent). In particular $f'(0) = 0$ for any solution to $f'' = Vf$. But if V satisfies the assumption in c) it must also satisfy that in a) so that there is a solution f to the scattering equation with $f'(0) = 1$ contradicting this. This proves the uniqueness part of c). The remaining assertions in c) and d) follow analogously to those in a) and b) by using instead of the results from Subsection 4.2.1 those from Subsection 4.2.2. □

4.3 The scattering length – definition and properties

We study in this section an object which we will call the scattering length of a certain class of potentials. From this point onwards we will use the notation
$$\mathscr{L} := \{V \in L^1(\mathbb{R}_+, (x \vee x^2)\,dx) \mid V \text{ is real-valued}\}$$
for this class, and since clearly $\mathscr{L} \subseteq L^1(\mathbb{R}_+, x\,dx)$ we know from Proposition 4.10(a) that the regular scattering solution f to the scattering equation $f'' = Vf$ exists for all $V \in \mathscr{L}$.

We take the topology on $\mathscr{L}$ to be that coming from the usual norm on $L^1(\mathbb{R}_+,(x\vee x^2)\,dx)$. Our entrance to this main topic of the present chapter is the following:

Theorem / Definition 4.11. If $V\in\mathscr{L}$ and f is the regular solution to the associated scattering equation then the limits

$$\alpha(V):=\lim_{x\to\infty} f(x)-xf'(x) \qquad \text{and} \qquad \beta(V):=\lim_{x\to\infty} f'(x)$$

exist, are real and not both 0. We define *the scattering length of* V to be the number $a(V):=\alpha(V)/\beta(V)$. In the cases where $\beta(V)=0$ we write $a(V)=\pm\infty$.

Proof. Consider the function $w(x):=xf(1/x)$. One can check that this satisfies the scattering equation with the potential[8] $W(x):=x^{-4}V(1/x)$. Moreover, by the substitution $z=1/y$ we get

$$\int_0^x |W(y)|\,dy=\int_{1/x}^\infty z^2|V(z)|\,dz<\infty$$

for all $x\in\mathbb{R}_+$. This means by Proposition 4.10(a) and (c) that there exist both a solution g with $g(0)=0$, $g'(0)=1$ and a solution h with $h(0)=1$, $h'(0)=0$ to the scattering equation $w''=Ww$. As these span the space of solutions to the equation (cf. Lemma A.3) we can write $w=\alpha g+\beta h$ for some $\alpha,\beta\in\mathbb{R}$ (not both 0) and observe that in particular w and w' extends continuously to 0 with $w(0)=\beta$ and $w'(0)=\alpha$. Since also $f(x)=xw(1/x)$ it follows that

$$f(x)-xf'(x)=xw(1/x)-x\left(w(1/x)-\frac{w'(1/x)}{x}\right)=w'(1/x)\longrightarrow\alpha$$

and

$$f'(x)=w(1/x)-\frac{w'(1/x)}{x}\longrightarrow\beta$$

as $x\to\infty$. From the construction of f in Subsection 4.2.1 it is clear that this is a real-valued function whenever V is real-valued. Consequently, also $\alpha(V)$ and $\beta(V)$ must be real when $V\in\mathscr{L}$. □

Theorem / Definition 4.12. Denoting by $\alpha(V)$ and $\beta(V)$ the limits from Theorem 4.11, the maps

$$\mathscr{L}\ni V\longmapsto\alpha(V)\in\mathbb{R} \quad \text{and} \quad \mathscr{L}\ni V\longmapsto\beta(V)\in\mathbb{R}$$

are continuous. In particular, if $I\subseteq\mathbb{R}$ is an interval and $I\ni t\mapsto V_t\in\mathscr{L}$ is a continuous curve in $\mathscr{L}$ then

$$\gamma: I\ni t\longmapsto\beta(V_t)+i\alpha(V_t)\in\mathbb{C}\backslash\{0\}$$

is a continuous curve in $\mathbb{C}\backslash\{0\}$. A continuous argument function of γ is called a *scattering argument* of the curve $t\mapsto V_t$.

[8] Assuming sufficient regularity of V this is an easy check. See Lemma A.1 and the Leibniz formula in a general set-up (Proposition A.4) in Appendix A for the technical details in the general case.

Remark 4.13. Let $I \subseteq \mathbb{R}$ be an interval and $I \ni t \mapsto V_t \in \mathscr{L}$ a continuous curve. If $\theta\colon I \to \mathbb{R}$ is a scattering argument of this curve then we make the following important observation: Letting γ be as above and writing $\gamma(t)/|\gamma(t)| = \cos\theta(t) + i\sin\theta(t)$ we obtain

$$a(V_t) = \frac{\alpha(V_t)}{\beta(V_t)} = \frac{\Im\mathfrak{m}\,\gamma(t)}{\Re\mathfrak{e}\,\gamma(t)} = \frac{\sin\theta(t)}{\cos\theta(t)} = \tan\theta(t)$$

where we put $\tan((n+1/2)\pi) = \pm\infty$ for $n \in \mathbb{Z}$. Consequently, away from the points where $\theta(t) = (n+1/2)\pi$, the scattering argument describes exactly the qualitative behaviour of the scattering lengths of the V_t's and vice versa. ■

Proof (of Theorem 4.12). We use the notation from the proof of Theorem 4.11 and additionally the fact that the Wronskian of two solutions to the same scattering equation is constant on $\mathbb{R}_+$ – see Lemma A.5 for the general result. We obtain

$$\alpha(V) = w'(0)h(0) - w(0)h'(0) = w'(1)h(1) - w(1)h'(1) = f(1)h(1) - f'(1)h(1) - f(1)h'(1),$$

and similarly

$$\beta(V) = g'(0)w(0) - g(0)w'(0) = g'(1)w(1) - g(1)w'(1) = g'(1)f(1) - g(1)f(1) + g(1)f'(1)$$

since all function are also in $C([0,\infty))$. Suppose now that $V_n \to V$ in $\mathscr{L}$. Then clearly this convergence holds also in $L^1(\mathbb{R}_+, x\,dx)$, and by Proposition 4.10(b) and (d) we thus need only to show that $W_n \to W$ in $L^1(\mathbb{R}_+, (1 \vee x)\,dx)$ where $W_n(x) := x^{-4}V_n(1/x)$ in order to prove the desired continuity. The convergence $W_n \to W$ is verified by the substitution $y = 1/x$ in the integral below, yielding

$$\begin{aligned}\int_0^\infty (1 \vee x)|W_n(x) - W(x)|\,dx &= \int_0^\infty (x^{-4} \vee x^{-3})|V_n(1/x) - V(1/x)|\,dx \\ &= \int_0^\infty (y \vee y^2)|V_n(y) - V(y)|\,dy \longrightarrow 0\end{aligned}$$

as $n \to \infty$. □

Our next aim is to prove relevant monotonicity properties of the scattering length and the scattering argument. For this we begin with some lemmas.

Lemma 4.14. Consider a potential $V \in \mathscr{L}$ and the regular solution f to the associated scattering equation.

a) For any non-zero solution $g \in C^1([0,\infty))$ to the equation $g'' = Vg$, the set $\{g = 0\}$ has no accumulation points.

b) The set $\{f = 0\}$ is finite.

Proof. a): Suppose for a contradiction that x_0 is an accumulation point of the set and consider a sequence $\{g = 0\} \ni x_n \to x_0$. Then $g(x_0) = \lim_{n\to\infty} g(x_n) = 0$, and furthermore $g'(x_0) = 0$: Indeed, if $g'(x_0) \neq 0$, it must be true that either $g' > 0$ or $g' < 0$ on an interval of the form $I = (x_0 - \varepsilon, x_0 + \varepsilon)$ (or $I = [0, \varepsilon)$ if $x_0 = 0$). Hence, g would be strictly monotone on this interval, meaning that $I \cap \{g = 0\} = \{x_0\}$. But this contradicts the fact that x_0 is an accumulation point of $\{g = 0\}$. Since $g(x_0) = g'(x_0) = 0$, one can proceed as in the proof of Proposition 4.5 or Lemma A.3 to obtain $g' \equiv 0$ and therefore $g \equiv 0$ contradicting the assumption.

b): By a) we only need to argue that $\{f = 0\}$ is bounded. However, if this is not the case 0 will be an accumulation point of the set $\{w = 0\}$ where $w(x) = xf(1/x)$. We have seen in the proof of Theorem 4.11 that $w \in C^1([0,\infty))$ (as a linear combination of two such functions). Moreover, on $(0,1)$ the function w solves $w'' = W\mathbb{1}_{(0,1)}w$ with $W(x) = x^{-4}V(1/x)$, and it is an easy check that $W\mathbb{1}_{(0,1)} \in \mathscr{L}$. From a) we see that $\{w = 0\} \cap [0,1)$ has no accumulation points at all which by the above observations implies that $\{f = 0\}$ is bounded. □

We need now a classical comparison result from the theory of Sturm-Liouville operators. Here we specialize as always to the case of Schrödinger operators (i.e. to the solutions of scattering equations).

Lemma 4.15 (Sturm comparison). Consider potentials $V, \widetilde{V} \in \mathscr{L}$ so that $\widetilde{V} \leq V$ pointwise almost everywhere and let f and $\widetilde{f}$ be the regular solutions to the respective associated scattering equations. Denote by $x_0 = 0 < x_1 < x_2 < \cdots < x_k$ the zeroes of f. Then $\widetilde{f}$ has at least one zero in each of the intervals $(x_{i-1}, x_i]$, $i = 1, \ldots, k$.

Proof. Note firstly that we use already in the formulation of the lemma the fact that f has finitely many zeroes, i.e. Lemma 4.14. Now fix an $i \in \{1, \ldots, k\}$. The result will follow if we can show that $\widetilde{f}(x) \neq 0$ for all $x \in (x_{i-1}, x_i)$ implies $\widetilde{f}(x_i) = 0$.

To this end suppose that indeed $\widetilde{f}(x) \neq 0$ for all $x \in (x_{i-1}, x_i)$ and notice that (using the Leibniz formula)

$$(f'\widetilde{f} - f\widetilde{f}')' = f''\widetilde{f} - f\widetilde{f}'' = [V - \widetilde{V}]f\widetilde{f}.$$

Observing that we can assume without loss of generality that $f, \widetilde{f} > 0$ on (x_{i-1}, x_i), this leads by the fundamental theorem of calculus for distributions to

$$f'(x_i)\widetilde{f}(x_i) - f'(x_{i-1})\widetilde{f}(x_{i-1}) = [f'\widetilde{f} - f\widetilde{f}']_{x_{i-1}}^{x_i} = \int_{x_{i-1}}^{x_i} [V - \widetilde{V}]f\widetilde{f}\,dx \geq 0,$$

and since both $f'(x_i)\widetilde{f}(x_i)$ and $-f'(x_{i-1})\widetilde{f}(x_{i-1})$ are non-positive they must both be 0. We have seen before that $f(x_i) = 0$ implies $f'(x_i) \neq 0$, and can conclude that $\widetilde{f}(x_i) = 0$ finishing the proof. □

Remark 4.16. We observe that the proof of Lemma 4.15 actually shows a more general result: If $\mathbb{1}_{(0,R)}V, \mathbb{1}_{(0,R)}\widetilde{V} \in \mathscr{L}$ for any $R > 0$ and $\widetilde{V} \leq V$ pointwise almost everywhere the regular solutions f and $\widetilde{f}$ still exist and have a finite number of zeroes on each $(0,R)$. If $x_{i-1} < x_i$ are two zeroes of f then $\widetilde{f}$ has at least one zero in $(x_{i-1}, x_i]$. ■

We are now in a position to prove our first monotonicity result. We use the notation $B_\varepsilon^{\mathscr{L}}(V)$ for the ε-ball in $\mathscr{L}$ around a potential $V \in \mathscr{L}$.

Proposition 4.17 (Local monotonicity of a). Let $V \in \mathscr{L}$ and assume $a(V) \neq \pm\infty$. Then there exists an $\varepsilon > 0$ (depending on V) so that

i) If $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ and $\widetilde{V} \leq V$ almost everywhere then $a(\widetilde{V}) \geq a(V)$,

ii) If $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ and $\widetilde{V} \geq V$ almost everywhere then $a(\widetilde{V}) \leq a(V)$.

Proof. We prove only i) as the proof of ii) is completely analogous. We denote as usual by f and $\widetilde{f}$ the regular solutions of the scattering equations associated to V and $\widetilde{V}$ respectively.

Denote by $x_0 = 0 < x_1 < \cdots < x_k$ the zeroes of f. We begin by proving the assertion by using a technical result to be proven below, namely:

$$\text{"There exists } \varepsilon > 0 \text{ so that } \widetilde{f} \text{ has exactly } k+1 \text{ zeroes whenever } \widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)\text{."} \tag{4.7}$$

Now for $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$, $\widetilde{V} \leq V$, one obtains from Lemma 4.15 the facts that the largest zero of $\widetilde{f}$ is smaller than x_k and that f and $\widetilde{f}$ has the same sign on (x_k, ∞). Since $\beta(V) \neq 0$ and β is continuous in $\mathscr{L}$ we can achieve by choosing an $\varepsilon > 0$ potentially smaller than above also $\beta(\widetilde{V}) \neq 0$ (and with the same sign as $\beta(V)$) for all $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$. Thus,

$$a(\widetilde{V}) - a(V) = \lim_{x\to\infty} \frac{\widetilde{f}(x) - x\widetilde{f}'(x)}{\widetilde{f}'(x)} - \lim_{x\to\infty} \frac{f(x) - xf'(x)}{f'(x)} = \lim_{x\to\infty} \frac{f'(x)\widetilde{f}(x) - f(x)\widetilde{f}'(x)}{\widetilde{f}'(x)f'(x)},$$

where the denominator converges towards $\beta(\widetilde{V})\beta(V) > 0$ and the numerator can be rewritten as in the proof of Lemma 4.15,

$$f'(x)\widetilde{f}(x) - f(x)\widetilde{f}'(x) = \int_{x_k}^{x} [V(y) - \widetilde{V}(y)] f(y)\widetilde{f}(y)\, dy + f'(x_k)\widetilde{f}(x_k).$$

This is non-negative for all $x \in (x_k, \infty)$ since $f\widetilde{f} > 0$ on (x_k, ∞) and similarly $f'(x_k)\widetilde{f}(x_k) \geq 0$. Hence, the assertion i) in the proposition is verified.

It remains to prove (4.7). For this note that Proposition 4.10(b) says in particular that the map $V \mapsto f'$ is continuous from $\mathscr{L}$ to $C([0,\infty), \mathbb{R})$ and that $V \mapsto f$ is continuous from $\mathscr{L}$ to $C([0,R], \mathbb{R})$ for any fixed $R > 0$. Here the spaces of continuous functions are equipped with the supremum-norm. These facts are used freely from this point onwards. As a first step we use the assumption $\beta(V) \neq 0$ to choose $R > 0$ so that $|f| > 1$, $|f'| > \beta(V)/2$ and f and f' have the same sign on (R, ∞). Then there is an $\varepsilon > 0$ so that, for all $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$, it is true that: $|\widetilde{f}(R)| > 1/2$, $|\widetilde{f}'| > \beta(V)/3 > 0$ on (R, ∞) and these quantities have the same signs when removing the absolute values as the their non-tilded counterparts. As a consequence, also f and $\widetilde{f}$ have the same sign on (R, ∞) for all such $\widetilde{V}$. In particular we have found an $\varepsilon > 0$ so that for any $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ all zeroes of both f and $\widetilde{f}$ are in $[0, R)$, and thus the problem is reduced to an interval on which both $\widetilde{f}$ and $\widetilde{f}'$ vary uniformly continuously with $\widetilde{V}$.

To deal with the problem on $[0, R]$ we choose $\delta > 0$ so small that

$$A_\delta := \min_{x \in \mathscr{J}_\delta} |f'(x)| > 0$$

where

$$\mathscr{J}_\delta := [0,\delta] \cup \Big(\bigcup_{i=1}^{k} [x_i - \delta, x_i + \delta]\Big) \subseteq [0,R]$$

and introduce additionally the constant

$$B_\delta := \min_{x\in[0,R]\setminus \mathscr{J}_\delta} |f(x)| > 0.$$

We claim that if

$$\sup_{x\in[0,R]} |f(x) - \widetilde{f}(x)| \leq \frac{B_\delta}{2} \qquad \text{and} \qquad \sup_{x\in[0,R]} |f'(x) - \widetilde{f}'(x)| \leq \frac{A_\delta}{2} \tag{4.8}$$

then $\widetilde{f}$ has exactly $k+1$ zeroes in $[0,R]$. Indeed, the first condition ensures both that $\widetilde{f}$ has no zeroes in $[0,R]\setminus\mathscr{J}_\delta$ and that it has at least one zero in $[x_i-\delta, x_i+\delta]$ for each $i = 1,\dots,k$ by the intermediate value theorem[9]. On the other hand, the second condition ensures that $\widetilde{f}$ is injective on $[0,\delta]$ and on every $[x_i-\delta,x_i+\delta]$ and thus that it has at most one zero on each of these intervals. As always $\widetilde{f}(0) = 0$, and we obtain the claimed result. By choosing $\varepsilon > 0$ smaller than above and so that the two conditions in (4.8) are fulfilled for all $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ we complete the proof of (4.7) and hence of the proposition. □

Let us now answer the in the light of Proposition 4.17 obvious question: What happens when $a(V) = \pm\infty$? The answer is in some sense the only sensible possibility, and it is proved through a related result concerning the scattering argument.

Proposition 4.18 (Monotonicity of θ). Let $I \subseteq \mathbb{R}$ be an interval and $I \ni t \mapsto V_t \in \mathscr{L}$ a continuous curve in $\mathscr{L}$ with the property that $V_t \leq V_s$ almost everywhere whenever $t \leq s$. Then any scattering argument $\theta\colon I \to \mathbb{R}$ of the curve is a non-increasing function. Similarly, if $V_t \geq V_s$ almost everywhere whenever $t \leq s$ then any scattering argument of the curve is non-decreasing.

Proof. We prove only the first part. Suppose for a contradiction that θ is not non-increasing, i.e. that there is $s_1, s_2 \in I$, $s_1 < s_2$ so that $\theta(s_1) < \theta(s_2)$, and consider a $\theta_0 \in (\theta(s_1), \theta(s_2))$ <u>not</u> of the form $\pi(n+1/2)$. Since the scattering argument is continuous, we can use the intermediate value theorem to find $t_0 \in (s_1,s_2)$ so that $\theta(t_0) = \theta_0$. Considering

$$t^* := \inf\{t \in [s_1,s_2] \mid \theta(t) \geq \theta_0\} \in (s_1,s_2)$$

it is not difficult, using again the continuity of θ, to realize that $\theta(t^*) = \theta_0$ and hence $a(V_{t^*}) \neq \pm\infty$. Proposition 4.17 then implies the existence of an $\varepsilon > 0$ so that $a(\widetilde{V}) \geq a(V_{t^*})$ for all $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V_{t^*})$ with $\widetilde{V} \leq V_{t^*}$ almost everywhere. However, this is violated by the sequence $\{V_{t^*-\frac{1}{n}}\}_{n=1}^{\infty} \subseteq \mathscr{L}$. Indeed, for any fixed $\delta > 0$ we have $\theta(t^* - 1/n) \in (\theta_0 - \delta, \theta_0)$ for large n, and for sufficiently small δ this implies $a(V_{t^*-\frac{1}{n}}) < a(V_{t^*})$ for large n (using the observations in Remark 4.13). By this contradiction we conclude that θ is indeed non-increasing as claimed. □

[9]This last point is actually a bit subtle. One needs in particular to realize that the choice of δ implies that the sign of f alternates on the connected components of $\mathscr{J}_\delta$.

Proposition 4.19 (Behaviour of a near critical potentials). Let $V \in \mathscr{L}$ and assume that $a(V) = \pm\infty$. Then there exists an $\varepsilon > 0$ (depending on V) so that

i) If $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ and $\widetilde{V} \le V$ almost everywhere then $a(\widetilde{V}) \in (-\infty, 0)$ or $a(\widetilde{V}) = \pm\infty$,

ii) If $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ and $\widetilde{V} \ge V$ almost everywhere then $a(\widetilde{V}) \in (0, \infty)$ or $a(\widetilde{V}) = \pm\infty$.

Proof. Again we prove only i). Since $\beta(V) = 0$ we must have $\alpha(V) \neq 0$, and, according to Theorem 4.12, $\alpha(\widetilde{V})$ must have the same sign for all $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ when $\varepsilon > 0$ is chosen sufficiently small. Now if we assume for a contradiction that i) is not true then there exists $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V)$ with $\widetilde{V} \le V$ almost everywhere and $a(\widetilde{V}) \in (0, \infty)$, and we can consider the continuous curve

$$[0,1] \ni t \longmapsto (1-t)\widetilde{V} + tV =: V_t \in B_\varepsilon^{\mathscr{L}}(V) \subseteq \mathscr{L}$$

which satisfies $V_t \le V_s$ almost everywhere whenever $t \le s$. We can choose a scattering argument $\theta\colon [0,1] \to \mathbb{R}$ of this curve so that either $\theta(1) = \pi/2$ or $\theta(1) = -\pi/2$ depending on the sign of $\alpha(V)$. Assume the former for definiteness. Then, since $a(\widetilde{V}) \in (0, \infty)$ and $\alpha(\widetilde{V}) > 0$, it must hold that $\theta(0) \in (2n\pi, 2n\pi + \pi/2)$ for some $n \in \mathbb{Z}$. But as $\alpha(V_t) > 0$ for all $t \in [0,1]$ this clearly contradicts Proposition 4.18 (if this is unclear, the reader is strongly encouraged to make a sketch of the scattering curve), proving the assertion. □

4.4 Oscillation theory in the scattering length

In this section, although this might not be strictly necessary, we stick to considering potentials V from the space

$$\mathscr{L}^{\mathrm{Reg}} := \mathscr{L} \cap L^2_{\mathrm{loc}}(\mathbb{R}_+)$$

of "regular"[10] $\mathscr{L}$-potentials with the topology inherited from $\mathscr{L}$. This space is primarily chosen to avoid drowning in technical details when considering the following construction: We define a self-adjoint Schrödinger operator H acting as $-d^2/dx^2 + V$ on the Hilbert space $L^2(\mathbb{R}_+)$ by putting

$$D(H) = D_{\min} \oplus \mathbb{C}\xi f$$

where $D_{\min}$ is the closure of $C_0^\infty(\mathbb{R}_+)$ with respect to the operator norm of H, $\xi \in C^\infty(\mathbb{R}_+)$ is a localizing function which is identically 1 on $(0,1)$ and vanishes on $(2,\infty)$. Finally, f is the regular solution to the scattering equation $f'' = Vf$. It can be shown that $\sigma_{\mathrm{ess}}(H) = [0,\infty)$. When we from this point refer to "the Schrödinger operator H associated to V" this is always meant in the sense of this construction.

[10] Regular in the sense that the theory from Section 1.3 applies directly when considering these potentials. To realize this one strictly speaking also has to verify that all solutions to the scattering equation are square integrable near the origin. This can be seen for example by applying Proposition 2.5(2) in [DG20].

Other constructions of associated Schrödinger operators exist for even wider classes of potentials – for example for $V \in \mathscr{L}$. These are discussed in Section 4 of [DG20].

4.4.1 The oscillation theorem

We show now through some intermediate steps that Sturm's Oscillation Theorem is true for the class of operators, which we study. The presentation of this result is loosely based on Section 3 of the highly recommended review article [Sim05]. However, for our purposes we need some modifications of the approach in [Sim05]. Thus, we will be: Working directly on all of $\mathbb{R}_+$ instead of on bounded intervals, and – perhaps more non-standard – treating Schrödinger operators constructed as above instead of those defined simply by Dirichlet boundary conditions[11].

Theorem 4.20 (Sturm oscillation). Suppose that the regular solution f to the scattering equation $f'' = Vf$ has k zeroes in $\mathbb{R}_+$ for some $V \in \mathscr{L}^{\mathrm{Reg}}$. Then the Schrödinger operator H associated to V has exactly k eigenvalues in $(-\infty, 0)$.

As a very useful technical step we have:

Lemma 4.21. Let $V \in \mathscr{L}^{\mathrm{Reg}}$. Then the Schrödinger operator H associated to V is bounded below, and we have

$$D(H) \subseteq H_0^1(\mathbb{R}_+) = Q(H)$$

where $Q(H)$ is the quadratic form domain of H. Moreover, H is the Friedrichs extension of H restricted to $C_0^\infty(\mathbb{R}_+)$.

Proof. As a warm up we prove the pointwise bound $|\psi(x)| \le \sqrt{x}\|\psi'\|$ which is valid for any $\psi \in H_0^1(\mathbb{R}_+)$. For fixed x both sides of the inequality are continuous with respect to the H^1-norm, so it suffices to prove the statement for $\psi \in C_0^\infty(\mathbb{R}_+)$, and for this we write

$$|\psi(x)| \le \int_0^x |\psi'(y)|\,dy \le \sqrt{x}\left(\int_0^x |\psi'(y)|^2\right)^{1/2} \le \sqrt{x}\|\psi'\|$$

where we use Cauchy-Schwartz in the middle inequality.

Denote now by q_H the quadratic form associated to H. We begin by considering this for $\psi \in C_0^\infty(\mathbb{R}_+)$ where we easily find

$$q_H(\psi) = \int_0^\infty |\psi'|^2 + V|\psi|^2\,dx. \tag{4.9}$$

Note that for such ψ, by the above inequality,

$$\left|\int_0^\infty V|\psi|^2\,dx\right| \le \int_0^\infty [|V| - C]_+ \cdot |\psi|^2\,dx + C\|\psi\|^2 \le \|\psi'\|^2 \int_0^\infty x\,[|V(x)| - C]_+\,dx + C\|\psi\|^2$$

for any number $C > 0$. The integrand on the right-hand side here clearly converges pointwise towards 0 almost everywhere as $C \to \infty$, and it is dominated by the integrable function $x \mapsto x|V(x)|$. Thus, by choosing a sufficiently large C, we obtain

$$-\varepsilon\|\psi'\|^2 - C\|\psi\|^2 \le \int_0^\infty V|\psi|^2\,dx \le \varepsilon\|\psi'\|^2 + C\|\psi\|^2$$

[11] Defining Schrödinger operators $-d^2/dx^2 + V$ by Dirichlet boundary conditions at the origin is morally what we do, but for $V \in \mathscr{L}^{\mathrm{Reg}}$ the construction is not as straightforward as it is for more regular potentials.

for some $\varepsilon \in (0,1)$ for all $\psi \in C_0^\infty(\mathbb{R}_+)$. This yields in particular $q_H(\psi) \geq -C\|\psi\|^2$ on this set so that the quadratic form is bounded below here. Moreover, introducing the quadratic-form-norm

$$\|\psi\|_{q_H} := \sqrt{q_H(\psi) + (C+1)\|\psi\|^2},$$

(initially only defined on $C_0^\infty(\mathbb{R}_+)$) one observes that

$$(1-\varepsilon)\|\psi'\|^2 + \|\psi\|^2 \leq \|\psi\|_{q_H}^2 \leq (1+\varepsilon)\|\psi'\|^2 + (2C+1)\|\psi\|^2$$

for $\psi \in C_0^\infty(\mathbb{R}_+)$. In particular $\|\cdot\|_{q_H}$ is equivalent to the H^1-norm on $C_0^\infty(\mathbb{R}_+)$. Since the operator norm $\|\cdot\|_H = \sqrt{\|H\cdot\|^2 + \|\cdot\|^2}$ of H satisfies

$$\|\psi\|_{q_H}^2 \leq |\langle\psi, H\psi\rangle| + (C+1)\|\psi\|^2 \leq \|\psi\|\,\|H\psi\| + (C+1)\|\psi\|^2 \leq (C+2)\|\psi\|_H^2$$

for all $\psi \in C_0^\infty(\mathbb{R}_+)$, we see that

$$D_{\min} = \overline{C_0^\infty(\mathbb{R}_+)}^{\|\cdot\|_H} \subseteq \overline{C_0^\infty(\mathbb{R}_+)}^{\|\cdot\|_{q_H}} = \overline{C_0^\infty(\mathbb{R}_+)}^{\|\cdot\|_{H^1}} = H_0^1(\mathbb{R}_+).$$

It is clear that also ξf from the construction of $D(H)$ is in $H_0^1(\mathbb{R}_+)$, and thus the inclusion $D(H) \subseteq H_0^1(\mathbb{R}_+)$ holds. If we manage to prove that the expression (4.9) is valid for all $\psi \in D(H)$ then the arguments above prove also (since we know now that $D(H) \subseteq H_0^1(\mathbb{R}_+)$ so that we have the inequality $|\psi(x)| \leq \sqrt{x}\|\psi'\|$ at our disposal) that

- q_H is bounded below on $D(H)$ and thus defines a norm $\|\cdot\|_{q_H}$ on this domain,
- moreover, $\|\cdot\|_{q_H}$ is equivalent to the H^1-norm on $D(H)$.

This will imply

$$Q(H) = \overline{D(H)}^{\|\cdot\|_{q_H}} = \overline{D(H)}^{\|\cdot\|_{H^1}} \begin{cases} \supseteq \overline{C_0^\infty(\mathbb{R}_+)}^{\|\cdot\|_{H^1}} = H_0^1(\mathbb{R}_+) \\ \subseteq \overline{H_0^1(\mathbb{R}_+)}^{\|\cdot\|_{H^1}} = H_0^1(\mathbb{R}_+) \end{cases}$$

and hence finish the proof of the main part of the lemma.

Let $\psi \in D(H)$. To prove (4.9) for ψ we aim to use generalized partial integration. As $\psi \in H_0^1(\mathbb{R}_+)$, we have (almost) seen above that $V|\psi|^2$ is integrable, so that $\psi'' = V\psi - H\psi$ is a $L^1_{\mathrm{loc}}(\mathbb{R}_+)$-function satisfying $\overline{\psi}\psi'' = V|\psi|^2 - \overline{\psi}H\psi \in L^1(\mathbb{R}_+)$. These are exactly the conditions needed (see Proposition A.6) to perform the partial integration in the equation

$$\begin{aligned} q_H(\psi) = \langle\psi, H\psi\rangle &= \int_0^\infty \overline{\psi}(-\psi'' + V\psi)\,dx = -\int_0^\infty \overline{\psi}\psi''\,dx + \int_0^\infty V|\psi|^2\,dx \\ &= \int_0^\infty |\psi'|^2\,dx + \int_0^\infty V|\psi|^2\,dx = \int_0^\infty |\psi'|^2 + V|\psi|^2\,dx \end{aligned}$$

as needed.

To see that H is the Friedrichs extension of H restricted to $C_0^\infty(\mathbb{R}_+)$ we simply note that

$$D(H) \subseteq H_0^1(\mathbb{R}_+) = \overline{C_0^\infty(\mathbb{R}_+)}^{\|\cdot\|_{q_H}}$$

which is a property characterizing the Friedrichs extension. □

Remark 4.22. From the proof of Lemma 4.21 we can derive also that the expression (4.9) is valid for all $\psi \in Q(H) = H^1_0(\mathbb{R}_+)$. To see that the right-hand side of (4.9) is well defined for such ψ's we simply use the inequality $|\psi(x)| \le \sqrt{x}\|\psi'\|$ as described in the proof. It is a standard check that $q_H(\psi)$ for $\psi \in Q(H)$ can be found as the limit of $q_H(\psi_n)$ with $\psi_n \in D(H)$ for all n and $\|\psi_n - \psi\|_{q_H} \to 0$, i.e. $\|\psi_n - \psi\|_{H^1} \to 0$, as $n \to \infty$. Evidently we need thus only to argue that the integral of $V|\psi_n|^2$ converges towards that of $V|\psi|^2$ in this set-up. For this, simply observe that

$$\begin{aligned}\left|\int_0^\infty V|\psi_n|^2\,dx - \int_0^\infty V|\psi|^2\,dx\right| &\le \int_0^\infty |V|\cdot|\psi_n - \psi|\cdot\big(|\psi_n| + |\psi|\big)\,dx \\ &\le \|\psi_n' - \psi'\|\cdot\big(\|\psi_n'\| + \|\psi'\|\big)\int_0^\infty x|V(x)|\,dx \longrightarrow 0\end{aligned}$$

as $n \to \infty$, where we have used one last time the inequalities $|\psi_n(x)| \le \sqrt{x}\|\psi_n'\|$ and $|\psi(x)| \le \sqrt{x}\|\psi'\|$ as well as $|\psi_n(x) - \psi(x)| \le \sqrt{x}\|\psi_n' - \psi'\|$. ■

Lemma 4.23. Let $V \in \mathscr{L}^{\mathrm{Reg}}$. The Schrödinger operator H associated to V has no eigenvalues with multiplicity larger than 1. Moreover, 0 is not an eigenvalue of H.

Proof. We prove both statements by using the fact that:

$$\textit{If } h \in C(\mathbb{R}_+) \textit{ and } xh(x) \longrightarrow c \neq 0 \textit{ as } x \to 0 \textit{ then } h \textit{ is not square integrable near } 0, \tag{4.10}$$

the proof of which is a simple estimation.

Assume firstly that there are $\psi_1, \psi_2 \in D(H) \subseteq H^1_0(\mathbb{R}_+)$ linearly independent so that $H\psi_1 = E\psi_1$ and $H\psi_2 = E\psi_2$ for some $E \in \mathbb{R}$. Then these will span the space of solutions to the equation $f'' = (V - E)f$ on $\mathbb{R}_+$ which are thus all in $H^1_0(\mathbb{R}_+)$. We recall that by Lemma A.3 all these solutions are additionally in $C^1(\mathbb{R}_+)$. Choosing now f_1 to be the regular solution to the equation and f_2 to be a solution satisfying $f_1 f_2' - f_1' f_2 \equiv 1$ on $\mathbb{R}_+$, we obtain $f_1(x)f_2'(x) \to 1$ as $x \to 0$ since clearly $f_1'(x)f_2(x) \to f_1'(0)f_2(0) = 0$ as $x \to 0$. Now writing $f_1(x) = xf_1'(\xi_x)$ for some $\xi_x \in (0,x)$ we find that

$$xf_2'(x) = f_1'(\xi_x)^{-1} f_1(x) f_2'(x) \longrightarrow 1 \cdot 1 = 1$$

as $x \to 0$. By (4.10) this contradicts $f_2 \in H^1(\mathbb{R}_+)$ and hence proves the first assertion in the lemma.

For the second assertion assume that $Hf = 0$ for some $f \in D(H)\backslash\{0\}$. Then a simple change of variables shows that the function $x \mapsto f(1/x)/x$ and hence also $x \mapsto f(1/x)$ are square integrable on $(0,1)$. However, we claim that we can use (4.10) to disprove this. Indeed, we have seen in the proof of Theorem 4.11 that the non-zero function $w(x) := xf(1/x)$ is in $C^1([0,\infty))$, and hence, as $x \to 0$, either $x \cdot f(1/x) = w(x) \to c \neq 0$ or $w(0) = 0$ so that

$$x \cdot \frac{f(1/x)}{x} = \frac{w(x)}{x} = w'(\xi_x) \longrightarrow c \neq 0$$

where ξ_x is some number in $(0,x)$. This finishes the proof. □

It turns out that the results obtained so far imply rather straightforwardly the one bound in the oscillation theorem:

Proof (of Theorem 4.20 – H has at least k eigenvalues). Denote by $x_0 = 0, x_1, x_2, \dots, x_k$ the zeroes of f and consider the functions $f_i = f \mathbb{1}_{(x_{i-1},x_i)} \in H_0^1(\mathbb{R}_+) = Q(H)$ for $i = 1, \dots, k$. Consider any

$$\psi = \sum_{i=1}^{k} b_i f_i \in \operatorname{span}\{f_1, \dots, f_k\} =: \mathcal{U}_0,$$

and recall the expression (4.9) for $q_H(\psi)$. We get now by a partial integration on each (x_{i-1}, x_i) – which can be justified by noticing that $f \in H_0^1((x_{i-1}, x_i))$ and[12] $f f'' = V|f|^2 \in L^1((x_{i-1}, x_i))$ – that

$$q_H(\psi) = \sum_{i=1}^{k} |b_i|^2 \int_{x_{i-1}}^{x_i} |f'|^2 + V|f|^2 \, dx = \sum_{i=1}^{k} |b_i|^2 \int_{x_{i-1}}^{x_i} (-f'' + Vf) f \, dx = 0,$$

and the variational principle tells us that H has at least k eigenvalues ≤ 0. Indeed, the k^{th} eigenvalue counting from below, E_k, satisfies

$$E_k = \inf_{\substack{\mathcal{U} \subseteq Q(H) \\ \dim \mathcal{U} = k}} \sup_{\substack{\psi \in \mathcal{U} \\ \|\psi\| = 1}} q_H(\psi) \leq \sup_{\substack{\psi \in \mathcal{U}_0 \\ \|\psi\| = 1}} q_H(\psi) = 0.$$

Since 0 is not an eigenvalue of H and all eigenvalues have multiplicities 1 by Lemma 4.23, this finishes this part of the proof. □

For the other bound in the oscillation theorem we need some more intermediate results. The first of these follows more or less directly from Lemmas 4.14 and 4.15 (see also Remark 4.16).

Lemma 4.24. Let $V \in \mathscr{L}$ and consider the regular solutions ψ and $\widetilde{\psi}$ to the equations $\psi'' = (V - E)\psi$ and $\widetilde{\psi}'' = (V - \widetilde{E})\widetilde{\psi}$ respectively where $E < \widetilde{E}$.

a) If $\widetilde{E} \leq 0$ then ψ and $\widetilde{\psi}$ has finitely many zeroes.

b) If $\psi(x) = 0 = \psi(y)$ for some $x < y$ then there exists $z \in (x, y]$ so that $\widetilde{\psi}(z) = 0$. In particular, $\widetilde{\psi}$ has as least as many zeroes as ψ. □

Lemma 4.25. Let $V \in \mathscr{L}^{\text{Reg}}$ be fixed and k_0 be any number. The Schrödinger operator H associated to V has at most one eigenfunction with strictly negative eigenvalue and exactly k_0 zeroes.

[12] For $i = 1$ one can for example recall that $f(x) = xr(x)$ for a continuous function r (cf. Subsection 4.2.1) to get the integrability of $V|f|^2$.

Proof. Suppose that $\psi_1, \psi_2 \in D(H)$ are two such functions, i.e. that $H\psi_1 = E_1\psi_1$ and $H\psi_2 = E_2\psi_2$ with $E_1 < E_2 < 0$ (this can be assumed due to Lemma 4.23) and that the functions have the same number of zeroes. Note that the latter is finite by Lemma 4.24(a). Also, it is non-zero since ψ_1 and ψ_2 must be orthogonal in $L^2(\mathbb{R}_+)$ as eigenfunctions of H with different eigenvalues, and hence at least one of ψ_1 and ψ_2 has to change sign yielding a zero of this function. Denote by z_1 and z_2 the last zero of ψ_1 and ψ_2 respectively. Using Lemma 4.24(b) together with our assumption we find that $z_2 \le z_1$.

The key step is now to introduce a new operator: The Schrödinger operator H_0 associated to $V(\cdot + z_2) \in \mathscr{L}^{\mathrm{Reg}}$. It can be proved[13] (and is indeed very plausible) that $\phi_2 := \psi_2(\cdot + z_2)$ lies in $D(H_0)$ and it is thus an easy check that this is an eigenfunction with eigenvalue E_2 for H_0. We observe moreover that $\phi_0 := \psi_1(\cdot + z_2)\mathbb{1}_{(z_1 - z_2, \infty)} \in H_0^1(\mathbb{R}_+) = Q(H_0)$ by Remark 4.22 satisfies

$$\begin{aligned} q_{H_0}(\phi_0) &= \int_{z_1 - z_2}^{\infty} |\phi_0'(x)|^2 + V(x + z_2)|\phi_0(x)|^2 \, dx = \int_{z_1}^{\infty} |\psi_1'|^2 + V|\psi_1|^2 \, dx \\ &= \int_{z_1}^{\infty} \overline{\psi_1}(-\psi_1'' + V\psi_1) \, dx = E_1 \int_{z_1}^{\infty} |\psi_1|^2 \, dx = E_1 \int_{z_1 - z_2}^{\infty} |\phi_0|^2 \, dx = E_1 \|\phi_0\|^2, \end{aligned}$$

where, as usual, the partial integration can be justified by checking the conditions in Proposition A.6. By the variational principle this tells us that H_0 has at least one eigenvalue $\widetilde{E}_1 \le E_1$ strictly smaller than E_2. However, Lemma 4.24(b) says that the eigenfunction[14] ϕ_1 corresponding to the eigenvalue $\widetilde{E}_1$ has no zeroes in $\mathbb{R}_+$ (since then so would ϕ_2, but this is not the case). This means that ϕ_1 and ϕ_2, on the one hand, have no chance of being orthogonal in $L^2(\mathbb{R}_+)$ but on the other hand must be so as eigenfunctions with different eigenvalues. This contradiction proves that no ψ_1 and ψ_2 as above can exist. □

Proposition 4.26. Let $V \in \mathscr{L}^{\mathrm{Reg}}$ and consider the ordered eigenvalues $E_0 < E_1 < \cdots$ of the associated Schrödinger operator H. For each $j \in \mathbb{N}_0$, the eigenfunction ψ_j with eigenvalue E_j has exactly j zeroes in $\mathbb{R}_+$.

Proof. Fix j. By Lemma 4.25 it suffices to show that ψ_j has at most j zeroes. Assume now that ψ_j has ℓ zeroes $x_1, \dots, x_\ell$ in $\mathbb{R}_+$ and consider as usual the functions $\phi_i = \psi_j \mathbb{1}_{(x_{i-1}, x_i)}$ for $i = 1, \dots, \ell$ where, as always, $x_0 = 0$. We put additionally $\phi_{\ell+1} = \psi_j \mathbb{1}_{(x_\ell, \infty)}$. Using Lemma 4.21 it can be seen that $\phi_i \in Q(H)$ for all i, and a calculation like in the first part of the proof of Theorem 4.20 shows that $q_H(\phi) = E_j \|\phi\|^2$ for all $\phi \in \operatorname{span}\{\phi_1, \dots, \phi_{\ell+1}\} =: \mathcal{U}_0$.

[13] The proof uses the theory from Section 1.3 and is as follows: We are in the more regular setting where the potential is even integrable near the origin. Thus, cf. Proposition 4.10, the space of solutions to the scattering equation is spanned by functions f and g with $f(0) = g'(0) = 0$ and $f'(0) = g(0) = 1$. It is an easy check that ϕ_2 lies in the domain of the maximal extension, but this means that $\phi_2 = \phi + \alpha\xi f + \beta\xi g$ with ϕ lying in the domain of the minimal extension $D(H_{0,\min}) \subseteq H_0^1(\mathbb{R}_+)$ (cf. Lemma 4.21) and $\alpha, \beta \in \mathbb{C}$. But since $\phi_2(0) = \phi(0) = f(0) = 0 \neq g(0)$ we must have $\beta = 0$ proving $\phi_2 \in D(H_{0,\min}) \oplus \mathbb{C}\xi f = D(H_0)$.

[14] Note that this has to be a multiple of the regular solution to the relevant equation since no other solutions has $\phi_1(0) = 0$.

Consequently,

$$E_\ell = \inf_{\substack{\mathcal{U}\subseteq Q(H)\\ \dim\mathcal{U}=\ell+1}} \sup_{\substack{\psi\in\mathcal{U}\\ \|\psi\|=1}} q_H(\psi) \le \sup_{\substack{\psi\in\mathcal{U}_0\\ \|\psi\|=1}} q_H(\psi) = E_j,$$

and thus $\ell \le j$ as we needed. □

Proof (of Theorem 4.20 – H has at most k eigenvalues). Consider an arbitrary eigenvalue $E < 0$ and the associated eigenfunction ψ. By Lemma 4.24 this ψ has at most k zeroes in $\mathbb{R}_+$, and in fact it has a most $k-1$ zeroes (meaning that it does not exists if $k = 0$). The proof of this is sketched below. Consequently, by Proposition 4.26, it must be among the first k eigenvalues counting from below. As $E < 0$ was arbitrary, this proves the theorem.

To exclude the possibility that ψ has k zeroes just as f (the regular solution to $f'' = Vf$) does, one considers, if $k \neq 0$, the situation on $[z,\infty)$ with z the largest zero of f. If ψ and f indeed had the same number of zeroes then, by Lemma 4.24, the largest zero of ψ would lie in this interval. As in the proof of Lemma 4.25, this implies the existence of an eigenfunction ϕ to the Schrödinger operator associated to $V(\,\cdot\,+z)$ with eigenvalue $\widetilde{E} \le E < 0$. However, an application of Corollary A.5 shows that $|\phi| \ge c\cdot|f(\,\cdot\,+z)|$ for some $c > 0$ on all of (z,∞) by comparing the logarithmic derivatives of these functions. This contradicts the fact that f is not square integrable (cf. Lemma 4.23) and thus proves the assertion. The proof when $k = 0$ is just the last part of this argument. □

4.4.2 Counting the negative eigenvalues

We now set up the machinery that will allow us to apply the oscillation theorem to the following important question: Consider two potentials $V_0, V_1 \in \mathscr{L}^{\mathrm{Reg}}$. We know by Lemma 4.14 and Theorem 4.20 that the Schrödinger operators associated to these have finitely many negative eigenvalues. But how can we detect the difference in the number of negative eigenvalues between the two operators?

To answer this we let V_0 and V_1 be the endpoints of a continuous curve $[0,1] \ni t \mapsto V_t \in \mathscr{L}^{\mathrm{Reg}}$. Such a curve always exists since $\mathscr{L}^{\mathrm{Reg}}$ is convex. We would like to associate to this curve another curve $s\colon [0,1] \to \mathbb{T} := \{z \in \mathbb{C} \mid |z| = 1\}$ (to be described below) on the unit circle in $\mathbb{C}$. The idea is that under some natural assumptions this curve will have $s(0) = s(1)$ and thus possess a winding number which happens to count exactly the difference in the number of negative eigenvalues of the associated Schrödinger operators.

Definition 4.27. Let $I \subseteq \mathbb{R}$ be an interval and $I \ni t \mapsto V_t \in \mathscr{L}$ a continuous curve in $\mathscr{L}$ and consider moreover the continuous curve $\gamma\colon I \to \mathbb{C}\backslash\{0\}$ from Theorem 4.12. We define the *scattering curve* of $t \mapsto V_t$ to be the curve

$$s\colon I \ni t \longmapsto \frac{\gamma(t)^2}{|\gamma(t)|^2} = \frac{\beta(V_t)^2 - \alpha(V_t)^2 + 2i\alpha(V_t)\beta(V_t)}{\alpha(V_t)^2 + \beta(V_t)^2} \in \mathbb{T}$$

which is continuous as well.

We note firstly some immediate properties of scattering curves on $\mathbb{T}$.

Lemma 4.28. Let $s\colon I \to \mathbb{T}$ be the scattering curve of a continuous curve $I \ni t \mapsto V_t \in \mathscr{L}$. Also, let $J \subseteq I$ be a subinterval.

a) $s(t) = -1$ if and only if $\beta(V_t) = 0$, i.e. if and only if $a(V_t) = \pm\infty$.

b) $s(t_1) = s(t_2)$ if and only if $a(V_{t_1}) = a(V_{t_2})$

c) If $V_t \le V_s$ almost everywhere whenever $t, s \in J$ and $t \le s$ then $s(t)$ moves clockwise on $\mathbb{T}$ as $t \in J$ increases.

d) If $V_t \ge V_s$ almost everywhere whenever $t, s \in J$ and $t \le s$ then $s(t)$ moves counter-clockwise on $\mathbb{T}$ as $t \in J$ increases.

Proof. The claim in a) is readily checked. For the remaining assertions note that if $\theta\colon I \to \mathbb{R}$ is a scattering argument of $t \mapsto V_t$ then $2\theta(t)$ is a continuous argument along the curve s. This proves through Proposition 4.18 immediately c) and d). If we moreover recall from Remark 4.13 that $a(V_t) = \tan\theta(t)$ and notice that

$$\begin{aligned} s(t_1) = s(t_2) \quad &\text{if and only if} \quad 2\theta(t_1) = 2\theta(t_2) \mod 2\pi \\ &\text{if and only if} \quad \theta(t_1) = \theta(t_2) \mod \pi \end{aligned}$$

we obtain b) as well. □

We formulate below a precise statement based on the slogan "the scattering curve counts the difference in the number of negative eigenvalues of the associated Schrödinger operators". To this end, we use the notation

$$n_-\colon \mathscr{L}^{\mathrm{Reg}} \ni V \longmapsto n_-(V) := \mathrm{Tr}[\mathbb{1}_{(-\infty,0)}(H)] \in \mathbb{N}_0$$

for the number of negative eigenvalues (here V and H are related as usual) and introduce for $a \in \mathbb{R} \cup \{\pm\infty\}$ the sets

$$\mathscr{L}_a := \{V \in \mathscr{L} \mid a(V) = a\} \qquad \text{and} \qquad \mathscr{L}_a^{\mathrm{Reg}} := \{V \in \mathscr{L}^{\mathrm{Reg}} \mid a(V) = a\}$$

of potentials with fixed scattering lengths. Note that if $I \ni t \mapsto V_t \in \mathscr{L}^{\mathrm{Reg}}$ is a continuous curve in $\mathscr{L}^{\mathrm{Reg}}$ with both endpoints in some fixed $\mathscr{L}_a^{\mathrm{Reg}}$ and $s\colon I \to \mathbb{T}$ is the associated scattering curve then Lemma 4.28(b) tells us that s has a well-defined winding number. This makes these subsets of $\mathscr{L}^{\mathrm{Reg}}$ the natural starting point when formulating statements of the desired form. The central result is in the above language:

Theorem 4.29. Let $V_0, V_1 \in \mathscr{L}_a^{\mathrm{Reg}}$ for some $a \in \mathbb{R}$ and let $[0,1] \ni t \mapsto V_t \in \mathscr{L}^{\mathrm{Reg}}$ be an arbitrary continuous curve connecting these two potentials. Then

$$n_-(V_1) - n_-(V_0) = \omega(s) \tag{4.11}$$

where $\omega(s)$ is the winding number of the scattering curve $s\colon [0,1] \to \mathbb{T}$ of $t \mapsto V_t$.

Before proving this theorem we observe some convenient properties of the set $\mathscr{L}\backslash\mathscr{L}_{\pm\infty}$ and a general fact about the zeroes of the scattering solutions. These facts will be needed in the proof of Theorem 4.29.

Lemma 4.30.

a) The function $n_-\colon \mathscr{L}^{\mathrm{Reg}} \to \mathbb{N}_0$ is locally constant on $\mathscr{L}^{\mathrm{Reg}}\backslash\mathscr{L}^{\mathrm{Reg}}_{\pm\infty}$.

b) The scattering length $V \mapsto a(V)$ considered as a map is continuous on $\mathscr{L}\backslash\mathscr{L}_{\pm\infty}$.

Proof. The statement (4.7) – which holds exactly for $V \in \mathscr{L}\backslash\mathscr{L}_{\pm\infty}$ – and the oscillation theorem yield straightforwardly a). The statement in b) is a consequence of the facts that $a = \alpha/\beta$ with $\alpha, \beta\colon \mathscr{L} \to \mathbb{R}$ continuous and $\mathscr{L}_{\pm\infty} = \{V \in \mathscr{L} \mid \beta(V) = 0\}$. □

Lemma 4.31. Let $I \subseteq \mathbb{R}$ be an interval and $I \ni t \mapsto V_t \in \mathscr{L}$ a continuous curve in $\mathscr{L}$. Consider also the regular solutions f_t to the scattering equations $f_t'' = V_t f_t$ and assume that there exists an $R > 0$ and $t_1 < t_2$ so that $f_t(R) \neq 0$ for all $t \in [t_1, t_2] \subseteq I$. Then f_{t_1} and f_{t_2} has the same number of zeroes in $(0, R)$.

Proof. Consider an arbitrary $t_0 \in [t_1, t_2]$. With our assumptions we can follow the last part of the proof of Proposition 4.17 exactly to show that a small perturbation (with respect to the $\mathscr{L}$-topology) of V_{t_0} does not change the number of zeroes of the regular solution to the scattering equation in $(0, R)$. If one in this context lets $x_1, \ldots, x_k$ be the zeroes of f_{t_0} lying in $(0, R)$ and defines δ, $\mathscr{J}_\delta$, A_δ and B_δ as it is done in the mentioned proof then this produces an $\varepsilon > 0$ so that the regular solution to the scattering equation with any potential from $B_\varepsilon^{\mathscr{L}}(V_{t_0})$ has the same number of zeroes in $(0, R)$ as f_{t_0}. Here the assumption $f_{t_0}(R) \neq 0$ is clearly essential since if $f_{t_0}(R) = 0$ we would have $B_\delta = 0$ and the proof breaks down.

This shows in particular that the function

$$[t_1, t_2] \ni t \longmapsto \text{number of zeroes of } f_t \text{ in } (0, R)$$

is locally constant. As it is defined on a connected space, it is constant and the lemma follows. □

Remark 4.32. Apart from being useful below, Lemma 4.31 also shed some light on how zeroes of the regular solutions f_t to scattering equations along a continuous path $t \mapsto V_t$ of potentials emerge and disappear. It tells us that this can only happen at infinity. Indeed, if we assume that all zeroes of the f_t's are smaller than some fixed constant R then by the lemma the total number of zeroes stays unchanged. Rephrasing this we see that if f_{t_1} and f_{t_2} have a different number of zeroes for some $t_1 < t_2$ then there must be $t^* \in (t_1, t_2)$ so that f_{t^*} has an arbitrarily large zero – zeroes come and go only at infinity! ■

With these lemmas in place we can move on to the

Proof (of Theorem 4.29). Step 1 (Independence of curve): Observe firstly that the right hand side of (4.11) is independent of the choice of curve $t \mapsto V_t$. Indeed, for example by the convexity of $\mathscr{L}^{\mathrm{Reg}}$, there exists an end-point preserving homotopy $F\colon [0,1]\times[0,1] \to \mathscr{L}^{\mathrm{Reg}}$ between any pair of continuous curves between V_0 and V_1. Clearly such homotopy gives rise to a homotopy $G\colon [0,1]\times[0,1] \to \mathbb{T}$ between the associated scattering curves on $\mathbb{T}$ also fixing the endpoints by Lemma 4.28(b). Since the winding number is preserved by the homotopy G this proves the assertion.

Step 2 (Choice of curve): Step 1 also implies that we can choose the curve $t \mapsto V_t$ freely when proving (4.11). We construct it in the following way: As a first step use Lemma 4.30 to find an $\varepsilon > 0$ so that all $V \in B_\varepsilon^{\mathscr{L}}(V_0) \cap \mathscr{L}^{\mathrm{Reg}}$ has $n_-(V) = n_-(V_0)$ and $a(V) \neq \pm\infty$ and all $\widetilde{V} \in B_\varepsilon^{\mathscr{L}}(V_1) \cap \mathscr{L}^{\mathrm{Reg}}$ has $n_-(\widetilde{V}) = n_-(V_1)$ and $a(\widetilde{V}) \neq \pm\infty$. Next, choose a large fixed $R > 0$ (depending on V_0 and V_1) so that $V_0\mathbb{1}_{(0,R)} \in B_\varepsilon^{\mathscr{L}}(V_0)$ and $V_1\mathbb{1}_{(0,R)} \in B_\varepsilon^{\mathscr{L}}(V_1)$. Finally, we can write down the expression

$$V_t = \begin{cases} V_0\mathbb{1}_{(0,\frac{1}{t}-4+R)} & \text{for } t \in (0,\frac{1}{4}] \\ (2-4t)V_0\mathbb{1}_{(0,R)} + (4t-1)(V_0 \wedge V_1)\mathbb{1}_{(0,R)} & \text{for } t \in [\frac{1}{4},\frac{1}{2}] \\ (3-4t)(V_0 \wedge V_1)\mathbb{1}_{(0,R)} + (4t-2)V_1\mathbb{1}_{(0,R)} & \text{for } t \in [\frac{1}{2},\frac{3}{4}] \\ V_1\mathbb{1}_{(0,\frac{1}{1-t}-4+R)} & \text{for } t \in [\frac{3}{4},1) \end{cases}$$

for a continuous curve in $\mathscr{L}^{\mathrm{Reg}}$ connecting V_0 and V_1. In words, the curve starts out by moving from V_0 to $V_0\mathbb{1}_{(0,R)}$ while staying inside $B_\varepsilon^{\mathscr{L}}(V_0)$. Then it moves from $V_0\mathbb{1}_{(0,R)}$ to $(V_0 \wedge V_1)\mathbb{1}_{(0,R)}$ in a way which is pointwise (almost everywhere) non-increasing before moving from $(V_0 \wedge V_1)\mathbb{1}_{(0,R)}$ to $V_1\mathbb{1}_{(0,R)}$ in a way which is pointwise (almost everywhere) non-decreasing and finally travelling from $V_1\mathbb{1}_{(0,R)}$ to V_1 while staying inside $B_\varepsilon^{\mathscr{L}}(V_1)$.

Step 3 (Behaviour of s): Consider now the scattering curve $s\colon [0,1] \to \mathbb{T}$ associated to the curve $t \mapsto V_t$ from Step 2. From Lemma 4.28 we learn that s stays away from -1 on $[0,1/4]$ and $[3/4,1]$. We learn also that it has on $[1/4,1/2]$ some well-defined and finite number of positive (counter-clockwise) crossing of -1 and on $[1/2,3/4]$ some well-defined and finite number of negative (clockwise) crossings of -1 (both of which might be 0). The winding number $\omega(s)$ must be the difference between these numbers of crossings[15]. Now, what we also need to study is the behaviour of $n_-(V_t)$ as t runs from 0 to 1. To this end note as a warm-up that for $t \in [0,1/4]$ and $t \in [3/4,1]$ respectively the potentials V_t stays inside $\mathscr{L}^{\mathrm{Reg}}\backslash\mathscr{L}^{\mathrm{Reg}}_{\pm\infty}$ and Lemma 4.30(a) tells us that $n_-(V_t)$ is unchanged on these intervals. We now begin the description of the behaviour of $n_-(V_t)$ for $t \in [1/4,3/4]$ which is in a sense the key element in the present proof.

Step 4 (Counting the eigenvalues I): We consider firstly $t \in [1/4,1/2]$ and assume that s has $k \in \mathbb{N}_0$ positive crossings of -1 on this interval. Recall that $s(1/4) \neq -1$. By the description in Step 3 we see further that there are numbers

$$\frac{1}{4} = t_0' < t_1 \leq t_1' < t_2 \leq t_2' < \cdots < t_k \leq t_k' < t^* \leq 1/2$$

so that $s(t) \neq -1$ for $t \in (t_{i-1}', t_i)$ and $s(t) = -1$ for $t \in [t_i, t_i']$ for $i = 1,\ldots,k$. Lastly, $s(t) \neq -1$ for $t \in (t_k', t^*)$ and either $t^* = 1/2$ and $s(t^*) \neq -1$ or $s(t) = -1$ for $t \in [t^*, 1/2]$. By Lemma 4.28(a)

[15] Here a positive crossing is really going across -1 and into $\mathbb{C}_-$ and a negative one is going across -1 and into $\mathbb{C}_+$

one has $V_t \in \mathscr{L}^{\mathrm{Reg}} \backslash \mathscr{L}^{\mathrm{Reg}}_{\pm\infty}$ for $t \in s^{-1}(\mathbb{T}\backslash\{-1\})$, and hence $t \mapsto n_-(V_t)$ is constant on each (t'_{i-1}, t_i) according to Lemma 4.30(a). We prove in Step 5 below that this is also true on the larger intervals $(t'_{i-1}, t'_i]$ and on $(t'_k, 1/2]$ but that $n_-(V_{\tilde{t}}) - n_-(V_t) = 1$ whenever $t \in (t'_{i-1}, t'_i]$ and $\tilde{t} \in (t'_i, t'_{i+1}]$ for some $i = 1, \ldots, k-1$ or $t \in (t'_{k-1}, t'_k]$ and $\tilde{t} \in (t'_k, 1/2]$. Consequently, $n_-(V_{1/2}) - n_-(V_{1/4}) = k$ since $n_-(V_t)$ is locally constant near $t = 1/4$. Considering then $t \in [1/2, 3/4]$ and assuming that s has ℓ (negative) crossings of -1 on this interval, we can run through this part of the curve backwards to obtain a curve on $\mathbb{T}$ with ℓ (positive) crossings of -1. Now by what we just did, $n_-(V_{1/2}) - n_-(V_{3/4}) = \ell$ and thus

$$\begin{aligned} n_-(V_1) - n_-(V_0) = n_-(V_{3/4}) - n_-(V_{1/4}) &= n_-(V_{1/2}) - n_-(V_{1/4}) - (n_-(V_{1/2}) - n_-(V_{3/4})) \\ &= k - \ell = \omega(s) \end{aligned}$$

which proves the theorem.

Step 5 (Counting the eigenvalues II): Let us finally prove the remaining assertion in Step 4, i.e. that the number $n_-(V_t)$ increases with 1 exactly when t has passed through a t'_i for some $i = 1, \ldots, k$. For this, consider any such t_i. If we as in Lemma 4.31 denote by f_t the regular solution to $f_t'' = V_t f_t$ then the assumption in this lemma is satisfied in a neighbourhood around $[t_i, t'_i] \subseteq (1/4, 1/2)$: Indeed, since all V_t with t near this interval (or point) is 0 on (R, ∞), we must have $f_t(x) = \alpha(V_t) + \beta(V_t)x$ for $x \in [R, \infty)$ up to an overall non-zero constant (depending on t) for all these t's. Now observe that for $t \in [t_i, t'_i]$ we have $a(V_t) = \pm\infty$ meaning $\beta(V_t) = 0$ and $\alpha(V_t) \neq 0$ so that consequently $f_t(R) \neq 0$ by the above. By continuity of the map $t \mapsto f_t(R)$ this is also true on a small neighbourhood $[t_i - \delta, t'_i + \delta]$ meaning that Lemma 4.31 is applicable on this interval. We conclude that the number of zeroes of f_t on $(0, R)$ is constant on $[t_i - \delta, t'_i + \delta]$, and thus $n_-(V_t)$ – which is the total number of zeroes of f_t by the oscillation theorem – only varies on this interval depending on the number of zeroes of f_t on $[R, \infty)$. As we have seen, determining this number amounts to finding the number of zeroes of the linear function $\alpha(V_t) + \beta(V_t)x$ on $[R, \infty)$. If $\beta(V_t) = 0$ (i.e. for $t \in [t_i, t'_i]$) this function has no zeroes at all, and if $\beta(V_t) \neq 0$ the only possible zero is $-\alpha(V_t)/\beta(V_t) = -a(V_t)$ so we are really asking whether this lies in $[R, \infty)$. As s moves counter-clockwise it must be the case that $\operatorname{Im} s(t) > 0$ on $[t_i - \delta, t_i)$ and $\operatorname{Im} s(t) < 0$ on $(t'_i, t'_i + \delta]$. Recalling the definition of s it is clear that this means $\alpha(V_t)\beta(V_t) > 0$ on $[t_i - \delta, t_i)$ and $\alpha(V_t)\beta(V_t) < 0$ on $(t'_i, t'_i + \delta]$. Therefore, $\alpha(V_t)$ and $\beta(V_t)$ have the same sign for $t \in [t_i - \delta, t_i)$ so that $-\alpha(V_t)/\beta(V_t) < 0$ is not in $[R, \infty)$ on this interval. For $t \in (t'_i, t'_i + \delta]$, on the other hand, $\alpha(V_t)$ and $\beta(V_t)$ have opposite signs, and choosing $\delta > 0$ sufficiently small we can have also $|\alpha(V_t)| > |\alpha(V_{t'_i})|/2$ and $|\beta(V_t)| < |\alpha(V_{t'_i})|/(2R)$ for all such t's by continuity. Consequently,

$$-\frac{\alpha(V_t)}{\beta(V_t)} = \frac{|\alpha(V_t)|}{|\beta(V_t)|} > \frac{|\alpha(V_{t'_i})|/2}{|\alpha(V_{t'_i})|/(2R)} = R$$

so that there is indeed a zero of f_t on $[R, \infty)$ for $t \in (t'_i, t'_i + \delta]$. The overall conclusion is the desired one: $n_-(V_t)$ is unchanged on $[t_i - \delta, t'_i]$ and hence on $(t'_{i-1}, t'_i]$ but it increases by 1 when t goes from $[t_i - \delta, t'_i]$ to $(t'_i, t'_i + \delta]$. Since it is really the passing of s through -1 that yields the change we see finally that $n_-(V_t)$ is also constant on $(t'_k, 1/2]$ completing the proof of all the assertions. □

Remark 4.33. With[16] the above theory in fresh memory we record here its implications for a particularly important class of examples. Fix a non-zero potential $V \in \mathscr{L}^{\mathrm{Reg}}$ which is pointwise non-positive almost everywhere and consider the continuous curve $[0,\infty) \ni t \mapsto tV \in \mathscr{L}^{\mathrm{Reg}}$ and its scattering curve $s\colon [0,\infty) \to \mathbb{T}$. Now, by Lemma 4.28(d), $s(t)$ moves counter-clockwise as t increases (so that it here makes sense to discuss the number of its positive crossings of -1 as we do below). Moreover, the Weyl law at least morally tells us that if additionally $V \in L^{1/2}(\mathbb{R}_+)$ then

$$n_-(tV) \approx \frac{\sqrt{t}}{\pi} \int_0^\infty \sqrt{-V(x)}\,dx,$$

and in particular that tV has arbitrarily many negative eigenvalues if one chooses t sufficiently large in this case.

In many cases, a more detailed analysis of the asymptotic behaviour of the scattering length also reveals that $a(tV) \neq \pm\infty$ for arbitrarily large t's. From this it follows that

$$\textit{there are arbitrarily large } t\textit{'s so that } a(tV) = 0. \tag{4.12}$$

To see this one can for any fixed $T > 0$ choose $T < t_1 < t_2 < t_3$ so that $a(t_i V) \neq \pm\infty$ and additionally $n_-(t_1 V) < n_-(t_2 V) < n_-(t_3 V)$. As is argued in the proof of Theorem 4.29 $n_-(tV)$ stays unchanged as long as $s(t) \neq -1$ so $s(t)$ must cross -1 between both t_1 and t_2 and between t_2 and t_3. But it is impossible for it to cross -1 twice without also crossing 1 – meaning that $a(tV) = 0$ – at least once between t_1 and t_3. This shows that (4.12) holds true and puts us in a position to apply Theorem 4.29 to "prove"[17] a statement about the time of emergence of new negative eigenvalues. That is,

$$\begin{gathered}\textit{The scattering curve } s \textit{ crosses } -1 \textit{ infinitely many times. Moreover, if } s(t_0) \neq -1\\ \textit{and } s(t) \textit{ is between its } n\textit{'th and } (n+1)\textit{'st crossing of } -1 \textit{ at } t = t_0 \textit{ then } n_-(t_0 V) = n.\end{gathered} \tag{4.13}$$

Indeed, for any natural number N we can use (4.12) and the Weyl law to find a $t' \in [0,\infty)$ satisfying $a(t'V) = 0$ and $n_-(t'V) \geq N$. An application of Theorem 4.29 to the restriction $[0,t'] \ni t \mapsto tV$ shows that the winding number of $s|_{[0,t']}$ is larger than N which implies by the monotonicity that $s(t)$ has at least N crossings of -1 even on this sub-interval of $[0,\infty)$. For the second assertion in (4.13) assume for definiteness[18] that $\operatorname{Im} s(t_0) \leq 0$ and note that there is a $t' \geq t_0$ so that $a(t'V) = 0$ and $s(t) \neq -1$ for $t \in [t_0, t']$, i.e. $s(t)$ have performed exactly n crossings of -1 at $t = t'$. By Theorem 4.29 this is to say that $n_-(t'V) = n$, and since we can clearly join $t_0 V$ and $t'V$ with a continuous curve within $\mathscr{L}^{\mathrm{Reg}} \backslash \mathscr{L}^{\mathrm{Reg}}_{\pm\infty}$ (we basically just did), Lemma 4.30(a) tells us that also $n_-(t_0 V) = n$.

Turning the picture around, (4.13) says also that when t grows larger and larger the "jumps" in $n_-(tV)$ from n to $n+1$ happens exactly at t_0's for which $s(t)$ is performing its n'th crossing of -1 at $t = t_0$. Or, put another way, exactly when $a(tV)$ is $\pm\infty$ for the n'th time. The asymptotics of these t_0's is therefore controlled by the asymptotics of the

[16] Consider this a teaser to Section 5.2.

[17] Since we are neither precise with the assumptions nor with the results we use, this should of course not be considered as a rigorous proof – but rather a heuristic argument.

[18] In the other case one needs to run the last part of the curve $t \mapsto tV$ backwards, but this is nothing but a technical problem.

scattering length which is in some cases computable and leads to nice results improving the more basic result from Weyl's law. ■

We end this chapter by arguing that for most relevant purposes the assumption $V \in \mathscr{L}^{\mathrm{Reg}} \cap L^{1/2}(\mathbb{R}_+)$ in Remark 4.33 can be replaced by $V \in L^1(\mathbb{R}_+, x^2\,dx) \cap L^{1/2}(\mathbb{R}_+)$ together with some local regularity which is more or less exactly the condition under which Weyl's law holds with added regularity at ∞ only – not at the origin. I learned the clever proof of this fact from Johannes Agerskov.

Proposition 4.34. Assume $V \in L^{1/2}(\mathbb{R}_+)$ and that $|V(x)|$ is non-increasing. Then also $V \in L^1(\mathbb{R}_+, x\,dx)$.

Proof. Let V be as in the proposition. The main part of the proof is to show that one has the pointwise bound $|V(x)| \le x^{-2}e^{2\|V\|_{1/2}}$ with the notation $\|V\|_{1/2} := \int |V|^{1/2}$. Now using this bound we learn that

$$\int_0^\infty x|V(x)|\,dx \le \int_0^\infty |V(x)|^{1/2}e^{\|V\|_{1/2}}\,dx \le \|V\|_{1/2}e^{\|V\|_{1/2}} < \infty$$

as needed.

To show the pointwise bound suppose for a contradiction that it does not hold, i.e. that $|V(x_0)| > x_0^{-2}e^{2\|V\|_{1/2}}$ for some $x_0 > 0$. Consequently, for $y \in (x_0e^{-\|V\|_{1/2}}, x_0)$,

$$|V(y)| \ge |V(x_0)| > \frac{e^{2\|V\|_{1/2}}}{x_0^2} > \frac{1}{y^2},$$

and hence

$$\int_{x_0e^{-\|V\|_{1/2}}}^{x_0} |V(y)|^{1/2}\,dy > \int_{x_0e^{-\|V\|_{1/2}}}^{x_0} \frac{1}{y}\,dy = \ln(x_0) - \ln\Big(\frac{x_0}{e^{\|V\|_{1/2}}}\Big) = \|V\|_{1/2}$$

which is clearly a contradiction. This finishes the proof. □

Chapter 5

Perspectives and outlook

5.1 Scattering length asymptotics

This section aims to provide reasonably simple asymptotic formulas for the scattering lengths of large negative potentials as the ones appearing in Chapter 2 (when we take $\kappa \to \infty$ here). We show firstly such a formula in a particularly convenient case as an example and then move on to discussing a more general setting covering many more potentials of interest.

Example 5.1. We consider for the moment a potential $V\colon \mathbb{R}_+ \to \mathbb{R}_+$ satisfying the Assumptions 2.1 from Chapter 2 with $\alpha = 0$ and $\beta = -4$ and the additional condition that the integral

$$\int_1^\infty x \left| \frac{d^2}{dx^2}\Big(V^{-1/4}\Big) \right| dx$$

is finite. Note that the integrand here is 0 wherever $V(x) = C_\infty x^{-4}$, and thus this is just another way of quantifying the asymptotic behaviour $V \sim C_\infty x^{-4}$ for large x. As a final extra assumption we demand that

$$\frac{d}{dx}\Big(V^{-1/4}\Big) \longrightarrow C_\infty^{-1/4} \qquad \text{and} \qquad V(x)^{-1/4} - x\frac{d}{dx}\Big(V^{-1/4}\Big) \longrightarrow 0$$

as $x \to \infty$. These do not seem to be very strict requirements since the former simply describes the "right" behaviour for the derivative of V and the latter equals identically 0 whenever $V(x) = C_\infty x^{-4}$ for any $C_\infty > 0$. On the other hand, we remark that they are actually stronger assumptions on the asymptotics of V than the Assumptions 2.1 from Chapter 2.

Now, for a large parameter $\kappa > 0$, the regular solution f_κ to the equation $f_\kappa'' = -\kappa V f_\kappa$ is actually well described <u>globally</u> by the Liouville-Green approximation – and this allows us to give very nice large κ asymptotics for the scattering length of the most natural transformation of the potential $-\kappa V$. More precisely, we can use the result of Olver, [Olv61] Theorem 4, parts of which are presented in Proposition 3.8 of Chapter 2, on all of $\mathbb{R}_+$, where the errors are controlled by functions ε_κ^1 and ε_κ^2 satisfying

$$|\varepsilon_\kappa^1(x)|, |\varepsilon_\kappa^2(x)| \lesssim \exp\left(\kappa^{-1/2}\int_0^x V(y)^{-1/4}\left|\frac{d^2}{dy^2}\Big(V^{-1/4}\Big)\right| dy\right) - 1, \tag{5.1}$$

the integral being convergent as $x \to \infty$ due to our assumptions. Note that consequently $\varepsilon_\kappa^1(x), \varepsilon_\kappa^2(x) \to 0$ uniformly on $\mathbb{R}_+$ as $\kappa \to \infty$. Moreover, it can be seen from the construction of the error functions in [Olv61] that they have well-defined finite limits as $x \to \infty$ for all

$\kappa > 0$. We denote these limits by $\varepsilon_\kappa^1(\infty)$ and $\varepsilon_\kappa^2(\infty)$ and observe that they must also satisfy (5.1) with x replaced by ∞. The statement from [Olv61] is then (slightly reformulated) that we can write

$$f_\kappa(x) = V(x)^{-1/4}\left[\sin\left(\kappa^{1/2}\int_0^x V(y)^{1/2}\,dy + \theta(\kappa)\right) + \varepsilon_\kappa^1(x)\right]$$

and

$$\begin{aligned} f_\kappa'(x) = \frac{d}{dx}\left(V^{-1/4}\right)\cdot\left[\sin\left(\kappa^{1/2}\int_0^x V(y)^{1/2}\,dy + \theta(\kappa)\right) + \varepsilon_\kappa^1(x)\right] \\ + \kappa^{1/2}V(x)^{1/4}\left[\cos\left(\kappa^{1/2}\int_0^x V(y)^{1/2}\,dy + \theta(\kappa)\right) + \varepsilon_\kappa^2(x)\right], \end{aligned}$$

up to an overall constant, for some a priori unknown number $\theta(\kappa)$. However, we see from (5.1) that $\varepsilon_\kappa^1(0) = \varepsilon_\kappa^2(0) = 0$ so that $0 = f_\kappa(0) = V(0)^{-1/4}\sin(\theta(\kappa))$ meaning that we can take $\theta(\kappa) = 0$ for all $\kappa > 0$. This together with our assumptions yield

$$\lim_{x\to\infty} f_\kappa'(x) = C_\infty^{-1/4}\left[\sin\left(\kappa^{1/2}\int_0^\infty V(x)^{1/2}\,dx\right) + \varepsilon_\kappa^1(\infty)\right]$$

and

$$\begin{aligned} f_\kappa(x) - x f_\kappa'(x) = \left[V(x)^{-1/4} - x\frac{d}{dx}\left(V^{-1/4}\right)\right]\cdot\left[\sin\left(\kappa^{1/2}\int_0^x V(y)^{1/2}\,dy\right) + \varepsilon_\kappa^1(x)\right] \\ - \kappa^{1/2} x V(x)^{1/4}\left[\cos\left(\kappa^{1/2}\int_0^x V(y)^{1/2}\,dy\right) + \varepsilon_\kappa^2(x)\right] \\ \longrightarrow -\kappa^{1/2}C_\infty^{1/4}\left[\cos\left(\kappa^{1/2}\int_0^\infty V(x)^{1/2}\,dx\right) + \varepsilon_\kappa^2(\infty)\right] \end{aligned}$$

as $x \to \infty$ up to a single constant multiplied on both limits.

By considering the construction also treated in Chapter 2, i.e. $V_\kappa(x) := \kappa^2 V(\kappa^{1/2}x)$, it can be seen by a simple calculation that $g_\kappa(x) := f_\kappa(\kappa^{1/2}x)$ solves the equation $g_\kappa'' = -V_\kappa g_\kappa$. Since also $g_\kappa(0) = 0$, this means that

$$\begin{aligned} a(-V_\kappa) &= \lim_{x\to\infty}\frac{g_\kappa(x) - x g_\kappa'(x)}{g_\kappa'(x)} = \lim_{x\to\infty}\frac{f_\kappa(x) - x f_\kappa'(x)}{\kappa^{1/2}f_\kappa'(x)} \\ &= -C_\infty^{1/2}\frac{\cos\left(\kappa^{1/2}\int_0^\infty V(x)^{1/2}\,dx\right) + \varepsilon_\kappa^2(\infty)}{\sin\left(\kappa^{1/2}\int_0^\infty V(x)^{1/2}\,dx\right) + \varepsilon_\kappa^1(\infty)} = C_\infty^{1/2}\frac{\sin\left(\int_0^\infty V_\kappa(x)^{1/2}\,dx - \pi/2\right) - \varepsilon_\kappa^2(\infty)}{\cos\left(\int_0^\infty V_\kappa(x)^{1/2}\,dx - \pi/2\right) + \varepsilon_\kappa^1(\infty)} \end{aligned}$$

implying the large κ asymptotics

$$a(-V_\kappa) = C_\infty^{1/2}\tan\left(\int_0^\infty V_\kappa(x)^{1/2}\,dx - \pi/2 + o_{\kappa\to\infty}(1)\right)$$

for the scattering length of $-V_\kappa$. Remarkably, the scattering length has this very nice asymptotic expression exactly for the family of potentials $\{-V_\kappa\}_{\kappa>0}$ which happen to also converge uniformly towards the potential $-C_\infty x^{-4}$ away from the origin as $\kappa \to \infty$. On the other hand, $a(-\kappa V) = \kappa^{1/2}a(-V_\kappa)$ cannot be written as a constant times tangent to a well-behaved expression for large κ's. On an intuitive level this combination of nice asymptotics of both the potentials (away from the origin) and of the scattering lengths can be seen as the key to achieving the strong resolvent convergence of the associated Schrödinger operators as in Chapter 2 along certain subsequences – with some particular assumptions on the potential V^1. ▲

As we will see below, the more general case of potentials from Chapter 2 that actually have a scattering length also has ties to rather explicit scattering length asymptotics. However, these ties are a bit more subtle than in Example 5.1, and they tell us only indirectly something about the scaled potentials Φ_κ (from Chapter 2). To explain this more precisely, we need firstly a computational result.

Lemma 5.2. Let $f_\pm(x) = \sqrt{x} J_{\pm\nu}(Cx^{\frac{1}{2\nu}})$ for some $\nu \in (-1, 0)$ and $C > 0$. Then we have

$$\lim_{x\to\infty} f_+'(x) = \frac{(C/2)^\nu}{\Gamma(1+\nu)}, \qquad \lim_{x\to\infty}[f_+(x) - x f_+'(x)] = 0,$$

$$\lim_{x\to\infty} f_-'(x) = 0 \qquad \text{and} \qquad \lim_{x\to\infty}[f_-(x) - x f_-'(x)] = \frac{(C/2)^{-\nu}}{\Gamma(1-\nu)}.$$

We observe initially that $f_\pm$ solve the equation $f_\pm'' = -(C/2)^2\nu^{-2}x^{\frac{1}{\nu}-2}f_\pm$, i.e. a scattering equation with a potential that is in $L^1(x^2\,dx)$ near infinity. Hence, it is almost immediate from Theorem 4.11 that the limits in the lemma exist.

Proof (of Lemma 5.2). In order to prove the convergences we need the power series expansion

$$J_\tau(x) = \left(\frac{x}{2}\right)^\tau \sum_{k=0}^\infty \frac{(-1)^k (x/2)^{2k}}{k!\Gamma(1+k+\tau)}$$

of the Bessel function of the first kind around the origin, cf. [AS72] p.360 or any other reference on special functions. This yields the large x behaviour

$$f_+(x) = \frac{(C/2)^\nu}{\Gamma(1+\nu)} x + \mathcal{O}_{x\to\infty}(x^{1+\frac{1}{\nu}}) \qquad \text{and} \qquad f_+'(x) = \frac{(C/2)^\nu}{\Gamma(1+\nu)} + \mathcal{O}_{x\to\infty}(x^{\frac{1}{\nu}})$$

from which the values of the limits concerning f_+ in the lemma follow straightforwardly since $1 + 1/\nu < 0$.

For f_- we can be a bit more sophisticated. From the power series we see that we have $f_-(x) \to (C/2)^{-\nu}/\Gamma(1-\nu)$ as $x \to \infty$. As mentioned above we know that $f_-'(x)$ and $f_-(x) - x f_-'(x)$ are convergent as $x \to \infty$ and thus so are $x f_-'(x)$. From this it is clear that $f_-'(x) \to 0$, but perhaps more surprisingly also $x f_-'(x) \to 0$. To see this, simply consider $g(x) := f_-(e^x)$ which is bounded for large x and has $g'(x) = e^x f_-(e^x)$ convergent as $x \to \infty$. Hence, $g'(x) \to 0$ which is exactly equivalent to the last claim finishing the proof. □

[1] An important observation here is that the scattering length on its own says absolutely nothing about the behaviour of the operators $H_{\kappa,\ell}$ in the ℓ-sectors where $\ell \neq 0$. Hence, when we in this section propose scattering length asymptotics as an explanation of the strong resolvent convergence in Chapter 2, we mean this only for the operators $H_{\kappa,0}$ acting in the $\ell = 0$ sector.

To tune in on the situation from Chapter 2 once again we would like to emphasize a particular aspect of the proof of the main result which is not explicitly mentioned in Chapter 2 itself: The fact that we at some point replace the original potential Φ by a modified version Ψ_λ and implicitly show strong resolvent convergence of the Schrödinger operators associated to Φ_κ through the corresponding convergence of operators associated to some modified versions of Φ_κ. The point being that in terms of the desired convergence there is no difference between these things since the modifications really approximate the Φ_κ's in L^2 (or in any reasonable weighted L^p-space one could think of) as $\kappa \to \infty$.

It is the convergence of the modified operators with potentials slightly different from Φ_κ that can be considered in the same light as it is done in Example 5.1, i.e. in terms of somewhat nice asymptotics of the scattering lengths of the potentials involved (recall, however, the content of the footnote in Example 5.1). Recalling the relation to the original potentials for later discussions we notice for the moment that in case Φ actually equals $C_\infty x^\beta$ from some point onwards then there is no modification made to this potential for sufficiently large κ. Thus, with this very strong assumption on the asymptotics of the potential (which we will from now again call V to be somewhat consistent within the present chapter) at infinity we can simply use the results obtained in Chapter 2 to find the asymptotic scattering lengths $a(-V_\kappa)$ of the suitably scaled potentials $V_\kappa(x) := \kappa^{-\beta} V(\kappa x)$ for large κ. From the proof of Theorem 2.4 in Chapter 2 we learn that the regular solutions g_κ to the scattering equations $g_\kappa'' = -V_\kappa g_\kappa$ from some point onwards, say for $x > 1$, and up to an overall constant is given by

$$g_\kappa(x) = \cos\theta_\kappa \cdot \sqrt{x} \cdot J_{\frac{1}{2+\beta}}\left(\frac{-2C_\infty^{1/2}}{2+\beta} x^{\frac{2+\beta}{2}}\right) + \sin\theta_\kappa \cdot \sqrt{x} \cdot Y_{\frac{1}{2+\beta}}\left(\frac{-2C_\infty^{1/2}}{2+\beta} x^{\frac{2+\beta}{2}}\right)$$

for some constants θ_κ satisfying

$$\theta_\kappa = \int_0^\infty V_\kappa(x)^{1/2}\,dx - \frac{\pi}{4+2\alpha} - \frac{\pi}{4+2\beta} - \frac{\pi}{2} + o_{\kappa\to\infty}(1).$$

We will need in a moment also the fact that from the definition of the Bessel function Y_τ of the second kind we have

$$\cos\theta \cdot J_\tau + \sin\theta \cdot Y_\tau = \cos\theta \cdot J_\tau + \sin\theta \frac{\cos(\tau\pi) J_\tau - J_{-\tau}}{\sin(\tau\pi)} = \frac{\sin(\theta+\tau\pi) J_\tau - \sin\theta J_{-\tau}}{\sin(\tau\pi)}$$

for any θ and any non-integer τ. Now in order for $-V_\kappa$ to have a scattering length we clearly must have $\beta < -3$ so we assume this from now onwards. Then Lemma 5.2 with $\nu = 1/(2+\beta) \in (-1,0)$ and $C = -2C_\infty^{1/2}/(2+\beta) > 0$ together with the above 3 equations yield the intriguing formula

$$
\begin{aligned}
a(-V_\kappa) &= \frac{\lim_{x\to\infty}[g_\kappa(x) - x g_\kappa'(x)]}{\lim_{x\to\infty} g_\kappa'(x)} = \frac{-\sin\theta_\kappa \cdot \left(\frac{-C_\infty^{1/2}}{2+\beta}\right)^{-\frac{1}{2+\beta}} \cdot \Gamma\left(\frac{1+\beta}{2+\beta}\right)^{-1}}{\sin\left(\theta_\kappa + \frac{\pi}{2+\beta}\right) \cdot \left(\frac{-C_\infty^{1/2}}{2+\beta}\right)^{\frac{1}{2+\beta}} \cdot \Gamma\left(\frac{3+\beta}{2+\beta}\right)^{-1}} \\
&= \left(\frac{-C_\infty^{1/2}}{2+\beta}\right)^{-\frac{2}{2+\beta}} \frac{\Gamma\left(\frac{3+\beta}{2+\beta}\right)}{\Gamma\left(\frac{1+\beta}{2+\beta}\right)} \cdot \frac{\sin\theta_\kappa}{\cos\left(\theta_\kappa + \frac{\pi}{2+\beta} + \frac{\pi}{2}\right)} \\
&= \left(\frac{-C_\infty^{1/2}}{2+\beta}\right)^{-\frac{2}{2+\beta}} \frac{\Gamma\left(\frac{3+\beta}{2+\beta}\right)}{\Gamma\left(\frac{1+\beta}{2+\beta}\right)} \cdot \frac{\sin\left(\int_0^\infty V_\kappa(x)^{1/2}\,dx - \frac{\pi}{4+2\alpha} - \frac{\pi}{4+2\beta} - \frac{\pi}{2} + o_{\kappa\to\infty}(1)\right)}{\cos\left(\int_0^\infty V_\kappa(x)^{1/2}\,dx - \frac{\pi}{4+2\alpha} + \frac{\pi}{4+2\beta} + o_{\kappa\to\infty}(1)\right)}
\end{aligned}
\tag{5.2}
$$

for the large κ asymptotics of the scattering length. We make some observations.

Remark 5.3. a) The picture where the correct scaling for making the potentials converge away from the origin and the one securing nice scattering length asymptotics agree – as discussed in Example 5.1 – is the same in the case above with more general β. It seems to be a pattern that one has a better understanding of the asymptotic scattering length the more one knows about the convergence of the potentials themselves. As mentioned above, this universally "nice" scaling of the potentials is very important for having the main results in Chapter 2.

b) Something that can be seen from (5.2) is that the scattering length $a(-V_\kappa)$ tend to be asymptotically increasing. Indeed, ignoring the error terms and using

$$
\frac{d}{dx}\frac{\sin(h(x)+c_1)}{\cos(h(x)+c_2)} = \frac{h'(x)\cos(c_1-c_2)}{\cos(h(x)+c_2)^2},
$$

we deduce relatively easily that $da(-V_\kappa)/d\kappa$ has the same sign as

$$
\cos\left(-\frac{\pi}{4+2\alpha} - \frac{\pi}{4+2\beta} - \frac{\pi}{2} + \frac{\pi}{4+2\alpha} - \frac{\pi}{4+2\beta}\right) = \cos\left(-\frac{\pi}{2+\beta} - \frac{\pi}{2}\right)
$$

which is positive since $-\pi/(2+\beta) \in (0,\pi)$. From the general theory, cf. Proposition 4.17, and the connection to the scattering length $a(-\kappa V)$ this is not a surprising result, but it nevertheless shows how we can re-observe the general theory in asymptotic expressions, this time in the derivative of the scattering length for large κ. ■

To end the section we include a discussion about the assumptions one needs to put on the potential V in order to have the asymptotic expression (5.2) for the scattering length of $-V_\kappa$.

Remark 5.4. Fortunately, the formula (5.2) matches with the result from Example 5.1. Indeed, in the case of $\alpha = 0$ and $\beta = -4$ one has

$$
-\frac{\pi}{4+2\alpha} - \frac{\pi}{4+2\beta} - \frac{\pi}{2} = -\frac{\pi}{4} + \frac{\pi}{4} - \frac{\pi}{2} = -\frac{\pi}{2}, \quad -\frac{\pi}{4+2\alpha} + \frac{\pi}{4+2\beta} = -\frac{\pi}{4} - \frac{\pi}{4} = -\frac{\pi}{2},
$$

and

$$
\left(\frac{-C_\infty^{1/2}}{2+\beta}\right)^{-\frac{2}{2+\beta}} \frac{\Gamma\left(\frac{3+\beta}{2+\beta}\right)}{\Gamma\left(\frac{1+\beta}{2+\beta}\right)} = \frac{C_\infty^{1/2}}{2} \cdot \frac{\Gamma(1/2)}{\Gamma(3/2)} = C_\infty^{1/2}.
$$

This is a strong indication that the formula (5.2) has some robustness in terms of conditions on the asymptotics of the potential near infinity – at least for some α's and β's. After all, we did not assume the perfect asymptotic expression for the potential in Example 5.1.

We believe that this combined with the fact that the asymptotics works with only very natural conditions on the asymptotics x^α near the origin gives an indication that (5.2) holds true more generally than for the cases treated above. At least it seems plausible that one needs only to control the behaviour of a couple of derivatives of the potential near infinity – both since this is the case near the origin but also considering the various refined WKB approximation techniques that might be applied to approximate solutions of the equation $f_\kappa'' = -\kappa V f_\kappa$ for large κ. By the latter we mean for example the "exact WKB method", cf. [GG88], or the analysis carried out by Feffermann and Seco in [FS92]. Using these methods there seems to be a rather clear connection between the number of well-controlled derivatives of the potential and the quality of the approximation. We ask only for the asymptotics of the scattering length which is really given by evaluating scattering solutions and their derivatives at some fixed point (as is seen in the proof of Theorem 4.12). Therefore, one should be able to determine this by the mentioned methods with way weaker assumptions than we have above, thus opening a way to improve our results.

Another possible approach[2] to broadening the class of potentials for which (5.2) holds true is strengthening the abstract theory on the scattering length. More precisely, any kind of uniform continuity of scattering length-related quantities will be an enormous help in this regard, since this might open the possibility of relating asymptotic scattering lengths of more general potentials and those for which we have (5.2). However, we do really need this kind of result – at least with our methods – to get all the way to having similar conditions at the origin and at infinity in the above. Indeed, while the modified potentials with which we are really working do approximate the "original" potentials in any relevant L^p-space, one has next to no control over the rate of this approximation: It depends on the asymptotics of the "original" potential at infinity in a very convoluted way (through the function η in Chapter 2). As a consequence, only true uniform continuity of some relevant quantity as a function of the potentials will be a real short-cut to weakening the assumptions above. ■

5.2 A conjecture about the asymptotic jumps of $n_-(-\kappa V)$

Consider a potential V which is everywhere non-negative and satisfies suitable conditions securing that $n_-(-\kappa V)$ from Section 4.4 is well-defined for all $\kappa > 0$ and Weyl's law (see Section 4.4 in [FLW22] for a standard treatment of slightly weaker forms of this) holds, i.e.

$$n_-(-\kappa V) = \frac{\sqrt{\kappa}}{\pi}\int_0^\infty V(x)^{1/2}\,dx + \mathcal{O}_{\kappa\to\infty}(1)$$

[2]It should be mentioned that we find this approach somewhat unlikely to work out. Actually, it would also be interesting to try to disprove uniform continuity of, say, the scattering curve from Definition 4.27 (note that this can similarly be defined on $\mathscr{L}$ directly).

as $\kappa \to \infty$. Introducing the "jumps" of the function $\kappa \mapsto n_-(-\kappa V)$ rigorously by putting

$$\kappa_n(V) := \inf\{\kappa > 0 \mid n_-(-\kappa V) \geq n\}$$

for $n = 1, 2, \ldots$, we claim that $n_-(-\kappa_n(V)V)$ is either $n-1$ or n. This can be seen from Remark 4.33 (where κ now plays the role of t) since by tracing the continuous scattering curve just before and after its n'th crossing of -1 respectively, it is apparent that $n_-(-\kappa V) = n-1$ for some $\kappa < \kappa_n(V)$ and $n_-(-\kappa V) = n$ for some $\kappa > \kappa_n(V)$. It is well known that $n_-(-\kappa V)$ is non-deceasing in κ by the variational principle, and thus the claim follows. This and the Weyl law combined with the fact that $\kappa_n(V) \to \infty$ as $n \to \infty$ yields the equation

$$\frac{\kappa_n(V)^{1/2}}{\pi} \int_0^\infty V(x)^{1/2}\, dx = n + \mathcal{O}_{n\to\infty}(1), \tag{5.3}$$

describing the asymptotic behaviour of $\kappa_n(V)$ up to errors of order n as $n \to \infty$. We conjecture that these asymptotics in many cases can be improved in the sense that $\mathcal{O}_{n\to\infty}(1)$ in (5.3) can be replaced by $C(V) + o_{n\to\infty}(1)$ with some explicit constant $C(V)$ depending on the behaviour of the potential near the origin and infinity. This will describe the asymptotics of $\kappa_n(V)$ including its order n behaviour exactly. More precisely, our primary conjecture is the following:

Conjecture 5.5. Suppose that V satisfies the Assumptions 2.1 in Chapter 2. Then, with $\kappa_n(V)$ defined as a above,

$$\frac{\kappa_n(V)^{1/2}}{\pi} \int_0^\infty V(x)^{1/2}\, dx = n + \frac{1}{4+2\alpha} - \frac{1}{4+2\beta} - \frac{1}{2} + o_{n\to\infty}(1) \tag{5.4}$$

which implies

$$\kappa_n(V) = \pi^2 \Big(\int_0^\infty V(x)^{1/2}\, dx \Big)^{-2} \Big[n^2 + \frac{n}{2+\alpha} - \frac{n}{2+\beta} - n \Big] + o_{n\to\infty}(n)$$

as $n \to \infty$.

As we will see below the conjecture about the next-to-leading order asymptotic term in (5.4) primarily stems from the fact that modulo 1 precisely this constant arises in the cases where we can find scattering length asymptotics (5.2) – thus making us almost able to prove the conjecture in these more regular cases.

Meanwhile, we also motivate the conjecture with an example that sheds some light on the mechanisms that should be driving the asymptotics in (5.4).

Example 5.6. Consider the simple potential

$$V(x) = \begin{cases} 1 & \text{for } x \in (0,1) \\ x^{-4} & \text{for } x \in (1,\infty) \end{cases}$$

which does not strictly speaking satisfy the regularity assumptions in the conjecture. On the other hand, it is still very plausible that the result holds also for this potential, and here we actually have a chance of computing (or at least of approximating) the numbers $\kappa_n(V)$ pretty well for almost all n. Now notice that, for any $\kappa > 0$, if $f_\kappa'' = -\kappa V f_\kappa$ is the regular solution to the scattering equation and $g_\kappa(x) := f_\kappa(\kappa^{1/2}x)$ then $g_\kappa'' = -V_\kappa g_\kappa$ with

$$V_\kappa(x) = \begin{cases} \kappa^2 & \text{for } x \in (0, \kappa^{-1/2}) \\ x^{-4} & \text{for } x \in (\kappa^{-1/2}, \infty), \end{cases}$$

and g_κ is a multiple of the regular solution of this equation. Now by the oscillation theorem this shows that $n_-(-\kappa V) = n_-(-V_\kappa)$ since f_κ and g_κ clearly have the same number of zeroes. Moreover, we have $a(-\kappa V) = \pm\infty$ if and only if $a(-V_\kappa) = \pm\infty$ since this corresponds to $f_\kappa'(x) \to 0$ and $g_\kappa'(x) \to 0$ as $x \to \infty$ respectively. As described in Remark 4.33 these κ's are exactly the $\kappa_n(V)$'s and thus a relatively thorough analysis of $\kappa \mapsto a(-V_\kappa)$ might very well give us an expression like (5.4). We now start this analysis.

Since we can consider the g_κ solving $g_\kappa'' = -V_\kappa g_\kappa$, $g_\kappa(0) = 0$, we choose the solution, up to a constant on one of the regions,

$$g_\kappa(x) = \begin{cases} \sin(\kappa x) & \text{for } x \in (0, \kappa^{-1/2}) \\ x\cos(\theta_\kappa - 1/x) & \text{for } x \in (\kappa^{-1/2}, \infty) \end{cases}$$

where θ_κ is determined by the condition $g \in C^1([0,\infty))$ (it is not difficult to check that all solutions to $g''(x) = -x^{-4}g(x)$ has the above form for some θ_κ). This solution has

$$g_\kappa'(x) = \begin{cases} \kappa\cos(\kappa x) & \text{for } x \in (0, \kappa^{-1/2}) \\ \cos(\theta_\kappa - 1/x) - \dfrac{1}{x}\sin(\theta_\kappa - 1/x) & \text{for } x \in (\kappa^{-1/2}, \infty), \end{cases}$$

up to a constant on one of the regions, which shows in particular

$$a(-V_\kappa) = \lim_{x\to\infty} \frac{g_\kappa(x) - x g_\kappa'(x)}{g_\kappa'(x)} = \lim_{x\to\infty} \frac{\sin(\theta_\kappa - 1/x)}{\cos(\theta_\kappa - 1/x)} = \tan(\theta_\kappa),$$

i.e. $\kappa \mapsto \theta_\kappa$ is a continuous scattering argument (from Definition 4.12 – continuity is relatively clear from the definitions above) of the pointwise non-increasing curve $\kappa \mapsto -V_\kappa$. Since we know from the general theory that this is non-decreasing, we conclude that $\kappa_n(V)$ is characterized by $\theta_{\kappa_n(V)} = n\pi - \pi/2$ when choosing[3] $\theta_0 \in (-\pi/2, \pi/2)$, and all there is left to do is to provide a sufficiently detailed description of the map $\kappa \mapsto \theta_\kappa$.

From equating the expressions for g_κ and g_κ' at $x = \kappa^{-1/2}$ and dividing them with each other – thus eliminating any overall constants – we arrive after minor algebraic manipulations at the equation[4]

$$\tan(\theta_\kappa - \kappa^{1/2}) - \tan(\kappa^{1/2} + \pi/2) = \kappa^{-1/2} \tag{5.5}$$

which together with $\theta_0 \in (-\pi/2, \pi/2)$ and the continuity completely describes $\kappa \mapsto \theta_\kappa$. To see that this is a possible choice of θ_0 simply notice that

$$\tan(\theta_\kappa - \kappa^{1/2}) = \tan(\kappa^{1/2} + \pi/2) + \kappa^{-1/2} \longrightarrow 0$$

[3] You will see in a moment that this is indeed possible.

[4] This should be understood in the sense that $\theta_\kappa - \kappa^{1/2} = \pi/2 \bmod \pi$ if and only if $\kappa^{1/2} = 0 \bmod \pi$.

as $\kappa \to 0$ and thus we can choose $\theta_\kappa - \kappa^{1/2} \to 0 =: \theta_0$. From (5.5) it follows that

$$|\theta_\kappa - 2\kappa^{1/2} + \pi/2 - k_\kappa \pi| = |\theta_\kappa - \kappa^{1/2} - (\kappa^{1/2} + \pi/2) - (k_\kappa - 1)\pi| \leq \kappa^{-1/2}$$

for some $k_\kappa \in \mathbb{Z}$ depending on κ. Combining this with the continuity yields

$$|\theta_\kappa - 2\kappa^{1/2} + \pi/2 - k\pi| \leq \kappa^{-1/2} \tag{5.6}$$

for some fixed $k \in \mathbb{Z}$ for all $\kappa \in (4/\pi^2, \infty)$. We claim that $k = 0$. To realize this, put $h_1(\kappa) = \theta_\kappa - \kappa^{1/2}$ and $h_2(\xi) = \tan(\xi + \pi/2) + \xi^{-1}$ and observe that the latter is well-defined on all of $(0, \pi)$ with

$$h_2'(\xi) = \frac{\xi^2 - \sin^2 \xi}{\xi^2 \sin^2 \xi} > 0$$

here. Together with the limits $h_2(\xi) \to 0$ as $\xi \to 0$ and $h_2(\xi) \to \infty$ as $\xi \to \pi$ this is to say that on $(0,\pi)$ it grows from 0 to ∞, and hence that $h_1(\kappa) = \arctan(h_2(\kappa^{1/2}))$ for $\kappa \in (0, \pi^2)$. Consequently, h_1 grows from 0 to $\pi/2$ on $(0, \pi^2)$ by the choice $\theta_0 = 0$. The important part is that by continuity of h_1 we have

$$\theta_{\pi^2} - 2\pi + \frac{\pi}{2} = h_1(\pi^2) - \frac{\pi}{2} = 0$$

so that indeed $k = 0$ in (5.6) (as clearly $\pi^2 > 4/\pi^2$ and $\pi > 1/\pi$).

We have thus obtained a very nice asymptotic expression for the scattering length as $a(-V_\kappa) = \tan \theta_\kappa$ with $\theta_\kappa = 2\kappa^{1/2} - \pi/2 + \mathcal{O}_{\kappa\to\infty}(\kappa^{-1/2})$. From this we obtain

$$n\pi - \frac{\pi}{2} = \theta_{\kappa_n(V)} = 2\kappa_n(V)^{1/2} - \frac{\pi}{2} + \mathcal{O}_{n\to\infty}(\kappa_n(V)^{-1/2})$$

and, rearranging, $2\kappa_n(V)^{1/2} = n\pi + \mathcal{O}_{n\to\infty}(\kappa_n(V)^{-1/2}) = n\pi + \mathcal{O}_{n\to\infty}(n^{-1})$. Correspondingly we easily find that

$$\int_0^\infty V(x)^{1/2}\, dx = 2$$

which confirms the correctness of Conjecture 5.5 for this particular potential since in this case

$$\frac{1}{4+2\alpha} - \frac{1}{4+2\beta} - \frac{1}{2} = \frac{1}{4+2\cdot 0} - \frac{1}{4+2\cdot(-4)} - \frac{1}{2} = 0.$$

We even have a smaller error term of order n^{-1} instead of $o_{n\to\infty}(1)$ which might be seen as a consequence of the fact that V satisfies exactly the asymptotics ~ 1 and $\sim x^{-4}$ at the origin and infinity respectively. ▲

Remark 5.7. One can – and should – notice several things about Example 5.6:

a) The equation (5.5) actually tells us that whenever $\kappa^{1/2} = k\pi$ for some $k \in \mathbb{N}$ then it forces $\theta_\kappa = \pi/2 \mod \pi$, i.e. $a(-V_\kappa) = \pm\infty$. From this it is possible to extract the equality $\kappa_{2n}(V)^{1/2} = n\pi$ for all $n \in \mathbb{N}$. These points of new eigenvalues are in other words quite easy to find; it is the $\kappa_n(V)$'s with odd n which take some effort to describe sufficiently well.

b) The entire analysis in the example could have been carried out without considering the transformed potentials V_κ. The reason for nevertheless performing the transformation is more of the aesthetic kind, yielding as usual the nice(r) formula $a = \tan\theta$ for the scattering length. We do believe that this approach makes the connection between scattering length asymptotics and the conjecture more transparent.

c) In the case of the potential V from the example there seems to be no obvious obstructions for using the Liouville-Green approximation to the regular solution f_κ to the scattering equation for large κ as in Example 5.1. Doing so one arrives at the expression $a(-\kappa V) \approx \kappa^{1/2}\tan(2\kappa^{1/2} - \pi/2)$ for large κ, and one can relatively easily extract the equality (5.4) – at least modulo 1. For the details see the discussion below the present remark. However, this approach to the problem also has massive issues in describing the small κ behaviour of the relevant quantities which was actually the most delicate part of the exact treatment of the example.

d) The error term of the form $\mathcal{O}_{n\to\infty}(n^{-1})$ in the example corresponding to $o_{n\to\infty}(1)$ in (5.4) is interesting in two ways. Perhaps most obviously it tells us, as we briefly mentioned above, that for sufficiently regular potentials the "natural" next term after the constant one in (5.4) is that of order n^{-1}. But on the other hand it is remarkable that, according to a), the error term is 0 for even n's while by (5.5) this is not the case for odd n's. In other words, the error is oscillating in a non-trivial way. Perhaps a bit speculative one could ask whether this is a consequence of the discontinuity of V' at $x = 1$. ■

Let us now see how close we can get to proving Conjecture 5.5. For this we unfortunately have to consider the set-up where we have shown the scattering length asymptotics (5.2). Analogously to Example 5.1 (with slightly different notation) it can be seen by standard calculations that $a(-\kappa V) = \tilde\kappa a(-V_{\tilde\kappa})$ with $\tilde\kappa = \kappa^{\frac{-1}{2+\beta}}$ and $V_{\tilde\kappa}(x) := \tilde\kappa^{-\beta} V(\tilde\kappa x)$. Further, as in Example 5.6, for each n, the number $\kappa_n(V)$ is exactly the $\kappa > 0$ in the n'th occurrence of $a(-V_{\tilde\kappa}) = \pm\infty$. Once $\tilde\kappa$ and thus κ is sufficiently large we can use that it follows from (5.2) and the above that all $\kappa_n(V)$'s are the κ's for which $\tilde\kappa$ satisfies

$$\int_0^\infty V_{\tilde\kappa}(x)^{1/2}\,dx - \frac{\pi}{4+2\alpha} + \frac{\pi}{4+2\beta} + o_{\kappa\to\infty}(1) = \frac{\pi}{2} \tag{5.7}$$

modulo π. Now, since

$$\int_0^\infty V_{\tilde\kappa}(x)^{1/2}\,dx = \tilde\kappa^{\frac{-2-\beta}{2}} \int_0^\infty V(x)^{1/2}\,dx = \sqrt{\kappa}\int_0^\infty V(x)^{1/2}\,dx,$$

we recover the formula (5.4) by rearranging (5.7) – except we only know about its validity modulo 1 (from the modulo π above).

We can extend this argument slightly to include potentials for which the "inverted potential" $V^{\mathrm{inv}}(x) := V(1/x)/x^4$ satisfies the assumptions needed to prove the asymptotics (5.2) (of course with α replaced by $-\beta-4$ and β by $-\alpha-4$). This means essentially that V should satisfy the β-part of Assumptions 2.1 in Chapter 2 together with very strong assumptions on the behaviour of V near the origin (i.e. that it is identically C_0x^α here).

To realize the connection between $\kappa_n(V)$ and $\kappa_n(V^{\text{inv}})$ observe that if f_κ is the regular solution to $f_\kappa'' = -\kappa V f_\kappa$ and $f_\kappa^{\text{inv}}(x) := x f_\kappa(1/x)$ then $(f_\kappa^{\text{inv}})'' = -\kappa V^{\text{inv}} f^{\text{inv}}$. Since f_κ and f_κ^{inv} has the exact same number of zeroes in $\mathbb{R}_+$ we learn by the oscillation theorem that $\kappa_n(V) = \kappa_n(V^{\text{inv}})$. By the above we obtain further

$$\begin{aligned}\frac{\kappa_n(V)}{\pi}\int_0^\infty V(x)^{1/2}\,dx &= \frac{\kappa_n(V^{\text{inv}})}{\pi}\int_0^\infty V^{\text{inv}}(x)^{1/2}\,dx \\ &= n + \frac{1}{4+2(-\beta-4)} - \frac{1}{4+2(-\alpha-4)} - \frac{1}{2} + o_{n\to\infty}(1) \\ &= n - \frac{1}{4+2\beta} + \frac{1}{4+2\alpha} - \frac{1}{2} + o_{n\to\infty}(1)\end{aligned}$$

modulo π which verifies the conjecture (modulo 1) also in the case of these assumptions.

Remark 5.8. In the light of the partial proof of Conjecture 5.5 just presented we can discuss how to get closer to proving the full conjecture. We mention both the directions for which we have concrete ideas for proceeding and the ones for which we do not.

a) The most obvious improvement to the proof above would be to be able to relax the assumptions on the behaviour of the potential near infinity needed for (5.2) to hold true. This is discussed in Remark 5.4, and we believe that it is the most difficult obstruction for proving Conjecture 5.5. It might be the case that one needs to assume a bit more than the β-part of Assumptions 2.1 in Chapter 2, for instance assumptions like those in Example 5.1, but it is remarkable that one can take so general behaviour near the origin and only very restricted ones near infinity (or vice versa). By the nature of the problem it seems unnatural that the asymmetry in assumptions about asymptotics near the origin and near infinity should be too large – as it is the case in the above proof.

b) A flaw in our scattering length approach above is that it needs the existence of a scattering length. In particular this means that it fails for $\beta \in [-3,-2)$. One way to fix this issue would be to generalize the theory of scattering lengths to a theory that include also these potentials. For most potentials from $L^1(\mathbb{R}_+, x\,dx)$ this does not seem impossible since a distinguished scattering solution, the Jost solution (cf. [RS79] XI.8.E) which converges towards 1 at infinity, exists for all potentials in this space. The problem is rather that a general scattering solution in its asymptotics near infinity contains terms between the leading order linear term and the constant term from the Jost solution. Thus, one cannot quantify the relationship between the contribution from each of these terms in an arbitrary scattering solution as it can be done in the more regular cases where the scattering length is well-defined as this relation exactly.

   However, it is still extremely plausible that the jumps $\kappa_n(V)$ in the number of negative eigenvalues are the κ's for which the regular solution to $f_\kappa'' = -\kappa V f_\kappa$ is a multiple of the Jost solution (actually we believe that this fact is part of the more advanced theory of the "Jost function" – not to be confused with the Jost solution – see [RS79] XI.8.E for the details). Thus, a closer examination of Wronskians like the ones defining $\beta(V)$ in the proof of Theorem 4.12 might very well be sufficient to determine the asymptotics of $\kappa_n(V)$ – even in the cases where the scattering length does not exist. In order to find asymptotic expressions for these Wronskians, one must of course additionally control the asymptotics of derivatives of scattering solutions. This does not seem like an impossible task since standard approximation results like those in [Olv61] actually include expressions for derivatives. However, the calculations in this approach could turn out to be tedious, and one still needs to strengthen the approximations also where the Liouville-Green method or similar methods do not apply.

c) Lastly there is the issue with our approach above that it only proves the assertion modulo 1. So one could reasonably ask: Then why do we conjecture the asymptotics 5.4 without "modulo 1"? This is based partly on the fact that it holds true in toy examples like Example 5.6 (see also Examples 5.11 and 5.12 below). But it also relies on more theoretical considerations. Considering for instance the Liouville-Green approximation in Example 5.1 for large κ's it is apparent from the oscillation theorem that the constant term in (5.4) is the desired one for potentials of this somewhat general type. We do believe that it is possible to obtain the same kind of results in the global approximation of scattering solutions in Chapter 2. Here, a large part of the approximation also comes from the Liouville-Green method where the number of zeroes of the solution – i.e. the contribution to the number of negative eigenvalues of the operator – is rather controllable as in Example 5.1. On the remaining parts of $\mathbb{R}_+$ the approximation is through exact solutions, described by Bessel functions, of "approximate scattering equations". In Chapter 2 only the asymptotic expressions of the Bessel functions for large variables are used, but in fact one also has some knowledge about the structure of zeroes of the Bessel functions – almost as for usual sine functions. Moreover, it seems likely that the expression for $\kappa_n(V)$ one would obtain from these asymptotics matches the one in (5.4). We believe that proving this is simply a matter of carrying out a rigorous analysis. ■

5.2.1 Generalizing the conjecture

We suggest also a slight generalization of Conjecture 5.5 to a class of potentials which is surprisingly difficult to handle with the methods of Chapter 2, but which are nonetheless standard objects in the theory of Schrödinger operators. A somewhat vague formulation of this is the following:

Conjecture 5.9. The result in Conjecture 5.5 extends to the cases $\alpha = \infty$ and $\beta = -\infty$ where this means that the potential V decays faster than any power at the origin and/or infinity and $1/\pm\infty := 0$ in the formula (5.4).

This conjecture is mostly motivated by the examples discussed below with exponentially decaying potentials, and in particular by the fact that the behaviour of the $\kappa_n(V)$'s fits so elegantly into (5.4) with the in this case very natural choice $\beta = -\infty$. It would be very interesting if one could even extend the conjecture to potentials with compact support where one must have both $\alpha = \infty$ and $\beta = -\infty$. Then the constant term in (5.4) would be the least possible in this case – i.e. the new eigenvalues would come "as fast as possible compared to the semi-classical term" exactly in this case. On the other end of the scale would be the potentials lying close to x^{-2} asymptotically near the origin and infinity.

For the final examples supporting Conjecture 5.9 we need a small lemma (which we surprisingly have not needed of so far).

Lemma 5.10. Consider a $V \in \mathscr{L}$ and let f be the regular solution to the scattering equation $f'' = Vf$. Then f is bounded on all of $\mathbb{R}_+$ if and only if $a(V) = \pm\infty$.

Proof. Recall the notation and content of the proof of Theorem 4.11. In particular let $w(x) := xf(1/x)$ so that $w(0) = \beta(V)$ and $w'(0) = \alpha(V)$. Now if $a(V) = \pm\infty$ then $\beta(V) = 0$ so that

$$f(x) = xw(1/x) = \frac{w(1/x) - w(0)}{1/x} = w'(\xi_x) \longrightarrow w'(0) = \alpha(V) \in \mathbb{R}$$

as $x \to \infty$ where $\xi_x \in [0, 1/x]$. This implies that f is bounded near infinity and hence on all of $\mathbb{R}_+$. If, on the other hand, $a(V) \neq \pm\infty$ then $f'(x) \to \beta(V) \neq 0$ as $x \to \infty$ and consequently f cannot be bounded at infinity. □

Example 5.11. Consider now the Pöschl-Teller potential defined by $V(x) = \cosh(x)^{-2}$. This has the to us very nice properties of being smooth and lying in the right L^p-spaces, and moreover the equations $f_\kappa'' = -\kappa V f_\kappa$ are completely solvable with all solutions being linear combinations of

$$g_\kappa(x) := P_{\frac{\sqrt{4\kappa+1}-1}{2}}(\tanh x) \qquad \text{and} \qquad h_\kappa(x) := Q_{\frac{\sqrt{4\kappa+1}-1}{2}}(\tanh x)$$

where P and Q are the Legendre functions of the first and second kind respectively. Letting f_κ be the regular solution to the scattering equation above, the condition $f_\kappa(0) = 0$ forces this to be, up to an (irrelevant) overall constant, of the form

$$f_\kappa(x) = P_{\frac{\sqrt{4\kappa+1}-1}{2}}(\tanh x) - \frac{P_{\frac{\sqrt{4\kappa+1}-1}{2}}(0)}{Q_{\frac{\sqrt{4\kappa+1}-1}{2}}(0)} Q_{\frac{\sqrt{4\kappa+1}-1}{2}}(\tanh x) =: g_\kappa(x) + C_\kappa h_\kappa(x)$$

in the sense that $f_\kappa(x) = ch_\kappa(x)$ whenever $h_\kappa(0) = 0$.

We notice in the spirit of Lemma 5.10 that g_κ is bounded on all of $\mathbb{R}_+$ while $h_\kappa(x) \to \infty$ as $x \to \infty$. Hence, $a(-\kappa V) = \pm\infty$ if and only if $C_\kappa = 0$, and by the general theory outlined above $\kappa_n(V)$ is exactly the value of κ for which this happens for the n'th time. A calculation shows that

$$C_\kappa = -\frac{2}{\pi}\tan\left(\frac{\pi}{4}\left(\sqrt{4\kappa+1}+1\right)\right)$$

yielding the equation

$$\frac{\pi}{4}\left(\sqrt{4\kappa_n(V)+1}+1\right) = n\pi$$

for $\kappa_n(V)$. Rewriting, we obtain $(\kappa_n(V)+1/4)^{1/2}/2 = n-1/4$, and further simple calculations result in the asymptotics

$$\frac{\kappa_n(V)^{\frac{1}{2}}}{\pi}\int_0^\infty V(x)^{\frac{1}{2}}\,dx = \frac{\kappa_n(V)^{\frac{1}{2}}}{2} = \frac{1}{2}\sqrt{\kappa_n(V)+\frac{1}{4}} + \mathcal{O}_{n\to\infty}(\kappa_n(V)^{-\frac{1}{2}}) = n-\frac{1}{4}+\mathcal{O}_{n\to\infty}(n^{-1})$$

which matches the conjecture with $\alpha = 0$ and $\beta = -\infty$. Comparing the error term we obtain here to Remark 5.7(d), further analysis will show quite easily that the error term for this very regular potential can be expanded as a power series in n^{-1} as one might find natural for smooth potentials. ▲

Example 5.12. As a final very simple example we take our potential to be $V(x) = e^{-x}$. If exponentially decaying potentials all have the same $\kappa_n(V)$-asymptotics then we should observe

$$n-\frac{1}{4}+\mathcal{O}_{n\to\infty}(n^{-1}) = \frac{\kappa_n(V)^{1/2}}{\pi}\int_0^\infty V(x)^{1/2}\,dx = \frac{2\kappa_n(V)^{1/2}}{\pi}$$

when determining $\kappa_n(V)$. We are basically doing so by following the procedure from Example 5.11. That is, if f_κ is the regular solution to $f_\kappa'' = -\kappa V f_\kappa$ then we find that

$$f_\kappa(x) = J_0(2\kappa^{1/2}e^{-x/2}) - \frac{J_0(2\kappa^{1/2})}{Y_0(2\kappa^{1/2})}Y_0(2\kappa^{1/2}e^{-x/2})$$

up to an overall constant. This is since $J_0(2\kappa^{1/2}e^{-x/2})$ and $Y_0(2\kappa^{1/2}e^{-x/2})$ span the space of solutions and we as usual force the boundary condition $f_\kappa(0) = 0$. Moreover, it can be seen that only the solution with the Bessel function of the first kind is bounded at infinity, and thus $\kappa_n(V)$ must be exactly the κ for which $2\kappa^{1/2}$ is the n'th zero of J_0. But this zero is well known to be $(n-1/4)\pi+\mathcal{O}_{n\to\infty}(n^{-1})$ (cf. [AS72] p.371) so we recover exactly the desired formula. ▲

5.3 Conclusion and some additional open problems

We here wrap up the key content of our work treated in this thesis and present some possible directions for further research.

In Chapter 2 we settled the periodicity question of the large Z behaviour of atoms H_Z^{TFMF} in the Thomas-Fermi mean-field model: The n^{th} period is asymptotically of length $3D_{\mathrm{cl}}^{-3}\pi^3 n^2$ to leading order for some fixed constant $D_{\mathrm{cl}} > 0$, and along certain sequences we really have convergence $H_{Z_n}^{\mathrm{TFMF}} \to H_{\infty,\theta}^{\mathrm{TFMF}}$ towards explicitly given "infinite atoms". There are several directions in which one could continue the research in this field.

Firstly, it would be interesting (but probably also difficult) to carry out a similar analysis in other mean-field models, or, more generally, to compare the periodicity in this model to that in other models for large atoms. Problems could be:

- Proving strong resolvent convergence in the other mean-field models introduced in Section 1.1. That is, $H_{Z_n}^{\star\mathrm{MF}} \to H_{\infty,\theta}^{\star\mathrm{MF}}$ along certain sequences in the strong resolvent sense for some "infinite atoms" $H_{\infty,\theta}^{\star\mathrm{MF}}$. Such results would significantly strengthen the hypothesis concerning a quite general periodicity in the many-body Schrödinger model for large atoms.

- A starting point could be to consider the Thomas-Fermi-von Weizsäcker mean-field model as also mentioned in Section 1.1 – and in particular the one-dimensional operators acting in the $\ell = 0$ angular momentum subspace corresponding to the $H^{\mathrm{TF}}_{Z,0}$'s from Chapter 2. Here it seems plausible that the scattering length theory from Chapter 4 and the convergence of the potentials away from the origin might prove abstractly (see the last bullet below for the details) convergence along *some* sequences of Z_n's. Perhaps one could manage to prove that these behave asymptotically like the corresponding Z_n's from the Thomas-Fermi mean-field model.

- Another related question is whether the sequences of Z_n's from the Thomas-Fermi mean-field model capture the (conjectured) oscillations in the radii $R^{\mathrm{HF}}_Q(Z)$ and ionization energy $I^{\mathrm{HF}}_Q(Z)$ as $Z \to \infty$.

Secondly, we suggest a further study of the limiting operators $H^{\mathrm{TFMF}}_{\infty,\theta}$, especially of its spectral properties. Here the problems are mathematically very appealing due to the very explicit form of the operators.

- The operators should have essential spectrum covering all of $[0,\infty)$. What about the part of the spectrum $\sigma(H^{\mathrm{TFMF}}_{\infty,\theta})$ lying in $(-\infty,0)$? Is this discrete? We can also ask whether 0 is an accumulation point of $\sigma(H^{\mathrm{TFMF}}_{\infty,\theta}) \cap (-\infty,0)$. If this is not the case, there will be a spectral gap below 0 which can be interpreted as the ionization energy of the infinite atom – and it will be natural to study its behaviour as a function of θ. For all these questions, one can start by answering the easier corresponding questions concerning the one-dimensional operators acting in the different angular momenta ℓ subspaces.

- A description of the asymptotic behaviour of large negative eigenvalues (if such exist, see above) of $H^{\mathrm{TFMF}}_{\infty,\theta}$ would be relevant. Since these eigenvalues describe the (infinitely many) electrons arbitrarily near the origin, their properties in the Thomas-Fermi mean-field model might actually tell us something about the corresponding quantities in the many-body Schrödinger model. This is unlike the previous question concerning the ionization energy in the infinite atoms which most likely depend only on the outermost electron(s).

In Chapter 3 we provided the exact relation between convergence of symmetric operators A_n, their self-adjoint extensions B_n and the operators U_n used in the construction of these extensions. We did this in terms of strong (resolvent) convergence of operators and strong convergence of graphs. Another natural convergence type of sequences of self-adjoint operators is norm resolvent convergence, and hence a relevant extension of our results would be:

- Proving the analogue of our results (say, Theorem 12 in Chapter 3) but where strong resolvent convergence of the B_n's is replaced by norm resolvent convergence. An educated guess is that one should then replace the strong convergence of the U_n's by norm convergence. Similarly the convergence conditions on the A_n's should be adapted to capture the nature of norm convergence.

We developed in Chapter 4 a general theory for the scattering length of real-valued potentials V lying in the class $L^1((x \vee x^2)\,dx, \mathbb{R}_+)$. Crucially, we constructed the scattering length $a(V)$ as a fraction $\alpha(V)/\beta(V)$ of two numbers, $\alpha(V)$ and $\beta(V)$, which are *continuous functions of* V. We proved also monotonicity of the scattering length and related quantities. Finally, we applied Sturm's oscillation theory to express the difference in the number of negative eigenvalues of $-d^2/dx^2+V$ and $-d^2/dx^2+\widetilde{V}$ (for suitable V and $\widetilde{V}$) as the winding number of a curve closely related to the scattering length. Some possible problems for further research on this topic are:

- Developing a theory similar to that of the scattering length for real-valued potentials from the class $L^1(x\,dx, \mathbb{R}_+)$. For many purposes this is a more natural class to consider, and in a sense $L^1((x \vee x^2)\,dx, \mathbb{R}_+)$ is primarily chosen in order to ensure the existence of the limit defining the scattering length. Furthermore, a wider class of possible potentials would automatically make us able to define also the ℓ^{th} scattering length $a_\ell(V)$ of such potentials for all $\ell \in \mathbb{N}_0$.[5]
- Determining whether the maps $V \mapsto \alpha(V)$ and $V \mapsto \beta(V)$ are not only continuous but uniformly continuous. If this is the case, it will, as noted in Section 5.1, be a major help for finding asymptotics of scattering lengths. If it is not the case, the proof of this will certainly still provide some insight into the nature of the continuity of these maps.
- Extending Theorem 4.29 to include the case $V_0, V_1 \in \mathscr{L}^{\text{Reg}}_{\pm\infty}$ (see Section 4.4 for the notation). This requires basically only to exclude some pathological behaviour of the number of negative eigenvalues n_- on $\mathscr{L}^{\text{Reg}}_{\pm\infty}$, but we have so far not been able to do so.

Chapter 5 proposed as a partial explanation of the strong resolvent convergence in Chapter 2 the asymptotic behaviour of the scattering length of the relevant potentials. These asymptotics were determined in some particular cases. Further, it was explained how they are related to a conjecture (Conjecture 5.5), which strengthens, in some cases, Weyl's law for the number of negative eigenvalues of Schrödinger operators. It is of course a goal to prove this conjecture. We mention here also one final result which we believe could quite easily be proved using the theory presented in this thesis.

- Consider a continuous curve $\mathbb{R}_+ \ni t \mapsto V_t \in \mathscr{L}^{\text{Reg}}$ of potentials as in Section 4.4. Then it is natural to conjecture that $-d^2/dx^2 + V_{t_n}$ converges in the strong resolvent sense if and only if V_{t_n} converges in $L^2_{\text{loc}}(\mathbb{R}_+)$ and $a(V_{t_n})$ is convergent. In this case, the limit should be a self-adjoint extension of $-d^2/dx^2 - \lim V_{t_n}$ (defined in terms of $\lim a(V_{t_n})$ if no natural extension exists). In case V_t gets arbitrarily negative – in an appropriate sense – for large t, we will be able to find sequences $\{t_n\}_{n=1}^\infty$ so that $a(V_{t_n}) \to a$ for any a. If, moreover, V_t converges as $t \to \infty$, this proves abstractly strong resolvent convergence of the Schrödinger operators along some subsequences. As mentioned above this could be a useful technical tool for some interesting problems.

[5] Although this is not discussed in this thesis, it is a perspective we find very interesting.

Appendix A

Selected results from the theory of distributions on $\mathbb{R}_+$

In this appendix we treat some facts from the theory of distributions adapted to our case of interest, i.e. functions on $\mathbb{R}_+$. Recommended general references on the topic are [Gru09] and [LL01].

Proposition A.1. Let $f \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ and suppose that $f' \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$. The function $g(x) := f(1/x)$ then has the derivative $g' \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ given by $g'(x) = -f'(1/x)/x^2$.

Proof. Let $\phi \in C_0^\infty(\mathbb{R}_+)$ and note that also the function $\eta(x) := \phi(1/x)$ is in $C_0^\infty(\mathbb{R}_+)$. Now a simple substitution $y = 1/x$ yields

$$\begin{aligned} g'(\phi) = -g(\phi') &= -\int_0^\infty g\phi'\,dx = -\int_0^\infty f(1/x)\phi'(x)\,dx = -\int_0^\infty \frac{f(y)\phi'(1/y)}{y^2}\,dy \\ &= \int_0^\infty f\eta'\,dy = f(\eta') = -f'(\eta) = -\int_0^\infty f'(x)\phi(1/x)\,dx = -\int_0^\infty \frac{f'(1/y)\phi(y)}{y^2}\,dy \end{aligned}$$

which is the desired result. □

Proposition A.2 (Fundamental Theorem of Calculus). If $g \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ and

$$f(x) := \int_a^x g(y)\,dy := \int_{a\wedge x}^x g(y)\,dy - \int_{a\wedge x}^a g(y)\,dy$$

for $x \in \mathbb{R}_+$ for some fixed $a \in \mathbb{R}_+$ then $f \in C(\mathbb{R}_+)$ and $f' = g$. If moreover $g \in L^1((0,1))$ then additionally $f \in C([0,\infty))$ and the a can be chosen to be 0 as well.

Conversely, for any f with $f' \in L^1_{\mathrm{loc}}(\mathbb{R}_+)$ it is true that $f \in C(\mathbb{R}_+)$ with

$$f(x) = f(a) + \int_a^x f'(y)\,dy$$

for all $x, a \in \mathbb{R}_+$. If, moreover, $f' \in L^1((0,1))$ then $f \in C([0,\infty))$ and the above equality holds also when $x = 0$ and/or $a = 0$.

Proof. Continuity is relatively clear. For any $\phi \in C_0^\infty(\mathbb{R}_+)$ we now observe that by the elementary identity

$$\mathbb{1}_{(a\wedge x,x)}(y) - \mathbb{1}_{(a\wedge x,a)}(y) = \mathbb{1}_{(0,y)}(a)\mathbb{1}_{(y,\infty)}(x) - \mathbb{1}_{(0,y)}(x)\mathbb{1}_{(y,\infty)}(a)$$

and Fubini's Theorem we can obtain

$$\begin{aligned} f'(\phi) = -f(\phi') &= -\int_0^\infty f\phi'\,dx = -\int_0^\infty \int_0^\infty g(y)[\mathbb{1}_{(a\wedge x,x)}(y) - \mathbb{1}_{(a\wedge x,a)}(y)]\phi'(x)\,dy\,dx \\ &= -\int_0^\infty g(y)\mathbb{1}_{(0,y)}(a)\int_y^\infty \phi'(x)\,dx\,dy + \int_0^\infty g(y)\mathbb{1}_{(y,\infty)}(a)\int_0^y \phi'(x)\,dx\,dy \\ &= \int_0^\infty g(y)[\mathbb{1}_{(0,y)}(a) + \mathbb{1}_{(y,\infty)}(a)]\phi(y)\,dy = \int_0^\infty g\phi\,dy = g(\phi) \end{aligned}$$

which means $f' = g$ as claimed. The additional results for $g \in L^1((0,1))$ follows from only very slight modifications of the above.

For the second part of the result we have just seen that f and the function

$$h(x) := \int_a^x f'(y)\,dy$$

have the same derivative, meaning that they differ at most by a constant. Since $h \in C(\mathbb{R}_+)$ with $h(a) = 0$ we conclude that $f \in C(\mathbb{R}_+)$ and

$$f(x) - \int_a^x f'(y)\,dy = f(x) - h(x) = f(a) - h(a) = f(a)$$

as claimed. Again the extension to the case $f' \in L^1((0,1))$ should be an easy check. □

Lemma A.3. Let $V \in L^1_{\text{loc}}(\mathbb{R}_+)$ and consider the space

$$\mathcal{N} := \{f \in L^1_{\text{loc}}(\mathbb{R}_+) \mid f'' = Vf \text{ in the distributional sense}\}.$$

This space is a two-dimensional subspace of $C^1(\mathbb{R}_+)$.

Proof. We argue firstly that $\mathcal{N} \subseteq C^1(\mathbb{R}_+)$. For any $f \in \mathcal{N}$ part of the condition $f'' = Vf$ is that $Vf \in L^1_{\text{loc}}(\mathbb{R}_+)$. Consequently, the fundamental theorem of calculus tells us that $f' \in C(\mathbb{R}_+)$, and consequently $f \in C^1(\mathbb{R}_+)$.

Now fix any point $x_0 \in \mathbb{R}_+$ and $f \in \mathcal{N}$. Then $f(x_0) = A$ and $f'(x_0) = B$ for some $A, B \in \mathbb{R}$, and we claim that these constants determine f completely which will clearly prove the last part of the lemma, i.e. that $\dim \mathcal{N} = 2$. For this we proceed basically as in the proof of Proposition 4.5, i.e. we prove that $A = B = 0$ implies $f \equiv 0$. In this case we can show by induction that

$$|f'(x)| \leq \frac{1}{n!x}\left(x\int_{x_0}^x |V(y)|\,dy\right)^n \sup_{y\in(x_0,x)} |f(y)|$$

for all $n \in \mathbb{N}$ and $x > x_0$. Hence, $f'(x) = 0$ for all $x > x_0$ and, since $f(x_0) = 0$, we must have $f \equiv 0$ on (x_0, ∞). The fact that $f \equiv 0$ on $(0, x_0)$ is proven completely analogously.

To show the inequality we see straightforwardly that, assuming the inequality for some n,

$$\begin{aligned}
|f'(x)| &\leq \int_{x_0}^{x} |V(y)||f(y)|\,dy \leq x\int_{x_0}^{x} |V(y)|\left|\frac{f(y)}{y-x_0}\right| dy \\
&\leq \frac{1}{n!}x^n \sup_{y\in(x_0,x)} |f(y)| \int_{x_0}^{x} |V(y)| \left(\int_{x_0}^{y} |V(z)|\,dz\right)^n dy \\
&= \frac{1}{(n+1)!x}\left(x\int_{x_0}^{x}|V(y)|\,dy\right)^{n+1} \sup_{y\in(x_0,x)} |f(y)|
\end{aligned}$$

as claimed. The case $n = 1$ is a simple estimate, and thus the proof is complete. □

Proposition A.4. If $f \in C^1(\mathbb{R}_+)$ and $g, g' \in L^1_{\text{loc}}(\mathbb{R}_+)$ then $(fg)' = f'g + fg'$.

Proof. The proof goes by a mollification argument. One can approximate f and f' by some $f_\varepsilon, f'_\varepsilon \in C^\infty(\mathbb{R}_+)$ uniformly on any bounded subset of $\mathbb{R}_+$ as $\varepsilon \to 0$ by taking suitable convolutions. Applying $(fg)'$ to a test function $\phi \in C_0^\infty(\mathbb{R}_+)$ we see that, as claimed,

$$\begin{aligned}
(fg)'(\phi) = -\int_0^\infty fg\phi'\,dx &= -\lim_{\varepsilon\to 0}\int_0^\infty f_\varepsilon g\phi'\,dx = \lim_{\varepsilon\to 0}\int_0^\infty f'_\varepsilon\phi g - (f_\varepsilon\phi)'g\,dx \\
&= \lim_{\varepsilon\to 0}\int_0^\infty f'_\varepsilon\phi g + f_\varepsilon\phi g'\,dx = \int_0^\infty (f'g+fg')\phi\,dx.
\end{aligned}$$ □

Corollary A.5. Let $V, \widetilde{V} \in L^1_{\text{loc}}(\mathbb{R}_+)$ and consider any solutions f and $\widetilde{f}$ to the equations $f'' = Vf$ and $\widetilde{f}'' = \widetilde{V}\widetilde{f}$ respectively. Then the wronskian $W := f'\widetilde{f} - f\widetilde{f}'$ has the distributional derivative $W' = [V - \widetilde{V}]f\widetilde{f}$. In particular, if f and g are both solutions to $f'' = Vf$ then $f'g - fg'$ is constant on $\mathbb{R}_+$.

Proof. We learn from Lemma A.3 that $f, \widetilde{f} \in C^1(\mathbb{R}_+)$ so that in particular $f', \widetilde{f}' \in L^1_{\text{loc}}(\mathbb{R}_+)$. Further, $(f')' = Vf$ and $(\widetilde{f}')' = \widetilde{V}\widetilde{f}$ lie in $L^1_{\text{loc}}(\mathbb{R}_+)$ as well. Therefore, Proposition A.4 yields

$$W' = f''\widetilde{f} + f'\widetilde{f}' - f'\widetilde{f}' - f\widetilde{f}'' = [V - \widetilde{V}]f\widetilde{f}$$

as needed. The last part of the corollary follows from the fact that in this case $W' \equiv 0$. □

Proposition A.6 (A particular partial integration). Let $0 \leq a < b \leq \infty$. If $f \in H_0^1((a,b))$, $f'' \in L^1_{\text{loc}}((a,b))$ and $\overline{f}f'' \in L^1((a,b))$ then the equality

$$\int_a^b \overline{f}f''\,dx = -\int_a^b |f'|^2\,dx$$

holds.

Proof. We prove the slightly more general statement that if $f \in H_0^1((a,b))$, $\widetilde{f}' \in L^2((a,b))$, $\widetilde{f}'' \in L^1_{\mathrm{loc}}((a,b))$ and $\overline{f}\widetilde{f}'' \in L^1((a,b))$ then

$$\int_a^b \overline{f}\widetilde{f}''\,dx = -\int_a^b \overline{f'}\widetilde{f}'\,dx$$

and suppose initially that f has compact support inside (a,b). By a convolution argument one can then find $\{h_n\}_{n=1}^\infty \subseteq C_0^\infty((a,b))$ so that $\sup|h_n| \le \sup|f|$ and $\operatorname{supp} h_n \subseteq (a+\varepsilon, b-\varepsilon)$ for all n for some $\varepsilon > 0$ (which is independent of n), and so that $h_n \to f$ in $H^1((a,b))$ and pointwise as $n \to \infty$. Thus, in this case,

$$\int_a^b \overline{f}\widetilde{f}''\,dx = \lim_{n\to\infty}\int_a^b \overline{h_n}\widetilde{f}''\,dx = -\lim_{n\to\infty}\int_a^b \overline{h_n'}\widetilde{f}'\,dx = -\int_a^b \overline{f'}\widetilde{f}'\,dx$$

where the first equality is by the dominated convergence theorem with $|\widetilde{f}''| \cdot \sup|f| \cdot \mathbb{1}_{(a+\varepsilon,b-\varepsilon)}$ as a dominating function.

For a $f \in H_0^1((a,b))$ with $\overline{f}\widetilde{f}'' \in L^1((a,b))$ which is additionally (real-valued) non-negative, consider a sequence $\{g_n\}_{n=1}^\infty \subseteq C_0^\infty((a,b))$ satisfying $g_n \to f$ in $H^1((a,b))$ and almost everywhere as $n \to \infty$. Define now for each n the function $f_n = (g_n \wedge f) \vee 0 \in H_0^1((a,b))$. These have compact support (since $g_n(x) = 0$ implies $f_n(x) = 0$) and their derivatives are (see [LL01] Corollary 6.18)

$$f_n' = \begin{cases} g_n' & \text{on } \{0 \le g_n < f\} \\ f' & \text{on } \{0 \le f \le g_n\} \cup \{g_n < 0 = f\} \\ 0 & \text{on } \{g_n < 0 < f\}. \end{cases}$$

Consequently,

$$\int_a^b |f_n' - f'|^2\,dx \le \int_a^b |g_n' - f'|^2 + \int_a^b \mathbb{1}_{\{g_n<0<f\}}|f'|^2\,dx,$$

where the first term on the right hand side clearly converges towards 0. The second term on the right hand side also converges towards 0. This is due to the dominated converge theorem, since $\mathbb{1}_{\{g_n<0<f\}} \to 0$ almost everywhere (on the set where g_n converges towards f), and $|f'|^2$ can be used as a dominating function. We conclude that $f_n' \to f'$ in $L^2((a,b))$. Hence,

$$\int_a^b \overline{f}\widetilde{f}''\,dx = \lim_{n\to\infty}\int_a^b \overline{f_n}\widetilde{f}''\,dx = -\lim_{n\to\infty}\int_a^b \overline{f_n'}\widetilde{f}'\,dx = -\int_a^b \overline{f'}\widetilde{f}'\,dx$$

where the first equality is by the dominated convergence theorem with $|f\widetilde{f}''|$ as a dominating function, and the second equality is due to the first part of the proof.

For a general f as introduced in the first lines of this proof we need now only notice that we can write $f = f_1 - f_2 + if_3 - if_4$ for four non-negative functions $f_i \in H_0^1((a,b))$ satisfying $|f_i| \le |f|$. Thus, they satisfy also $\overline{f_i}\widetilde{f}'' \in L^1((a,b))$. As both sides of the equality we want to prove is linear in f, this decomposition of the general f finishes the proof. □

Appendix B

Properties of H_κ and $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$

In this appendix we prove Proposition 2.3 of Chapter 2. We need firstly some preliminary results.

Lemma B.1. Consider abstractly a sequence of Hilbert spaces $\mathcal{H}_n$ and for each n a densely defined symmetric operator A_n on $\mathcal{H}_n$. Define the densely defined and symmetric operator A acting on the orthogonal direct sum $\mathcal{H} = \bigoplus_n \mathcal{H}_n$ by

$$D(A) = \left\{ \sum_{n=1}^{M} \phi_n \,\middle|\, M \in \mathbb{N},\ \phi_n \in D(A_n) \right\}, \quad A \sum_{n=1}^{M} \phi_n = \sum_{n=1}^{M} A_n \phi_n.$$

Then the deficiency indices $d_\pm(A)$ of A equal the sums of the deficiency indices $d_\pm(A_n)$ of the A_n's,

$$d_\pm(A) = \sum_{n=1}^{\infty} d_\pm(A_n).$$

If, moreover, there exists a constant $C > 0$ so that $\langle A_n\phi_n, \phi_n\rangle \geq -C\|\phi_n\|^2$ for all $n \in \mathbb{N}$ and $\phi_n \in D(A_n)$ then A is bounded below, and its Friedrichs' extension is the closure of the operator A_{F}^0 given by

$$D(A_{\mathrm{F}}^0) = \left\{ \sum_{n=1}^{M} \phi_n \,\middle|\, M \in \mathbb{N},\ \phi_n \in D((A_n)_{\mathrm{F}}) \right\}, \quad A_{\mathrm{F}}^0 \sum_{n=1}^{M} \phi_n = \sum_{n=1}^{M} (A_n)_{\mathrm{F}} \phi_n$$

where $(A_n)_{\mathrm{F}}$ is the Friedrichs' extension of A_n.

Proof. We prove only the case where finitely many of the A_n's have non-zero deficiency indices and these are all finite. This is the only case we will use below.

The first part of the lemma is Problem 1(a) in [RS75] X. We denote by P_n the orthogonal projection in $\mathcal{H}$ onto $\mathcal{H}_n$. Now, if ψ lies in the deficiency subspace $Z(A^* \pm i)$ then, for all $\phi_n \in D(A_n) \subseteq D(A)$,

$$\langle P_n\psi, A_n\phi_n\rangle_{\mathcal{H}_n} = \langle \psi, A\phi_n\rangle_{\mathcal{H}} = \langle A^*\psi, \phi_n\rangle_{\mathcal{H}} = \langle P_nA^*\psi, \phi_n\rangle_{\mathcal{H}_n}.$$

That is, $P_n\psi \in D(A_n^*)$ with $A_n^*P_n\psi = P_nA^*\psi = \mp iP_n\psi$, i.e. $P_n\psi \in Z(A_n^* \pm i)$ for all n. We conclude that any $\psi \in Z(A^* \pm i)$ can be written as

$$\psi = \sum_{n=1}^{\infty} P_n\psi$$

where the sum is finite and the n^{th} term lies in $Z(A_n^* \pm i)$. Conversely, one can straightforwardly check that all ψ on this form lie in $Z(A^* \pm i)$. This decomposition proves the first part of the lemma.

For the second part notice firstly that the assumptions imply rather directly that A is bounded below by $-C$ and thus has a Friedrichs' extension. Observe further that on $D(A)$ the quadratic form q_A is given by

$$q_A\Big(\sum_{n=1}^M \phi_n\Big) = \Big\langle A\sum_{n=1}^M \phi_n, \sum_{n=1}^M \phi_n\Big\rangle = \sum_{n=1}^M \langle A_n\phi_n, \phi_n\rangle$$

From here it is an easy verification that $D(A_{\mathrm{F}}^0)$ lies inside the closure of $D(A)$ with respect to the quadratic form norm given by $\|\cdot\|_{q_A}^2 = (C+1)\|\cdot\|_{\mathcal{H}} + q_A(\cdot)$, and that the extended quadratic form (still denoted q_A) acts as $q_A(\phi) = \langle A_{\mathrm{F}}^0\phi, \phi\rangle$ for $\phi \in D(A_{\mathrm{F}}^0)$. That is, it is the quadratic form of A_{F}^0. Hence, we have

$$D\big(\overline{A_{\mathrm{F}}^0}\big) \subseteq \overline{D(A_{\mathrm{F}}^0)}^{\|\cdot\|_{q_A}} = \overline{D(A)}^{\|\cdot\|_{q_A}}$$

by the standard bound $\|\phi\|_{q_A}^2 \le (C+2)(\|A_{\mathrm{F}}^0\phi\|^2 + \|\phi\|^2)$. As A_{F}^0 is essentially self-adjoint by the first part of the lemma, this proves that the closure $\overline{A_{\mathrm{F}}^0}$ is indeed the Friedrichs' extension of A. □

In the following we use the notation that $\mathcal{D} = C_0^\infty(\mathbb{R}^3\backslash\{0\})$ and $\mathcal{D}_0$ is the space of functions $\psi \in \mathcal{D}$ of the form

$$\psi(r\omega) = \sum_{\ell=0}^M \sum_{m=-\ell}^{\ell} \psi_\ell^m(r) Y_\ell^m(\omega)$$

for some $M \in \mathbb{N}$ and $\psi_\ell^m \in C_0^\infty(\mathbb{R}_+)$ where $r \in \mathbb{R}_+$, $\omega \in S^2 \subseteq \mathbb{R}^3$ and Y_ℓ^m are the spherical harmonics from Chapter 2. In this notation we have:

Lemma B.2. The space $\mathcal{D}_0$ is a dense subspace of $\mathcal{D}$ with respect to the $H^2(\mathbb{R}^3)$-norm.

Proof. Consider the symmetric operators A and B on $L^2(\mathbb{R}^3)$ both acting as $-\Delta$ with domains $D(A) = \mathcal{D}_0$ and $D(B) = \mathcal{D}$. As it is discussed in Section 2 of Chapter 2 this A is unitarily equivalent to an operator UAU^{-1} of the form from Lemma B.1 (indexed by ℓ instead of n) with $\mathcal{H}_\ell = L^2(\mathbb{R}_+) \otimes \operatorname{span}_m Y_\ell^m$, $A_\ell = (-d^2/dx^2 + \ell(\ell+1)x^{-2}) \otimes I$ and

$$D(A_\ell) = \Big\{ \sum_{m=-\ell}^{\ell} \psi_\ell^m \otimes Y_\ell^m \;\Big|\; \psi_\ell^m \in C_0^\infty(\mathbb{R}_+) \Big\} = C_0^\infty(\mathbb{R}_+) \otimes \operatorname{span}_{m=-\ell,\dots,\ell} Y_\ell^m.$$

Using Weyl's limit point/limit circle criterion on its non-trivial factor it is easily seen that A_ℓ is essentially self-adjoint for $\ell = 1, 2, \dots$ and that it has deficiency indices $d_\pm(A_0) = 1$ for $\ell = 0$. From Lemma B.1 we conclude that $d_\pm(A) = 1$.

Correspondingly, the extension theory for B has been completely studied, for example in [Alb+12] I.1.1. In particular it is known that B has deficiency indices $d_\pm(B) = 1$. As $A \subseteq B$ and these have the same finite deficiency indices, they must in turn (since $B^* \subseteq A^*$)

have the same deficiency subspaces. This implies that the closure of A equals the closure of B. The operator norm of A and B is simply the H^2-norm, and consequently the H^2-closure of $\mathcal{D}_0$ in particular contains $\mathcal{D}$, proving the lemma. □

Corollary B.3. Let A and B be the operators on $L^2(\mathbb{R}^3)$ acting as $-\Delta + V$ for some real-valued continuous potential $V\colon \mathbb{R}^3\backslash\{0\} \to \mathbb{R}$ on $D(A) = \mathcal{D}_0$ and $D(B) = \mathcal{D}$ respectively. Assuming further that V is uniformly bounded on any set of the form $\mathbb{R}^3\backslash B_\varepsilon(0)$, the closure of A coincides with the closure of B.

Proof. We need clearly only to argue that the closure of $\mathcal{D}$ is contained in the closure of $\mathcal{D}_0$ with respect to the operator norm of A. To this end we fix an arbitrary $\phi \in \mathcal{D}$ and choose $\varepsilon > 0$ so that $\phi \in C_0^\infty(\mathbb{R}^3\backslash B_{3\varepsilon}(0))$. By Lemma B.2 we can find a sequence $\{\phi_n\}_{n=1}^\infty \subseteq \mathcal{D}_0$ so that $\phi_n \to \phi$ with respect to the H^2-norm. Letting χ be a smooth radially symmetric function on $\mathbb{R}^3$ which is 0 on $B_{2\varepsilon}(0)$ and 1 on $\mathbb{R}^3\backslash B_{3\varepsilon}(0)$ it is not difficult to realize that $\{\chi\phi_n\}_{n=1}^\infty \subseteq \mathcal{D}_0 \cap C_0^\infty(\mathbb{R}^3\backslash B_\varepsilon(0))$ and $\chi\phi_n \to \chi\phi = \phi$ with respect to the H^2-norm. But on the space $\mathcal{D}_0 \cap C_0^\infty(\mathbb{R}^3\backslash B_\varepsilon(0))$ the H^2-norm and the operator norm of A are equivalent due to our assumptions on V. This proves the corollary. □

We arrive finally at:

Proof (of Proposition 2.3 in Chapter 2). a): Fix $\kappa > 0$. Let A and B be the operators on $L^2(\mathbb{R}^3)$ acting as $-\Delta + \Phi_\kappa$ on $D(A) = \mathcal{D}_0$ and $D(B) = \mathcal{D}$ respectively. According to Corollary B.3 these have the same closures and thus the same Friedrichs' extension. Hence, for the first part of the assertion, it suffices to prove that H_κ is the Friedrichs' extension of A. For this observe that UAU^{-1} is on the form from Lemma B.1 with the same $\mathcal{H}_\ell$ and $D(A_\ell)$ as in the proof of Lemma B.2 and with

$$A_\ell = \Big(-\frac{d^2}{dx^2} + \frac{\ell(\ell+1)}{x^2} - \Phi_\kappa\Big) \otimes I$$

on these domains. Now, according to Lemma B.1, the Friedrichs' extension of UAU^{-1} is the closure of

$$D(A_{\mathrm{F}}^0) = \Big\{ \sum_{\ell=0}^{M} \phi_\ell \,\Big|\, M \in \mathbb{N},\ \phi_\ell \in D((A_\ell)_{\mathrm{F}}) \Big\}, \quad A_{\mathrm{F}}^0 \sum_{\ell=0}^{M} \phi_\ell = \sum_{\ell=0}^{M} (A_\ell)_{\mathrm{F}} \phi_\ell$$

where $(A_\ell)_{\mathrm{F}}$ is the Friedrichs' extension of A_ℓ. Since $(A_\ell)_{\mathrm{F}} = (\widetilde{A}_\ell)_{\mathrm{F}} \otimes I$ with $(\widetilde{A}_\ell)_{\mathrm{F}}$ the Friedrichs' extension of $\widetilde{A}_\ell = -d^2/dx^2 + \ell(\ell+1)x^{-2} - \Phi_\kappa$ on $D(\widetilde{A}_\ell) = C_0^\infty(\mathbb{R}_+)$, we learn from the limit point/limit circle criterion and Lemma 4.21 that A_{F}^0 equals $\widetilde{H}_\kappa^0$ from Definition 2.2 in Chapter 2. This proves the first assertion, showing that $\widetilde{H}_\kappa$ is the Friedrichs' extension of UAU^{-1} so that $H_\kappa = U^{-1}\widetilde{H}_\kappa U$ is the Friedrichs' extension of A.

For the second assertion we need $\alpha > -3/2$. Then $\Phi_\kappa \in L^2(\mathbb{R}^3)$ so that one can define the operators B and $\widetilde{B}$ acting as $-\Delta - \Phi_\kappa$ on both $D(B) = \mathcal{D}$ and on $D(\widetilde{B}) = C_0^\infty(\mathbb{R}^3)$. As it is discussed in Subsection 1.2 in Chapter 2, $\widetilde{B}$ is well known to be essentially self-adjoint.

Moreover, since $\Phi_\kappa \in L^{3/2}(\mathbb{R}^3)$, this potential is[1] infinitesimally form bounded with respect to $-\Delta$ on $\mathcal{D}$ and $C_0^\infty(\mathbb{R}^3)$. Consequently, the quadratic form norms of B and $\widetilde{B}$ are equivalent to that of $-\Delta$, i.e. to the H^1-norm. We conclude that the closures of $D(B)$ and $D(\widetilde{B})$ with respect to the respective quadratic form norms are both $H^1(\mathbb{R}^3\backslash\{0\}) = H^1(\mathbb{R}^3)$. In particular, the closure of $\widetilde{B}$ is a self-adjoint operator with domain inside the closure of $D(B)$ with respect to its quadratic form norm, and we can conclude that the closure of $\widetilde{B}$ is the Friedrichs' extension of B – which by the first part of the Proposition is exactly H_κ.

b): When recalling that all $H_{\infty,\ell,\theta_\ell}$ (and hence $H_{\infty,\ell,\theta_\ell} \otimes I$) have deficiency indices 0 by construction, the fact that $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ is self-adjoint is a consequence of Lemma B.1 and considerations completely similar to in the proof of (a) above. The fact that $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ is an extension of $-\Delta-\Phi_\infty$ defined on $\mathcal{D}$ follows from Corollary B.3 since $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty}$ is clearly a closed extension of $-\Delta-\Phi_\infty$ defined on $\mathcal{D}_0$. Finally, we must have $H_{\infty,\{\theta_\ell\}_{\ell=0}^\infty} \neq H_{\infty,\{\theta'_\ell\}_{\ell=0}^\infty}$ whenever $\{\theta_\ell\}_{\ell=0}^\infty \neq \{\theta'_\ell\}_{\ell=0}^\infty$: This can be seen by considering the restrictions to an angular momentum subspace corresponding to an ℓ for which $\theta_\ell \neq \theta'_\ell$. □

[1] This is true for any potential of Rollnik class, see [RS75] Theorem X.19.

Bibliography

[Fer27] Enrico Fermi. "Un metodo statistico per la determinazione di alcune priorieta dell'atome". In: *Rend. Accad. Naz. Lincei* 6 (1927), pp. 602–607.

[Tho27] Llewellyn H Thomas. "The calculation of atomic fields". In: *Mathematical proceedings of the Cambridge philosophical society*. Vol. 23. 5. Cambridge University Press. 1927, pp. 542–548.

[LHY57] Tsin D Lee, Kerson Huang, and Chen N Yang. "Eigenvalues and eigenfunctions of a Bose system of hard spheres and its low-temperature properties". In: *Physical Review* 106.6 (1957), p. 1135.

[Zhi60] Grigorii M Zhislin. "Discussion of the spectrum of Schrödinger operators for systems of many particles". In: *Trudy Moskovskogo matematiceskogo obscestva* 9 (1960), pp. 81–120.

[Olv61] F. W. J. Olver. "Error bounds for the Liouville–Green (or WKB) approximation". In: *Mathematical Proceedings of the Cambridge Philosophical Society* 57.4 (1961), pp. 790–810.

[AS72] Milton Abramowitz and Irene A Stegun. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. Tenth Printing.* (As it appears on https://personal.math.ubc.ca/~cbm/aands/abramowitz_and_stegun.pdf). National Bureau of Standards, 1972.

[LS73] Elliott H Lieb and Barry Simon. "Thomas-Fermi theory revisited". In: *Physical Review Letters* 31.11 (1973), pp. 681–683.

[RS75] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics. II Fourier Analysis, Self-adjointness*. Academic Press, 1975.

[LS77] Elliott H Lieb and Barry Simon. "The Thomas-Fermi theory of atoms, molecules and solids". In: *Advances in mathematics* 23.1 (1977), pp. 22–116.

[RS79] Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics. III Scattering theory*. Academic Press, 1979.

[Won79] D Pan Wong. "Theoretical justification of madelung's rule". In: *Journal of Chemical Education* 56.11 (1979), pp. 714–717.

[Lie81] Elliott H. Lieb. "Thomas-fermi and related theories of atoms and molecules". In: *Review of Modern Physics* 53.4 (1981), pp. 603–641.

[Hug86] Barnwell Webster Hughes. *An atomic energy lower bound that proves Scott's correction (Dissertation)*. Princeton University, 1986.

[SW87] Heinz Siedentop and Rudi Weikard. "On the leading energy correction for the statistical model of the atom: Interacting case". In: *Communications in Mathematical Physics* 112.3 (1987), pp. 471–490.

[GG88] Christian Gérard and Alain Grigis. "Precise estimates of tunneling and eigenvalues near a potential barrier". In: *Journal of differential equations* 72.1 (1988), pp. 149–177.

[FS90] Charles L Fefferman and Luis A Seco. "On the energy of a large atom". In: *Bulletin of the American Mathematical Society* 23.2 (1990), pp. 525–530.

[Sol90] Jan Philip Solovej. "Universality in the Thomas-Fermi-von Weizsäcker model of atoms and molecules". In: *Communications in mathematical physics* 129.3 (1990), pp. 561–598.

[FS92] Charles Fefferman and Luis Seco. "Eigenvalues and eigenfunctions of ordinary differential operators". In: *Advances in Mathematics* 95.2 (1992), pp. 145–305.

[Sim00] Barry Simon. "Schrödinger operators in the twenty-first century". In: *Mathematical physics* 2000 (2000), pp. 283–288.

[LL01] Elliott H Lieb and Michael Loss. *Analysis*. American Mathematical Soc., 2001.

[LY01] Elliott H. Lieb and Jakob Yngvason. "The ground state energy of a dilute two-dimensional Bose gas". In: *Journal of Statistical Physics* 103 (2001).

[Sol03] Jan Philip Solovej. "The ionization conjecture in Hartree-Fock theory". In: *Annals of mathematics* (2003), pp. 509–576.

[BB04] Philippe Bénilan and Haim Brezis. "Nonlinear problems related to the Thomas-Fermi equation". In: *Nonlinear Evolution Equations and Related Topics: Dedicated to Philippe Bénilan*. Springer, 2004, pp. 673–770.

[Lie+05] Elliott H. Lieb et al. *The Mathematics of the Bose Gas and its Condensation*. Birkhäuser, 2005.

[Sim05] Barry Simon. "Sturm Oscillation and Comparison Theorems". In: *Sturm-Liouville Theory: Past and Present*. Ed. by Werner O. Amrein, Andreas M. Hinz, and David P. Pearson. Birkhäuser Basel, 2005, pp. 29–43.

[Gru09] Gerd Grubb. *Distributions and Operators*. Springer, 2009.

[Yaf10] D. R. Yafaev. *Mathematical Scattering Theory: Analytic Theory*. American Mathematical Soc., 2010.

[BDG11] Laurent Bruneau, Jan Dereziński, and Vladimir Georgescu. "Homogeneous Schrödinger operators on half-line". In: *Annales Henri Poincaré* 12 (2011), pp. 547–590.

[Alb+12] Sergio Albeverio et al. *Solvable models in quantum mechanics*. Springer Science & Business Media, 2012.

[Tes14] Gerald Teschl. *Mathematical methods in quantum mechanics*. American Mathematical Soc., 2014.

[Sol16] Jan Philip Solovej. "A new look at Thomas–Fermi theory". In: *Molecular Physics* 114.7-8 (2016), pp. 1036–1040.

[FNV18] Rupert L Frank, Phan Thành Nam, and Hanne Van Den Bosch. "The ionization conjecture in Thomas–Fermi–Dirac–von Weizsäcker theory". In: *Communications on Pure and Applied Mathematics* 71.3 (2018), pp. 577–614.

[DG20] Jan Dereziński and Vladimir Georgescu. "One-Dimensional Schrödinger Operators with Complex Potentials". In: *Annales Henri Poincaré* 21.6 (2020), pp. 1947–2008.

[BCS21] Giulia Basti, Serena Cenatiempo, and Benjamin Schlein. "A new second-order upper bound for the ground state energy of dilute Bose gases". In: *Forum of Mathematics, Sigma* 9 (2021), e74.

[FLW22] Rupert L Frank, Ari Laptev, and Timo Weidl. *Schrödinger operators: eigenvalues and Lieb–Thirring inequalities*. Cambridge University Press, 2022.

[Nam22] Phan Thành Nam. "The ionization problem in quantum mechanics". In: *The Physics and Mathematics of Elliott Lieb – The 90th Anniversary Volume II*. Ed. by Rupert L. Frank et al. EMS Publishing House, 2022, pp. 93–120.

[Bje23] August Bjerg. "Convergence of operators with deficiency indices (k,k) and of their self-adjoint extensions". In: *Annales Henri Poincaré* (2023). URL: https://doi.org/10.1007/s00023-023-01397-9.

[FS23] Søren Fournais and Jan Philip Solovej. "The energy of dilute Bose gases II: The general case". In: *Inventiones mathematicae* 232.2 (2023), pp. 863–994.