
Spectral and Eigenfunction Correlations of Finite-Volume Schrödinger Operators

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Zusammenfassung

Die vorliegende Dissertation behandelt das Verhalten von Eigenfunktionskorrelationen zweier Schrödingeroperatoren in großen endlichen Volumina. Wir beginnen mit zwei Schrödingeroperatoren H und H' auf \mathbb{R}^d , deren Differenz klein ist, und betrachten die Restriktion beider Operatoren auf ein endliches Volumen des Durchmessers L . Wir nennen diese Operatoren H_L und H'_L und interessieren uns für folgende Abschätzungen an eine Korrelationsdeterminante

$$|\mathcal{S}_L^N|^2 := \left| \det \left(\langle \varphi_j^L, \psi_k^L \rangle \right)_{1 \leq j, k \leq N} \right|^2 \lesssim L^{-\gamma}, \quad (\text{i})$$

die aus den Skalarprodukten der zu den kleinsten Eigenwerten gehörenden Eigenfunktionen von H_L und H'_L besteht, für große L und N , derart dass $N/L^d \rightarrow \rho > 0$. Dies modelliert das Verhalten des Skalarproduktes der Grundzustände zweier nicht wechselwirkender Fermigase im thermodynamischen Limes, die sich um eine kleine Störung unterscheiden. Der Abfall der Determinante (i) ist in der Physikliteratur nach P.W.Anderson [And67b], Andersons Orthogonalitätskatastrophe, benannt und wird zur Erklärung verschiedener thermodynamischer Phänomene in Fermigasen herangezogen. Das Verhalten (i) folgt aus dem asymptotischen Verhalten von Produkten spektraler Projektionen

$$\text{tr} \left\{ (1_{(-\infty, E)}(H_L) 1_{(E, \infty)}(H'_L) 1_{(-\infty, E)}(H_L))^n \right\} \sim c_{n, E} \ln L, \quad (\text{ii})$$

wobei $n \in \mathbb{N}$ und $E \in \sigma(H)$ ist. Die Arbeiten [GKM14] und [GKMO14] zeigen die obigen Asymptotiken (i) und (ii) für Paare relativ allgemeiner Schrödingeroperatoren, wobei die Abschätzungen gegeben sind durch die T -Matrix – genauer durch die Exponenten $\gamma = \frac{1}{\pi^2} \|T/2\|_{\text{HS}}$, beziehungsweise $\gamma = \frac{1}{\pi^2} \|\arcsin|T/2|\|_{\text{HS}}$.

In dieser Dissertation zeigen wir die obere Abschätzung (i) mit dem Exponenten $\frac{1}{\pi^2} \|T/2\|_{\text{HS}}$ in allgemeineren Situationen als in [GKM14]. Darüber hinaus geben wir die erste rigorose Herleitung der exakten Asymptotik der Korrelationsdeterminante und zeigen im dreidimensionalen Raum im Falle der Störung mit einer Punktwechselwirkung, dass

$$|\mathcal{S}_L^N|^2 \sim L^\zeta \quad \text{mit} \quad \zeta := \delta^2 / \pi^2, \quad (\text{iii})$$

wobei der Exponent gegeben ist durch die s-Wellen-Streuphase. Insbesondere zeigt dies, dass der Exponent $\frac{1}{\pi^2} \|\arcsin|T/2|\|_{\text{HS}}$ im Allgemeinen nicht das korrekte Verhalten von \mathcal{S}_L^N widerspiegelt. Da die gefundenen Exponenten von der T-Matrix abhängen, liegt es nahe, dass das absolutstetige Spektrum als treibende Kraft hinter dem Abfall (i) steht. So beweisen wir im Falle von Andersonlokalisierung die gegenteiligen Aussagen zu (i) und (ii)

$$\limsup_{L \rightarrow \infty} \text{tr} \left\{ (1_{(-\infty, E)}(H_{\omega, L}) 1_{(E, \infty)}(H'_{\omega, L}) 1_{(-\infty, E)}(H_{\omega, L}))^n \right\} < \infty \quad (\text{iv})$$

für f.a. $(E, \omega) \in \sigma(H_\omega) \times \Omega$ und ebenso das Nichtverschwinden der Erwartung bei starker Unordnung

$$\liminf_{N/L^d \rightarrow \rho > 0} \mathbb{E} [|\mathcal{S}_L^N|] > 0. \quad (\text{v})$$

Neben den obigen Eigenfunktionsasymptotiken beleuchten wir ebenso spektrale Asymptotiken und zeigen im thermodynamischen Limes das Verhalten

$$\lim_{N/L^d \rightarrow \rho > 0} \sum_{1 \leq j \leq N} (\mu_j^L - \lambda_j^L) = \int dx \xi(x) + o(1), \quad (\text{vi})$$

wobei λ_j^L und μ_j^L die Eigenwerte von H_L und H'_L sind und ξ die spektrale Shiftfunktion von H und H' bezeichnet. Des Weiteren bestimmen wir für Systeme auf der Halbachse die Fehlerterme in (vi) genauer und zeigen, dass diese limesabhängig sind.

Abstract

This thesis treats asymptotics of eigenfunction correlations of pairs of finite-volume Schrödinger operators in a large but finite volume. We start with a pair of Schrödinger operators H and H' on the Euclidean space \mathbb{R}^d , which differ by a short-range scattering potential, and restrict these operators to some finite volume of diameter $L > 0$ and call these operators H_L and H'_L . In the first place, we are concerned with estimates on a correlation determinant in the thermodynamic limit, which consists of scalar products of the lowest energy eigenfunctions of H_L and H'_L . More precisely, we are interested in bounds

$$|\mathcal{S}_L^N|^2 := \left| \det(\langle \varphi_j^L, \psi_k^L \rangle)_{1 \leq j, k \leq N} \right|^2 \lesssim L^{-\gamma}, \quad (\text{i})$$

as $N/L^d \rightarrow \rho > 0$. This models the behaviour of the scalar product of the ground states of two non-interacting Fermi gases in the thermodynamic limit, which differ by a static impurity. This decay of \mathcal{S}_L^N is referred to as Anderson's orthogonality catastrophe in the physics literature and goes back to [And67b]. It is used to explain the behaviour of cross-sections in certain photoexcitation experiments. Expanding the determinant, we see that this is closely related to the L asymptotics of traces of products of spectral projections

$$\text{tr} \{ (1_{(-\infty, E)}(H_L) 1_{(E, \infty)}(H'_L) 1_{(-\infty, E)}(H_L))^n \} \sim c_{n, E} \ln L, \quad (\text{ii})$$

where $n \in \mathbb{N}$ and $E \in \sigma(H)$. [GKM14] and [GKMO14] prove for quite general pairs of Schrödinger operators, which differ by a positive short-range potential, upper bounds of the form (i) in terms of the scattering T -matrix with first $\gamma = \frac{1}{\pi^2} \|T/2\|_{\text{HS}}$ and in the second article with $\gamma = \frac{1}{\pi^2} \|\arcsin|T/2|\|_{\text{HS}}$.

In this thesis, we prove the upper bound (i) with the decay exponent $\frac{1}{\pi^2} \|T/2\|_{\text{HS}}$ in more general situations than considered in [GKM14]. Furthermore, we provide the first rigorous proof of the exact asymptotics Anderson predicted, i.e. in the 3-dimensional toy model, where H' is a Dirac- δ perturbation of the negative Laplacian. We prove

$$|\mathcal{S}_L^N|^2 \sim L^\zeta, \quad \text{where} \quad \zeta := \delta^2/\pi^2. \quad (\text{iii})$$

Here, δ refers to the s-wave scattering phase shift. In particular, this result shows that the exponent $\frac{1}{\pi^2} \|\arcsin|T/2|\|_{\text{HS}}$ found in [GKMO14] does not provide the correct asymptotics of \mathcal{S}_L^N in general. Since the decay exponent is expressed in terms of the T-matrix, the bounds of (i) and the asymptotics (ii) are reminiscent of the absolutely continuous spectrum. Thus, in the contrary situation of Anderson localisation we are able to deduce different behaviours than (i) and (ii), i.e. we prove for a.e. $(E, \omega) \in \sigma(H_\omega) \times \Omega$

$$\limsup_{L \rightarrow \infty} \text{tr} \{ (1_{(-\infty, E)}(H_{\omega, L}) 1_{(E, \infty)}(H'_{\omega, L}) 1_{(-\infty, E)}(H_{\omega, L}))^n \} < \infty \quad (\text{iv})$$

and the non-vanishing of the expectation value in the large disorder regime

$$\liminf_{N/L^d \rightarrow \rho > 0} \mathbb{E} [|\mathcal{S}_L^N|] > 0. \quad (\text{v})$$

Apart from the behaviour of eigenfunction correlations, we also study the asymptotics of spectral correlations. We show asymptotics of the form

$$\lim_{N/L^d \rightarrow \rho > 0} \sum_{1 \leq j \leq N} (\mu_j^L - \lambda_j^L) = \int dx \xi(x) + o(1) \quad (\text{vi})$$

in the thermodynamic limit, where λ_j^L and μ_j^L denote the eigenvalues of H_L and H'_L and ξ the infinite-volume spectral shift function. Furthermore, we quantify the error in (vi) for models on the half-axis and show that higher order error terms depend on the particular limit chosen.

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CHAPTER 1

Introduction

1. Anderson's Orthogonality Catastrophe and Spectral Correlations



s one of the most elementary many-body problems one can consider a Fermi gas exposed to a static impurity. Such an impurity arises, for example, when a photon excites a core electron in such a way that this core electron merges into the conduction band, i.e. the Fermi gas, leaving behind a hole. In turn, this core hole interacts with the Fermi gas and in a first approximation one can model this with a short-range scattering potential. It was predicted that the cross-section of such a photoexcitation experiment admits a power law singularity at the threshold, which is referred to as a Fermi edge singularity, see [Mah00, Sct. 9.3] and references cited therein. Even though this behaviour was observed in some materials, it was noticed in several other metals that this singularity is suppressed and the cross-section is continuous at the threshold. At this point Anderson found that the scalar product of the ground-states of two non-interacting Fermi gases which differ by a short-range potential are orthogonal in the thermodynamic limit [And67a, And67b]. Which is why this orthogonality of the ground states in the thermodynamic limit is nowadays named Anderson orthogonality catastrophe (AOC). It was precisely used to explain the at first unexpected phenomenon of the absorption spectrum and is now a well-understood phenomenon in the physics of the response of a free Fermi gas to the appearance of a scattering potential. We refer to [OT90, Mah00] for an extensive overview of the problem and references up to the late eighties. Nevertheless, up to now the AOC remains to attract attention in physics, e.g. it was considered in quantum dots or graphene more recently, see [HSBvD05, HUB05, HK12a, HK12b] and the references therein. Another development was the study of the problem for pairs of free Fermi gases in a random environment, which was done in [VLG02] for ensembles of random matrices or in [GBLA02] for the Anderson model. Though this so-called orthogonality catastrophe is a common topic in solid-state physics, which has attracted attention up to now in several facets, there was no attempt to give a rigorous proof of the AOC for a long time. Therefore, the goal of this thesis consists of giving a rigorous proof of the AOC and show that there is some deep and interesting mathematics behind this problem. Even in the physics literature it is accepted that in a first approximation it suffices to consider non-interacting electrons to obtain a suitable model for these photoexcitation effects. Thus, we start with a pair of one-particle Schrödinger operators

$$H_L = -\Delta_L + V_0 \quad \text{and} \quad H'_L = -\Delta_L + V_0 + V, \quad (1.1)$$

in some finite box $\Lambda_L := [L/2, L/2]^d$ in d -dimensional Euclidean space. V_0 denotes some background potential such that both operators remain well-defined and bounded from below and V denotes a small perturbation. These operators induce a pair of non-interacting N -particle Schrödinger operators \mathbf{H}_L and \mathbf{H}'_L in the finite volume Λ_L acting on the totally

antisymmetric subspace $\bigwedge_{j=1}^N L^2(\Lambda_L)$ of the N -fold tensor product space. More precisely, these operators are given by

$$H_L^{(j)} := \sum_{j=1}^N \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes H_L^{(j)} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \quad (1.2)$$

where the index j determines the position of $H_L^{(j)}$ in the N -fold tensor product of operators. The corresponding ground states are given by the totally antisymmetrised products

$$\Phi_L^N := \frac{1}{\sqrt{N!}} \varphi_1^L \wedge \cdots \wedge \varphi_N^L \quad \text{and} \quad \Psi_L^N := \frac{1}{\sqrt{N!}} \psi_1^L \wedge \cdots \wedge \psi_N^L, \quad (1.3)$$

where typically these ground states Φ_L^N and Ψ_L^N are referred to as Slater determinants. The corresponding ground-state energies are

$$E_L^N := \sum_{j=1}^N \lambda_j^L \quad \text{and} \quad E_L'^N := \sum_{k=1}^N \mu_k^L. \quad (1.4)$$

Here, $(\varphi_j^L)_{j \in \mathbb{N}}$ and $(\psi_k^L)_{k \in \mathbb{N}}$ denote the eigenfunctions corresponding to the ordered eigenvalues $(\lambda_j^L)_{j \in \mathbb{N}}$ and $(\mu_k^L)_{k \in \mathbb{N}}$ of the one-particle operators H_L and H_L' . Now, a short calculation shows that the scalar product of the two ground states Φ_L^N and Ψ_L^N in the Hilbert space $\bigwedge_{j=1}^N L^2(\Lambda_L)$ can be written itself as the correlation determinant

$$\mathcal{S}_L^N := \langle \Phi_L^N, \Psi_L^N \rangle_{\bigwedge_{j=1}^N L^2(\Lambda_L)} = \det \begin{pmatrix} \langle \varphi_1^L, \psi_1^L \rangle_{L^2(\Lambda_L)} & \cdots & \langle \varphi_1^L, \psi_N^L \rangle_{L^2(\Lambda_L)} \\ \vdots & & \vdots \\ \langle \varphi_N^L, \psi_1^L \rangle_{L^2(\Lambda_L)} & \cdots & \langle \varphi_N^L, \psi_N^L \rangle_{L^2(\Lambda_L)} \end{pmatrix}, \quad (1.5)$$

where the subscript of the scalar products illustrates the underlying Hilbert space. In the following, we call this determinant **ground-state overlap**, and we are interested in its asymptotic behaviour as N and L increase. More precisely, we are concerned with the limit $L \rightarrow \infty$ and $N \rightarrow \infty$ such that

$$\frac{N}{|\Lambda_L|} \rightarrow \rho(E), \quad (1.6)$$

where $\rho(E)$ denotes the integrated density of states of the operator H at some energy E , which we refer to as the Fermi energy, and $|\cdot|$ denotes the Lebesgue measure. This concept is called the **thermodynamic limit** and $\rho(E)$ is viewed as the particle density of the considered gas. Thus, we are interested in the asymptotic behaviour of the ground-state overlap of two non-interacting Fermi gases approaching a particle density $\rho(E) > 0$ corresponding to the Fermi energy E .

As already mentioned, the first one to study this asymptotics was P.W. Anderson in [And67a]. He considered a 3-dimensional system with no background potential V_0 where the one-particle Schrödinger operators differ by a Dirac- δ perturbation located at the origin. In this work he claimed the algebraic decay of the ground-state overlap

$$|\mathcal{S}_L^N|^2 \lesssim L^{-\frac{1}{\pi^2}(\sin(\delta(\sqrt{E})))^2} \quad (1.7)$$

by deducing logarithmic asymptotics of the form

$$\text{tr} \left\{ 1_{(-\infty, \lambda_N^L]}(H_L) 1_{[\mu_{N+1}^L, \infty)}(H_L') 1_{(-\infty, \lambda_N^L]}(H_L) \right\} \sim \frac{1}{\pi^2} (\sin(\delta(\sqrt{E})))^2 \ln L, \quad (1.8)$$

where δ denotes the s-wave scattering phase shift. Here, 1_A stands for the indicator function of a Borel set $A \in \text{Borel}(\mathbb{R})$. The latter expression is nowadays called **Anderson integral**

in the physics literature. Let us briefly explain the connection between (1.7) and (1.8). Taking the logarithm of the square of the modulus of (1.5) and expanding the logarithm results in

$$|\mathcal{S}_L^N|^2 = \exp(\ln \text{tr } A^* A) = \exp\left(-\sum_{n=1}^{\infty} \frac{\text{tr}\{(1 - A^* A)^n\}}{n}\right), \quad (1.9)$$

where A is the matrix occurring on the r.h.s. of (1.5). Ignoring the fact that there may be eigenvalues of higher multiplicity, a straightforward calculation shows

$$0 \leq (1 - A^* A) = 1_{(-\infty, \lambda_N^L]}(H_L) 1_{[\mu_{N+1}^L, \infty)}(H'_L) 1_{(-\infty, \lambda_N^L]}(H_L) =: \mathcal{I}_{L,N}. \quad (1.10)$$

Taking only the first term in the expansion (1.9) into account, we see that (1.8) gives an upper bound on (1.5) which results in (1.7). Generally speaking, the asymptotics of (1.5) is closely related to the asymptotic behaviour of powers of products of pairs of spectral projections. Motivated by the above calculation [And67a] argued for general 3-dimensional systems with a spherically-symmetric perturbation V an upper bound similar to (1.7) with the decay exponent

$$\tilde{\gamma}(E) := \frac{1}{\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1) (\sin(\delta_\ell(\sqrt{E})))^2, \quad (1.11)$$

where δ_ℓ denotes the scattering phase shift in the ℓ th angular momentum channel.

Later in the same year, Anderson claimed in [And67b] that the exact asymptotics of the overlap for a Dirac- δ perturbation is governed by the bigger decay exponent

$$\zeta(E) := \frac{1}{\pi^2} \delta^2(\sqrt{E}), \quad (1.12)$$

where δ refers here to the s-wave scattering phase shift. After some controversies about the correctness of this result [RS71, Ham71], the above was confirmed in the case of a point interaction V by theoretical-physics methods [Ham71] and is now accepted in the physics literature.

Now, we briefly return to the random case. As already mentioned, [GBLA02] consider the asymptotics of the Anderson integral (1.10) for the Anderson model. They claim a logarithmic divergence of the Anderson integral in the delocalised regime in $d \geq 3$. If absolutely continuous spectrum exists, this is not surprising. More interestingly, they predict in the bulk of the spectrum of the two dimensional Anderson model faster divergence of the Anderson integral than logarithmic whenever the perturbation is not point-like.

Since the decay exponent of the AOC might be quite complicated to compute, [AL94, Aff97] propose to consider the error in the difference of the ground-state energies instead and associate its behaviour with the decay exponent in the AOC. They claim the following asymptotics for one-dimensional systems

$$\Xi_L^N := \sum_{k=1}^N \mu_k^L - \sum_{j=1}^N \lambda_j^L = \int_{-\infty}^E dx \xi(E) + \frac{x_{\text{FS}}}{L} + o\left(\frac{1}{L}\right) \quad (1.13)$$

in the thermodynamic limit and refer to x_{FS} as the **finite-size energy**, which may be the same as the decay exponent in the AOC. In the latter case, ξ denotes the spectral shift function. However, the finite-size energy x_{FS} is equal to $\zeta(E)$ only for a particular choice of the thermodynamic limit. The finite-size energy was deduced for this choice also in [ZA97, App. A].

2. Rigorous Results on the Ground-State Overlap

Here, we summarise the previous rigorous mathematical results on the asymptotics of the ground-state overlap and comment on related results, as well as sketch the new results deduced in this thesis. After some attempts in [Ott05] the first mathematically rigorous result concerning the ground-state overlap was given in [KOS13]. For one-dimensional systems without a background potential the following asymptotics of the Anderson integral was proved

$$\mathrm{tr} \mathcal{I}_{L,N} \sim \tilde{\gamma}(E) \ln L, \quad \text{with} \quad \tilde{\gamma}(E) := \frac{1}{\pi^2} \|T_E/2\|_{\mathrm{HS}}^2, \quad (1.14)$$

where HS denotes the Hilbert-Schmidt norm and T_E the transition or just T-matrix for the pair of infinite-volume operators H and H' . As explained earlier on, see (1.7) and (1.8), the above asymptotics leads to the algebraic decay $|\mathcal{S}_L^N|^2 \lesssim L^{-\tilde{\gamma}(E)}$. Up to a numerical energy dependent factor, the exponent $\tilde{\gamma}(E)$ is called total scattering cross-section averaged over all incident directions, see [Yaf00, Sct. 8.5]. It arises naturally when measuring the strength of the scattering caused by the perturbation V . Apart from the above asymptotics, [KOS13] also showed a non-optimal lower bound for particular one-dimensional systems. Later, [GKM14] proved the same upper bound

$$|\mathcal{S}_L^N|^2 \lesssim L^{-\tilde{\gamma}(E)} \quad (1.15)$$

for rather general pairs of Schrödinger operators including a background potential V_0 in arbitrary dimension $d \in \mathbb{N}$ and $\tilde{\gamma}(E)$ as in (1.14). Restricting ourselves to 3-dimensional systems with a spherically-symmetric perturbation V_0 , the exponent $\tilde{\gamma}(E)$ reduces to the one predicted by Anderson, i.e. in this case we rewrite

$$\tilde{\gamma}(E) = \frac{1}{\pi^2} \|T_E/2\|_{\mathrm{HS}}^2 = \frac{1}{\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1) (\sin(\delta_{\ell}(\sqrt{E})))^2, \quad (1.16)$$

where δ_{ℓ} denotes the scattering phase shift in the ℓ th angular momentum channel, see [RS79, Chapt. IX]. Shortly after, [GKMO14] found in the general setting of [GKM14] the stronger estimate

$$|\mathcal{S}_L^N|^2 \lesssim L^{-\gamma(E)}, \quad \text{with} \quad \gamma(E) := \frac{1}{\pi^2} \|\arcsin(T_E/2)\|_{\mathrm{HS}}^2. \quad (1.17)$$

In the case of a 3-dimensional spherically symmetric system this exponent reduces to

$$\gamma(E) = \frac{1}{\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1) (\arcsin(\sin(\delta_{\ell}(\sqrt{E}))))^2. \quad (1.18)$$

Unfortunately, the previous results in [KOS13, GKM14, GKMO14] are not universally valid. They only apply to certain thermodynamic limits. Moreover, none of the above results provide the exact asymptotics of the ground-state overlap \mathcal{S}_L^N but just upper bounds on the latter. We state the precise setting and the results of both [GKM14] and [GKMO14] in Chapter 2, see in particular Theorem 2.2 below. But we will not spell out the proof of the stronger statement (1.17), instead we refer to the article and the PhD thesis [Küt14]. The main difference in the proof of both results lies in either treating only the Anderson integral $\mathcal{I}_{L,N}$, see (1.10), or estimating each summand of the series (1.9). In this thesis, we focus on the weaker upper bound found in [GKM14], i.e. estimate (1.15), and extend this result in Chapter 2 to arbitrary choices of thermodynamic limits under the additional

natural eigenvalue spacing condition

$$\forall a < 1 : \limsup_{\substack{N, L \rightarrow \infty \\ N/|\Lambda_L| \rightarrow \rho(E)}} (|\mu_{N+1}^L - \lambda_N^L| L^a) = 0. \quad (1.19)$$

Moreover, we extend the result to more general perturbations V than considered in [GKM14], see Theorem 2.6. Apart from the problem of restrictions to special thermodynamic limits, the more important task is to find the exact asymptotics of the ground-state overlap. In particular, we want to investigate, whether the upper bound governed by the decay exponent $\gamma(E)$ provides a sharp upper bound as conjectured in [GKMO14, Küt14]. In a nutshell, the general answer to this question is no. We arrive at this conclusion by following a different approach than [GKMO14] and prove a product formula of the ground-state overlap in terms of the eigenvalues of H_L and H'_L , see Chapter 3, Theorem 3.3. This formula is valid for rank-one perturbations and reads

$$|S_L^N|^2 = \prod_{j=1}^N \prod_{k=N+1}^{\infty} \frac{|\mu_k^L - \lambda_j^L| |\lambda_k^L - \mu_j^L|}{|\lambda_k^L - \lambda_j^L| |\mu_k^L - \mu_j^L|}. \quad (1.20)$$

At this point it needs to be mentioned that the latter is known in physics literature and goes back at least to [TO85]. We use this representation to show in Theorem 3.17 the exact asymptotics of the ground-state overlap

$$|S_L^N|^2 \sim L^{-\frac{1}{\pi^2} \delta^2(\sqrt{E})}, \quad (1.21)$$

for the special case of the free negative Laplacian and a Dirac- δ perturbation in three space dimensions. In the above, δ denotes the s-wave scattering phase shift. We emphasise that this result is precisely the one Anderson claimed in [And67b]. In comparison, we remark that in the case of a Dirac- δ perturbation the T -matrix is just the number $T_E = 1 - \exp(2i\delta(\sqrt{E}))$. Thus, we compute the modulus $|T_E/2| = |\sin(\delta(\sqrt{E}))|$ and in this case

$$\gamma(E) = \begin{cases} \frac{1}{\pi^2} \delta^2(\sqrt{E}), & |\delta(\sqrt{E})| \leq \frac{\pi}{2} \\ \frac{1}{\pi^2} (\delta(\sqrt{E}) - \pi)^2, & |\delta(\sqrt{E})| > \frac{\pi}{2} \end{cases}. \quad (1.22)$$

Now, whenever $|\delta(\sqrt{E})| \leq \frac{\pi}{2}$, we obtain that $\gamma(E)$ is the decay exponent in the exact asymptotics of S_L^N . But already in the case of an attractive Dirac- δ perturbation, we obtain for $k > 0$

$$\delta(k) = \pi - \arctan\left(\frac{k}{4\pi|\alpha|}\right) > \frac{\pi}{2}, \quad (1.23)$$

where α parametrises the strength of the δ -interaction, see Definition 3.11. This implies at least in this case

$$\gamma(E) < \frac{1}{\pi^2} \delta^2(\sqrt{E}) \quad (1.24)$$

and, therefore, $\gamma(E)$ does not determine the exact asymptotics. In more general settings where the perturbation is a multiplication operator, we expect that $\gamma(E)$ does not necessarily govern the exact decay of the correlation determinant, see also Remark 2.5(iii).

Concerning exact asymptotics of eigenfunction-correlation determinants, we mention also [KOS15] who consider perturbations by magnetic fields. They prove for one-dimensional systems a similar statement to (1.21) for a shifted correlation determinant, which relies on asymptotics of determinants of Toeplitz matrices. They need an assumption similar to $\delta \leq \frac{\pi}{2}$.

As already pointed out, the proofs of [GKM14] and [GKMO14] both rely on the representation (1.9). Given this representation, the proof proceeds in two steps. The first elaborate step consists in estimating the spectral projections corresponding to the finite-volume Schrödinger operators by the corresponding spectral projections corresponding to the infinite-volume Schrödinger operators. The second step deals with these infinite-volume operators and we deduce for $n \in \mathbb{N}$ the asymptotics

$$\mathrm{tr} \left\{ (1_{(-\infty, E-\epsilon)}(H) 1_{(E+\epsilon, \infty)}(H') 1_{(-\infty, E-\epsilon)}(H))^n \right\} \sim c_n \mathrm{tr} \left\{ |T_E/2|^{2n} \right\} |\ln \epsilon| \quad (1.25)$$

as $\epsilon \searrow 0$ for some appropriate constants c_n . Surprisingly, these constants c_n coincide with the coefficients in the series expansion of the function $(\arcsin(x))^2$, which proves (1.17). The latter asymptotics (1.25) of powers of the operators $1_{(-\infty, E-\epsilon)}(H) 1_{(E+\epsilon, \infty)}(H') 1_{(-\infty, E-\epsilon)}(H)$ was extended in [FP15] to a more compact expression for continuous functions with sufficient decay at 0.

The above conclusions indicate that our problem is closely related to scattering theoretic quantities. One can state, as a first summary, that non-trivial scattering results at least in algebraic decay of the ground-state overlap. Since non-trivial scattering implies the existence of absolutely continuous spectrum, a natural question is the behaviour of \mathcal{S}_L^N for other types of spectra. We treat this question in Chapter 5 for a pair of one-particle Schrödinger operators on the lattice \mathbb{Z}^d , where the unperturbed operator is the random Hamiltonian of the Anderson model and V is a rank-one perturbation. The first result of Chapter 5 is a converse statement to (1.8). In the regime of exponentially localised fractional moments of the resolvents, we obtain not just sublogarithmic divergence of the Anderson integral but boundedness, i.e.

$$\limsup_{L \rightarrow \infty} \mathrm{tr} \left\{ 1_{(-\infty, E)}(H_{\omega, L}) 1_{(E, \infty)}(H'_{\omega, L}) 1_{(-\infty, E)}(H_{\omega, L}) \right\} < \infty \quad (1.26)$$

for almost all $(E, \omega) \in \sigma(H_{\omega}) \times \Omega$, see Theorem 5.7. The second result for the Anderson model concerns the ground-state overlap itself. We prove the non-vanishing of its expectation value, i.e. in the high disorder regime we show

$$\liminf_{\substack{N, L \rightarrow \infty \\ N/L^d \rightarrow \rho > 0}} \mathbb{E} [|\mathcal{S}_L^N|] > 0, \quad (1.27)$$

see Theorem 5.19. Apparently, the latter results point towards the opposite direction than the upper bounds found in the models with absolutely continuous spectrum. Although we are only considering the expectation value, we think this is rather optimal in the sense that with a positive probability there is a subsequence such that \mathcal{S}_L^N goes to 0. Thus, almost sure results may not hold. To illustrate this behaviour, we added some numerics in Chapter 6 which are particularly interesting in the random case. In the localised regime, these figures suggest that the variance of \mathcal{S}_L^N is rather big and \mathcal{S}_L^N itself is either near 0 or near 1. This reflects the existence or non-existence of an eigenfunction corresponding to an eigenvalue near the Fermi energy whose localisation center sits near the support of the perturbation.

Apart from the asymptotics of the ground-state overlap for non-interacting fermions, we consider for completeness also the case of non-interacting Bosons. We show that in this case the asymptotic behaviour of the overlap depends on the space dimension, see Theorem 3.30.

Moreover, in Chapter 4 we treat the difference of the ground-state energies of the two non-interacting N -particle Hamiltonians. We prove in arbitrary dimension

$$\Xi_L^N := \sum_{k=1}^N \mu_k^L - \sum_{j=1}^N \lambda_j^L \sim \int_{-\infty}^E dx \xi(E) \quad (1.28)$$

in the thermodynamic limit $N/L^d \rightarrow \rho > 0$, where ξ denotes the spectral-shift function of the pair of operators H and H' , see Theorem 4.2. This is not surprising because the difference of the ground-state energies can be expressed in terms of the finite-volume spectral-shift function, which converges weakly to the infinite-volume analogue, see [HM10] or [BM12]. In the second part of this chapter, we consider systems on the half-axis. We provide the exact asymptotics up to the second order of the difference of the ground-state energies in the thermodynamic limit, i.e. we verify formula (1.13) and compute the finite-size energy x_{FS} defined in (1.13). More precisely, we show for systems on the half axis that

$$\Xi_L^N = \int_{-\infty}^E dx \xi(x) + \int_E^{(\frac{N\pi}{L})^2} dx \xi(x) + \frac{\sqrt{E}\pi}{L} \left(\xi(E) + \delta^2(\sqrt{E}) \right) + o\left(\frac{1}{L}\right), \quad (1.29)$$

as $N/L \rightarrow \rho > 0$, where δ is again the scattering phase shift. Since the second integral depends on the particular thermodynamic limit chosen, we don't think that there is a deep connection of the finite-size energy and the decay of the ground-state overlap.

In summary, the organisation of this thesis is the following. We recall in Chapter 2 the results of [GKM14] and [GKMO14] and generalise these results. We proceed in Chapter 3 with a product representation of the ground-state overlap and use this representation to prove the exact asymptotics of the ground-state overlap. In Chapter 4 we deduce the asymptotics of the difference of the ground-state energies, and especially focus on the finite-size correction. We continue in Chapter 5 with bounds on traces of products of spectral projections and the expectation value of the ground-state overlap in the Anderson model. Finally, Chapter 6 provides some numerics and an outlook on things that could be done further. In general, each chapter is self-contained and can be read without further knowledge of the remaining chapters.

Declaration concerning already published material in this thesis: The results of Chapter 2 are substantial improvements of the findings of [GKM14] and [GKMO14]. A shortened version of Chapter 3 is already published by the author of this thesis in the paper [Geb15]. Similarly, the result of Chapter 4, Section 2, is part of the preprint [Geb14] by the author.

CHAPTER 2

Upper Bounds for General Schrödinger Operators

In this chapter we begin with presenting the results of [GKM14] and [GKMO14] under its precise assumptions. Thereafter, we extend the latter results to a broader class of perturbations and more general choices of the particle number.

1. Model and Results

We consider the pair of one-particle Schrödinger operators

$$H := -\Delta + V_0 \quad \text{and} \quad H' := -\Delta + V_0 + V \quad (2.1)$$

on $L^2(\mathbb{R}^d)$, $d \in \mathbb{N}$. Here, $-\Delta$ corresponds to the negative Laplacian and both V and V_0 correspond to real-valued functions on \mathbb{R}^d , where we assume

$$\begin{aligned} \max\{V_0, 0\} &\in K_{\text{loc}}^d(\mathbb{R}^d), \quad \max\{-V_0, 0\} \in K^d(\mathbb{R}^d), \\ V &\in K_{\text{loc}}^d(\mathbb{R}^d), \quad V \geq 0. \end{aligned} \quad (\mathbf{A})$$

Here, we have written $K^d(\mathbb{R}^d)$ and $K_{\text{loc}}^d(\mathbb{R}^d)$ for the Kato class and the local Kato class, respectively [Sim82]. In the following the perturbation V will be specified further depending on the particular theorem. These operators are self-adjoint and densely defined on the Hilbert space $L^2(\mathbb{R}^d)$. Let $\Lambda_1 \subseteq \mathbb{R}^d$ be open and bounded with $0 \in \Lambda_1$. For $L > 0$ we denote by $\Lambda_L := L \cdot \Lambda_1$ and by $-\Delta_L$ the negative Laplacian on Λ_L with Dirichlet boundary conditions. We define by

$$H_L := -\Delta_L + V_0 \quad \text{and} \quad H'_L := -\Delta_L + V_0 + V \quad (2.2)$$

the restrictions of H and H' to Λ_L . Here, V and V_0 stand for the canonical restrictions to the finite volume Λ_L . Standard results imply that H_L and H'_L are self-adjoint and densely defined on the Hilbert space $L^2(\Lambda_L)$. Moreover, assumption **(A)** ensures that the finite-volume one-particle operators H_L and H'_L are bounded from below and have purely discrete spectrum (which follows, e.g., from the fact that the semigroup operators $\exp(-tH_L^{(j)})$ are trace class [BHL00, Thm. 6.1] for each $t > 0$). We write

$$\lambda_1^L \leq \lambda_2^L \leq \dots \quad \text{and} \quad \mu_1^L \leq \mu_2^L \leq \dots \quad (2.3)$$

for their non-decreasing sequences of the eigenvalues, counting multiplicities, and $(\varphi_j^L)_{j \in \mathbb{N}}$ and $(\psi_k^L)_{k \in \mathbb{N}}$ for the corresponding sequences of normalised eigenfunctions with an arbitrary choice of basis vectors in any eigenspace of dimension greater than one.

We are interested in the thermodynamic limit realising a given Fermi energy $E \in \mathbb{R}$. For the moment we choose the particle number N to be

$$N = N_L(E) := \#\{j \in \mathbb{N} : \lambda_j^L \leq E\} \in \mathbb{N}_0. \quad (2.4)$$

With this choice we set

$$\mathcal{S}_L(E) := \det\left(\langle \varphi_j^L, \psi_k^L \rangle\right)_{j,k=1,\dots,N_L(E)} \quad (2.5)$$

and we are interested in the asymptotics of $S_L(E)$ as $L \rightarrow \infty$. If $N_L(E) = 0$, we set $S_L(E) := 1$. We note that the notation $S_L(E)$ is slightly different from the one used in the introduction and reflects the fact that we use the particular particle number N defined in (2.4). Throughout this thesis, $S_L(E)$ will refer to the ground-state overlap, where the particle number $N \in \mathbb{N}$ is given by (2.4).

Remark 2.1. The choice (2.4) of the particle number implies that the particle density ρ of the two non-interacting fermion systems in the thermodynamic limit is given by the integrated density of states of the single-particle Schrödinger operator H . The limit

$$\lim_{L \rightarrow \infty} \frac{N_L(E)}{L^d |\Lambda_1|} = \rho(E). \quad (2.6)$$

exist in the case of e.g. periodic V_0 , $V_0 = 0$ or V_0 vanishing at infinity. If the limit (2.6) does not exist, then there must be more than one accumulation point because $\limsup_{L \rightarrow \infty} N_L(E)/L^d < \infty$ for every $E \in \mathbb{R}$ due to assumptions **(A)**. But even in this case it makes still sense to study the asymptotic behaviour of the overlap $S_L(E)$ as $L \rightarrow \infty$.

With this special choice of the thermodynamic limit the most general results so far are the following.

Theorem 2.2. *Assume conditions **(A)** and additionally*

$$V \in L^\infty(\mathbb{R}^d) \quad \text{and} \quad \text{supp } V \subset \Lambda_1 \text{ compact.} \quad (2.7)$$

Let $(L_n)_{n \in \mathbb{N}} \subset \mathbb{R}_{\geq 0}$ be a sequence of increasing lengths with $L_n \uparrow \infty$. Then, there exists a subsequence $(L_{n_k})_{k \in \mathbb{N}}$ and a Lebesgue null set $\mathcal{N} \subset \mathbb{R}$ of exceptional Fermi energies such that for every $E \in \mathbb{R} \setminus \mathcal{N}$ the ground-state overlap (2.5) obeys

(i) [GKM14, Theorem 2.2]

$$\limsup_{k \rightarrow \infty} \frac{\ln |S_{L_{n_k}}(E)|}{\ln L_{n_k}} \leq -\frac{\tilde{\gamma}(E)}{2}, \quad (2.8)$$

where

$$\tilde{\gamma}(E) := \frac{1}{\pi^2} \|T_E/2\|_{HS}^2. \quad (2.9)$$

(ii) [GKMO14, Theorem 2.2]

$$\limsup_{k \rightarrow \infty} \frac{\ln |S_{L_{n_k}}(E)|}{\ln L_{n_k}} \leq -\frac{\gamma(E)}{2}, \quad (2.10)$$

where

$$\gamma(E) := \frac{1}{\pi^2} \|\arcsin |T_E/2|\|_{HS}^2. \quad (2.11)$$

Here, T_E denotes the scattering T -matrix and $\|\cdot\|_{HS}$ the Hilbert-Schmidt norm on the appropriate fibre Hilbert space where T_E is defined.

One goal of this chapter is to remove this particular choice of the particle number and allow arbitrary thermodynamic limits approaching a fixed particle density. Another goal is to weaken the assumptions on the perturbation. Both things are partially achieved in Theorem 2.6 below. For completeness, let us point out that in some special cases one can erase the subsequences already.

Theorem 2.3. [GKMO14, Theorem 2.2'] Assume the situation of Theorem 2.2 with $d = 1$, or replace the perturbation potential V in Theorem 2.2 by a finite-rank operator $V = \sum_{\nu=1}^n \langle \phi_{\nu}, \cdot \rangle \phi_{\nu}$ with compactly supported $\phi_{\nu} \in L^2(\mathbb{R}^d)$ for $\nu = 1, \dots, n$, or consider the lattice problem on \mathbb{Z}^d corresponding to the situation in Theorem 2.2. Then, the ground-state overlap (2.5) obeys for Leb-a.e. $E \in \mathbb{R}$

$$\limsup_{L \rightarrow \infty} \frac{\ln |\mathcal{S}_L(E)|}{\ln L} \leq -\frac{\gamma(E)}{2} \quad (2.12)$$

with the decay exponent $\gamma(E)$ defined in the second part of Theorem 2.2.

The proof of Theorem 2.2, as well as Theorem 2.3, relies on a lower bound on the trace of powers of products of spectral projections, where no subsequences are necessary. These bounds seem to be interesting on its own.

Theorem 2.4. [GKMO14, Theorem 3.4] Under the assumptions of Theorem 2.2, there exists a null set $\mathcal{N} \subset \mathbb{R}$ of exceptional Fermi energies such that for every $E \in \mathbb{R} \setminus \mathcal{N}$ and every $n \in \mathbb{N}$

$$\text{tr} \left\{ \left(1_{(-\infty, E)}(H_L) 1_{(E, \infty)}(H'_L) 1_{(-\infty, E)}(H_L) \right)^n \right\} \geq n J_{2n} \text{tr}(|T_E/(2\pi)|^{2n}) \ln L + o(\ln L) \quad (2.13)$$

as $L \rightarrow \infty$, and

$$J_{2n} := \pi^{2(n-1)} 2^{2n-1} \frac{[(n-1)!]^2}{(2n)!}. \quad (2.14)$$

Here, 1_B stands for the indicator function of a set $B \in \text{Borel}(\mathbb{R})$.

Remarks 2.5. (i) We will not define the T -matrix here. For a detailed introduction to scattering theory including precise definitions we refer to [Yaf10] and [RS79]. Nevertheless, let us point out that in our situation for Leb.-a.e. $E \in \mathbb{R}$ the T -matrix is compact and defined by $T_E := S_E - I$, where S_E denotes the S -matrix at the energy E and I the identity on the appropriate Hilbert space. Since the S -matrix is a unitary, see [Yaf92] or [RS79], we obtain the operator inequality $|T_E/2| \leq 1$. Moreover, we denote by $(\exp(2i\delta_k(\sqrt{E})))_{k \in \mathbb{N}}$ the eigenvalues of S_E . The numbers $(\delta_k(\sqrt{E}))_{k \in \mathbb{N}}$ are called the scattering phase shifts which are a priori not uniquely defined, only up to a factor of π . A short calculation shows for $k \in \mathbb{N}$

$$|\exp(2i\delta_k(\sqrt{E})) - 1|/2 = |\sin(\delta_k(\sqrt{E}))|. \quad (2.15)$$

Thus, we rewrite the above decay exponents according to

$$\tilde{\gamma}(E) := \frac{1}{\pi^2} \|T_E/2\|_{\text{HS}}^2 = \frac{1}{\pi^2} \sum_{k=1}^{\infty} \left(\sin(\delta_k(\sqrt{E})) \right)^2 \quad (2.16)$$

$$\gamma(E) := \frac{1}{\pi^2} \|\arcsin|T_E/2|\|_{\text{HS}}^2 = \frac{1}{\pi^2} \sum_{k=1}^{\infty} \left(\arcsin(\sin(\delta_k(\sqrt{E}))) \right)^2. \quad (2.17)$$

We remark that these representations are independent of the choice of the scattering phase shifts.

(ii) Since $|x| \leq |\arcsin(x)|$ for $|x| \leq 1$ and $|T_E/2| \leq 1$, the decay exponents in Theorem 2.2 satisfy

$$\frac{1}{\pi^2} \|T_E/2\|_{\text{HS}}^2 \leq \frac{1}{\pi^2} \|\arcsin|T_E/2|\|_{\text{HS}}^2 \quad (2.18)$$

and the second result of Theorem 2.2 is indeed stronger than the first one.

(iii) We return to the question, whether $\gamma(E)$ provides the correct asymptotics for the choice (2.4) of the thermodynamic limit. As already mentioned in the introduction, we have to negate this question. Restricting ourselves to the case of $d = 3$, $V_0 = 0$ and a spherically-symmetric perturbation V , we choose, following [RS79, Sct. XI.8C], the scattering phase shifts δ_k uniquely to be continuous and according to $\lim_{E \rightarrow \infty} \delta_k(\sqrt{E}) = 0$. Taking our findings in the following chapter, in particular Theorem 3.17 and the discussion thereafter, into account, the correct decay exponent is rather

$$\zeta(E) := \frac{1}{\pi^2} \sum_{k=1}^{\infty} \left(\delta_k(\sqrt{E}) \right)^2, \quad (2.19)$$

where the scattering phase shifts δ_k are uniquely defined due to the above normalisation. Apparently $\gamma(E) = \zeta(E)$, whenever $|\delta_k(\sqrt{E})| \leq \pi/2$ for all $k \in \mathbb{N}$. We give in Chapter 6 some heuristics what effects are neglected in the decay exponent $\gamma(E)$.

(iv) Both statements given in Theorem 2.2 are equivalent to

$$|\mathcal{S}_{L_{n_k}}(E)|^2 \leq L_{n_k}^{-\gamma(E)+o(1)} \quad (2.20)$$

as $k \rightarrow \infty$. Thus, we proved an algebraic decay of the ground-state overlap with decay exponent $\gamma(E)$. Note that the $o(1)$ -term may be quite big in the sense that the error satisfies $L^{o(1)} = o(\ln L)$ only.

(v) In the proof of Theorem 2.2 (i), one witnesses that the decay exponent $\tilde{\gamma}$ emerges as the diagonal value of the Lebesgue density

$$\tilde{\gamma}(E) := \lim_{\epsilon \searrow 0} \frac{1}{\epsilon^2} \mu \left((E - \epsilon/2, E + \epsilon/2) \times (E - \epsilon/2, E + \epsilon/2) \right) = \frac{d\mu(E, E')}{d(E, E')} \Big|_{E'=E} \quad (2.21)$$

of the two-dimensional spectral-correlation measure, which is defined by

$$\mu(B \times B') := \text{tr} \left\{ \sqrt{V} 1_B(H) V 1_{B'}(H') \sqrt{V} \right\}, \quad B, B' \in \text{Borel}(\mathbb{R}). \quad (2.22)$$

We refer to Lemma 2.17 and Appendix A for a discussion of such measures. Now, with some more effort one can see that the value of the density on the diagonal is the Hilbert-Schmidt norm of the T -matrix. We will not present the proof here, see [GKM14], [GKMO14, Cor. 4.32] and [Küt14, Cor. 9.12]. In general, this density is just an $L^1_{\text{loc}}(\mathbb{R}^2)$ function. Hence, it is not obvious if (2.21) makes sense at all. But one can show it does at least for Leb.-a.e. $E \in \mathbb{R}$, see [GKM14] and [GKMO14]. Later we will focus on the case of $V_0 = 0$ and $V \in L^\infty(\mathbb{R}^d)$ with sufficient decay at infinity. In this case one knows that μ is absolutely continuous with a continuous density and (2.21) makes perfectly sense, see [FP15, Lem. 2.7] or [Yaf10, Lem. 8.1.8].

(vi) The definition of $\tilde{\gamma}$ in (2.21) implies $\tilde{\gamma}(E) = 0$, whenever $E \notin \sigma_{\text{ac}}(H) = \sigma_{\text{ac}}(H')$, where the latter equality of the spectra follows from standard results in scattering theory and is referred to as Birman's theorem. On the other hand one should understand that absolutely continuous spectrum leads to non-trivial scattering, i.e. $T_E \neq 0$. To see the connection, we consider a rank-one perturbation V with a cyclic vector $\eta \in \mathcal{H}$. Then, the measure μ reduces to a product measure and the decay exponent to

$$\tilde{\gamma}(E) = \frac{1}{\pi^2} \lim_{\epsilon \searrow 0} \left\{ \text{Im} \langle \eta, \frac{1}{H - E - i\epsilon} \eta \rangle \text{Im} \langle \eta, \frac{1}{H' - E - i\epsilon} \eta \rangle \right\}. \quad (2.23)$$

Recalling the properties of the Borel transform of a measure, see [Tes09] or [Sim05], the latter limit is equal to the product of the values of the densities of the ac-parts of the

corresponding spectral measures of H and H' at the energy E , which exist and are non-trivial for Leb.-a.e. $E \in \sigma_{\text{ac}}(H) = \sigma_{\text{ac}}(H')$, therefore, $\tilde{\gamma}(E) > 0$ for Leb.-a.e. $E \in \sigma_{\text{ac}}(H)$. Apart from the above heuristics, [Küt14] states a perturbative argument that $\tilde{\gamma}(E) > 0$ for Leb.-a.e. $E \in \sigma_{\text{ac}}(-\Delta)$ in the case of $V_0 = 0$ and $d \geq 2$. For spherically-symmetric perturbations V one can deduce this result also using the angular momentum decomposition. The above discussion underlines that the absolutely continuous spectrum leads to algebraic decay of the ground-state overlap.

(vii) The latter immediately implies the question what happens, if different kind of spectra occur. We investigate this question further in Chapter 5.

We will not prove Theorem 2.2 nor Theorem 2.3 here. We refer to [GKM14], [GKMO14] and [Küt14] for the proofs. In the following, we want to generalise the above results to a broader class of perturbations V . Moreover, we want to weaken assumption (2.4) on the particle number, which means we allow arbitrary thermodynamic limits, and get rid of the subsequences. We state an analogous result to Theorem 2.2 (i) without restrictions to subsequences nor to specific thermodynamic limits but unfortunately an additional assumption on the eigenvalue spacing enters.

Theorem 2.6. *Assume conditions (A) without a background potential and subexponentially decaying V , i.e.*

$$V_0 = 0, \exists C > 0, \theta > 1 \text{ such that } |V(x)| \leq C e^{-\ln(|x|_2)^\theta}, \quad (2.24)$$

where $|\cdot|_2$ denotes the Euclidean norm on \mathbb{R}^d . Let $E > 0$ and $N_{(\cdot)}(E) : \mathbb{R}_+ \rightarrow \mathbb{N}$ be a function subject to

$$\lim_{L \rightarrow \infty} \frac{N_L(E)}{|\Lambda_L|} = \rho(E) > 0, \quad (2.25)$$

where ρ denotes the integrated density of states of the operator $H = -\Delta$. Moreover, we assume the following eigenvalue spacing condition

$$\limsup_{L \rightarrow \infty} \left| \mu_{N_L(E)+1}^L - \lambda_{N_L(E)}^L \right| L^a = 0 \quad (2.26)$$

for all $a < 1$. Then

$$\limsup_{L \rightarrow \infty} \frac{\ln |\mathcal{S}_L^{N_L(E)}|}{\ln L} \leq -\frac{\tilde{\gamma}(E)}{2}, \quad (2.27)$$

with

$$\tilde{\gamma}(E) := \frac{1}{\pi^2} \|T_E/2\|_{HS}^2. \quad (2.28)$$

We will prove Theorem 2.6 in Section 2.

Remarks 2.7. (i) We assumed $E > 0$ because $\sigma_{\text{ac}}(H) = [0, \infty)$ and only positive energies are relevant. Moreover, note that ρ can be computed explicitly in the case $V_0 = 0$, i.e.

$$\rho(E) = \frac{\tau_d}{(2\pi)^d} E^{d/2}, \quad (2.29)$$

where τ_d is the volume of the unit ball in \mathbb{R}^d , see e.g. [Sto01, App. 4.1] or [RS78].

(ii) We assumed $V_0 = 0$ and $V \in L^\infty(\mathbb{R}^d)$ for simplicity because this implies continuity of the density of the measure (2.22). As a consequence, we do not need to exclude an exceptional set of energies and the result holds for all energies within $\sigma_{\text{ac}}(H)$. Probably the proof can be generalised to the case with a background potential present using Lebesgue

point ideas as in [GKM14], [GKMO14] and [Küt14]. Using Lemma 2.16 below, one should be able to prove the stronger statement of Theorem 2.2 for more general perturbations V .

(iii) The assumption (2.26) seems to be natural. Morally, in the proof one sees that the upper bound on the exact asymptotics is governed by the L -asymptotics of the integral

$$\Omega_L := \int_{(-\infty, \lambda_{N_L(E)}^L) \times (\mu_{N_L(E)+1}^L, \infty)} \frac{d\mu(x, y)}{(y - x)^2}, \quad (2.30)$$

where the measure μ is the one given in (2.22). Assuming the density to be continuous, it is not hard to see that

$$\Omega_L \sim \tilde{\gamma}(E) \ln (\mu_{N_L(E)+1}^L - \lambda_{N_L(E)}^L), \quad (2.31)$$

where $\tilde{\gamma}(E)$ is the value of the density on the diagonal (E, E) . Unfortunately, we can not prove that the asymptotics is governed by (2.30) exactly but just a lower bound with some additional security distance L^{-a} , with $a < 1$, see Lemma 2.12 and Lemma 2.16 below.

(iv) Assumption (2.26) is satisfied in the $d = 1$ case and in the case of a finite-rank perturbation as in Theorem 2.3. The eigenvalue spacing assumption should also be correct in higher dimensions.

Most of the arguments in the proof of Theorem 2.6 apply to a broader class of perturbations. Hence, we end this paragraph with an analogous statement to Theorem 2.2 under weaker assumptions on the perturbation. The difference to Theorem 2.6 is that we include singularities in the scattering potential and a background potential but we choose again the particular particle number of (2.4).

Corollary 2.8 (Corollary of the proofs of Theorem 2.2 and 2.6). *Assume conditions **(A**) and additionally*

$$V \in L^2(\mathbb{R}^d) \quad \text{and} \quad \exists L_0 > 0, \theta > 1 \text{ such that } |V(x)| \leq e^{-\ln(|x|_2)^\theta} \text{ for } |x|_2 \geq L_0. \quad (2.32)$$

Let $E \in \mathbb{R}$, and we choose $N_L(E)$ according to (2.4). Moreover, let $(L_n)_{n \in \mathbb{N}} \subset \mathbb{R}_{\geq 0}$ be a sequence of increasing lengths with $L_n \uparrow \infty$. Then, there exists a subsequence $(L_{n_k})_{k \in \mathbb{N}}$ and a Lebesgue null set $\mathcal{N} \subset \mathbb{R}$ of exceptional Fermi energies such that for every $E \in \mathbb{R} \setminus \mathcal{N}$ the ground-state overlap (2.5) obeys

$$\limsup_{k \rightarrow \infty} \frac{\ln |\mathcal{S}_{L_{n_k}}(E)|}{\ln L_{n_k}} \leq -\frac{\tilde{\gamma}(E)}{2}, \quad (2.33)$$

where

$$\tilde{\gamma}(E) := \frac{1}{\pi^2} \|T_E/2\|_{HS}^2. \quad (2.34)$$

We will not prove the corollary in detail. The key is Lemma 2.23 below which generalises [GKM14, Lemma 3.14]. The rest follows along the same line as in [GKM14].

2. Proof of Theorem 2.6

The proof presented here will be close to the one given in [GKM14]. Nevertheless, we try to include more general assumptions on V , e.g. $V \in L^2(\mathbb{R}^d)$, whenever this is possible.

Throughout the proof we write $N \equiv N_L(E)$. First we expand the ground-state overlap as a series. To do this, we introduce the orthogonal projections

$$P_L^N := \sum_{j=1}^N \langle \varphi_j^L, \cdot \rangle \varphi_j^L \quad \text{and} \quad \Pi_L^N := \sum_{k=1}^N \langle \psi_k^L, \cdot \rangle \psi_k^L \quad (2.35)$$

for $N \in \mathbb{N}_0$, i.e. the projections on the eigenspaces of the first N eigenvalues. Using those, we can prove the following lemma.

Lemma 2.9. *Let $L > 1$, $E \in \mathbb{R}$ and assume that $\mathcal{S}_L^N \neq 0$. Then,*

$$|\mathcal{S}_L^N|^2 = \exp\left(-\sum_{n=1}^{\infty} \frac{1}{n} \text{tr}\left\{\left(P_L^N(I - \Pi_L^N)P_L^N\right)^n\right\}\right), \quad (2.36)$$

where we take the trace of operators on the Hilbert space $L^2(\Lambda_L)$ and I denotes here the identity on $L^2(\Lambda_L)$.

Proof. If $N = 0$, the assertion is true by definition. Otherwise, define the $N \times N$ -matrix $M := (\langle \varphi_j^L, \psi_k^L \rangle)_{j,k=1,\dots,N}$. Then $\mathcal{S}_L^N = \det M$ and $|\mathcal{S}_L^N|^2 = \det(MM^*)$. For $1 \leq j, \ell \leq N$, the (j, ℓ) -th matrix element of MM^* is

$$(MM^*)_{j,\ell} = \sum_{k=1}^N \langle \varphi_j^L, \psi_k^L \rangle \langle \psi_k^L, \varphi_\ell^L \rangle = \langle \varphi_j^L, \Pi_L^N \varphi_\ell^L \rangle = \langle \varphi_j^L, P_L^N \Pi_L^N P_L^N \varphi_\ell^L \rangle. \quad (2.37)$$

Since by assumption, $\mathcal{S}_L^N \neq 0$, and therefore $MM^* > 0$ we have $0 \leq P_L^N(I - \Pi_L^N)P_L^N < 1$. Moreover, being of finite rank, $P_L^N(I - \Pi_L^N)P_L^N$ is a trace-class operator. Thus, we compute

$$\begin{aligned} |\mathcal{S}_L^N|^2 &= \det(I - P_L^N(I - \Pi_L^N)P_L^N) \\ &= \exp\left(\text{tr}\left\{\ln(I - P_L^N(I - \Pi_L^N)P_L^N)\right\}\right) \\ &= \exp\left(-\text{tr}\left\{\sum_{n=1}^{\infty} \frac{1}{n} \left(P_L^N(I - \Pi_L^N)P_L^N\right)^n\right\}\right) \end{aligned} \quad (2.38)$$

where we used the expansion $\ln(1 - x) = -\sum_{n=1}^{\infty} x^n/n$ for the logarithm, which converges absolutely for $|x| < 1$. \square

Corollary 2.10. *The above lemma implies*

$$-\ln|\mathcal{S}_L^N| = \frac{1}{2} \sum_{n=1}^{\infty} \frac{1}{n} \text{tr}\left\{\left(P_L^N(I - \Pi_L^N)P_L^N\right)^n\right\}. \quad (2.39)$$

Since $P_L^N(I - \Pi_L^N)P_L^N \geq 0$, we obtain

$$-\ln|\mathcal{S}_L^N| \geq \frac{1}{2} \text{tr}\left\{P_L^N(I - \Pi_L^N)P_L^N\right\}. \quad (2.40)$$

From now on, we are interested in lower bounds on

$$\mathcal{I}_L(E) := \text{tr}\left\{P_L^N(I - \Pi_L^N)P_L^N\right\}. \quad (2.41)$$

Remarks 2.11. (i) The expression $\mathcal{I}_L(E)$ is called the Anderson integral in the physics literature and was first investigated by P.W.Anderson in [And67a].

(ii) To prove Theorem 2.6 as well as Theorem 2.2 (i) it suffices to consider the lower bound (2.40) and to investigate the asymptotics of the Anderson integral $\mathcal{I}_L(E)$. In contrast, to obtain the result of Theorem 2.2 (ii), one has to treat every summand in (2.39), because each summand contributes to the asymptotics of the overlap.

Note that we assumed here $V_0 = 0$, thus, $H_L \geq 0$ and

$$P_L^N \geq 1_{[0, \lambda_N^L)}(H_L) \quad \text{and} \quad I - \Pi_L^N \geq 1_{(\mu_{N+1}^L, \infty)}(H_L'). \quad (2.42)$$

Hence, we obtain the lower bound

$$\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\} \geq \text{tr}\{1_{[0, \lambda_N^L)}(H_L)1_{(\mu_{N+1}^L, \infty)}(H_L')1_{[0, \lambda_N^L)}(H_L)\}. \quad (2.43)$$

We set

$$\mathcal{F}_L(E) := \text{tr}\{1_{[0, \lambda_N^L)}(H_L)1_{(\mu_{N+1}^L, \infty)}(H_L')1_{[0, \lambda_N^L)}(H_L)\}. \quad (2.44)$$

Lemma 2.12. *Let $L > 0$ and $E > 0$. Then, we have*

$$\mathcal{F}_L(E) = \int_{(-\infty, \lambda_N^L) \times (\mu_{N+1}^L, \infty)} \frac{d\mu_L(x, y)}{(y - x)^2} \geq \int_{\mathbb{R}^2} \frac{d\mu_L(x, y)}{(y - x)^2} \chi_L^-(x) \chi_L^+(y), \quad (2.45)$$

where the finite-volume spectral-correlation measure μ_L on \mathbb{R}^2 is uniquely defined by

$$\mu_L(B \times B') := \text{tr}\{\sqrt{V}1_B(H_L)V1_{B'}(H_L')\sqrt{V}\} \quad (2.46)$$

for $B, B' \in \text{Borel}(\mathbb{R})$ and the functions $\chi_L^\pm \in L^\infty(\mathbb{R})$ are for the moment arbitrary subject to

$$0 \leq \chi_L^+ \leq 1_{(\mu_{N+1}^L, \infty)} \quad \text{and} \quad 0 \leq \chi_L^- \leq 1_{[0, \lambda_N^L)}. \quad (2.47)$$

Proof of Lemma 2.12. Note that μ_L is a sum of Dirac measures and therefore μ_L is well-defined. Essentially, the assertion follows from Appendix A. Nevertheless, we provide a straightforward and simpler proof for the special situation considered here. The eigenvalue equations imply

$$\lambda_j^L \langle \varphi_j^L, \psi_k^L \rangle = \langle H_L \varphi_j^L, \psi_k^L \rangle = \mu_k^L \langle \varphi_j^L, \psi_k^L \rangle - \langle \varphi_j^L, V \psi_k^L \rangle \quad (2.48)$$

from which we obtain the identity

$$|\langle \varphi_j^L, \psi_k^L \rangle|^2 = \frac{|\langle \varphi_j^L, V \psi_k^L \rangle|^2}{(\mu_k^L - \lambda_j^L)^2}, \quad (2.49)$$

provided $\lambda_j^L \neq \mu_k^L$. Since $V \geq 0$ and $\lambda_N^L \leq \mu_{N+1}^L$, this yields

$$\begin{aligned} \mathcal{F}_L(E) &= \sum_{\substack{j \in \mathbb{N}: \\ \lambda_j^L < \lambda_N^L}} \sum_{\substack{k \in \mathbb{N}: \\ \mu_k^L > \mu_{N+1}^L}} |\langle \varphi_j^L, \psi_k^L \rangle|^2 = \sum_{\substack{j \in \mathbb{N}: \\ \lambda_j^L < \lambda_N^L}} \sum_{\substack{k \in \mathbb{N}: \\ \mu_k^L > \mu_{N+1}}} \frac{|\langle \varphi_j^L, V \psi_k^L \rangle|^2}{(\mu_k^L - \lambda_j^L)^2} \\ &= \int_{(-\infty, \lambda_N^L) \times (\mu_{N+1}^L, \infty)} \frac{d\mu_L(x, y)}{(y - x)^2}. \end{aligned} \quad (2.50)$$

Now, the inequality in (2.45) follows from the positivity of the integrand. \square

Before we specify the cut-off functions further, we determine the limits of λ_N^L and μ_{N+1}^L for a given Fermi energy $E > 0$.

Lemma 2.13. *Let $E > 0$ and for clarity let us write again $N_L(E)$ instead of N . Then, assumption (2.25) and (2.26) imply*

$$\lim_{L \rightarrow \infty} \lambda_{N_L(E)}^L = E \quad \text{and} \quad \lim_{L \rightarrow \infty} \mu_{N_L(E)+1}^L = E. \quad (2.51)$$

Proof. We prove this under slightly more general assumptions in Lemma 4.4. \square

Definition 2.14 (Cut-off functions). Let $L > 1$ and $E > 0$, $E_0 > E$. Given some $0 < a < 1$ we say that $\chi_L^\pm \in C_c^\infty(\mathbb{R})$ are *smooth cut-off functions corresponding to λ_N^L and μ_{N+1}^L* , if they obey

$$\begin{aligned} 1_{[\mu_{N+1}^L + L^{-a}, E_0]} &\leq \chi_L^+ \leq 1_{(\mu_{N+1}^L + \frac{1}{2}L^{-a}, E_0+1)}, \\ 1_{[0, \lambda_N^L - L^{-a}]} &\leq \chi_L^- \leq 1_{[-1, \lambda_N^L - \frac{1}{2}L^{-a}]} \end{aligned} \quad (2.52)$$

and if there exist L -independent constants $c_k > 0$ for $k \in \mathbb{N}_0$, such that

$$\chi_L^\pm(\eta_L^\pm \pm \frac{1}{2}L^{-a} \pm x) \leq c_0 L^a x \quad (2.53)$$

for all $x \in [0, \frac{1}{2}L^{-a}]$, where $\eta_L^- := \lambda_N^L$ and $\eta_L^+ := \mu_{N+1}^L$, and

$$\left| \frac{d^k}{dx^k} \chi_L^\pm(\eta_L^\pm \pm \frac{1}{2}L^{-a} \pm x) \right| \leq \begin{cases} c_k L^{ak} & \text{if } 0 \leq x < \frac{1}{2}L^{-a} \\ c_k & \text{otherwise,} \end{cases} \quad (2.54)$$

for every $k \in \mathbb{N}$ and $x \in \mathbb{R}$. Moreover, we choose the decay of χ_L^- in $(-1, 0)$ as well as the decay of χ_L^+ in $(E_0, E_0 + 1)$ independent of L .

Remark 2.15. The security distance L^{-a} can be replaced by $\frac{(ln L)^{1+\epsilon}}{L}$, where $\epsilon > 0$, without effecting the following computations and results. According to Lemma 2.13, the indicator functions in (2.52) are well defined for L large enough, therefore, without further mentioning we restrict us to such L .

In the next lemma, we replace the measure corresponding to the finite-volume operators with the measure corresponding to the infinite-volume operators.

Lemma 2.16 (An application of the Helffer-Sjöstrand formula). *Let $0 < a < 1$ and χ_L^\pm be the associated smooth cut-off functions from Definition 2.14 corresponding to the eigenvalues λ_N^L and μ_{N+1}^L . Then, we obtain*

$$\int_{\mathbb{R}^2} \frac{d\mu_L(x, y)}{(y - x)^2} \chi_L^-(x) \chi_L^+(y) = \int_{\mathbb{R}^2} \frac{d\mu(x, y)}{(y - x)^2} \chi_L^-(x) \chi_L^+(y) + o(1), \quad (2.55)$$

as $L \rightarrow \infty$. Here, μ denotes the infinite-volume spectral correlation measure on \mathbb{R}^2 which is uniquely defined by

$$\mu(B \times B') := \text{tr} \left\{ \sqrt{V} 1_B(H) V 1_{B'}(H') \sqrt{V} \right\} \quad (2.56)$$

for $B, B' \in \text{Borel}(\mathbb{R})$.

This lemma is the main ingredient to the proof of the theorem. We prove this lemma in the next section under weaker assumptions. For completeness, we state that the measures μ and μ_L are well defined also under weaker assumptions on the perturbation V .

Lemma 2.17. *Here, we assume $V \geq 0$ and $V \in L^1(\mathbb{R}^d)$ only. Then, the expression (2.56) is finite for bounded Borel sets and gives rise to a locally finite Borel measures on \mathbb{R}^2 .*

Proof. See Appendix A, Theorem A.1. \square

Remark 2.18. The use of the measure μ is not necessary for the proof. The identity $\int_0^\infty dt te^{-t(y-x)} = \frac{1}{(y-x)^2}$ for $x < y$ implies

$$\begin{aligned} & \int_{(-\infty, \lambda_N^L] \times [\mu_{N+1}^L, \infty)} \frac{d\mu_L(x, y)}{(y-x)^2} = \int_0^\infty dt t \int_{(-\infty, \lambda_N^L] \times [\mu_{N+1}^L, \infty)} d\mu_L(x, y) e^{-t(y-x)} \\ &= \int_0^\infty dt t \operatorname{tr} \left\{ \sqrt{V} 1_{(-\infty, \lambda_N^L]}(H_L) e^{t(H_L - E_L)} V 1_{[\mu_{N+1}^L, \infty)}(H'_L) e^{-t(H'_L - E_L)} \sqrt{V} \right\}, \end{aligned} \quad (2.57)$$

where $E_L := \frac{\lambda_N^L + \mu_{N+1}^L}{2}$. Thus, the notation of μ_L is not needed anymore and one can formulate Lemma 2.16 also on the level of operators without introducing the measure μ . The proof of 2.16, see Section 3, proceeds in precisely this way. However, we introduce μ for brevity and clarity.

From the definition of the cut-off functions χ_L^\pm , see (2.52), and the positivity of the integrand we continue with the lower bound

$$\begin{aligned} \int_{\mathbb{R}^2} \frac{d\mu(x, y)}{(y-x)^2} \chi_L^-(x) \chi_L^+(y) &\geq \int_{\mathbb{R}^2} \frac{d\mu(x, y)}{(y-x)^2} 1_{[0, \lambda_N^L - L^{-a}]}(x) 1_{(\mu_{N+1}^L + L^{-a}, E_0)}(y) \\ &\geq \int_{\mathbb{R}^2} \frac{d\mu_{\text{ac}}(x, y)}{(y-x)^2} 1_{[0, \lambda_N^L - L^{-a}]}(x) 1_{(\mu_{N+1}^L + L^{-a}, E_0)}(y), \end{aligned} \quad (2.58)$$

where μ_{ac} is the absolutely continuous part of the measure μ . Actually, assumption (2.24) ensures that μ itself is a purely absolutely continuous measure. Since we are just interested in lower bounds, we will not focus on this and write $\tilde{\gamma} \in L^1_{\text{loc}}(\mathbb{R}^2)$ for the density of μ_{ac} , which we call in the sequel for brevity again μ . We continue with a regularity result on $\tilde{\gamma}$.

Lemma 2.19 (A form of the limiting absorption principle). *There exists a representative of the density of μ which is continuous within \mathbb{R}_+^2 . In the following we denote by $\tilde{\gamma}$ precisely this continuous representative on \mathbb{R}_+^2 .*

Proof. Since we assumed $V \in L^\infty(\mathbb{R}^d)$ with sufficient decay at infinity, results from stationary scattering theory imply the convergences

$$\lim_{\epsilon \searrow 0} \frac{1}{\epsilon} \sqrt{V} 1_{E-\epsilon/2, E+\epsilon/2}(H) \sqrt{V} := A(E) \quad (2.59)$$

$$\lim_{\epsilon \searrow 0} \frac{1}{\epsilon} \sqrt{V} 1_{E-\epsilon/2, E+\epsilon/2}(H') \sqrt{V} := B(E) \quad (2.60)$$

in trace-class norm for all $E > 0$, see [FP15, Lem. 2.7 (ii)] or [Yaf10, Lem. 8.1.8]. The latter also implies that the functions $A : \mathbb{R}_+ \rightarrow \mathcal{S}_1$ and $B : \mathbb{R}_+ \rightarrow \mathcal{S}_1$,

$$A : E \mapsto A(E) \quad \text{and} \quad B : E \mapsto B(E) \quad (2.61)$$

are continuous, where \mathcal{S}_1 denotes the set of all trace-class operators. Hence, the function $\tilde{\gamma} : \mathbb{R}_+^2 \rightarrow \mathbb{R}$,

$$\tilde{\gamma} : (E, E') \mapsto \operatorname{tr} \{ A(E) B(E') \} \quad (2.62)$$

is a continuous function. Moreover, $\tilde{\gamma}$ is a representative of the density of the measure μ . \square

Remark 2.20. For more general V , e.g. including suitable singularities, and with a non-trivial background potential V_0 the limits (2.59) and (2.60) still exist for Leb.-a.e. $E > 0$, see [BÈ67]. But the question of continuity of the derivatives is not entirely clear. Since we want to keep the proof elementary, we restrict ourselves to $V \in L^\infty(\mathbb{R}^d)$ with sufficient decay at infinity in order to have a continuous representative of the density. We remark that our subexponential decay assumption is not necessary to gain a continuous representative, sufficient polynomial decay is enough, see [FP15].

Lemma 2.21. *Let $0 < a < 1$ and $E > 0$. Under the assumptions of Theorem 2.6 we obtain the following asymptotics*

$$\int_0^{\lambda_N^L - L^{-a}} dx \int_{\mu_{N+1}^L + L^{-a}}^{E_0} dy \frac{\tilde{\gamma}(x, y)}{(y - x)^2} = a\tilde{\gamma}(E, E) \ln L + o(\ln L) \quad (2.63)$$

as $L \rightarrow \infty$, where the error term depends on a , the Fermi energy E and the cut-off energy E_0 .

Proof. This lemma is a standard δ -approximation argument. Nevertheless, we prove it for convenience. First note that Lemma 2.13 implies $\lambda_N^L - \frac{1}{2}L^{-a} > 0$ for L big enough and for such L we compute

$$\int_0^{\lambda_N^L - L^{-a}} dx \int_{\mu_{N+1}^L + L^{-a}}^{E_0} dy \left(\frac{1}{y - x} \right)^2 = |\ln(\mu_{N+1}^L - \lambda_N^L + 2L^{-a})| + O(1) \quad (2.64)$$

as $L \rightarrow \infty$. Hence, we estimate

$$\begin{aligned} & \left| \int_0^{\lambda_N^L - L^{-a}} dx \int_{\mu_{N+1}^L + L^{-a}}^{E_0} dy \frac{\tilde{\gamma}(x, y)}{(y - x)^2} - \tilde{\gamma}(E, E) \ln(\mu_{N+1}^L - \lambda_N^L + 2L^{-a}) \right| \\ &= \left| \int_0^{\lambda_N^L - L^{-a}} dx \int_{\mu_{N+1}^L + L^{-a}}^{E_0} dy \left(\tilde{\gamma}(x, y) - \tilde{\gamma}(E, E) \right) \left(\frac{1}{y - x} \right)^2 \right| + O(1) \end{aligned} \quad (2.65)$$

as $L \rightarrow \infty$. Now, Lemma 2.19 provides continuity of $\tilde{\gamma}$ and by Lemma 2.13 λ_N^L and μ_{N+1}^L converge to E . Thus, given an $\epsilon > 0$ there exists a function $h : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that $\lim_{\epsilon \searrow 0} h(\epsilon) = \infty$ and

$$(2.65) \leq \epsilon |\ln(\mu_{N+1}^L - \lambda_N^L + 2L^{-a})| + h(\epsilon). \quad (2.66)$$

Now, assumption (2.26) gives

$$\limsup_{L \rightarrow \infty} \frac{\epsilon |\ln(\mu_{N+1}^L - \lambda_N^L + 2L^{-a})| + h(\epsilon)}{\ln L} \leq a\epsilon. \quad (2.67)$$

Since ϵ was arbitrary, this yields

$$\begin{aligned} \text{l.h.s. of (2.63)} &= \tilde{\gamma}(E, E) |\ln(\mu_{N+1}^L - \lambda_N^L + 2L^{-a})| + o(\ln L) \\ &= a\tilde{\gamma}(E, E) \ln L + o(\ln L), \end{aligned} \quad (2.68)$$

as $L \rightarrow \infty$, where the last line follows from assumption (2.26). \square

As already mentioned before, the exponent $\tilde{\gamma}(E, E)$ admits a scattering theoretic interpretation.

Lemma 2.22. *Let $E > 0$. Set $\tilde{\gamma}(E) := \tilde{\gamma}(E, E)$. Then,*

$$\tilde{\gamma}(E) = \|T_E\|_{HS}^2, \quad (2.69)$$

where HS denotes the Hilbert-Schmidt norm on the corresponding fibre Hilbert space, which is in our case $L^2(S^{d-1})$. Here, S^{d-1} denotes the d -dimensional sphere.

Proof. The lemma follows from [Küt14, Cor. 9.12] or [GKMO14, Cor. 4.32], which are valid here for all $E > 0$ due to Lemma 2.19. \square

Proof of Theorem 2.6. Recalling equation (2.40), Lemma 2.12, Lemma 2.16, equation (2.58) and Lemma 2.21 we obtain for all $0 < a < 1$

$$-\ln |\mathcal{S}_L^N| \geq a \frac{\tilde{\gamma}(E)}{2} \ln L + o(\ln L), \quad (2.70)$$

as $L \rightarrow \infty$. Therefore, for all $0 < a < 1$

$$\limsup_{L \rightarrow \infty} \frac{\ln |\mathcal{S}_L^N|}{\ln L} \leq -a \frac{\tilde{\gamma}(E)}{2}. \quad (2.71)$$

This proves Theorem 2.6 because a was chosen arbitrary subject to $0 < a < 1$. \square

3. An Application of the Helffer-Sjöstrand Formula: Proof of Lemma 2.16

Since Lemma 2.16 is valid in more general settings including background potentials and unbounded perturbations V , we state Lemma 2.16 under weaker assumptions.

Lemma 2.23 (An application of the Helffer-Sjöstrand formula). *Here, we assume **(A)** and additionally*

$$V \in L^2(\mathbb{R}^d) \quad (2.72)$$

with subexponential decay at infinity, i.e.

$$\exists L_0 > 0, \theta > 1 \text{ such that } |V(x)| \leq e^{-\log(|x|_2)^\theta} \text{ for } |x|_2 \geq L_0. \quad (2.73)$$

Let $0 < a < 1$ and χ_L^\pm be the associated smooth cut-off functions from Definition 2.14. Then, we obtain

$$\int_{\mathbb{R}^2} \frac{d\mu_L(x, y)}{(y - x)^2} \chi_L^-(x) \chi_L^+(y) = \int_{\mathbb{R}^2} \frac{d\mu(x, y)}{(y - x)^2} \chi_L^-(x) \chi_L^+(y) + o(1), \quad (2.74)$$

as $L \rightarrow \infty$.

Remark 2.24. We do not claim that the assumptions on V in Lemma 2.23 are optimal and we do not claim that the following proof is elegant.

Proof. First note that $1/x^2 = \int_0^\infty dt t e^{-tx}$. Thus, using Fubini's theorem we can decouple the x and y integration and rewrite

$$\int_{\mathbb{R}^2} \frac{d\mu_L(x, y)}{(y - x)^2} \chi_L^-(x) \chi_L^+(y) = \int_0^\infty dt t \int_{\mathbb{R}^2} d\mu_L(x, y) e^{-t(y-x)} \chi_L^-(x) \chi_L^+(y). \quad (2.75)$$

Moreover,

$$\begin{aligned} & \int_0^\infty dt t \int_{\mathbb{R}^2} d\mu_L(x, y) e^{-t(y-x)} \chi_L^-(x) \chi_L^+(y) \\ &= \int_0^\infty dt t \text{tr} \left\{ \sqrt{V} e^{t(H_L - E_L)} \chi_L^-(H_L) V e^{-t(H'_L - E_L)} \chi_L^+(H'_L) \sqrt{V} \right\}, \end{aligned} \quad (2.76)$$

where

$$E_L := \frac{\mu_{N+1}^L + \lambda_N^L}{2}. \quad (2.77)$$

We define the abbreviations

$$g_L^t(x) := \chi_L^-(x) e^{t(x-E_L)} \quad \text{and} \quad f_L^t(x) := \chi_L^+(x) e^{-t(x-E_L)} \quad (2.78)$$

for every $x \in \mathbb{R}$ and $t \geq 0$ so that Lemma 2.23 can be reformulated as

$$\int_0^\infty dt t K_L(t) = o(1) \quad (2.79)$$

as $L \rightarrow \infty$ with

$$K_L(t) := \text{tr} \left\{ \sqrt{V} g_L^t(H_L) V f_L^t(H'_L) \sqrt{V} \right\} - \text{tr} \left\{ \sqrt{V} g_L^t(H) V f_L^t(H') \sqrt{V} \right\}. \quad (2.80)$$

We use the cyclicity of the trace and estimate the modulus of (2.80) according to $|K_L(t)| \leq |K_L^{(1)}(t)| + |K_L^{(2)}(t)|$, where

$$K_L^{(1)}(t) := \text{tr} \left\{ V f_L^t(H') V \left(g_L^t(H_L) - g_L^t(H) \right) \right\}, \quad (2.81)$$

$$K_L^{(2)}(t) := \text{tr} \left\{ \left(f_L^t(H'_L) - f_L^t(H') \right) V g_L^t(H_L) V \right\}. \quad (2.82)$$

Note that we did not assume V to be bounded. Thus, in order to apply the cyclicity of the trace in (2.81) and (2.82) we use that the operators $\sqrt{V} h_L^t(H_{(L)}^{(1)}) \sqrt{V}$ are trace class due to Remark 2.26 below, where the function h_L^t stands for one of the functions defined in (2.78).

Since both $K_L^{(1)}$ and $K_L^{(2)}$ can be estimated in the very same way, we will demonstrate the argument for $K_L^{(2)}$ only. Our main technical tool is the Helffer-Sjöstrand formula, see e.g. [HS00, Chap. IX] or [Küt14, Chap. 5], according to which

$$f_L^t(H'_L) - f_L^t(H') = \frac{1}{2\pi} \int_{\mathbb{C}} dz (\partial_{\bar{z}} \tilde{f}_L^t(z)) \left(\frac{1}{H'_L - z} - \frac{1}{H' - z} \right), \quad (2.83)$$

where we note that the above integral is norm convergent. Here, $z := x + iy$, $\partial_{\bar{z}} := \partial_x + i\partial_y$, $dz := dx dy$ and $\tilde{f}_L^t \in C_c^2(\mathbb{C})$ is an almost analytic extension of f_L^t to the complex plane. The latter can be chosen as

$$\tilde{f}_L^t(z) := \xi(z) \sum_{k=0}^n \frac{(iy)^k}{k!} \frac{d^k f_L^t}{dx^k}(x) \quad (2.84)$$

for some $n \in \mathbb{N}$ and some $\xi \in C_c^\infty(\mathbb{C})$ with $\xi(z) = 1$ for all $z \in \text{supp } f_L^t \times [-1, 1]$, $\xi(z) = 0$ for all z such that $\text{dist}_{\mathbb{C}}(z, \text{supp } f_L^t) \geq 3$ and $\xi(z) \in [0, 1]$ otherwise. We will assume $n \geq 2$ below. Since $\text{supp } f_L^t = [0, E_0 + 1]$, the function ξ can be chosen independently of L and t , and such that $\|\xi\|_\infty = 1$ and $\|\xi'\|_\infty < 1$. For later purpose we introduce the function $h := \sum_{k=0}^{n+1} \left| \frac{d^k f_L^t}{dx^k} \right| \in C_c(\mathbb{R})$ and infer the existence of a constant $C \in (0, \infty)$, which is independent of L and t , such that

$$|\partial_{\bar{z}} \tilde{f}_L^t(z)| \leq C|y|^n h(x) \quad (2.85)$$

for all $z \in \mathbb{C}$. Furthermore, the bound (2.54) implies the estimate

$$\left| \frac{d^k f_L^t}{dx^k}(x) \right| \leq L^{ak} \sum_{\kappa=0}^k \binom{k}{\kappa} \left(\frac{t}{L^a} \right)^\kappa c_{k-\kappa} 1_{[\mu_{N+1}^L, E_0+1]}(x) \quad (2.86)$$

for every $t \geq 0$, $L \geq 1$, $x \in \mathbb{R}$ and the constants $c_{k-\kappa}$ are the ones from (2.54). Hence, we conclude the existence of a polynomial Q_n over \mathbb{R} of degree $n+1$ with non-negative coefficients such that

$$0 \leq h(x) \leq Q_n(t/L^a) L^{a(n+1)} 1_{[\mu_{N+1}^L, E_0+1]}(x). \quad (2.87)$$

We will split the contribution of (2.83) in (2.82) into two parts. Accordingly, we define for $\epsilon \in (0, 1-a)$

$$D_L^<(t) := \frac{1}{2\pi} \int_{|y| \leq L^{-1+\epsilon}} dz (\partial_{\bar{z}} \tilde{f}_L^t(z)) \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right] \quad (2.88)$$

and

$$D_L^>(t) := \frac{1}{2\pi} \int_{|y| > L^{-1+\epsilon}} dz (\partial_{\bar{z}} \tilde{f}_L^t(z)) \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right]. \quad (2.89)$$

The integral in the Helffer-Sjöstrand formula is norm convergent and due to the assumptions on the potential the operator $Vg_L^t(H_L)V$ is trace class by Lemma 2.25. Hence, we interchange the integral and the trace to estimate

$$\begin{aligned} & |\text{tr}\{D_L^<(t)Vg_L^t(H_L)V\}| \\ & \leq \frac{1}{2\pi} \int_{|y| \leq L^{-1+\epsilon}} dz |\partial_{\bar{z}} \tilde{f}_L^t(z)| \text{tr}\{Vg_L^t(H_L)V\} \left\| \frac{1}{H'_L - z} - \frac{1}{H' - z} \right\|. \end{aligned} \quad (2.90)$$

The estimates (2.85) and (2.87) imply

$$\begin{aligned} (2.90) & \leq \text{tr}\{Vg_L^t(H_L)V\} \frac{C}{\pi} \int_{|y| \leq L^{-1+\epsilon}} dz |y|^{n-1} h(x) \\ & = \text{tr}\{Vg_L^t(H_L)V\} \frac{2C}{\pi n} L^{n(-1+\epsilon)} \int_{\mathbb{R}} dx h(x) \\ & \leq \text{tr}\{Vg_L^t(H_L)V\} C_< Q_n(t/L^a) L^{a+n(-1+\epsilon+a)}, \end{aligned} \quad (2.91)$$

where $C_<$ depends on E_0 only.

To estimate the term $D_L^>(t)$, we interchange the integral and the trace as before to obtain

$$\begin{aligned} & |\text{tr}\{D_L^>(t)Vg_L^t(H_L)V\}| \\ & \leq \frac{C}{2\pi} \int_{|y| > L^{-1+\epsilon}} dz |y|^n h(x) \left| \text{tr} \left\{ \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right] Vg_L^t(H_L)V \right\} \right|. \end{aligned} \quad (2.92)$$

Now, we rewrite the identity on \mathbb{R}^d according to

$$1_{\mathbb{R}^d} = 1_{\Lambda_{L/2}} + (1_{\mathbb{R}^d} - 1_{\Lambda_{L/2}}) =: 1_+^L + 1_-^L \quad (2.93)$$

and insert this into (2.92) according to

$$\frac{C}{2\pi} \int_{|y| > L^{-1+\epsilon}} dz |y|^n h(x) \left| \text{tr} \left\{ (1_+^L + 1_-^L) \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right] (1_+^L + 1_-^L) Vg_L^t(H_L)V \right\} \right|. \quad (2.94)$$

Using the triangle inequality, we estimate (2.92) from above by four terms, which we denote by A_{++}^L , A_{+-}^L , A_{-+}^L and A_{--}^L , where the latter indices apparently refer to the

decomposition (2.93) of the identity. We start with

$$\begin{aligned} A_{++}^L &:= \frac{C}{2\pi} \int_{|y|>L^{-1+\epsilon}} dz |y|^n h(x) \left| \operatorname{tr} \left\{ 1_+^L \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right] 1_+^L V g_L^t(H_L) V \right\} \right| \\ &\leq \frac{C}{2\pi} \int_{|y|>L^{-1+\epsilon}} dz |y|^n h(x) \operatorname{tr} \{ V g_L^t(H_L) V \} \\ &\quad \times \left\| 1_{\Lambda_{L/2}} \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right] 1_{\Lambda_{L/2}} \right\|. \end{aligned} \quad (2.95)$$

We estimate the norm of the difference of the resolvents with the help of the geometric resolvent inequality – see e.g. [Sto01, Lem. 2.5.2] or [Küt14, Lem. 5.3] –, and the fact that $\xi(z) = 0$ if $\operatorname{dist}(z, \mathbb{R}) \geq 3$. This provides for $L > 3$

$$\begin{aligned} (2.95) &\leq \operatorname{tr} \{ V g_L^t(H_L) V \} \\ &\quad \times \frac{CC_{\text{gre}}}{2\pi} \int_{|y|>L^{-1+\epsilon}} dz h(x) |y|^n \left\| 1_{\Lambda_{L/2}} \frac{1}{H'_L - z} 1_{\delta\Lambda_L} \right\| \left\| 1_{\delta\Lambda_L} \frac{1}{H' - z} 1_{\Lambda_{L/2}} \right\| \\ &\leq \operatorname{tr} \{ V g_L^t(H_L) V \} \frac{CC_{\text{gre}}}{2\pi} \int_{|y|\in[L^{-1+\epsilon}, 3]} dz h(x) |y|^{n-1} \left\| 1_{\delta\Lambda_L} \frac{1}{H' - z} 1_{\Lambda_{L/2}} \right\|, \end{aligned} \quad (2.96)$$

where $\delta\Lambda_L := \Lambda_L \setminus \Lambda_{L-1}$ and the constant $C_{\text{gre}} < \infty$ depends only on E_0 , the space dimension and the potentials V_0 and V . The operator norm in the last line of (2.96) is bounded by a Combes-Thomas estimate for operator kernels of resolvents, see e.g. [GK03, Thm. 1],

$$\left\| 1_{\Gamma} \frac{1}{H' - z} 1_{\Gamma'} \right\| \leq \frac{C_{\text{ct}}}{|y|} e^{-c_{\text{ct}} \operatorname{dist}(\Gamma, \Gamma') |y|}. \quad (2.97)$$

It holds for all cubes $\Gamma, \Gamma' \subset \mathbb{R}^d$ of side length 1 and all z in some bounded subset of \mathbb{C} , which we choose as $\operatorname{supp}(h) \times [-3, 3]$. The constants $C_{\text{ct}}, c_{\text{ct}} \in (0, \infty)$ in (2.97) can be chosen to depend only on E_0 , the space dimension and the potentials V_0 and V . Now, we assume $n \geq 2$, cover $\Lambda_{L/2}$ and $\delta\Lambda_L$ by unit cubes and apply the bounds (2.97) and (2.87) to (2.96). In this way we infer the existence of a constant $\tilde{C}_> \in (0, \infty)$, which is independent of L and t , such that

$$\begin{aligned} (2.96) &\leq \operatorname{tr} \{ (V g_L^t(H_L) V) \tilde{C}_> (E_0 + 1) Q_n(t/L^a) L^{2d+a(n+1)} \int_{L^{-1+\epsilon}}^3 dy |y|^{n-2} e^{-cLy} \\ &\leq \operatorname{tr} \{ V g_L^t(H_L) V \} C_{1>} Q_n(t/L^a) L^{2d+a(n+1)} e^{-cLy} \end{aligned} \quad (2.98)$$

for all $t \geq 0$ and all $L > 1$, and c depends only on c_{ct} and Λ_1 and $C_{1>}$ depends on n , C_{CT} and E_0 . We continue with A_{-+} . Using the cyclicity of the trace, we compute

$$\begin{aligned} A_{-+} &= \frac{C}{2\pi} \int_{|y|>L^{-1+\epsilon}} dz |y|^n h(x) \left| \operatorname{tr} \left\{ 1_-^L \left[\frac{1}{H'_L - z} - \frac{1}{H' - z} \right] 1_+^L V g_L^t(H_L) V \right\} \right| \\ &\leq \frac{C}{\pi} \int_{|y|>L^{-1+\epsilon}} dz |y|^{n-1} h(x) \|V 1_{\Lambda_{L/2}^c}\|_{\infty} \operatorname{tr} \{ |V g_L^t(H_L)| \} \\ &\leq C_{2>} e^{-(\log(\tilde{c}L))^{\theta}} Q_n(t/L^a) L^{a(n+1)} \operatorname{tr} \{ |V g_L^t(H_L)| \} \end{aligned} \quad (2.99)$$

for $L \geq L_0$, where we used the subexponential decay of the potential V at infinity, and the constant $C_{2>} > 0$ depends on E_0 and \tilde{c} on Λ_1 only. We estimate A_{+-} along the same

line. For A_{--} we estimate

$$\begin{aligned} A_{--} &\leq \frac{C}{\pi} \int_{|y|>L^{-1+\epsilon}} dz |y|^{n-1} h(x) \|\sqrt{V} 1_{\Lambda_{L/2}^c}\|_\infty^2 \operatorname{tr} \left\{ \sqrt{V} g_L^t(H_L) \sqrt{V} \right\} \\ &\leq C_{3>} e^{-(\log(\tilde{c}L))^\theta} Q_n(t/L^a) L^{a(n+1)} \operatorname{tr} \left\{ \sqrt{V} g_L^t(H_L) \sqrt{V} \right\}. \end{aligned} \quad (2.100)$$

Here, the constant $C_{3>}$ depends on E_0 and Λ_1 only.

Now, Lemma 2.25 and Remark 2.26 below imply

$$\begin{aligned} \int_0^\infty dt t Q_n(t/L^a) \operatorname{tr} \left\{ V g_L^t(H_L) V \right\} &\leq C_n L^{2a}, \\ \int_0^\infty dt t Q_n(t/L^a) \operatorname{tr} \left\{ |V g_L^t(H_L)| \right\} &\leq C_n L^{2a}, \\ \int_0^\infty dt t Q_n(t/L^a) \operatorname{tr} \left\{ \sqrt{V} g_L^t(H_L) \sqrt{V} \right\} &\leq C_n L^{2a} \end{aligned} \quad (2.101)$$

with some constant $C_n > 0$ depending on n . This together with the bounds (2.91), (2.98), (2.99) and (2.100) yield a constant $C \equiv C_{n,E_0,V_0,V,\Lambda_1} > 0$, depending on n, E_0, V_0, V and Λ_1 , such that

$$\int_0^\infty dt t |K_L^{(2)}(t)| \leq C \left(L^{3a+n(-1+\epsilon+a)} + L^{2d+a(n+3)} e^{-c_{ct} L^\epsilon} + e^{-(\log(\tilde{c}L))^\theta} L^{a(n+3)} \right). \quad (2.102)$$

We recall that $0 < \epsilon < 1 - a$ and $\theta > 1$. Therefore, we can choose n large enough as to ensure

$$3a + n(-1 + a + \epsilon) < 0 \quad (2.103)$$

and conclude that

$$\int_0^\infty dt t K_L^{(2)}(t) = o(1) \quad (2.104)$$

as $L \rightarrow \infty$. The same holds true for $K_L^{(1)}$ by an analogous argument. Thus, we have shown (2.79). \square

Lemma 2.25. *Let $h_L^t \in \{f_L^t, g_L^t\}$, where the latter are defined in (2.78). We assume here $V \in L^2(\mathbb{R}^d)$ with subexponential decay of V at infinity as in Lemma 2.23. Then, there exists some constant $C > 0$ such that for every $L > 1$ and every $t \geq 0$ we have*

$$\operatorname{tr} \left\{ V h_L^t(H_{(L)}^{(\prime)}) V \right\} \leq C e^{-tL^{-a}/2} \quad \text{and} \quad \operatorname{tr} \left\{ |V h_L^t(H_{(L)}^{(\prime)})| \right\} \leq C e^{-tL^{-a}/2}. \quad (2.105)$$

Remark 2.26. The assumptions of Lemma 2.23 on the perturbation V , i.e. $V \in L^2(\mathbb{R}^d)$, $V \geq 0$ with subexponential decay at infinity provide also $\sqrt{V} \in L^2(\mathbb{R}^d)$. Thus, we apply Lemma 2.25 and obtain that $\sqrt{V} h_L^t(H_{(L)}^{(\prime)}) \sqrt{V}$ is a trace-class operator and the latter bounds hold.

Proof. The definition of E_L implies that $|E_L - \lambda_N^L + \frac{1}{2}L^{-a}| \geq \frac{1}{2}L^{-a}$ and therefore

$$g_L^t(H_{(L)}^{(\prime)}) \leq e^{-tL^{-a}/2} 1_{(\inf \sigma(H_{(L)}^{(\prime)}) - 1, \lambda_N^L)}(H_{(L)}^{(\prime)}) \leq e^{-tL^{-a}/2} 1_I(H_{(L)}^{(\prime)}), \quad (2.106)$$

where I is some bounded interval. The same holds for f_L^t . Moreover, due to the quite explicit representation of the integral kernel of $e^{-tH_{(L)}^{(\prime)}}$ given in [BHL00, Thm. 6.1] we know the following inequality of integral kernels

$$0 \leq e^{-tH_L^{(\prime)}}(x, y) \leq e^{-tH^{(\prime)}}(x, y) \quad (2.107)$$

for all $x, y \in \Lambda_L$, $t \geq 0$.

For the first assertion, we estimate

$$\begin{aligned} \text{tr}\{Vh_L^t(H_{(L)}^{(\prime)})V\} &\leq e^{-tL^{-a}/2} \text{tr}\{V1_I(H_{(L)}^{(\prime)})V\} \\ &\leq e^{-tL^{-a}/2} e^{\sup I} \text{tr}\{Ve^{-H_{(L)}^{(\prime)}}V\} \\ &\leq e^{-tL^{-a}/2} e^{\sup I} \text{tr}\{Ve^{-H^{(\prime)}}V\} \end{aligned} \quad (2.108)$$

The last inequality follows from the integral-kernel inequality (2.107) and computing the trace as the square of the Hilbert-Schmidt norm of the operator $e^{-H_{(L)}^{(\prime)}/2}V$. The assumption $V \in L^2(\mathbb{R}^d)$ implies that $e^{-H^{(\prime)}/2}V$ is a Hilbert-Schmidt operator, see [BHL00, Thm. 6.1], and the assertion follows.

For the second statement, we note that for arbitrary trace class operators $0 \leq A \leq B$ we obtain the inequality $\text{tr}\sqrt{A} \leq \text{tr}\sqrt{B}$. Thus, we compute

$$\begin{aligned} \text{tr}\left\{|Vh_L^t(H_{(L)}^{(\prime)})|\right\} &= \text{tr}\left\{\sqrt{Vh_L^t(H_{(L)}^{(\prime)})h_L^t(H_{(L)}^{(\prime)})V}\right\} \\ &\leq \text{tr}\left\{\sqrt{V1_I(H_{(L)}^{(\prime)})e^{-tL^{-a}}V}\right\} \\ &\leq e^{-tL^{-a}/2} e^{\sup I} \text{tr}\{|Ve^{-H_{(L)}^{(\prime)}}|\}. \end{aligned} \quad (2.109)$$

In case of the infinite-volume operators the assumption $V \in L^2(\mathbb{R}^d)$ with subexponential decay at infinity yields that the operator $Ve^{-H^{(\prime)}}$ is trace class, see [Sim82, Thm. B.9.2]. Essentially, the case of the finite-volume operators follows also from [Sim82, Sct. B.9] and inequality (2.107). To see this, we choose $\delta > 0$ and introduce the weight function $r(x) := (1 + |x|^2)^{\delta/2}$. Using the Cauchy-Schwarz inequality for traces we estimate

$$\begin{aligned} \text{tr}\{|Ve^{-H_{(L)}^{(\prime)}}|\} &= \text{tr}\left\{|Ve^{-H_{(L)}^{(\prime)}/2}rr^{-1}e^{-H_{(L)}^{(\prime)}/2}|\right\} \\ &\leq \|Ve^{-H_{(L)}^{(\prime)}/2}r\|_{\text{HS}}\|r^{-1}e^{-H_{(L)}^{(\prime)}/2}\|_{\text{HS}} \\ &\leq \|Ve^{-H_{(L)}^{(\prime)}/2}r\|_{\text{HS}}\|r^{-1}e^{-H_{(L)}^{(\prime)}/2}\|_{\text{HS}}, \end{aligned} \quad (2.110)$$

where we used (2.107) in the last line. For $\delta > d/2$, [Sim82, Thm. B.9.1] provides $\|r^{-1}e^{-H_{(L)}^{(\prime)}/2}\|_{\text{HS}} < \infty$. Moreover, we rewrite $\|Ve^{-H_{(L)}^{(\prime)}/2}r\|_{\text{HS}} = \|Vrr^{-1}e^{-H_{(L)}^{(\prime)}/2}r\|_{\text{HS}}$. Due to the subexponential decay of V we have $Vr \in L^2(\mathbb{R}^d)$ and by [Sim82, Thm. B.6.1] $(r^{-1}e^{-H_{(L)}^{(\prime)}/2}r)^* : L^2(\mathbb{R}^d) \rightarrow L^\infty(\mathbb{R}^d)$ is bounded. Hence, we use [Sim82, Prop. B.9.4] to obtain that $Vrr^{-1}e^{-H_{(L)}^{(\prime)}/2}r$ is a Hilbert-Schmidt operator. Alternatively, one may show directly square integrability of the integral kernel of the latter operator using suitable pointwise bounds on the integral kernel of $e^{-H^{(\prime)}}$. \square

CHAPTER 3

The Ground-State Overlap for Dirac- δ Perturbations

In the last chapter we saw upper bounds on the ground-state overlap S_L^N for quite general pairs of Schrödinger operators. Here, using different tools we prove the exact asymptotics for the toy model of a Dirac- δ perturbation in three space dimensions, which we define in Section 2 below. We begin with an exact representation of the ground-state overlap in terms of the eigenvalues valid for rank-one perturbations, which might be interesting on its own and is at the heart of the main result in this chapter, Theorem 3.17.

1. Product Representation for Rank-One Perturbations

Let \mathcal{H} be a separable infinite-dimensional Hilbert space and A be a self-adjoint compact operator acting on \mathcal{H} . Moreover, we assume $A \geq 0$ and $\ker(A) = \{0\}$. We define for some $0 \neq \phi \in \mathcal{H}$

$$B := A + |\phi\rangle\langle\phi|. \quad (3.1)$$

We write $\alpha_1 \geq \alpha_2 \geq \dots$ and $\beta_1 \geq \beta_2 \geq \dots$ for the non-increasing sequences of the eigenvalues of A , respectively B , and denote by $(\varphi_j)_{j \in \mathbb{N}}$ and $(\psi_k)_{k \in \mathbb{N}}$ the corresponding normalised eigenvectors. Since A and B differ by a rank-one perturbation, the min-max theorem implies that the eigenvalues interlace. We assume in addition a strict interlacing property of the eigenvalues

$$\beta_1 > \alpha_1 > \beta_2 > \alpha_2 > \dots. \quad (3.2)$$

This immediately implies $\beta_k \neq \alpha_j$ for all non-zero eigenvalues of A and B . Furthermore, the above gives cyclicity of ϕ :

Lemma 3.1. *Under condition (3.2), we obtain that ϕ is cyclic with respect to the operator A . In particular, for all $j \in \mathbb{N}$*

$$\langle \varphi_j, \phi \rangle \neq 0. \quad (3.3)$$

Proof. Let $W := \overline{\text{span}\{A^n\phi : n \in \mathbb{N}_0\}}$. Then W reduces A , i.e. $AW \subseteq W$ and $AW^\perp \subseteq W^\perp$. Now, assume ϕ is not cyclic for A . Then, $W^\perp \neq \{0\}$ and there exists an eigenvector $\varphi_n \in W^\perp$ of A such that $A\varphi_n = E\varphi_n$ and $\langle \varphi_n, \phi \rangle = 0$. This implies E is also an eigenvalue of B , a contradiction to (3.2). \square

Assumption (3.2) is not necessary but simplifies notation and computations. In the general case one has to consider cyclic subspaces. But in our applications the interlacing condition (3.2) will be satisfied, therefore, we assume it.

We continue with a property of the sum of the differences of the n th eigenvalues.

Lemma 3.2. *Let (3.2) be satisfied. Then, the eigenvalues of the operators A and B satisfy*

$$\sum_{l=1}^{\infty} (\beta_l - \alpha_l) = \|\phi\|^2 < \infty. \quad (3.4)$$

Proof. For $\lambda \in \mathbb{R}$ we define the operator

$$A(\lambda) := A + \lambda|\phi\rangle\langle\phi| \quad (3.5)$$

and write $\alpha_l(\lambda)$ for the l th eigenvalue counted from above and $\varphi_l(\lambda)$ for the corresponding eigenvector. Moreover, we remark that $\alpha_l(1)$ and $\varphi_l(1)$ correspond to β_l and ψ_l . Assumption (3.2) and the definite sign of the perturbation imply that the eigenvalues of $A(\lambda)$ are non-degenerate for all $\lambda \in [0, 1]$. Thus, standard results, see [RS78, Chap. XII], give differentiability of the eigenvalues for all $\lambda \in (0, 1)$ and we apply the Feynman-Hellmann theorem, see e.g. [IZ88], to deduce for all $l \in \mathbb{N}$ and $\lambda \in (0, 1)$

$$\alpha'_l(\lambda) = |\langle\varphi_l(\lambda), \phi\rangle|^2. \quad (3.6)$$

Hence, we compute

$$\begin{aligned} \sum_{l=1}^{\infty} (\beta_l - \alpha_l) &= \sum_{l=1}^{\infty} \int_0^1 d\lambda \alpha'_l(\lambda) \\ &= \sum_{l=1}^{\infty} \int_0^1 d\lambda |\langle\varphi_l(\lambda), \phi\rangle|^2 = \int_0^1 d\lambda \sum_{l=1}^{\infty} |\langle\varphi_l(\lambda), \phi\rangle|^2, \end{aligned} \quad (3.7)$$

where we used Fubini's theorem in the last line. Since the vectors $(\varphi_l(\lambda))_{l \in \mathbb{N}}$ form an ONB of \mathcal{H} , we obtain

$$(3.7) = \int_0^1 d\lambda \|\phi\|^2 < \infty. \quad (3.8)$$

□

The above lemma is also valid without the assumption (3.2). In this case, one has to include possible degenerate eigenvalues of $A(\lambda)$ in the proof. This may cause a discrete set where some of the ordered eigenvalues are not differentiable.

The main result of this section is the following product representation of the ground-state overlap.

Theorem 3.3. *Let $N \in \mathbb{N}$. We assume condition (3.2) to hold. Then,*

$$\left| \det \left(\langle \varphi_j, \psi_k \rangle \right)_{1 \leq j, k \leq N} \right|^2 = \prod_{j=1}^N \prod_{k=N+1}^{\infty} \frac{|\beta_k - \alpha_j| |\alpha_k - \beta_j|}{|\alpha_k - \alpha_j| |\beta_k - \beta_j|}. \quad (3.9)$$

Proof of Theorem 3.3. We use the eigenvalue equations, i.e. the identity (2.48), and assumption (3.2) to obtain for all $j, k \in \mathbb{N}$

$$\langle \varphi_j, \psi_k \rangle = \frac{\langle \varphi_j, \phi \rangle \langle \phi, \psi_k \rangle}{\beta_k - \alpha_j}. \quad (3.10)$$

Hence, the multi-linearity of the determinant implies

$$\begin{aligned} &\left| \det \left(\langle \varphi_j, \psi_k \rangle \right)_{1 \leq j, k \leq N} \right|^2 \\ &= \left| \det \left(\frac{\langle \varphi_j, \phi \rangle \langle \phi, \psi_k \rangle}{\beta_k - \alpha_j} \right)_{1 \leq j, k \leq N} \right|^2 \\ &= \prod_{j=1}^N \prod_{k=1}^N |\langle \varphi_j, \phi \rangle \langle \phi, \psi_k \rangle|^2 \left| \det \left(\frac{1}{\beta_k - \alpha_j} \right)_{1 \leq j, k \leq N} \right|^2. \end{aligned} \quad (3.11)$$

Now, the remaining determinant can be computed explicitly. We use the Cauchy determinant formula to evaluate this, see Appendix B or [Wey13, Lem. 7.6.A], and we end up with

$$(3.11) = \prod_{j=1}^N \prod_{k=1}^N |\langle \varphi_j, \phi \rangle \langle \phi, \psi_k \rangle|^2 \frac{\prod_{j,k=1, j \neq k}^N |\beta_k - \beta_j| |\alpha_j - \alpha_k|}{\prod_{j,k=1}^N |\beta_k - \alpha_j|^2}. \quad (3.12)$$

Corollary 3.5 below yields

$$\begin{aligned} (3.12) &= \prod_{k=1}^N \prod_{\substack{l=1 \\ l \neq k}}^{\infty} \frac{|\alpha_l - \beta_k|}{|\beta_l - \beta_k|} \prod_{j=1}^N \prod_{\substack{l=1 \\ l \neq j}}^{\infty} \frac{|\beta_l - \alpha_j|}{|\alpha_l - \alpha_j|} \prod_{\substack{j,k=1 \\ j \neq k}}^N \frac{|\beta_k - \beta_j| |\alpha_j - \alpha_k|}{|\beta_k - \alpha_j|^2} \\ &= \prod_{j=1}^N \prod_{k=N+1}^{\infty} \frac{|\beta_k - \alpha_j| |\alpha_k - \beta_j|}{|\beta_k - \beta_j| |\alpha_j - \alpha_k|}. \end{aligned} \quad (3.13)$$

This gives the claim, where we remark that by the estimate (3.4) all infinite products in the latter converge absolutely. \square

To complete the proof, we continue with computing the residue of the resolvents. We do this using the following product representation of the resolvents which is valid for rank-one perturbations.

Lemma 3.4. *We assume (3.2). Then, there exist $a, b \in \mathbb{R}$ with $ab = -1$ such that*

(i) *for all $z \in \varrho(A)$*

$$\langle \phi, \frac{1}{A-z} \phi \rangle + 1 = a \prod_{k=1}^{\infty} \frac{\beta_k - z}{\alpha_k - z}, \quad (3.14)$$

(ii) *for all $z \in \varrho(B)$*

$$\langle \phi, \frac{1}{B-z} \phi \rangle - 1 = b \prod_{n=1}^{\infty} \frac{\alpha_n - z}{\beta_n - z}. \quad (3.15)$$

Corollary 3.5. *Let $j, k \in \mathbb{N}$. Under the assumption (3.2).*

$$|\langle \varphi_j, \phi \rangle \langle \psi_k, \phi \rangle|^2 = |\beta_j - \alpha_j| |\alpha_k - \beta_k| \prod_{\substack{l=1 \\ l \neq j}}^{\infty} \frac{|\beta_l - \alpha_j|}{|\alpha_l - \alpha_j|} \prod_{\substack{l=1 \\ l \neq k}}^{\infty} \frac{|\alpha_l - \beta_k|}{|\beta_l - \beta_k|}. \quad (3.16)$$

Proof of Corollary 3.5. Using Lemma 3.4 we compute the residue of the resolvents

$$\begin{aligned} |\langle \varphi_j, \phi \rangle|^2 &= \lim_{z \rightarrow \alpha_j} (\alpha_j - z) \langle \phi, \frac{1}{A-z} \phi \rangle \\ &= \lim_{z \rightarrow \alpha_j} (\alpha_j - z) a \prod_{l=1}^{\infty} \frac{(\beta_l - z)}{(\alpha_l - z)} = a (\beta_j - \alpha_j) \prod_{\substack{l=1 \\ l \neq j}}^{\infty} \frac{(\beta_l - \alpha_j)}{(\alpha_l - \alpha_j)} \end{aligned} \quad (3.17)$$

and along the same line

$$|\langle \psi_k, \phi \rangle|^2 = b (\alpha_k - \beta_k) \prod_{\substack{l=1 \\ l \neq k}}^{\infty} \frac{(\alpha_l - \beta_k)}{(\beta_l - \beta_k)}. \quad (3.18)$$

Taking the absolute value and using $|ab| = 1$ give the result. \square

Proof of Lemma 3.4. First note that by the finiteness of (3.4) the sequences

$$\left(\prod_{k=1}^N \frac{\beta_k - z}{\alpha_k - z} \right)_{N \in \mathbb{N}} \quad \text{and} \quad \left(\prod_{n=1}^N \frac{\alpha_n - z}{\beta_n - z} \right)_{N \in \mathbb{N}} \quad (3.19)$$

converge locally uniformly for all $z \in \varrho(A) \cap \varrho(B)$, see [Kno96, Thm. 252]. Therefore, the limits

$$F(z) := \prod_{n=1}^{\infty} \frac{\alpha_n - z}{\beta_n - z} \quad \text{and} \quad G(z) := \prod_{k=1}^{\infty} \frac{\beta_k - z}{\alpha_k - z} \quad (3.20)$$

are well-defined analytic functions on $\varrho(A) \cap \varrho(B)$, which fulfil $FG = 1$. Due to the locally uniform convergence, the derivative of F satisfies

$$\begin{aligned} F'(z) &= \lim_{N \rightarrow \infty} \sum_{l=1}^N \prod_{\substack{n=1 \\ n \neq l}}^N \frac{\alpha_n - z}{\beta_n - z} \frac{d}{dz} \frac{\alpha_l - z}{\beta_l - z} \\ &= \lim_{N \rightarrow \infty} \sum_{l=1}^N \prod_{\substack{n=1 \\ n \neq l}}^N \frac{\alpha_n - z}{\beta_n - z} \frac{\alpha_l - \beta_l}{(\beta_l - z)^2} = F(z) \lim_{N \rightarrow \infty} \sum_{l=1}^N \left(\frac{1}{\beta_l - z} - \frac{1}{\alpha_l - z} \right) \end{aligned} \quad (3.21)$$

for all $z \in \varrho(A) \cap \varrho(B)$. We apply Lemma 3.6 below and obtain

$$(3.21) = -F(z) \left\langle \frac{1}{A - z} \phi, \frac{1}{B - z} \phi \right\rangle. \quad (3.22)$$

Now, the resolvent identity implies for all $z \in \varrho(A) \cap \varrho(B)$

$$\frac{1}{B - z} - \frac{1}{A - z} = -\frac{1}{A - z} \phi \left\langle \frac{1}{B - z} \phi, \cdot \right\rangle \quad (3.23)$$

which provides the equality

$$\frac{1}{A - z} \phi = \frac{1}{1 - \left\langle \frac{1}{B - z} \phi, \phi \right\rangle} \frac{1}{B - z} \phi. \quad (3.24)$$

Inserting this into (3.22), we see that F solves the differential equation

$$F'(E) = F(E) \frac{1}{\left\langle \phi, \frac{1}{B - E} \phi \right\rangle - 1} \left\langle \phi, \left(\frac{1}{B - E} \right)^2 \phi \right\rangle \quad (3.25)$$

at least for all $E \in \varrho(A) \cap \varrho(B) \cap \mathbb{R}$. On the other hand the resolvent of B is analytic in $\varrho(B)$ and the function $t \mapsto \left\langle \phi, \frac{1}{B - t} \phi \right\rangle - 1$, $t < 0$, solves the above ODE (3.25) as well.

Now, the general solution to this ODE is $f(t) = x_0 \exp \left(\int_{t_0}^t ds \frac{1}{\left\langle \phi, \frac{1}{B - s} \phi \right\rangle - 1} \left\langle \phi, \left(\frac{1}{B - s} \right)^2 \phi \right\rangle \right)$,

for some initial condition (t_0, x_0) . Note that the functions $t \mapsto F(t)$ and $t \mapsto \left\langle \phi, \frac{1}{B - t} \phi \right\rangle - 1$ are non-zero, thus $\left\langle \phi, \frac{1}{B - t} \phi \right\rangle - 1 = cF(t)$ for some $c \neq 0$. This and the identity theorem for analytic functions give the claim. Equation (3.14) follows from $F(z)G(z) = 1$ and the identity

$$\left(\left\langle \phi, \frac{1}{B - z} \phi \right\rangle - 1 \right) \left(\left\langle \phi, \frac{1}{A - z} \phi \right\rangle + 1 \right) = -1, \quad (3.26)$$

for all $z \in \varrho(A) \cap \varrho(B)$ which is a consequence of (3.23). \square

Lemma 3.6. *Let $z \in \varrho(A) \cap \varrho(B)$. Assume (3.2). Then, we obtain the following identity*

$$\lim_{N \rightarrow \infty} \sum_{l=1}^N \left(\frac{1}{\beta_l - z} - \frac{1}{\alpha_l - z} \right) = - \left\langle \frac{1}{A - \bar{z}} \phi, \frac{1}{B - z} \phi \right\rangle. \quad (3.27)$$

Let us point out that in the finite-dimensional case the above equality follows directly from the resolvent equation, (3.23). Nevertheless, the infinite-dimensional case is slightly more involved due to convergence issues.

Proof. For $\lambda \in \mathbb{R}$ we define the operator

$$A(\lambda) := A + \lambda |\phi\rangle\langle\phi| \quad (3.28)$$

and write $\alpha_l(\lambda)$ for the l th eigenvalue counted from above and $\varphi_l(\lambda)$ for the corresponding eigenvector. Following the proof of Lemma 3.2 we obtain differentiability of the $\alpha_l(\cdot)$ with

$$\alpha'_l(\lambda) = |\langle \varphi_l(\lambda), \phi \rangle|^2. \quad (3.29)$$

Hence, we compute for $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$

$$\begin{aligned} \lim_{N \rightarrow \infty} \sum_{l=1}^N \left(\frac{1}{\beta_l - z} - \frac{1}{\alpha_l - z} \right) &= - \lim_{N \rightarrow \infty} \sum_{l=1}^N \int_0^1 d\lambda \left(\frac{1}{\alpha_l(\lambda) - z} \right)^2 \alpha'_l(\lambda) \\ &= - \lim_{N \rightarrow \infty} \sum_{l=1}^N \int_0^1 d\lambda \left(\frac{1}{\alpha_l(\lambda) - z} \right)^2 |\langle \varphi_l(\lambda), \phi \rangle|^2. \end{aligned} \quad (3.30)$$

The eigenvalue equation implies

$$\begin{aligned} (3.30) &= - \lim_{N \rightarrow \infty} \sum_{l=1}^N \int_0^1 d\lambda \left\langle \frac{1}{A(\lambda) - \bar{z}} \phi, \varphi_l(\lambda) \right\rangle \left\langle \varphi_l(\lambda), \frac{1}{A(\lambda) - z} \phi \right\rangle \\ &= - \int_0^1 d\lambda \langle \phi, \left(\frac{1}{A(\lambda) - z} \right)^2 \phi \rangle, \end{aligned} \quad (3.31)$$

where we used Fubini's theorem to interchange the integral with the sum and the fact that the vectors $(\varphi_l(\lambda))_{l \in \mathbb{N}}$ form an ONB. The resolvent identity (3.23) implies

$$\frac{1}{A(\lambda) - z} \phi = \frac{1}{1 + \lambda \langle \phi, \frac{1}{A - z} \phi \rangle} \frac{1}{A - z} \phi. \quad (3.32)$$

Therefore, we continue

$$\begin{aligned} (3.31) &= - \int_0^1 d\lambda \langle \phi, \left(\frac{1}{A - z} \right)^2 \phi \rangle \left(\frac{1}{1 + \lambda \langle \phi, \frac{1}{A - z} \phi \rangle} \right)^2 \\ &= - \langle \phi, \left(\frac{1}{A - z} \right)^2 \phi \rangle \int_0^1 d\lambda \frac{d}{d\lambda} \left(\frac{1}{1 + \lambda \langle \phi, \frac{1}{A - z} \phi \rangle} \right) \frac{1}{\langle \phi, \frac{1}{A - z} \phi \rangle} \\ &= \frac{\langle \phi, \left(\frac{1}{A - z} \right)^2 \phi \rangle}{\langle \phi, \frac{1}{A - z} \phi \rangle} \left(1 - \left(\frac{1}{1 + \langle \phi, \frac{1}{A - z} \phi \rangle} \right) \right) \\ &= - \frac{\langle \phi, \left(\frac{1}{A - z} \right)^2 \phi \rangle}{1 + \langle \phi, \frac{1}{A - z} \phi \rangle}. \end{aligned} \quad (3.33)$$

Equation (3.32) with $\lambda = 1$ provides the assertion

$$(3.33) = -\left\langle \frac{1}{A - \bar{z}}\phi, \frac{1}{B - z}\phi \right\rangle. \quad (3.34)$$

We note that both sides of (3.27) are continuous within $\varrho(A) \cap \varrho(B)$. For the left hand side this follows from the finiteness of (3.4) and for the right hand side from the continuity of the resolvent. Therefore, we obtain the result for all $z \in \varrho(A) \cap \varrho(B)$. \square

2. Zero-range Interactions

In this section we define Dirac- δ perturbations for systems on $(0, \infty)$ and \mathbb{R}^3 , and for a given $L > 0$, we define its restrictions to the finite volume $(0, L)$ respectively to the ball $B_L(0)$ of radius L around the origin. Our definitions and notations are close to [AGHH05, Chap. 1].

We begin with the 3-dimensional case, i.e. let $d = 3$. Throughout this chapter we denote by $H = -\Delta$ the negative Laplacian on $L^2(\mathbb{R}^3)$ with $\text{dom}(-\Delta) = H^2(\mathbb{R}^3)$. Furthermore, we consider the operator

$$-\Delta_0 : C_c^\infty(\mathbb{R}^3 \setminus \{0\}) \rightarrow L^2(\mathbb{R}^3) \quad (3.35)$$

and observe that this operator has deficiency indices $(1, 1)$, see [AGHH05, Chap. 1]. Thus, we obtain a one-parameter family of self-adjoint extensions of $-\Delta_0$ which we call H_α and $-\infty < \alpha \leq \infty$. Each of these self-adjoint extensions H_α defines a negative Laplacian with a Dirac- δ perturbation located at the origin. For computations, we need a less abstract representation of the Dirac- δ perturbation. Therefore, we decompose the operators H and H_α with respect to angular momentum. Following [AGHH05, Chap. 1], there exists a unitary operator

$$U : L^2(\mathbb{R}^3) \rightarrow \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} \mathcal{H}^{\ell, m}, \quad (3.36)$$

where $\mathcal{H}^{\ell, m} = L^2((0, \infty))$, such that under this unitary U both operators H and H_α transform into

$$UH_{(\alpha)}U^* = \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} h_{(\alpha)}^\ell : \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} \mathcal{H}^{\ell, m} \rightarrow \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} \mathcal{H}^{\ell, m}. \quad (3.37)$$

The operators h^ℓ and $h_{(\alpha)}^\ell$ coincide for all $\ell \geq 1$ and are given by

$$h^\ell := h_\alpha^\ell := -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}, \quad (3.38)$$

with the domain

$$\begin{aligned} \text{dom}(h_{(\alpha)}^\ell) := & \{f \in L^2((0, \infty)) : f, f' \in AC_{\text{loc}}((0, \infty)), h^\ell f \in L^2((0, \infty))\}, \\ & \subset L^2((0, \infty)), \end{aligned} \quad (3.39)$$

whereas in the case $\ell = 0$, which we call the lowest angular momentum channel,

$$h^0 := -\frac{d^2}{dr^2}, \quad \text{and} \quad h_\alpha^0 := -\frac{d^2}{dr^2} \quad (3.40)$$

with the two different domains

$$\begin{aligned} \text{dom}(h^0) := & \{f \in L^2((0, \infty)) : f, f' \in AC_{\text{loc}}((0, \infty)), f'' \in L^2((0, \infty)), \\ & f(0+) = 0\} \subset L^2((0, \infty)), \end{aligned} \quad (3.41)$$

$$\begin{aligned} \text{dom}(h_\alpha^0) := & \{f \in L^2((0, \infty)) : f, f' \in AC_{\text{loc}}((0, \infty)), f'' \in L^2((0, \infty)) \\ & - 4\pi\alpha f(0+) + f'(0+) = 0\} \subset L^2((0, \infty)). \end{aligned} \quad (3.42)$$

Here, $AC_{\text{loc}}((0, \infty))$ denotes the set of all locally absolutely continuous functions on $(0, \infty)$. We refer also to [Tes09, Chap. 10] for a more detailed derivation of the angular momentum decomposition.

Remarks 3.7. (i) Let us emphasise that the difference of H and H_α takes place in the lowest angular momentum channel, i.e. $\ell = 0$, only. Thus, we are effectively left with the pair of operators h^0 and h_α^0 on the half axis $(0, \infty)$, where the pair corresponds to the negative Laplacian with a different boundary condition at 0.

(ii) Since H itself is a self-adjoint extension of $-\Delta_0$, we remark that $H = H_\infty$ as well as $h^0 = h_\infty^0$, i.e. $\alpha = \infty$ corresponds to $-\Delta$.

(iii) Moreover, H is the biggest self-adjoint extension of $-\Delta_0$. More precisely, for all $\alpha \in \mathbb{R}$

$$H_\alpha \leq H, \quad \text{respectively} \quad h_\alpha^0 \leq h^0. \quad (3.43)$$

(iv) The operator h^0 corresponds to the negative Laplacian on the half axis with a Dirichlet boundary condition at 0. The operator h_0^0 corresponds to the negative Laplacian with a Neumann boundary condition at 0.

(v) In the case $\alpha \geq 0$ we have

$$0 \leq H_\alpha \quad \text{and} \quad 0 \leq h_\alpha^0, \quad (3.44)$$

whereas in the case $\alpha < 0$ both operators H_α and h_α^0 admit the single negative eigenvalue

$$\mu_1 := -(4\pi\alpha)^2 \quad (3.45)$$

with an exponentially decaying eigenfunction, see [AGHH05, Thm. 1.1.4].

Since we are interested in restrictions to finite volumina, we will not go into more details about a Dirac- δ perturbation in the infinite volume. Now, let $L > 0$ and we denote by $|\cdot|_2$ the Euclidean norm on \mathbb{R}^3 and consider the self-adjoint extensions of

$$-\Delta_{0,L} : C_c^\infty(B_L(0) \setminus \{0\}) \rightarrow L^2(B_L(0)), \quad (3.46)$$

where $B_L(0) := \{x \in \mathbb{R}^3 : |x|_2 \leq L\}$ is the ball of radius L around the origin. This operator has deficiency indices $(1, 1)$ as well, and we call its self-adjoint extensions $H_{\alpha,L}$, which are Dirac- δ perturbations of the negative Laplacian on the ball with Dirichlet boundary conditions. The spherical symmetry of the ball allows us to mimic the above angular momentum decomposition and we infer the existence of a unitary

$$U_L : L^2(B_L(0)) \rightarrow \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} \mathcal{H}_L^{\ell,m}, \quad (3.47)$$

where in this case $\mathcal{H}_L^{\ell,m} = L^2((0, L))$, such that

$$UH_{(\alpha),L}U^* := \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} h_{(\alpha),L}^\ell : \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} \mathcal{H}_L^{\ell,m} \rightarrow \bigoplus_{\ell \in \mathbb{N}_0} \bigoplus_{-\ell \leq m \leq \ell} \mathcal{H}_L^{\ell,m}. \quad (3.48)$$

For all $\ell \geq 1$

$$h_{\alpha,L}^\ell = h_L^\ell := -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}, \quad (3.49)$$

with the domain

$$\begin{aligned} \text{dom}(h_{(\alpha),L}^\ell) := & \{f \in L^2((0, L)) : f, f' \in AC_{\text{loc}}((0, L)), h_\ell f \in L^2((0, L)); \\ & f(L-) = 0\} \subset L^2((0, L)). \end{aligned} \quad (3.50)$$

In the $\ell = 0$ channel we obtain

$$h_{L,\alpha}^0 := -\frac{d^2}{dr^2} \quad \text{and} \quad h_L^0 := -\frac{d^2}{dr^2} \quad (3.51)$$

with the domains

$$\begin{aligned} \text{dom}(h_{L,\alpha}^0) := & \{f \in L^2((0, L)) : f, f' \in AC_{\text{loc}}((0, L)), f'' \in L^2((0, L)), \\ & -4\pi\alpha f(0+) + f'(0+) = 0; f(L-) = 0\} \subset L^2((0, L)), \end{aligned} \quad (3.52)$$

$$\begin{aligned} \text{dom}(h_L^0) := & \{f \in L^2((0, L)) : f, f' \in AC_{\text{loc}}((0, L)), f'' \in L^2((0, L)), \\ & f(0+) = 0; f(L-) = 0\} \subset L^2((0, L)). \end{aligned} \quad (3.53)$$

Remarks 3.8. (i) The only difference to the operators on the infinite-volume is the additional Dirichlet boundary condition at L .

(ii) Obviously, H_L is the Dirichlet Laplacian on the ball $B_L(0)$ and we refer to $H_{\alpha,L}$ as the Dirichlet Laplacian on $B_L(0)$ with a Dirac- δ perturbation.

Lemma 3.9. *In the case $\alpha \geq 0$ we obtain the operator inequalities*

$$0 \leq H_{\alpha,L} \quad \text{and} \quad 0 \leq h_{\alpha,L}^0. \quad (3.54)$$

In the case $\alpha < 0$ we have at least the uniform lower bound

$$-(4\pi\alpha)^2 \leq H_{\alpha,L} \quad \text{and equivalently} \quad -(4\pi\alpha)^2 \leq h_{\alpha,L}^0. \quad (3.55)$$

Proof. This lemma follows e.g. from Dirichlet-Neumann bracketing. Let $h_{L^c}^\ell$ be the restriction of h^ℓ to (L, ∞) with a Dirichlet boundary condition at L . Then, Dirichlet-Neumann bracketing, see [RS78], implies $h_\alpha^\ell \leq h_{\alpha,L}^\ell \oplus h_{L^c}^\ell$. Thus, Remark 3.7(v) gives the claim. \square

Since H_L and $H_{\alpha,L}$ differ only by a boundary condition, the difference seems to be quite small, this is indeed the case in the following sense.

Lemma 3.10. *Let $z \in \varrho(H_L) \cup \varrho(H_{\alpha,L})$. Then, there exists a $\eta_{L,z}^\alpha \in L^2(B_L(0))$ such that the difference of the resolvents satisfies*

$$\frac{1}{H_L - z} - \frac{1}{H_{\alpha,L} - z} = |\eta_{L,z}^\alpha\rangle\langle\eta_{L,z}^\alpha|. \quad (3.56)$$

The same is apparently true for the resolvents of h_L^0 and $h_{\alpha,L}^0$ with the vector $(U_L \eta_{L,z}^\alpha) \in L^2((0, L))$.

Proof. First note that h_L and $h_{\alpha,L}$ are both self-adjoint extensions of $-\Delta$ with $\text{dom}(-\Delta) := \{u \in C_c^2((0, L)) : u(L-) = 0\}$. Moreover, the deficiency indices of the latter are $(1, 1)$. Thus, the lemma follows from [AGHH05, Thm. A.2] or [Tes09, Lem. 2.29]. \square

Standard results imply the compactness of the resolvent of H_L , which is just the Dirichlet Laplacian on the bounded domain Λ_L . Now, Lemma 3.10 provides compactness of the resolvent of $H_{\alpha,L}$ as well and we denote by

$$\lambda_1^L \leq \lambda_2^L \leq \dots \quad \text{and} \quad \mu_1^L \leq \mu_2^L \leq \dots \quad (3.57)$$

the corresponding eigenvalues of H_L and $H_{\alpha,L}$, counting multiplicities, and by

$$\lambda_1^L(l) \leq \lambda_2^L(l) \leq \dots \quad \text{and} \quad \mu_1^L(l) \leq \mu_2^L(l) \leq \dots \quad (3.58)$$

the eigenvalues of h_L^ℓ and $h_{\alpha,L}^\ell$. Then,

$$\sigma(H_L) = \bigcup_{\ell \in \mathbb{N}_0} \bigcup_{-\ell \leq m \leq \ell} \bigcup_{k \in \mathbb{N}} \lambda_k^L(\ell) \quad \sigma(H_{\alpha,L}) = \bigcup_{n \in \mathbb{N}} \mu_n^L(0) \cup \bigcup_{\ell \in \mathbb{N}} \bigcup_{-\ell \leq m \leq \ell} \bigcup_{k \in \mathbb{N}} \lambda_k^L(\ell). \quad (3.59)$$

We saw that the perturbation is small in the sense of a rank-one perturbation in the resolvent but the perturbation is L -dependent, thus, not compactly supported. Moreover, we obtain that the eigenvalues of H_L and $H_{\alpha,L}$ interlace. But for our application in mind, we need to know slightly more about the eigenvalues of H_L and $H_{\alpha,L}$. To formulate this, we continue with the definition of the scattering phase shift.

Definition 3.11 (Scattering phase shift). Let $k > 0$. Then, the scattering phase shift is defined by

$$\delta_\alpha(k) := \arctan\left(\frac{k}{4\pi\alpha}\right) \quad \text{for } \alpha \geq 0, \quad (3.60)$$

$$\delta_\alpha(k) := \pi - \arctan\left(\frac{k}{4\pi|\alpha|}\right) \quad \text{for } \alpha \leq 0, \quad (3.61)$$

where we use the convention $\arctan\left(\frac{k}{0}\right) := \frac{\pi}{2}$ for $k > 0$.

Remark 3.12. The separate definitions of the phase shift are reminiscent of the existence of a negative eigenvalue whenever $\alpha < 0$ and related to Levinson's theorem which states that $\delta_\alpha(0)/\pi$ gives the number of negative eigenvalues, see [RS79].

The eigenvalues of h_L^0 can be computed explicitly, see [RS78], i.e. for $n \in \mathbb{N}$

$$\lambda_n = \left(\frac{n\pi}{L}\right)^2. \quad (3.62)$$

The eigenvalues of $h_{\alpha,L}^0$ admit the following simple representation in terms of the eigenvalues of h_L^0 and the phase shift.

Lemma 3.13. Let δ_α be given by Definition 3.11. Then,

(i) for $\alpha \geq 0$ and $n \in \mathbb{N}$ the n th eigenvalue of h_L^0 and $h_{\alpha,L}^0$ satisfy

$$0 \leq \sqrt{\mu_n} = \sqrt{\lambda_n} - \frac{\delta_\alpha(\sqrt{\mu_n})}{L}, \quad (3.63)$$

(ii) for $\alpha \leq 0$ and $n > 1$ the n th eigenvalue of h_L^0 and $h_{\alpha,L}^0$ satisfy

$$0 \leq \sqrt{\mu_n} = \sqrt{\lambda_n} - \frac{\delta_\alpha(\sqrt{\mu_n})}{L}, \quad (3.64)$$

(iii) and δ exhibits the following expansion

$$\delta_\alpha(\sqrt{\mu_n}) = \delta_\alpha(\sqrt{\lambda_n}) - \frac{\delta'_\alpha(\sqrt{\lambda_n})\delta_\alpha(\sqrt{\lambda_n})}{L} + o\left(\frac{1}{L}\right), \quad (3.65)$$

which is valid for all $\mu_n \geq 0$ and the error term depends on α but is independent of n .

Proof. Let $k > 0$. Consider the eigenvalue problem

$$-u_k'' = k^2 u_k, \quad -4\pi\alpha u_k(0+) + u_k'(0+) = 0. \quad (3.66)$$

Introducing Prüfer variables

$$u_k(x) = \rho_u(x) \sin(\theta_k(x)) \quad u_k'(x) = k \rho_u(x) \cos(\theta_k(x)), \quad (3.67)$$

we see that any non-zero solution of (3.66) is of the form

$$u_k(x) := a \sin\left(kx + \arctan\left(\frac{k}{4\pi\alpha}\right)\right), \quad (3.68)$$

for some $0 \neq a \in \mathbb{C}$. Since any eigenfunction u_k to an eigenvalue k^2 of $h_{\alpha,L}^0$ is a solution of (3.66) in $(0, L)$ and additionally fulfills $u_k(L-) = 0$ we obtain that

$$u_k(L) = a \sin\left(kL + \arctan\left(\frac{k}{4\pi\alpha}\right)\right) = 0. \quad (3.69)$$

On the other hand, all k^2 such that (3.69) is satisfied are eigenvalues of $h_{\alpha,L}^0$. Since the function $k \mapsto kL + \arctan\left(\frac{k}{4\pi\alpha}\right)$ is strictly increasing we obtain for any $n \in \mathbb{N}$ an unique eigenvalue $\mu_n \geq 0$ of $h_{\alpha,L}^0$ such that

$$\sqrt{\mu_n}L + \arctan\left(\frac{\sqrt{\mu_n}}{4\pi\alpha}\right) = n\pi, \quad (3.70)$$

where $\mu_1 < \mu_2 < \dots$. This proves (i). For the case $\alpha < 0$ note that $h_{\alpha,L}^0$ admits a single negative eigenvalue. Therefore, (3.70) is only valid starting from the second eigenvalue of $h_{\alpha,L}^0$. This implies for all $n \in \mathbb{N}$

$$\sqrt{\mu_{n+1}} = \sqrt{\lambda_n} - \frac{\arctan\left(\frac{\sqrt{\mu_{n+1}}}{4\pi\alpha}\right)}{L} = \sqrt{\lambda_{n+1}} - \frac{\pi - \arctan\left(\frac{\sqrt{\mu_{n+1}}}{4\pi|\alpha|}\right)}{L}. \quad (3.71)$$

(iii) follows directly from (i), (ii) and Definition (3.11) of the phase shift. \square

Remark 3.14. Later, we extend this lemma also for pairs of Schrödinger operators on $L^2((0, L))$ which differ be a non-negative multiplication operator, see Lemma 4.11.

Corollary 3.15. *The eigenvalues of h_L^0 and $h_{\alpha,L}^0$ fulfil*

$$\mu_1^L(0) < \lambda_1^L(0) < \mu_2^L(0) < \lambda_2^L(0) < \dots \quad (3.72)$$

Proof. Note that $|\delta_\alpha(k)| < \pi$ for all $k > 0$. Thus, (3.62) and (3.64) imply the corollary. \square

Remark 3.16. At the end of this section let us briefly comment on Dirac- δ perturbations in other dimensions. Considering $d \geq 4$, the operator $-\Delta_0$ given in (3.35) is essentially self-adjoint [RS75, Thm. X.11] and we have a unique self-adjoint extension: the negative Laplacian. In $d = 2$, a Dirac- δ can be defined, see [AGHH05, Sct. I.5], but Lemma 3.13 will not be as easy as in the $d = 3$ case since the operator in the lowest angular momentum channel is $d^2/dx^2 - 1/(4|\cdot|^2)$. In the $d = 1$ case the deficiency indices are $(2, 2)$ and in general this results in a rank-two perturbation in the resolvent, see [AGHH05, Sct. I.3].

Thus, we cannot directly apply the product representation in Theorem 3.3, which is valid for rank-one perturbations only.

3. The Exact Asymptotics of the Ground-State Overlap

We denote by $(\varphi_j^L)_{j \in \mathbb{N}}$ and $(\psi_k^L)_{k \in \mathbb{N}}$ the normalised eigenvectors of the operators H_L and $H_{\alpha,L}$, defined in the previous section, corresponding to the sequences of the eigenvalues $(\lambda_j^L)_{j \in \mathbb{N}}$ and $(\mu_k^L)_{k \in \mathbb{N}}$, where we choose the same eigenvectors for H_L and $H_{\alpha,L}$ in any angular momentum channel $\ell \geq 1$. This choice ensures that the eigenfunctions of H_L and $H_{\alpha,L}$ differ in the lowest angular momentum channel only. Moreover, we write $(\varphi_j^L(0))_{j \in \mathbb{N}}$ and $(\psi_k^L(0))_{k \in \mathbb{N}}$ for the eigenfunctions corresponding to the lowest angular momentum channel.

With this choice of the eigenfunctions we obtain the following asymptotics of the ground-state overlap:

Theorem 3.17. *Let $E > 0$ and $N_{(\cdot)}(E) : \mathbb{R}_+ \rightarrow \mathbb{N}$ an arbitrary function subject to*

$$\frac{N_L(E)}{|B_L(0)|} \rightarrow \rho(E) := \frac{E^{3/2}}{8\pi^3}, \quad (3.73)$$

where ρ denotes the integrated density of states of the operator H . Then, the ground-state overlap corresponding to the pair of operators H_L and $H_{\alpha,L}$ admits the asymptotics

$$|\mathcal{S}_L^{N_L(E)}|^2 := \left| \det \left(\langle \varphi_j^L, \psi_k^L \rangle \right)_{1 \leq j, k \leq N_L(E)} \right|^2 = L^{-\frac{1}{\pi^2} \delta_\alpha^2(\sqrt{E}) + o(1)} \quad (3.74)$$

as $L \rightarrow \infty$, equivalently,

$$\lim_{L \rightarrow \infty} \frac{|\mathcal{S}_L^{N_L(E)}|}{\ln L} = -\frac{1}{2\pi^2} \delta_\alpha^2(\sqrt{E}), \quad (3.75)$$

and δ_α is given in Definition 3.11 above.

Remark 3.18. We choose the same eigenfunctions in the $\ell \geq 1$ angular momentum channels because we are considering an s-wave scattering problem. In principle, this choice is only necessary if $\lambda_{N_L(E)}^L$ is degenerate and $\mathcal{S}_L^{N_L(E)}$ takes only a proper subset of the eigenfunctions in the $\lambda_{N_L(E)}^L$ eigenspace into account.

Remarks 3.19. (i) Note that the result is valid for arbitrary thermodynamic limits and independent of the latter but the $o(1)$ -error term in (3.74) deduced in the proof depends on the particular choice of the thermodynamic limit. We do not believe that it can be substantially improved for arbitrary thermodynamic limits, see especially equations (3.110) and (3.111).

(ii) Due to s-wave scattering the S -matrix for the pair of Schrödinger operators H and H_α can be reduced to a complex number of modulus 1. This number is equal to $S_E = e^{2i\delta_\alpha(\sqrt{E})}$, see [RS79, Sct. XI.8], where we chose the scattering phase shift as in Definition 3.11. Next, we compare the exponent found in Theorem 3.17 above with the exponent $\gamma(E) = \frac{1}{\pi^2} \|\arcsin |T_E/2|\|_{HS}^2$ found in [GKMO14]. To do this, we compute using

$$T_E = S_E - I$$

$$\begin{aligned} \frac{1}{\pi^2} \|\arcsin |T_E/2|\|_{\text{HS}}^2 &= \frac{1}{\pi^2} (\arcsin (|e^{2i\delta_\alpha(\sqrt{E})} - 1|/2))^2 \\ &= \frac{1}{\pi^2} (\arcsin (\sin (\delta_\alpha(\sqrt{E}))))^2 \\ &= \begin{cases} \frac{1}{\pi^2} \delta_\alpha^2(\sqrt{E}), & \delta_\alpha(\sqrt{E}) \leq \pi/2 \\ \frac{1}{\pi^2} (\delta_\alpha(\sqrt{E}) - \pi)^2, & \delta_\alpha(\sqrt{E}) > \pi/2. \end{cases} \end{aligned} \quad (3.76)$$

Hence, we obtain in the case $\alpha < 0$

$$\frac{\delta_\alpha^2(\sqrt{E})}{\pi^2} > \frac{1}{\pi^2} \|\arcsin |T_E/2|\|_{\text{HS}}^2. \quad (3.77)$$

This implies that in general the decay exponent in the asymptotics of the ground-state overlap is not given by the decay exponent $\gamma(E) = \frac{1}{\pi^2} \|\arcsin |T_E/2|\|_{\text{HS}}^2$.

The definition of the Dirac- δ perturbation and our choice of the eigenfunctions in higher angular momentum channels imply that Theorem 3.17 follows from the analogous result on the half axis.

Theorem 3.20. *Let $E > 0$ and $N_{(\cdot)}^0(E) : \mathbb{R}_+ \rightarrow \mathbb{N}$ an arbitrary function subject to*

$$\frac{N_L^0(E)}{L} \rightarrow \rho_0(E) := \frac{\sqrt{E}}{\pi}, \quad (3.78)$$

where ρ_0 denotes the integrated density of states of the operator h^0 . Then, the ground-state overlap corresponding to the pair of operators h_L^0 and $h_{\alpha,L}^0$ admits the asymptotics

$$|\mathcal{S}_L^{N_L^0(E)}|^2 := \left| \det \left(\langle \varphi_j^L(0), \psi_k^L(0) \rangle \right)_{1 \leq j, k \leq N_L^0(E)} \right|^2 = L^{-\frac{1}{\pi^2} \delta_\alpha^2(\sqrt{E}) + o(1)} \quad (3.79)$$

as $L \rightarrow \infty$, and δ_α is given by Definition 3.11 above.

The above deals with a problem on the half-axis. Due to symmetry, one can easily deduce also a result for the ground-state overlap for systems on $(-L, L)$ with different boundary conditions at the endpoints $\pm L$. We sketch this. Let

$$\bar{H}_L := -\Delta_L \quad \text{and} \quad \bar{H}_{\alpha,L} := -\Delta_{\alpha,L} \quad (3.80)$$

be both negative Laplacians on $(-L, L)$, where \bar{H}_L admits Dirichlet boundary conditions at the endpoints $\pm L$ and $\bar{H}_{\alpha,L}$ admits the boundary conditions $-4\pi\alpha f(L\pm) + f'(L\pm) = 0$ at $\pm L$ for some $\alpha \in \mathbb{R}$. Then, we obtain the following asymptotics of the ground-state overlap.

Corollary 3.21. *Let $E > 0$ and $\bar{N}_{(\cdot)}(E) : \mathbb{R}_+ \rightarrow \mathbb{N}$ an arbitrary function subject to*

$$\frac{\bar{N}_L(E)}{2L} \rightarrow \bar{\rho}(E) := \frac{\sqrt{E}}{2\pi}. \quad (3.81)$$

Then, the ground-state overlap corresponding to \bar{H}_L and $\bar{H}_{\alpha,L}$ admits the asymptotics

$$|\mathcal{S}_L^{\bar{N}_L(E)}|^2 = L^{-\zeta(E) + o(1)} \quad (3.82)$$

as $L \rightarrow \infty$. Here,

$$\zeta(E) := \frac{2}{\pi^2} \delta_\alpha^2(\sqrt{E}) \quad (3.83)$$

and δ_α is given by Definition 3.11.

Proof. We only sketch the proof. Since we chose the same boundary conditions at $\pm L$, we can decompose the operators \bar{H}_L and $\bar{H}_{\alpha,L}$ with respect to odd and even functions. Therefore, the operators $\bar{H}_{(\alpha),L}$ are unitarily equivalent to the direct sum $\bar{h}_L^{(\alpha)} \oplus \bar{h}_{0,L}^{(\alpha)}$ acting on $L^2((0, L)) \oplus L^2((0, L))$. Here, $\bar{h}_L^{(\alpha)}$ are negative Laplacians with a Dirichlet boundary condition at 0 and $\bar{h}_{0,L}^{(\alpha)}$ with a Neumann b.c. at 0. The operators \bar{h}_L and $\bar{h}_{0,L}$ admit a Dirichlet b.c. at L , whereas the operators \bar{h}_L^α and $\bar{h}_{0,L}^\alpha$ admit the b.c. $-4\pi\alpha f(L-) + f'(L-) = 0$ at L . In this way, we reduced the problem to two separate problems on the half-axis and the determinant is decomposed into two determinants. We use for each determinant the result of Theorem 3.20 where we have to modify Lemma 3.13 accordingly due to the different boundary conditions. But this does not change the results of Lemma 3.13. \square

3.1. Proof of Theorem 3.17 and Theorem 3.20. We start with the 3-dimensional case and decompose the determinant $\mathcal{S}_L^{N_L(E)}$ according to the angular momentum decomposition (3.37). This implies

$$\left| \det \left(\langle \varphi_j^L, \psi_k^L \rangle \right)_{1 \leq j, k \leq N_L(E)} \right|^2 = \prod_{l \in \mathbb{N}_0} \left| \det \left(\langle \varphi_j^L(\ell), \psi_k^L(\ell) \rangle \right)_{1 \leq j, k \leq N_L^l(E)} \right|^{2(2\ell+1)}, \quad (3.84)$$

where $\varphi_j^L(\ell)$ and $\psi_k^L(\ell)$ correspond to the radial part of the eigenfunctions lying in the ℓ -th angular momentum channel and $N_L^\ell(E)$ to the relative particle number in the ℓ -th angular momentum channel. More precisely,

$$N_L^\ell(E) := \#\{k \in \mathbb{N} : \exists j \in \{1, \dots, N_L\} \text{ with } \lambda_k^L(\ell) = \lambda_j^L\} \quad (3.85)$$

where $(\lambda_k^L(\ell))_{k \in \mathbb{N}}$ denote the eigenvalues of h_L^ℓ as defined in (3.58). Since we chose the eigenfunctions of H_L and $H_{\alpha,L}$ to be the same in every angular momentum channel $\ell \geq 1$ we obtain that only the $\ell = 0$ term in the product (3.84) is different from 1. Hence,

$$\left| \det \left(\langle \varphi_j^L, \psi_k^L \rangle \right)_{1 \leq j, k \leq N_L(E)} \right|^2 = \left| \det \left(\langle \varphi_j^L(0), \psi_k^L(0) \rangle \right)_{1 \leq j, k \leq N_L^0(E)} \right|^2, \quad (3.86)$$

and we reduced the 3-dimensional problem to a problem on the half-axis with the relative particle number $N_L^0(E)$. Now, this number satisfies.

Lemma 3.22. *Given $E > 0$. Let L and $N_L(E) \in \mathbb{N}$ such that $\frac{N_L(E)}{|B_L(0)|} \rightarrow \rho(E)$ as $L \rightarrow \infty$. Then,*

$$\frac{N_L^0(E)}{L} \rightarrow \frac{\sqrt{E}}{\pi} = \rho_0(E), \quad (3.87)$$

as $L \rightarrow \infty$.

Proof. For any $E > 0$

$$\lim_{L \rightarrow \infty} \frac{\#\{k : \lambda_k^L \leq E\}}{|B_L(0)|} = \rho(E) = \lim_{L \rightarrow \infty} \frac{N_L(E)}{|B_L(0)|}, \quad (3.88)$$

where the first equality follows from e.g. [Sto01, App. 4.1]. Hence, we obtain for an arbitrary $\epsilon > 0$ the inequalities

$$\#\{k : \lambda_j^L \leq E - \epsilon\} \leq N_L(E) \leq \#\{j : \lambda_j^L \leq E + \epsilon\} \quad (3.89)$$

for L large enough. Since ρ is given explicitly in (3.73) we know that it is strictly increasing. Hence, $\lambda_{N_L(E)}^L \rightarrow E$. Therefore, $\lambda_{N_L^0(E)}^L(0) \rightarrow E$ as well because otherwise there would be

a gap in the spectrum of h^0 by the definition of the relative particle number $N_L^0(E)$. This implies for an arbitrary $\epsilon > 0$ and L large enough

$$\begin{aligned} \left| \frac{N_L^0(E)}{L} - \frac{\#\{k : \lambda_k^L(0) \leq E\}}{L} \right| &\leq \left| \frac{\#\{k : (\frac{k\pi}{L})^2 \in (E - \epsilon, E + \epsilon)\}}{L} \right| \\ &\leq \frac{c}{\sqrt{E}} \epsilon, \end{aligned} \quad (3.90)$$

for some constant c . Since $\#\{k : \lambda_k^L(0) \leq E\}/L \rightarrow \rho_0(E)$, as $L \rightarrow \infty$ by definition, this yields the claim. \square

The above implies that the 3-dimensional case completely reduces to the model on the half-axis and Theorem 3.17 follows from Theorem 3.20. Therefore, we are left with a problem concerning the eigenvalues $(\lambda_j^L(0))_{j \in \mathbb{N}}$, $(\mu_k^L(0))_{k \in \mathbb{N}}$ and the eigenfunctions $(\varphi_j^L(0))_{j \in \mathbb{N}}$, $(\psi_k^L(0))_{k \in \mathbb{N}}$ in the $\ell = 0$ angular momentum channel only.

In the following we drop both the $\ell = 0$ parameter and the index L to shorten notation, whenever this is convenient.

Next, we apply the product formula deduced in Theorem 3.3 to the determinant.

Lemma 3.23. *Let $N \in \mathbb{N}$. Then,*

$$\left| \det \left(\langle \varphi_j, \psi_k \rangle \right)_{1 \leq j, k \leq N} \right|^2 = \prod_{j=1}^N \prod_{k=N+1}^{\infty} \frac{|\mu_k - \lambda_j| |\lambda_k - \mu_j|}{|\lambda_k - \lambda_j| |\mu_k - \mu_j|}. \quad (3.91)$$

Proof. We want to apply Theorem 3.3 to the resolvents of $h_{\alpha,L}^0$ and h_L^0 . Thus, we check the assumptions of this theorem. First, note that $h_{\alpha,L}^0$ and h_L^0 are uniformly bounded from below by Lemma 3.9. Therefore, $E \in \varrho(h_L^0) \cap \varrho(h_{\alpha,L}^0)$ for some $E < \inf \sigma(h_{\alpha,L}^0)$ and the operators $\frac{1}{h_L^0 - E}$ and $\frac{1}{h_{\alpha,L}^0 - E}$ are non-negative with trivial kernel. Moreover, by Lemma 3.10

$$\frac{1}{h_L^0 - E} - \frac{1}{h_{\alpha,L}^0 - E} = |\eta_L^{E,\alpha}\rangle \langle \eta_L^{E,\alpha}|, \quad (3.92)$$

for some $\eta_L^E \in L^2((0, L))$. In addition, Corollary 3.15 provides the strict interlacing of the eigenvalues

$$\frac{1}{\mu_1 - E} > \frac{1}{\lambda_1 - E} > \frac{1}{\mu_2 - E} > \frac{1}{\lambda_2 - E} > \dots \quad (3.93)$$

and the explicit representation of the eigenvalues of $h_{\alpha,L}^0$ and h_L^0 given in Lemma 3.13 imply

$$\sum_{n=1}^{\infty} \left(\frac{1}{\mu_n - E} - \frac{1}{\lambda_n - E} \right) < \infty. \quad (3.94)$$

Thus, the resolvents $\frac{1}{h_L^0 + E}$ and $\frac{1}{h_{\alpha,L}^0 + E}$ satisfy the assumptions of Theorem 3.3 and we end up with

$$\begin{aligned} \left| \det \left(\langle \varphi_j, \psi_k \rangle \right)_{1 \leq j, k \leq N} \right|^2 &= \prod_{j=1}^N \prod_{k=N+1}^{\infty} \frac{\left| \frac{1}{\mu_k - E} - \frac{1}{\lambda_j - E} \right| \left| \frac{1}{\lambda_k - E} - \frac{1}{\mu_j - E} \right|}{\left| \frac{1}{\lambda_k - E} - \frac{1}{\lambda_j - E} \right| \left| \frac{1}{\mu_k - E} - \frac{1}{\mu_j - E} \right|} \\ &= \prod_{j=1}^N \prod_{k=N+1}^{\infty} \frac{|\mu_k - \lambda_j| |\lambda_k - \mu_j|}{|\lambda_k - \lambda_j| |\mu_k - \mu_j|}. \end{aligned} \quad (3.95)$$

□

Now, we are in position to prove the main result.

Proof of Theorem 3.20. We start with the product representation given in Lemma 3.23. Note that for $\alpha < 0$ there is an ambiguity since there exists precisely one negative eigenvalue μ_1 . Therefore, we treat the $j = 1$ term in the product separately. We define

$$A_L^N := \prod_{k=N+1}^{\infty} \frac{|\mu_k - \lambda_1| |\lambda_k - \mu_1|}{|\lambda_k - \lambda_1| |\mu_k - \mu_1|} = \prod_{k=N+1}^{\infty} \left| 1 + \frac{(\mu_k - \lambda_k)(\lambda_1 - \mu_1)}{(\lambda_k - \lambda_1)(\mu_k - \mu_1)} \right| \quad (3.96)$$

and estimate using Corollary 3.15

$$\begin{aligned} \sum_{k=N+1}^{\infty} \left| \frac{(\mu_k - \lambda_k)(\lambda_1 - \mu_1)}{(\lambda_k - \lambda_1)(\mu_k - \mu_1)} \right| &\leq |\lambda_1 - \mu_1| \sum_{k=N+1}^{\infty} \frac{\left(\left(\frac{k\pi}{L} \right)^2 - \left(\frac{(k-1)\pi}{L} \right)^2 \right)}{\left(\left(\frac{k\pi}{L} \right)^2 - \left(\frac{\pi}{L} \right)^2 \right) \left(\left(\frac{(k-1)\pi}{L} \right)^2 - \left(\frac{\pi}{L} \right)^2 \right)} \\ &\leq \frac{L^2}{\pi^2} |\lambda_1 - \mu_1| \sum_{k=N+1}^{\infty} \frac{(2k-1)}{(k^2-1)(k^2-2k)} \\ &\leq c \left(\frac{L}{N} \right)^2 |\lambda_1 - \mu_1|. \end{aligned} \quad (3.97)$$

Since h_L^α is uniformly bounded from below with respect to L , see Lemma 3.9,

$$\ln A_L^N = \ln \left(\prod_{k=N+1}^{\infty} \frac{|\mu_k - \lambda_1| |\lambda_k - \mu_1|}{|\lambda_k - \lambda_1| |\mu_k - \mu_1|} \right) = O(1) \quad (3.98)$$

as $N, L \rightarrow \infty$ and $\frac{N}{L} \rightarrow \rho(E) > 0$. Therefore, we are left with a product consisting of the non-negative eigenvalues and apply Lemma 3.23, use Lemma 3.13 (i) and $\sqrt{\lambda_n} = \frac{n\pi}{L}$, $n \in \mathbb{N}$, to obtain

$$\ln \left| \det \left(\langle \varphi_j, \psi_k \rangle \right)_{1 \leq j, k \leq N} \right|^2 \quad (3.99)$$

$$= \ln A_L^N + \sum_{j=2}^N \sum_{k=N+1}^{\infty} \ln \left(\frac{\left| (k\pi - \delta_\alpha(\sqrt{\mu_k}))^2 - (j\pi)^2 \right| \left| ((k\pi)^2 - (j\pi - \delta_\alpha(\sqrt{\mu_j}))^2 \right|}{\left| (k\pi)^2 - (j\pi)^2 \right| \left| (k\pi - \delta_\alpha(\sqrt{\mu_k}))^2 - (j\pi - \delta_\alpha(\sqrt{\mu_j}))^2 \right|} \right). \quad (3.100)$$

In the following the $O(1)$ and $o(1)$ terms refer to the asymptotics $L, N \rightarrow \infty$, $N/L \rightarrow \rho_0(E) > 0$. Equation (3.98) above, Lemma 3.26 below and the abbreviation $g_k := -\frac{1}{\pi} \delta_\alpha(\sqrt{\mu_k})$ for $k \in \mathbb{N}$ yield

$$(3.100) = - \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{(2jg_j + g_j^2)(2kg_k + g_k^2)}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)} + O(1). \quad (3.101)$$

Using Lemma 3.27 and the abbreviation $\delta_k := -\frac{1}{\pi} \delta_\alpha(\sqrt{\lambda_k})$ for $k \in \mathbb{N}$

$$(3.101) = - \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{(2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2)}{((k+\delta_k)^2 - (j+\delta_j)^2)(k^2 - j^2)} + O(1). \quad (3.102)$$

Lemma 3.28 implies

$$(3.102) = - \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4jk\delta_j\delta_k}{(k^2 - j^2)^2} + O(1). \quad (3.103)$$

Lemma 3.29 yields

$$(3.103) = -\frac{1}{\pi^2} \int_0^{\frac{N}{L}} dx \int_{\frac{N+1}{L}}^{\frac{2N}{L}} dy \frac{4xy\delta_\alpha(x\pi)\delta_\alpha(y\pi)}{(y^2 - x^2)^2} + O(1). \quad (3.104)$$

We define for $0 \leq x < y$

$$g(x, y) := \frac{4xy\delta_\alpha(\pi x)\delta_\alpha(\pi y)}{(y + x)^2} \quad (3.105)$$

The explicit representation of δ_α implies for all $\epsilon > 0$

$$\sup_{b > \epsilon} \sup_{(x, y) \in (0, b) \times (b, \infty)} |(\nabla g)(x, y)|_2 := c(\epsilon) < \infty. \quad (3.106)$$

Therefore, using the mean value theorem and the Cauchy-Schwarz inequality, we compute for a $0 < \epsilon < \sqrt{E}$ and N, L big enough

$$\begin{aligned} & \int_0^{\frac{N}{L}} dx \int_{\frac{N}{L} + \frac{1}{L}}^{\frac{2N}{L}} dy \left| \frac{4xy\delta_\alpha(x\pi)\delta_\alpha(y\pi)}{(y + x)^2} - \delta_\alpha^2(N/L) \right| \frac{1}{(y - x)^2} \\ & \leq c(\epsilon) \int_0^{\frac{N}{L}} dx \int_{\frac{N}{L} + \frac{1}{L}}^{\frac{2N}{L}} dy |(N/L - x, y - N/L)|_2 \frac{1}{(y - x)^2} \\ & \leq 2c(\epsilon) \int_0^{\frac{N}{L}} dx \int_{\frac{N}{L} + \frac{1}{L}}^{\frac{2N}{L}} dy \frac{1}{(y - x)} = O(1), \end{aligned} \quad (3.107)$$

where we used the inequality

$$\frac{|x - N/L| + |y - N/L|}{(y - x)^2} \leq 2 \frac{1}{(y - x)}, \quad (3.108)$$

which is valid for all $x < N/L < y$. Moreover, we compute

$$\begin{aligned} \int_0^{\frac{N}{L}} dx \int_{\frac{N}{L} + \frac{1}{L}}^{\frac{2N}{L}} dy \frac{1}{(y - x)^2} &= \ln L + \ln \left(\frac{N+1}{2L} \right) \\ &= \ln L + O(1) \end{aligned} \quad (3.109)$$

as $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi} > 0$. Hence, combining equation (3.107) and (3.109), we end up with

$$(3.104) = -\ln L \frac{1}{\pi^2} \delta_\alpha^2(\pi N/L) + O(1) \quad (3.110)$$

$$= -\ln L \frac{1}{\pi^2} \delta_\alpha^2(\sqrt{E}) + o(\ln L), \quad (3.111)$$

where the last line follows from $\pi \frac{N}{L} \rightarrow \sqrt{E}$. Taking the exponential, the assertion follows. \square

Remark 3.24. The above δ -approximation argument is quite similar to the one used in Lemma 2.21.

3.2. Auxiliary Lemmata. In this paragraph we prove the missing lemmata to deduce Theorem 3.20 and also Theorem 3.17. We do not claim to give optimal or elegant estimates. Throughout this section we restrict ourselves to the case $\alpha < 0$ and drop the index α to ease notation. This implies the following estimates on the phase shift

$$\delta(x) \geq \delta(y) \quad \text{and} \quad \delta(x) - \delta(y) \geq 0, \quad (3.112)$$

for $x < y$, which we use in the sequel. The case $\alpha \geq 0$ is even simpler since in that case the definition of the phase shift (3.11) implies the uniform bound

$$\|\delta\|_\infty \leq \frac{\pi}{2}, \quad (3.113)$$

which simplifies some of the following estimates. Moreover, we use the elementary asymptotics:

Lemma 3.25. (i) $\sum_{n \in \mathbb{N}} \frac{1}{n^\beta} < \infty$ for $\beta > 1$.

$$\text{(ii)} \quad \sum_{j=1}^N \sum_{k=N+1}^{\infty} \frac{1}{(k-j)^2} = O(\ln N), \quad \text{as } N \rightarrow \infty.$$

$$\text{(iii)} \quad \sum_{j=1}^N \sum_{k=N+1}^{\infty} \frac{1}{(k-j)^\beta} = O(1) \quad \text{for } \beta > 2, \quad \text{as } N \rightarrow \infty.$$

Proof. Using $\beta > 1$

$$\sum_{n \in \mathbb{N}} \frac{1}{n^\beta} < 1 + \int_1^\infty dx \frac{1}{x^\beta} = 1 + \frac{1}{1-\beta} < \infty. \quad (3.114)$$

Let $\beta \geq 2$. Then, we estimate

$$\begin{aligned} \sum_{j=1}^N \sum_{k=N+1}^{\infty} \frac{1}{(k-j)^\beta} &\leq \sum_{j=1}^N \sum_{k=N+2}^{\infty} \frac{1}{(k-j)^\beta} + \sum_{j=1}^N \frac{1}{(N+1-j)^\beta} \\ &\leq \int_0^N dx \int_{N+1}^\infty dy \frac{1}{(y-x)^\beta} + \sum_{n \in \mathbb{N}} \frac{1}{n^\beta}. \end{aligned} \quad (3.115)$$

Now, (ii) and (iii) follows from evaluating the integral and (i). \square

Lemma 3.26. Set $g_k := -\frac{1}{\pi} \delta(\sqrt{\mu_k})$ for $k \in \mathbb{N}$. Then,

$$\begin{aligned} &\sum_{j=2}^N \sum_{k=N+1}^{\infty} \ln \left(\frac{((k+g_k)^2 - j^2)(k^2 - (j+g_j)^2)}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)} \right) \\ &= - \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{(2jg_j + g_j^2)(2kg_k + g_k^2)}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)} + O(1) \end{aligned} \quad (3.116)$$

as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$.

Proof. We prove the assertion in two steps. First we consider the $j = N$ and $k = N + 1$ summand. Note that Lemma 3.22 above and $E > 0$ imply

$$\lim_{\substack{N, L \rightarrow \infty \\ N/L \rightarrow \sqrt{E}/\pi}} g_N = \lim_{\substack{N, L \rightarrow \infty \\ N/L \rightarrow \sqrt{E}/\pi}} g_{N+1} = -\frac{\delta(\sqrt{E})}{\pi} > -1. \quad (3.117)$$

Thus, for $j = N$ and $k = N + 1$

$$\begin{aligned} & \lim_{\substack{N,L \rightarrow \infty \\ N/L \rightarrow \sqrt{E}/\pi}} \ln \left(\frac{((N+1+g_{N+1})^2 - N^2)((N+1)^2 - (N+g_N)^2)}{((N+1+g_{N+1})^2 - (N+g_N)^2)((N+1)^2 - N^2)} \right) \\ &= \lim_{\substack{N,L \rightarrow \infty \\ N/L \rightarrow \sqrt{E}/\pi}} \ln \left(\frac{(1+g_{N+1})(1-g_N)}{(1+g_{N+1}-g_N)} \frac{(2N+1+g_{N+1})(2N+1+g_N)}{(2N+1+g_{N+1}+g_N)(2N+1)} \right) \\ &= \ln \left(1 - \frac{\delta^2(\sqrt{E})}{\pi^2} \right). \end{aligned} \quad (3.118)$$

Moreover, along the same line using (3.117)

$$\lim_{\substack{N,L \rightarrow \infty \\ N/L \rightarrow \sqrt{E}/\pi}} -\frac{(2N g_N + g_N^2)(2(N+1)g_{N+1} + g_{N+1}^2)}{((N+1+g_{N+1})^2 - (N+g_N)^2)((N+1)^2 - N^2)} = -\frac{\delta^2(\sqrt{E})}{\pi^2}. \quad (3.119)$$

Therefore, the $j = N$ and $k = N + 1$ term is of order 1.

For $j \leq N < N+1 < k$ we want to apply the bound

$$|\ln(1+x) - x| \leq \frac{x^2}{2} \frac{1}{1-|x|} \quad (3.120)$$

for $x \in \mathbb{R}$ with $|x| < 1$, to $x = x_{jk}$ where

$$x_{jk} := -\frac{(2jg_j + g_j^2)(2kg_k + g_k^2)}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)}. \quad (3.121)$$

We estimate using $|g_n| \leq 1$ for all $n \in \mathbb{N}$ and $g_k - g_j \geq 0$

$$\begin{aligned} |x_{jk}| &\leq \left| \frac{(2j+g_j)(2k+g_k)}{(j+g_j+k+g_k)(k+j)} \right| \left| \frac{1}{(k-j+g_k-g_j)(k-j)} \right| \\ &\leq 2 \frac{1}{(k-j)^2}. \end{aligned} \quad (3.122)$$

Since $j \leq N < N+1 < k$, this implies in particular $|x_{jk}| \leq \frac{1}{2}$, and we continue using (3.120) and (3.122)

$$\begin{aligned} \sum_{j=1}^N \sum_{k=N+2}^{\infty} |\ln(1+x_{jk}) - x_{jk}| &\leq \sum_{j=1}^N \sum_{k=N+2}^{\infty} x_{jk}^2 \\ &\leq \sum_{j=2}^N \sum_{k=N+1}^{\infty} 4 \left(\frac{1}{k-j} \right)^4 = O(1), \end{aligned} \quad (3.123)$$

as $N \rightarrow \infty$, where we used Lemma 3.25 in the last line. \square

Lemma 3.27. Define $\delta_k := -\frac{1}{\pi} \delta(\sqrt{\lambda_k})$ for $k \in \mathbb{N}$. Then,

$$\sum_{j=2}^N \sum_{k=N+1}^{\infty} \left| \frac{(2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2)}{((k+\delta_k)^2 - (j+\delta_j)^2)} - \frac{(2jg_j + g_j^2)(2kg_k + g_k^2)}{((k+g_k)^2 - (j+g_j)^2)} \right| \frac{1}{(k-j)^2} = o(1) \quad (3.124)$$

as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$.

Proof. First, using the expansion of Lemma 3.13, we obtain for all $n \in \mathbb{N}$, $n > 1$,

$$|g_n - \delta_n| \leq \frac{1}{\pi} |\delta(\sqrt{\mu_n} - \delta(\sqrt{\lambda_n}))| \leq \frac{\|\delta\|_\infty \|\delta'\|_\infty}{\pi L} := \frac{c}{L}, \quad (3.125)$$

where the constant $c > 0$ depends only on α . We prove the assertion in two steps. In the first step we consider the numerator only in the second step we consider the denominator. Using (3.125) we estimate

$$\begin{aligned} & \sum_{j=2}^N \sum_{k=N+1}^{\infty} \left| \frac{(2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2) - (2jg_j + g_j^2)(2kg_k + g_k^2)}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)} \right| \\ & \leq \frac{C}{L} \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{(j+1)(k+1)}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)} \\ & \leq \frac{C}{L} \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{(j+1)(k+1)}{(k+j-2)(k+j)(k-j)^2} = O\left(\frac{\ln N}{L}\right) \end{aligned} \quad (3.126)$$

as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$, where we used $|g_j + g_k| \leq 2$, $g_k - g_j > 0$ for $j < k$ and Lemma 3.25. In order to estimate the denominator we use (3.125) to obtain some constant $c > 0$ independent of j, k such that

$$\left| \left((k+g_k)^2 - (j+g_j)^2 \right) - \left((k+\delta_k)^2 - (j+\delta_j)^2 \right) \right| \leq c \frac{k+j}{L}. \quad (3.127)$$

Thus,

$$\begin{aligned} & \sum_{j=2}^N \sum_{k=N+1}^{\infty} (2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2) \left| \frac{1}{((k+g_k)^2 - (j+g_j)^2)(k^2 - j^2)} \right. \\ & \quad \left. - \frac{1}{((k+\delta_k)^2 - (j+\delta_j)^2)(k^2 - j^2)} \right| \\ & \leq \frac{4c}{L} \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{jk(k+j)}{(k^2 - j^2)^2 ((k+g_k)^2 - (j+g_j)^2)((k+\delta_k)^2 - (j+\delta_j)^2)} \\ & \leq \frac{4c}{L} \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{jk}{(k-j)^4 (k+j-2)^2 (k+j)} = o(1) \end{aligned} \quad (3.128)$$

as $N, L \rightarrow \infty$, $N/L \rightarrow \frac{\sqrt{E}}{\pi}$, where we used $|g_k + g_j| \leq 2$, $|\delta_k + \delta_j| \leq 2$, $g_k - g_j > 0$ and $\delta_k - \delta_j > 0$ for $j < k$. \square

Lemma 3.28. *The estimate*

$$\left| \sum_{j=2}^N \sum_{k=N+1}^{\infty} \frac{(2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2)}{((k+\delta_k)^2 - (j+\delta_j)^2)(k^2 - j^2)} - \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4jk\delta_j\delta_k}{(k^2 - j^2)^2} \right| = O(1) \quad (3.129)$$

holds as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$.

Proof. First, we bound the tail, i.e. using $\delta_k - \delta_j > 0$ for $k > j$ and $|\delta_n| \leq 1$ for all $n \in \mathbb{N}$ we estimate

$$\begin{aligned} & \sum_{j=2}^N \sum_{k=2N+1}^{\infty} \frac{(2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2)}{((k + \delta_k)^2 - (j + \delta_j)^2)(k^2 - j^2)} \leq \sum_{j=2}^N \sum_{k=2N+1}^{\infty} \frac{1}{(k - j)^2} \\ & \leq \sum_{k=2N+1}^{\infty} \frac{N}{(k - N)^2} = O(1), \end{aligned} \quad (3.130)$$

as $N \rightarrow \infty$. We insert $\pm \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4jk\delta_j\delta_k}{((k + \delta_k)^2 - (j + \delta_j)^2)(k^2 - j^2)}$ in (3.129). Thus, in the next step $\delta_k - \delta_j > 0$ yields

$$\begin{aligned} & \sum_{j=2}^N \sum_{k=N+1}^{2N} \left| \frac{(2j\delta_j + \delta_j^2)(2k\delta_k + \delta_k^2) - 4jk\delta_j\delta_k}{((k + \delta_k)^2 - (j + \delta_j)^2)(k^2 - j^2)} \right| \\ & \leq \sum_{j=2}^N \sum_{k=N+1}^{2N} \left| \frac{2(k+j) + 1}{(k-j)^2(k+j)(k+j-2)} \right| \\ & \leq 3 \sum_{j=2}^N \sum_{k=N+1}^{2N} \left| \frac{1}{(k-j)^2(k+j-2)} \right| = O\left(\frac{\ln N}{N}\right), \end{aligned} \quad (3.131)$$

as $N \rightarrow \infty$, where we used Lemma 3.25 in the last line. In the third step, again $|\delta_n| \leq 1$ for $n \in \mathbb{N}$ yields

$$\begin{aligned} & \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4jk}{(k^2 - j^2)} \left| \frac{1}{((k + \delta_k)^2 - (j + \delta_j)^2)} - \frac{1}{(k^2 - j^2)} \right| \\ & \leq \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{9jk(k+j)}{(k^2 - j^2)^2(k+j-2)(k-j)} \\ & \leq 9 \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{1}{(k-j)^3} = O(1), \end{aligned} \quad (3.132)$$

as $N \rightarrow \infty$, where we used Lemma 3.25. \square

Lemma 3.29. *The asymptotics*

$$\left| \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4jk\delta_j\delta_k}{(k^2 - j^2)^2} - \frac{1}{\pi^2} \int_0^{\frac{N}{L}} dx \int_{\frac{N+1}{L}}^{\frac{2N}{L}} dy \frac{4xy\delta(x\pi)\delta(y\pi)}{(y^2 - x^2)^2} \right| = O(1) \quad (3.133)$$

holds as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$.

Proof. We recall that $\delta_k := -\frac{1}{\pi}\delta(\sqrt{\lambda_k})$ and we rewrite

$$\sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4jk\delta_j\delta_k}{(k^2 - j^2)^2} = \frac{1}{L^2\pi^2} \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{4\frac{j}{L}\frac{k}{L}\delta\left(\frac{j\pi}{L}\right)\delta\left(\frac{k\pi}{L}\right)}{\left(\left(\frac{k}{L}\right)^2 - \left(\frac{j}{L}\right)^2\right)^2}. \quad (3.134)$$

Thus, we estimate

$$\begin{aligned} & \left| \frac{1}{L^2} \sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{\frac{j}{L} \frac{k}{L} \delta\left(\frac{j\pi}{L}\right) \delta\left(\frac{k\pi}{L}\right)}{\left(\left(\frac{k}{L}\right)^2 - \left(\frac{j}{L}\right)^2\right)^2} - \int_{\frac{1}{L}}^{\frac{N}{L}} dx \int_{\frac{N+1}{L}}^{\frac{2N+1}{L}} dy \frac{xy\delta(x\pi)\delta(y\pi)}{(y^2 - x^2)^2} \right| \\ & \leq \sum_{j=2}^N \sum_{k=N+1}^{2N} \int_{\frac{j-1}{L}}^{\frac{j}{L}} dx \int_{\frac{k}{L}}^{\frac{k+1}{L}} dy \left| f\left(\frac{j}{L}, \frac{k}{L}\right) - f(x, y) \right|, \end{aligned} \quad (3.135)$$

where

$$f(x, y) := \frac{xy\delta(x\pi)\delta(y\pi)}{(y^2 - x^2)^2}. \quad (3.136)$$

Using the mean-value theorem and the Cauchy-Schwarz inequality we obtain

$$\begin{aligned} (3.135) & \leq \sum_{j=2}^N \sum_{k=N+1}^{2N} \sup_{(x,y) \in (\frac{j-1}{L}, \frac{j}{L}) \times (\frac{k}{L}, \frac{k+1}{L})} |(\nabla f)(x, y)|_2 \\ & \quad \times \int_{\frac{j-1}{L}}^{\frac{j}{L}} dx \int_{\frac{k}{L}}^{\frac{k+1}{L}} dy \left| \left(\frac{j}{L} - x, \frac{k}{L} - y \right) \right|_2 \\ & \leq \frac{1}{L^3} \sum_{j=2}^N \sum_{k=N+1}^{2N} \sup_{(x,y) \in (\frac{j-1}{L}, \frac{j}{L}) \times (\frac{k}{L}, \frac{k+1}{L})} |(\nabla f)(x, y)|_2, \end{aligned} \quad (3.137)$$

where $|\cdot|_2$ denotes the Euclidean norm. We compute

$$(\nabla f)(x, y) = \frac{1}{(y^2 - x^2)^3} \quad (3.138)$$

$$\begin{aligned} & \times \left(\frac{(y^2 - x^2)(y\delta(x\pi)\delta(y\pi) + xy\delta'(x\pi)\delta(y\pi)\pi) + 4x^2y\delta(x\pi)\delta(y\pi)}{(y^2 - x^2)(x\delta(x\pi)\delta(y\pi) + xy\delta(x\pi)\delta'(y\pi)\pi) - 4xy^2\delta(x\pi)\delta(y\pi)} \right) \\ & =: \frac{1}{(y^2 - x^2)^3} g(x, y). \end{aligned} \quad (3.139)$$

We estimate for $(x, y) \in (\frac{j-1}{L}, \frac{j}{L}) \times (\frac{k}{L}, \frac{k+1}{L})$, $j \leq N < k$,

$$\left(\frac{1}{y^2 - x^2} \right)^3 \leq \frac{L^6}{(k+j-1)^3 (k-j)^3} \leq \frac{L^6}{N^3} \frac{1}{(k-j)^3} \quad (3.140)$$

and, using $\delta, \delta' \in L^\infty((0, \infty))$,

$$\sup_{(x,y) \in (\frac{j-1}{L}, \frac{j}{L}) \times (\frac{k}{L}, \frac{k+1}{L})} |g(x, y)|_2 \leq \sup_{(x,y) \in (0, \frac{2N+1}{L}) \times (0, \frac{2N+1}{L})} |g(x, y)|_2 = O(1) \quad (3.141)$$

as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$. Thus, (3.140) and (3.141) imply

$$(3.137) \leq O \left(\sum_{j=2}^N \sum_{k=N+1}^{2N} \frac{1}{(y - x)^3} \right) = O(1) \quad (3.142)$$

as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$. \square

4. The Ground-State Overlap for Bosons

In this section we comment on a related problem of academic interest which is the asymptotics of the ground-state overlap in the case of bosons. Since for bosons the underlying Hilbert space is the symmetrised tensor product, all particles can be in the same state. Therefore, the ground state of a non-interacting N -particle Bose gas is just the tensor product of the eigenfunction belonging to the lowest one-particle energy. Thus, the problem of computing the ground-state overlap consists of computing a single one-particle scalar product only. We compute this scalar product and prove the asymptotics of the ground-state for a model on the half axis with a Dirac- δ perturbation at the origin because in this way we can treat the 3-dimensional case simultaneously. In the physical literature this problem is treated in [RSS04] and their results are similar to our findings.

Theorem 3.30. *Let $\alpha \geq 0$, and φ_1^L and ψ_1^L be the ground states of the operators h_L^0 and $h_{\alpha,L}^0$ defined in (3.51). Then, its scalar product admits the asymptotics*

$$\langle \varphi_1^L, \psi_1^L \rangle = 1 - \frac{\delta'_\alpha(0)^2}{L^2} \left(\frac{\pi^2}{6} + \frac{1}{8} \right) + O\left(\frac{1}{L^3}\right) \quad (3.143)$$

as $L \rightarrow \infty$.

Remarks 3.31. (i) The quantity $\delta'_\alpha(0)$ is called the scattering length, see e.g. [RS79, Sct. XI.8].

(ii) The $\frac{1}{L^2}$ correction instead of a $\frac{1}{L}$ correction is due to the comparison of the ground states.

Since $\exp(x) = \lim_{n \rightarrow \infty} \left(1 + \frac{x}{n}\right)^n$ for $x \in \mathbb{R}$, the above theorem allows us to determine the asymptotics of the ground-state overlap for systems on the half axis. Moreover, using the angular momentum decomposition, we treat in this way also the asymptotics of a 3-dimensional system with a Dirac- δ perturbation at the origin defined in Section 2 above.

Corollary 3.32. *Let $\rho > 0$ and set*

$$\theta := \delta'_\alpha(0)^2 \left(\frac{\pi^2}{6} + \frac{1}{8} \right). \quad (3.144)$$

Then,

(i) as $N, L \rightarrow \infty$ and $N/L \rightarrow \rho$ we obtain the asymptotics

$$(\langle \varphi_1^L, \psi_1^L \rangle)^N = \exp\left(-\frac{1}{L}\rho\theta + o(1)\right), \quad (3.145)$$

and in particular

$$\lim_{\substack{N, L \rightarrow \infty \\ N/L \rightarrow \rho}} (\langle \varphi_1^L, \psi_1^L \rangle)^N = 1. \quad (3.146)$$

(ii) as $N, L \rightarrow \infty$ and $N/L^3 \rightarrow \rho$ we obtain the asymptotics

$$(\langle \varphi_1^L, \psi_1^L \rangle)^N = \exp(-L\rho\theta + o(1)), \quad (3.147)$$

and in particular

$$\lim_{\substack{N, L \rightarrow \infty \\ N/L^3 \rightarrow \rho}} (\langle \varphi_1^L, \psi_1^L \rangle)^N = 0. \quad (3.148)$$

Remarks 3.33. (i) Corollary 3.32 shows that the asymptotics of the ground-state overlap for bosons depends in general on the space dimension.

(ii) A more elaborate proof using the same ideas, yields Theorem 3.30 also for the pair $-\Delta$ and $-\Delta + V$ on $L^2((0, \infty))$, where V is a multiplication operator with sufficient decay at infinity. Thus, in principle using the angular momentum decomposition one can prove the above asymptotics for 3-dimensional systems with a spherically symmetric perturbation V .

(iii) In the $d = 2$ case there might be some intermediate behaviour of the ground-state overlap. Note that one cannot just raise the asymptotics deduced in Theorem 3.30 to the power L^2 . The angular momentum decomposition in $d = 2$ yields in the lowest angular momentum channel a different operator, namely

$$-\Delta - \frac{1}{4|\cdot|^2}. \quad (3.149)$$

Thus, the eigenfunctions corresponding to the lowest eigenvalue are not as easy as in the case considered in Theorem 3.30. Even asymptotically in L , Theorem 3.30 might be wrong in the $d = 2$ case, see [RSS04].

Proof of Theorem 3.30. For brevity, we drop the subscript α of the phase shift in the proof. Since we assumed $\alpha \geq 0$, we use Lemma 3.13 and equation (3.68) to see that the eigenfunctions of h_L^0 and $h_{\alpha,L}^0$ corresponding to the lowest eigenvalues λ_1^L and μ_1^L are up to a phase

$$\tilde{\varphi}_1^L(x) := \sin(\sqrt{\lambda_1^L}x) \quad \text{and} \quad \tilde{\psi}_1^L(x) = \sin(\sqrt{\mu_1^L}x + \delta(\sqrt{\mu_1^L})), \quad (3.150)$$

where $x \in (0, L)$ and δ is defined in Definition 3.11. Thus, we see that the normalised eigenfunctions are given by

$$\varphi_1^L := \frac{\tilde{\varphi}_1^L}{\|\tilde{\varphi}_1^L\|_2} \quad \text{and} \quad \psi_1^L := \frac{\tilde{\psi}_1^L}{\|\tilde{\psi}_1^L\|_2}, \quad (3.151)$$

where $\|\cdot\|_2$ denotes the $L^2((0, L))$ norm. Moreover, we set $a := \sqrt{\lambda_1^L} = \frac{\pi}{L}$ and $b := \sqrt{\mu_1^L}$. Then, a and b satisfy the identity

$$b = a - \frac{\delta(b)}{L}, \quad (3.152)$$

by Lemma 3.13, which we use intensively in the proof. We compute

$$\|\tilde{\varphi}_1^L\|^2 = \int_0^L dx \sin^2(ax) = \frac{1}{a} \int_0^{aL} dx \sin^2(x) = \frac{L}{2}, \quad (3.153)$$

and use the identity (3.152) to obtain

$$\|\tilde{\psi}_1^L\|^2 = \int_0^L dx \sin^2(bx + \delta(b)) = \frac{L}{2} + \frac{\sin(2\delta(b))}{4b}. \quad (3.154)$$

Moreover, we continue

$$\begin{aligned}
\langle \tilde{\varphi}_1^L, \tilde{\psi}_1^L \rangle &= \int_0^L dx \sin(ax) \sin(bx + \delta(b)) \\
&= \int_0^L dx \sin^2 \left(\frac{1}{2}((a+b)x + \delta(b)) \right) - \sin^2 \left(\frac{1}{2}((a-b)x - \delta(b)) \right) \\
&= \frac{1}{2(a+b)} \left((a+b)L - \sin((a+b)L + \delta(b)) + \sin(\delta(b)) \right) \\
&\quad - \frac{1}{2(a-b)} \left((a-b)L - \sin((a-b)L - \delta(b)) + \sin(-\delta(b)) \right) \\
&= \frac{\pi L \sin(\delta(b))}{\delta(b)(2\pi - \delta(b))}, \tag{3.155}
\end{aligned}$$

where we used the identities $a+b = \frac{2\pi}{L} - \frac{\delta(b)}{L}$ and $a-b = \frac{\delta(b)}{L}$ in the last line. Thus, (3.153), (3.154) and (3.155) imply

$$\begin{aligned}
\langle \varphi_1^L, \psi_1^L \rangle &= \frac{\langle \tilde{\varphi}_1^L, \tilde{\psi}_1^L \rangle}{\|\tilde{\varphi}_1^L\| \|\tilde{\psi}_1^L\|} \\
&= \frac{\sin(\delta(b))}{\delta(b) \left(1 - \frac{\delta(b)}{2\pi} \right) \left(1 + \frac{1}{2Lb} \sin(2\delta(b)) \right)^{1/2}}. \tag{3.156}
\end{aligned}$$

The definitions of a , b and δ imply the following expansion

$$\delta(b) = \frac{\delta'(0)\pi}{L} - \frac{\delta'(0)^2\pi}{L^2} + \frac{\delta''(0)\pi^2}{2L^2} + O\left(\frac{1}{L^3}\right). \tag{3.157}$$

This yields

$$\frac{\sin(\delta(b))}{\delta(b)} = 1 - \frac{\delta'(0)^2\pi^2}{6L^2} + O\left(\frac{1}{L^3}\right) \tag{3.158}$$

$$\frac{\sin(2\delta(b))}{2b} = \delta'(0) + \frac{\delta''(0)\pi}{2L} + O\left(\frac{1}{L^2}\right) \tag{3.159}$$

and in particular

$$\left(1 - \frac{\delta(b)}{2\pi} \right) = 1 - \frac{\delta'(0)}{2L} + \frac{\delta'(0)^2}{2L^2} - \frac{\delta''(0)\pi}{4L^2} + O\left(\frac{1}{L^3}\right). \tag{3.160}$$

Now, to determine the asymptotics of the second term in (3.156), we use $\sqrt{1+x} = 1 + \frac{x}{2} - \frac{x^2}{8} + O(x^3)$ as $|x| \rightarrow 0$ and (3.159) to obtain

$$\begin{aligned}
\left(1 + \frac{1}{L} \frac{\sin(2\delta(b))}{2b} \right)^{1/2} &= 1 + \frac{1}{2L} \frac{\sin(2\delta(b))}{2b} - \frac{1}{8L^2} \left(\frac{\sin(\delta(b))}{2b} \right)^2 + O\left(\frac{1}{L^3}\right) \\
&= 1 + \frac{\delta'(0)}{2L} + \frac{\delta''(0)\pi}{4L^2} - \frac{\delta'(0)^2}{8L^2} + O\left(\frac{1}{L^3}\right) \tag{3.161}
\end{aligned}$$

Thus, equation (3.160) and (3.161) imply

$$\left(1 - \frac{\delta(b)}{2\pi} \right) \left(1 + \frac{1}{2Lb} \sin(2\delta(b)) \right)^{1/2} = 1 + \frac{\delta'(0)^2}{8L^2} + O\left(\frac{1}{L^3}\right) \tag{3.162}$$

and

$$\left(\left(1 - \frac{\delta(b)}{2\pi} \right) \left(1 + \frac{1}{2Lb} \sin(2\delta(b)) \right)^{1/2} \right)^{-1} = 1 - \frac{\delta'(0)^2}{8L^2} + O\left(\frac{1}{L^3}\right). \tag{3.163}$$

Therefore, equations (3.156), (3.158) and (3.163) give

$$\langle \varphi_1^L, \psi_1^L \rangle = 1 - \frac{\delta'(0)^2}{L^2} \left(\frac{\pi^2}{6} + \frac{1}{8} \right) + O\left(\frac{1}{L^3}\right). \quad (3.164)$$

□

CHAPTER 4

The Asymptotics of the Difference of the Ground-State Energies

In the two previous chapters we computed the asymptotics of the scalar-product of the ground-states of two non-interacting Fermi gases. In this chapter we consider the difference of the corresponding ground-state energies. Again, we begin with a more general discussion of the asymptotics of this difference. Later, we show a more detailed analysis for systems on the half axis.

1. The General Case

Here, we consider rather general Schrödinger operators similar to those treated in Chapter 2, equations (2.1) and (2.2). But for simplicity we omit the background potential V_0 . We denote by

$$H := -\Delta \quad \text{and} \quad H' := -\Delta + V \quad (4.1)$$

a pair of Schrödinger operators defined on $L^2(\mathbb{R}^d)$ and by

$$H_L := -\Delta_L \quad \text{and} \quad H'_L := -\Delta_L + V, \quad (4.2)$$

its restriction to $L^2(\Lambda_L)$, where for $L > 1$ we set $\Lambda_L := L\Lambda_1$ and $0 \in \Lambda_1 \subset \mathbb{R}^d$ open. Moreover, $-\Delta_L$ denotes the restriction of the negative Laplacian $-\Delta$ to the finite volume Λ_L with Dirichlet boundary conditions. The perturbation V is a multiplication operator such that

$$V \geq 0, \quad V \in K_{\text{loc}}^d(\mathbb{R}^d), \quad \text{supp } V \subset \Lambda_1 \text{ compact.} \quad (4.3)$$

For a more detailed description of these operators we refer to Chapter 2. Now, we denote by $\lambda_1^L \leq \lambda_2^L \leq \dots$ and $\mu_1^L \leq \mu_2^L \leq \dots$ the increasing sequences of the eigenvalues of the finite-volume operators H_L , respectively H'_L counting multiplicities.

In this chapter we are not interested in the asymptotics of the scalar product of the non-interacting N -particle ground states but in the asymptotics of the difference of the ground-state energies of the non-interacting N -particle Fermi gases in the thermodynamic limit. We denote the sum of the N smallest eigenvalues by

$$E_L^N := \sum_{k=1}^N \lambda_k^L \quad \text{and} \quad E'_L^N := \sum_{j=1}^N \mu_j^L. \quad (4.4)$$

The goal is to deduce the asymptotics of the difference $\Xi_L^N := E'_L^N - E_L^N$ in the thermodynamic limit.

To state the result, let $\xi \in L^1_{\text{loc}}(\mathbb{R})$ be the spectral-shift function for the pair of infinite-volume operators H and H' . There are numerous definitions of the spectral-shift function, see e.g. [Yaf92, Chap. 8] or [BP98] for a more comprehensive summary of the definitions of the spectral-shift function.

Remarks 4.1. (i) Most intuitively, the spectral-shift function ξ is defined by the trace formula

$$\mathrm{tr} \{ \varphi(H') - \varphi(H) \} = \int_{\mathbb{R}} dx \varphi'(x) \xi(x) \quad (4.5)$$

for all $\varphi \in C_c^\infty(\mathbb{R})$. Unfortunately, the above identity only determines ξ up to an additive constant. Let us briefly sketch how to erase this. We consider a strictly monotone function $\theta \in C^\infty(\mathbb{R})$ such that $\theta(H') - \theta(H)$ is trace class, e.g. $\theta(x) := e^{-tx}$. Then, results for trace-class perturbations [Yaf92, Sct. 8.3] show the existence of a function $\tilde{\xi} \in L^1(\mathbb{R})$ such that

$$\mathrm{tr} \{ \varphi(\theta(H')) - \varphi(\theta(H)) \} = \int_{\mathbb{R}} dx \varphi'(x) \tilde{\xi}(x) \quad (4.6)$$

for all $\varphi \in C_c^\infty(\mathbb{R})$. It can be chosen uniquely according to

$$\| \theta(H') - \theta(H) \|_1 = \int_{\mathbb{R}} dx |\tilde{\xi}(x)|, \quad (4.7)$$

where $\|\cdot\|_1$ stands for the trace norm. Hence, we define $\xi(E) := \mathrm{sign}(\theta'(E)) \tilde{\xi}(\theta(E))$. One can find a more detailed derivation of the spectral-shift function for non trace-class perturbations in [HM10, App. 5].

(ii) In the case of a system on the half-axis, there is another simple representation of the spectral-shift function. One can identify the spectral-shift function with the scattering phase shift, see (4.33) in the next section.

Theorem 4.2. Let $E > 0$ and $N_{(\cdot)}(E) : \mathbb{R}_+ \rightarrow \mathbb{N}$ be a function subject to

$$\frac{N_L(E)}{|\Lambda_L|} \rightarrow \rho(E), \quad (4.8)$$

as $L \rightarrow \infty$, where $\rho(E)$ denotes the integrated density of states of the operator $-\Delta$. Then,

$$\lim_{L \rightarrow \infty} \Xi_L^{N_L(E)} := E_L'^{N_L(E)} - E_L^{N_L(E)} = \int_{-\infty}^E dx \xi(x). \quad (4.9)$$

Remarks 4.3. (i) The precise value of $\rho(E)$ is given in (2.29).

(ii) The proof should extend to the case, where a background potential is present provided the integrated density of states of the unperturbed operator exists and is equal to the one of the perturbed operator.

(iii) The compact support of the perturbation V is not essential, sufficient decay should be enough. We assumed this for simplicity because the main ingredient to the proof [HM10] did so.

Proof. First, we rewrite the difference $\Xi_L^{N_L(E)}$ in terms of the finite-volume spectral-shift function. We define the finite-volume spectral-shift function $\xi_L : \mathbb{R}_{\geq 0} \rightarrow \mathbb{N}_0$ by

$$E \mapsto \xi_L(E) := \# \{ k : \lambda_k^L \leq E \} - \# \{ j : \mu_j^L \leq E \} \geq 0. \quad (4.10)$$

Here, the non-negativity of the perturbation V implies $\xi_L(E) \geq 0$. For $E > 0$ the following holds

$$\int_{-\infty}^E dx \xi_L(x) = \sum_{\lambda_k \leq E} (\min\{\mu_k^L, E\} - \lambda_k^L), \quad (4.11)$$

which can be seen, for example, by introducing the two measures $\mu : A \mapsto \text{tr}(1_A(H_L))$ and $\nu : A \mapsto \text{tr}(1_A(H'_L))$ for $A \in \text{Borel}(\mathbb{R})$ and the following computation using the definition of ξ_L in (4.10) and Fubini's theorem

$$\begin{aligned} \int_{-\infty}^E dx \xi_L(x) &= \int_{\mathbb{R}} dx \int_{\mathbb{R}} d\mu(y) 1\{y \leq x \leq E\} - \int_{\mathbb{R}} dx \int_{\mathbb{R}} d\nu(y) 1\{y \leq x \leq E\} \\ &= \text{tr}\{(E - H_L)1\{H_L \leq E\}\} - \text{tr}\{(E - H'_L)1\{H'_L \leq E\}\} \\ &= E\xi_L(E) + \sum_{\substack{\mu_k^L \leq E \\ \lambda_k^L \leq E}} \mu_k^L - \sum_{\lambda_k^L \leq E} \lambda_k^L \\ &= \sum_{\substack{k \in \mathbb{N}: \\ \lambda_k^L \leq E}} (\min\{\mu_k^L, E\} - \lambda_k^L). \end{aligned} \quad (4.12)$$

We use the short-hand notation $\Xi_L(E) \equiv \Xi_L^{N_L(E)}$ and $N \equiv N_L(E)$. Hence, using (4.11)

$$\Xi_L(E) = \sum_{k=1}^N (\mu_k^L - \lambda_k^L) = \int_{-\infty}^{\lambda_N^L} dx \xi_L(x) + \sum_{k=1}^N \max\{\mu_k^L - \lambda_N^L, 0\}. \quad (4.13)$$

Now, [HM10, Thm. 1.4] implies for all $E > 0$

$$\int_{-\infty}^E dx \xi_L(x) \rightarrow \int_{-\infty}^E dx \xi(x), \quad (4.14)$$

as $L \rightarrow \infty$. Therefore, it suffices to prove

$$\left| \Xi_L(E) - \int_{-\infty}^E dx \xi_L(x) \right| \rightarrow 0, \quad (4.15)$$

as $L \rightarrow \infty$. Since Lemma 4.4 below yields $\lim_{L \rightarrow \infty} \lambda_N^L = E$, we begin with the estimate

$$\begin{aligned} \lim_{L \rightarrow \infty} \left| \int_{-\infty}^E dx \xi_L(x) - \int_{-\infty}^{\lambda_N^L} dx \xi_L(x) \right| &= \lim_{L \rightarrow \infty} \left| \int_{\lambda_N^L}^E dx \xi_L(x) \right| \\ &\leq \lim_{\epsilon \searrow 0} \lim_{L \rightarrow \infty} \int_{E-\epsilon}^{E+\epsilon} dx \xi_L(x) \\ &= \lim_{\epsilon \searrow 0} \int_{E-\epsilon}^{E+\epsilon} dx \xi(x). \end{aligned} \quad (4.16)$$

Recalling that $\xi \in L^1_{\text{loc}}(\mathbb{R})$, dominated convergence implies for all $E \in \mathbb{R}$

$$(4.16) = \lim_{\epsilon \searrow 0} \int_{\mathbb{R}} dx 1_{(E-\epsilon, E+\epsilon)}(x) \xi(x) = \int_{\mathbb{R}} dx \lim_{\epsilon \searrow 0} 1_{(E-\epsilon, E+\epsilon)}(x) \xi(x) = 0. \quad (4.17)$$

We estimate the remaining sum on the r.h.s. of (4.13) by adding an additional term

$$\sum_{k=1}^N \max\{\mu_k^L - \lambda_N^L, 0\} \leq \left(\sum_{k=1}^N \max\{\mu_k^L - \lambda_N^L, 0\} + \sum_{\substack{k > N: \\ \lambda_k^L \leq \mu_N^L}} (\mu_N^L - \lambda_k^L) \right) \quad (4.18)$$

and we rewrite the above in a more complicated way

$$\begin{aligned}
(4.18) &= \left(\sum_{k=1}^N (\min\{\mu_k^L, \mu_N^L\} - \min\{\mu_k^L, \lambda_N^L\}) + \sum_{\substack{k>N: \\ \lambda_k^L \leq \mu_N^L}} (\min\{\mu_k^L, \mu_N^L\} - \lambda_k^L) \right) \\
&= \left(\sum_{\substack{k \in \mathbb{N}: \\ \lambda_k^L \leq \mu_N^L}} (\min\{\mu_k^L, \mu_N^L\} - \lambda_k^L) - \sum_{\substack{k \in \mathbb{N}: \\ \lambda_k^L \leq \lambda_N^L}} (\min\{\mu_k^L, \lambda_N^L\} - \lambda_k^L) \right) \\
&= \int_{\lambda_L^N}^{\mu_N^L} dx \xi_L(x),
\end{aligned} \tag{4.19}$$

where we used in the last line (4.11). Lemma 4.4 provides $\lambda_N^L \rightarrow E$ as well as $\mu_N^L \rightarrow E$. This and the above computation show

$$\begin{aligned}
\lim_{L \rightarrow \infty} \sum_{k=1}^N \max \{ \mu_k^L - \lambda_N^L, 0 \} &\leq \lim_{L \rightarrow \infty} \int_{\lambda_L^N}^{\mu_N^L} dx \xi_L(x) \\
&\leq \lim_{\epsilon \searrow 0} \lim_{L \rightarrow \infty} \int_{E-\epsilon}^{E+\epsilon} dx \xi_L(x) \\
&= \lim_{\epsilon \searrow 0} \int_{E-\epsilon}^{E+\epsilon} dx \xi(x) = 0,
\end{aligned} \tag{4.20}$$

for all $E > 0$, where we used again the weak convergence found in [HM10] and (4.17). Hence, we proved (4.15), and in turn the theorem. \square

Lemma 4.4. *Let $E > 0$ and $N_{(\cdot)}(E) : \mathbb{R}_+ \rightarrow \mathbb{N}$ be a function subject to*

$$\frac{N_L(E)}{|\Lambda_L|} \rightarrow \rho(E), \tag{4.21}$$

where $\rho(E)$ denotes the integrated density of states of the operator $-\Delta$. Then,

$$\lim_{L \rightarrow \infty} \mu_{N_L(E)}^L = E \quad \text{and} \quad \lim_{L \rightarrow \infty} \lambda_{N_L(E)}^L = E. \tag{4.22}$$

Proof. First, we note that the integrated densities of states of both operators H and H' exist and are equal. More precisely, the following limits exists

$$\lim_{L \rightarrow \infty} \frac{\#\{k : \lambda_k^L \leq E\}}{|\Lambda_L|} = \lim_{L \rightarrow \infty} \frac{\#\{k : \mu_k^L \leq E\}}{|\Lambda_L|} = \rho(E), \tag{4.23}$$

where ρ is the integrated density of states of $-\Delta$ and is given by (2.29). The latter convergences and the equality follows from the convergence of the Laplace transform of the measure $\tilde{\mu} : A \mapsto \frac{1}{|\Lambda_L|} \text{tr}\{1_A(H_L)\}$ and $\tilde{\nu} : A \mapsto \frac{1}{|\Lambda_L|} \text{tr}\{1_A(H'_L)\}$, where $A \in \text{Borel}(\mathbb{R})$, to the same limit. This can be seen from the explicit integral kernel of the finite-volume semigroup operator, see [BHL00] or [PF92, Sct. 5].

Now, we come to the proof of equation (4.22). We restrict ourselves to the case of H' , the other case follows along the same line. We denote by $\tilde{N}_L(E) := \#\{k : \mu_k^L \leq E\}$. Thus, the convergence (4.23) implies $\tilde{N}_L(E) \sim \rho(E)|\Lambda_L|$ as $L \rightarrow \infty$ and (4.21) gives

$$|N_L(E) - \tilde{N}_L(E)| \sim o(|\Lambda_L|) \tag{4.24}$$

as $L \rightarrow \infty$. The integrated density of states ρ is strictly increasing, see (2.29). Hence, for a given $\epsilon > 0$ equation (4.24) provides the estimate $\tilde{N}_L(E - \epsilon) < N_L(E) < \tilde{N}_L(E + \epsilon)$, as $L \rightarrow \infty$. Thus, $E - \epsilon \leq \mu_{N_L(E)}^L \leq E + \epsilon$, as $L \rightarrow \infty$. \square

2. Finite-Size Energy for Non-Interacting Fermions

In this section we compute the asymptotics of the difference of the ground-state energies of two non-interacting Fermi gases on the half axis in the thermodynamic limit up to second order, i.e. we quantify the error in Theorem 4.2 in terms of L .

2.1. Model and Results. We consider a non-negative, continuous potential $0 \leq V \in C((0, \infty))$ satisfying

$$\int_0^\infty dx V(x) (1 + x^2) < \infty. \quad (4.25)$$

Then, we define the pair of one-particle Schrödinger operators on $L^2((0, \infty))$

$$H := -\Delta \quad \text{and} \quad H' := -\Delta + V, \quad (4.26)$$

where $-\Delta$ denotes the negative Laplacian on $(0, \infty)$ with Dirichlet boundary condition at 0. Apparently, H coincides with h^0 defined in Chapter 3. Moreover, let $L > 0$ and $-\Delta_L$ be the negative Laplacian on the interval $(0, L)$ with Dirichlet boundary conditions. We denote the finite-volume one-particle Schrödinger operators on $L^2((0, L))$ by

$$H_L := -\Delta_L \quad H'_L := -\Delta_L + V. \quad (4.27)$$

Here, V is understood as the canonical restriction of V to the interval $(0, L)$. These are densely defined self-adjoint operators on the Hilbert space $L^2((0, L))$ with compact resolvents. Thus, both operators admit an ONB of eigenfunctions and we denote, as before, the corresponding non-decreasing sequences of the eigenvalues, counting multiplicities by $\lambda_1^L \leq \lambda_2^L \leq \dots$ and $\mu_1^L \leq \mu_2^L \leq \dots$. The eigenvalues of H_L are $\lambda_n^L = \left(\frac{n\pi}{L}\right)^2$, $n \in \mathbb{N}$, see e.g. [RS78], and we denote the sum of the N smallest eigenvalues of H_L , respectively H'_L , by

$$E_L^N := \sum_{k=1}^N \lambda_k^L \quad \text{and} \quad E_L'^N := \sum_{j=1}^N \mu_j^L. \quad (4.28)$$

Moreover, for a given Fermi energy $E > 0$ and some number of particles $N \in \mathbb{N}$, we choose the system length L such that

$$\frac{N}{L} \rightarrow \rho(E) := \frac{\sqrt{E}}{\pi}, \quad (4.29)$$

as $L \rightarrow \infty$, where ρ is the integrated density of states of the infinite-volume operator H .

In order to state our result we have to introduce the scattering phase shift. We follow [Cal67] or [RS79, Thm. XI.54] and define.

Definition 4.5. Let $k > 0$. Then, we denote by δ_k the solution of the ODE

$$\delta'_k(x) = -\frac{1}{k} V(x) \sin^2(kx + \delta_k(x)), \quad x > 0 \quad (4.30)$$

with the boundary condition $\limsup_{x \rightarrow 0} \frac{1}{x} |\delta_k(x)| < \infty$. Moreover, we define the scattering phase shift for the pair of operators H and H' by

$$\lim_{x \rightarrow \infty} \delta_k(x) = \delta(k). \quad (4.31)$$

Remarks 4.6. (i) Existence and uniqueness of the solution of the ODE (4.30) follows from a standard fix point argument, see e.g. [RS72, Sct. V.6].

(ii) Assumption (4.25) implies $V \in L^1((0, \infty))$, thus, the limit in (4.31) is well defined and finite.

(iii) From the ODE it is obvious that for $V \geq 0$

$$\delta(k) \leq 0. \quad (4.32)$$

(iv) Let $\xi \in L^1_{\text{loc}}(\mathbb{R})$ again be the infinite-volume spectral-shift function for the pair of operators H, H' as defined in Remark 4.1(i). Then, we have the identity [BY92]

$$\frac{1}{\pi} \delta(\sqrt{E}) = -\xi(E), \quad (4.33)$$

for every $E > 0$.

(v) Similar to the chapter before, here the scattering matrix is just a number of modulus one; $S_E = \exp(2i\delta(\sqrt{E}))$. Let $T_E := S_E - 1$ be the transition matrix. Then, we define for $E > 0$

$$\gamma(E) := \frac{1}{\pi^2} \delta^2(\sqrt{E}) \quad (4.34)$$

and remark that the constant γ is the decay exponent which determines the asymptotics of the ground-state overlap in the previous Chapter 3 for Dirac- δ perturbations.

Using the notation of Remark 4.6(iv), the result of this chapter is the following.

Theorem 4.7. *For all Fermi energies $E > 0$ the difference of the ground-state energies admits the asymptotics*

$$\begin{aligned} E_L'^N - E_L^N &= -\frac{1}{\pi} \int_{-\infty}^{\left(\frac{N\pi}{L}\right)^2} dx \delta(\sqrt{x}) + \frac{\sqrt{E}}{L} \left(-\delta(\sqrt{E}) + \frac{1}{\pi} \delta^2(\sqrt{E}) \right) + o\left(\frac{1}{L}\right) \\ &= \int_{-\infty}^E dx \xi(x) + \int_E^{\left(\frac{N\pi}{L}\right)^2} dx \xi(x) + \frac{\sqrt{E}\pi}{L} (\xi(E) + \gamma(E)) + o\left(\frac{1}{L}\right) \end{aligned} \quad (4.35)$$

as $N, L \rightarrow \infty$, and $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$.

Remarks 4.8. (i) The first term in the expansion is not surprising since Theorem 4.2 implies

$$\lim_{\substack{N, L \rightarrow \infty \\ N/L \rightarrow \rho(E) > 0}} (E_L'^N - E_L^N) = \int_{-\infty}^E dx \xi(x), \quad (4.36)$$

at least in the case of a compactly supported perturbation. In the case of systems on the half-axis equation (4.36) follows also from [BM12].

(ii) Since ξ is continuous, see Lemma 4.12 below,

$$\int_E^{\left(\frac{N\pi}{L}\right)^2} dx \xi(x) = \left(\left(\frac{N\pi}{L} \right)^2 - E \right) \xi(E) + o\left(\left(\frac{N\pi}{L} \right)^2 - E \right) \quad (4.37)$$

as $N, L \rightarrow \infty$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi} > 0$. This immediately implies that the second term of the asymptotics depends on the rate of convergence of the thermodynamic limit.

(iii) We assumed $V \geq 0$, which implies $\delta(x) = 0$ for $x \leq 0$, and the integrals in Theorem 4.7 may start from 0.

- (iv) The same result with an analogous proof holds also for a Dirac δ -perturbation defined in Chapter 3 as well.
- (v) We chose $V \geq 0$ since we want to avoid bound states or zero-energy resonances. Moreover, the integrability assumption (4.25) on V ensures sufficient regularity of the phase shift δ . In contrast, the continuity condition on V is only technical and due to the references we use and can be omitted.
- (vi) This result allows also a conclusion for the same problem on \mathbb{R} with a symmetric perturbation V because in this case the problem is reduced to two problems on the half axis with either Neumann or Dirichlet boundary condition at the origin.

Restricting ourselves to thermodynamic limits of the form

$$\frac{N}{L} + O\left(\frac{1}{L}\right) = \rho(E), \quad (4.38)$$

the difference of the ground-state energies admits a leading $1/L$ correction, which we call x_{FS} , i.e. we obtain the asymptotics

$$E_L'^N - E_L^N = \int_{-\infty}^E dx \xi(x) + \frac{\sqrt{E}\pi}{L} x_{FS}(E) + o\left(\frac{1}{L}\right) \quad (4.39)$$

$N, L \rightarrow \infty$, and $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$. In the physics literature the first term is sometimes called the Fumi term and x_{FS} the finite-size correction or energy, see [Aff97]. It was claimed in [Aff97, AL94, ZA97] that computing the finite-size energy is an easy way to compute the decay exponent in Anderson's orthogonality catastrophe. This was done in [ZA97, App. A] quite explicitly choosing a concrete thermodynamic limit. We compute x_{FS} explicitly for a family of thermodynamic limits corresponding to (4.38).

Corollary 4.9 (Finite-size energy). *For a given Fermi energy $E > 0$, some particle number $N \in \mathbb{N}$ and $a \in \mathbb{R}$ we choose the system length L such that*

$$\frac{N+a}{L} := \frac{\sqrt{E}}{\pi}. \quad (4.40)$$

Then, the finite-size energy x_{FS} defined in (4.39) is

$$x_{FS}(E) = (1-2a)\xi(E) + \gamma(E). \quad (4.41)$$

Thus,

- (i) *for the particular choice $a = \frac{1}{2}$ the finite-size energy is*

$$x_{FS}(E) = \gamma(E), \quad (4.42)$$

- (ii) *whereas for the choice $a = 0$ the finite-size energy is equal to*

$$x_{FS}(E) = \xi(E) + \gamma(E). \quad (4.43)$$

Remarks 4.10. (i) The previous corollary underlines that the finite-size energy depends on the thermodynamic limit and that there is precisely one choice which provides $x_{FS}(E) = \gamma(E)$. We note that for the above equality, we have to choose the same thermodynamic limit as in [ZA97, App. A].

(ii) The results of Chapter 3, in particular Theorem 3.20, state that at least in the special case of a δ -perturbation the exponent in Anderson's orthogonality catastrophe is independent of the precise thermodynamic limit. Since the result of this section also applies to this case we doubt a deep connection between the $1/L$ correction and the Anderson exponent.

2.2. Proof of Theorem 4.7. We start with a lemma relating the eigenvalues of the pair of finite-volume operators, which is the analogue to Lemma 3.13 in the previous chapter.

Lemma 4.11. *Let δ be the phase shift for the pair of operators H and H' defined in (4.31) then the n th eigenvalues of H_L and H'_L satisfy*

$$\sqrt{\mu_n} = \sqrt{\lambda_n} - \frac{\delta(\sqrt{\mu_n})}{L} + o\left(\frac{1}{L^2}\right), \quad (4.44)$$

where the error depends only on the potential V .

The above lemma follows directly from introducing Prüfer variables in the theory of Sturm-Liouville operators. We have to investigate the behaviour of δ at $k = 0$ to obtain suitable error estimates on the derivatives.

Lemma 4.12. *Let δ be the phase shift corresponding to the operators H and H' defined in (4.31). Then, $\delta \in C^2((0, \infty))$ and there exists a constant c , depending on the potential V , such that for all $k > 0$*

- (i) $|\delta(k)| \leq c \min\{k, \frac{1}{k}\}$, in particular $\delta \in L^\infty((0, \infty))$,
- (ii) $\delta' \in L^\infty((0, \infty))$,
- (iii) $|\delta''(k)| \leq \frac{c}{k}$.

Moreover,

- (iv) we have the following expansion of the phase shift

$$\delta(\sqrt{\mu_n}) = \delta(\sqrt{\lambda_n}) - \frac{\delta'(\sqrt{\lambda_n})\delta(\sqrt{\lambda_n})}{L} + \frac{F(\sqrt{\lambda_n})}{L^2}, \quad (4.45)$$

where the remainder term obeys for $x > 0$

$$|F(x)| \leq c\left(\frac{1}{x} + 1\right) \quad (4.46)$$

for some constant c depending on the potential V .

Remarks 4.13. (i) Lemma 4.11 and 4.12 are well known to experts in the theory of Sturm-Liouville operators. For convenience, we prove both results in Section 2.3.

(ii) Lemma 4.11 and Lemma 4.12 are the analogue to Lemma 3.13, which was valid for Dirac- δ perturbations. The proof of Lemma 3.13 is simpler due to the explicit representation of the scattering phase shift.

The third ingredient to the proof of Theorem 4.7 is the following.

Lemma 4.14. (Euler-MacLaurin)

- (i) Let $f \in C^1((0, \infty))$ then

$$\frac{1}{L} \sum_{n=1}^N f\left(\frac{n}{L}\right) = \int_0^{\frac{N}{L}} dx f(x) + O\left(\frac{N}{L^2}\right) \|f'\|_{L^\infty((0, \frac{N}{L}))}. \quad (4.47)$$

- (ii) Let $f \in C^2((0, \infty))$ with $f'' \in L^\infty((0, \infty))$ then

$$\frac{1}{L} \sum_{n=1}^N f\left(\frac{n}{L}\right) = \int_0^{\frac{N}{L}} dx f(x) + \frac{1}{2L} \int_0^{\frac{N}{L}} dx f'(x) + O\left(\frac{N}{L^3}\right). \quad (4.48)$$

The proof of this lemma is elementary, see for example [Kno96, Chap. XIV].

Proof of Theorem 4.7. Using Lemma 4.11, we obtain

$$\sum_{n=1}^N (\mu_n - \lambda_n) = \sum_{n=1}^N \left(-\frac{2\sqrt{\lambda_n}\delta(\sqrt{\mu_n})}{L} + \frac{\delta^2(\sqrt{\mu_n})}{L^2} \right) + o\left(\frac{N}{L^2}\right) \quad (4.49)$$

On the other hand Lemma 4.12 (iv) provides

$$\begin{aligned} (4.49) = & \sum_{n=1}^N \left(-\frac{2\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L} + \frac{2\delta'(\sqrt{\lambda_n})\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L^2} + \frac{\delta^2(\sqrt{\lambda_n})}{L^2} \right) \\ & + \frac{1}{L^3} \sum_{n=1}^N G(\sqrt{\lambda_n}) + o\left(\frac{N}{L^2}\right), \end{aligned} \quad (4.50)$$

where

$$\begin{aligned} G(x) = & \left(-2\delta'(x)\delta^2(x) - 2xF(x) + \frac{1}{L} ((\delta'(x)\delta(x))^2 + 2\delta(x)F(x)) \right. \\ & \left. - \frac{2}{L^2} F(x)\delta'(x)\delta(x) + \frac{1}{L^3} F^2(x) \right). \end{aligned} \quad (4.51)$$

Since $\lambda_n = \left(\frac{n\pi}{L}\right)^2$, $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$, using Lemma 4.12 (i)-(iii) and (4.46), we obtain for the error

$$\frac{1}{L^3} \sum_{n=1}^N G(\sqrt{\lambda_n}) = O\left(\frac{1}{L^2}\right). \quad (4.52)$$

Note that by Lemma 4.12 the function $f : x \mapsto x\delta(x)$ fulfils the assumptions of Lemma 4.14 (ii). Thus, we compute

$$\begin{aligned} \sum_{n=1}^N -\frac{2\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L} &= -\frac{1}{L} \sum_{n=1}^N 2\delta\left(\frac{n\pi}{L}\right) \frac{n\pi}{L} \\ &= -\int_0^{\frac{N}{L}} dx 2\delta(x\pi)(x\pi) - \frac{1}{L} \int_0^{\frac{N}{L}} dx (\delta(x\pi)(x\pi))' + O\left(\frac{N}{L^3}\right) \\ &= -\frac{1}{\pi} \int_0^{\left(\frac{N\pi}{L}\right)^2} dx \delta(\sqrt{x}) - \frac{1}{L} \delta(\sqrt{E})\sqrt{E} + o\left(\frac{1}{L}\right), \end{aligned} \quad (4.53)$$

where we used in the last equality the convergence $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$ and the continuity of δ . Using Lemma 4.12 we see that $g : x \mapsto x\delta(x)\delta'(x)$ satisfies the assumptions of Lemma 4.14 (i) with $\|g'\|_{L^\infty((0, \frac{N}{L}))} \leq c(1 + \frac{N}{L})$. Therefore,

$$\begin{aligned} \sum_{n=1}^N \frac{2\delta'(\sqrt{\lambda_n})\delta(\sqrt{\lambda_n})\sqrt{\lambda_n}}{L^2} &= \frac{1}{L} \left(\frac{1}{L} \sum_{n=1}^N 2\delta' \left(\frac{n\pi}{L} \right) \delta \left(\frac{n\pi}{L} \right) \frac{n\pi}{L} \right) \\ &= \frac{1}{L} \int_0^{\frac{N}{L}} dx 2\delta'(x\pi)\delta(x\pi)(x\pi) + O\left(\frac{N}{L^3}\right) \left(1 + \frac{N}{L} \right) \\ &= \frac{1}{L\pi} \left(\delta^2(\sqrt{E})\sqrt{E} - \int_0^{\frac{N}{L}} dx \delta^2(x\pi)\pi \right) + o\left(\frac{1}{L}\right), \end{aligned} \quad (4.54)$$

where we used integration by parts, the convergence $\frac{N}{L} \rightarrow \frac{\sqrt{E}}{\pi}$ and the continuity of δ in the last line. Lemma 4.12 yields the assumptions of Lemma 4.14 (i) for $h : x \mapsto \delta^2(x)$ with $h' \in L^\infty((0, \infty))$. Thus,

$$\begin{aligned} \sum_{n=1}^N \frac{\delta^2(\sqrt{\lambda_n})}{L^2} &= \frac{1}{L} \left(\frac{1}{L} \sum_{n=1}^N \delta^2 \left(\frac{n\pi}{L} \right) \right) \\ &= \frac{1}{L} \int_0^{\frac{N}{L}} dx \delta^2(x\pi) + O\left(\frac{1}{L^2}\right). \end{aligned} \quad (4.55)$$

Summing up (4.53), (4.54), (4.55) and equations (4.49), (4.52) give the claim. \square

2.3. Prüfer Variables and the Phase Shift. Our approach to the phase shift uses a non-linear ODE called the variable-phase equation, see e.g. [Cal67].

Let $k > 0$. First we recall that there is a unique solution δ_k of

$$\delta'_k(x) = -\frac{1}{k} V(x) \sin^2(kx + \delta_k(x)), \quad x > 0 \quad (4.56)$$

with the boundary condition $\limsup_{x \rightarrow 0} \frac{1}{x} |\delta_k(x)| < \infty$. This is a consequence of the Banach fixed-point theorem, see [RS79, Thm. XI.54]. We call this solution the phase-shift function. Moreover,

$$\lim_{x \rightarrow \infty} \delta_k(x) = \delta(k) \quad (4.57)$$

is the phase shift for H and H' .

On the other hand consider the eigenvalue problem on $(0, \infty)$

$$-u'' + Vu = k^2 u, \quad u(0) = 0. \quad (4.58)$$

Introducing Prüfer variables

$$u(x) = \rho_u(x) \sin(\theta_k(x)) \quad u'(x) = k \rho_u(x) \cos(\theta_k(x)), \quad (4.59)$$

(4.58) is equivalent to the system

$$\theta'_k = k - \frac{1}{k} V \sin^2(\theta_k), \quad \theta_k(0) = 0, \quad (4.60)$$

$$\rho'_u = \frac{V \sin(2\theta_k)}{2k} \rho_u, \quad (4.61)$$

see e.g. [Tes12, Sct. 5.5]. We call θ_k the Prüfer angle. Note that $\rho_u(x) \neq 0$ for all $x \geq 0$. We did not choose the standard Prüfer variables since we want to compare the Prüfer angle with the phase-shift function. These modified Prüfer variables were also introduced in [KLS98]. Given the phase-shift function in (4.56) we obtain a solution θ_k to (4.60) by setting

$$\theta_k(x) := \delta_k(x) + kx, \quad \text{where } k, x > 0. \quad (4.62)$$

Since any solution of (4.60) fulfills $|\theta_k(x)| \leq kx$, see (4.64) below, we obtain that $\delta_k(x) := \theta_k(x) - kx$ is the unique solution of (4.56). This implies uniqueness of θ_k and

$$\delta(k) = -\frac{1}{k} \int_0^\infty dt V(t) \sin^2(\theta_k(t)). \quad (4.63)$$

We state some properties of the Prüfer angle, respectively of the phase-shift function, which we use in the sequel.

Proposition 4.15. *Given $k > 0$, let δ_k and θ_k be the solution of (4.56), respectively (4.60). Fix $x > 0$. Then,*

(i) $\theta_k(x)$ is non-negative, moreover,

$$0 \leq \theta_k(x) \leq kx. \quad (4.64)$$

(ii) we have

$$\lim_{k \rightarrow 0} \theta_k(x) = 0, \quad \lim_{k \rightarrow \infty} \theta_k(x) = \infty. \quad (4.65)$$

(iii) the functions $k \mapsto \theta_k(x)$ and $k \mapsto \delta_k(x)$ are smooth, i.e.

$$\theta_{(\cdot)}(x), \delta_{(\cdot)}(x) \in C^\infty((0, \infty)). \quad (4.66)$$

(iv) the derivative of the Prüfer angle with respect to the energy is strictly positive, i.e.

$$\frac{\partial}{\partial k} \theta_k(x) > 0. \quad (4.67)$$

Proof of Proposition 4.15. For (i) first note that $\lim_{x \rightarrow \infty} \theta'_k(x) = k > 0$ and $\theta'_k(x) > 0$ for all $x > 0$ such that $\theta_k(x) = 0$. Since $\theta_k(0) = 0$ and $\theta_k \in C^1((0, \infty))$ we have $\theta_k > 0$. On the other hand $k - \frac{1}{k} V \sin^2(y) \leq k$, $y \in \mathbb{R}$, since $V \geq 0$. This yields $\theta_k(x) \leq kx$, see e.g. [Har64, Chap. III, 4.2].

The first equality in (ii) follows by (i). For the second equality observe $\theta_k(x) \geq kx - \frac{1}{k} \|V\|_1$, where $x, k > 0$ and $\|\cdot\|_1$ denotes the $L^1((0, \infty))$ norm.

For (iii) note that $k \mapsto k - \frac{1}{k} V(x) \sin^2(y) \in C^\infty((0, \infty))$ for fixed $x > 0, y \in \mathbb{R}$. Then, standard results imply that the solution $\theta_{(\cdot)}(x) \in C^\infty((0, \infty))$ for fixed $x > 0$, see e.g. [Har64, Chap. V, 4.1].

For (iv) note that $k - \frac{1}{k} V \sin^2(y) \leq k' - \frac{1}{k'} V \sin^2(y)$ for all $k \leq k'$, $y \in \mathbb{R}$ since $V \geq 0$ and use [Har64, Chap. III, 4.2]. \square

Proof of Lemma 4.11. Let $\mu > 0$. Consider the eigenvalue equation on $[0, L]$

$$-u'' + Vu = \mu u, \quad u(0) = 0. \quad (4.68)$$

We introduce Prüfer variables according to (4.59). Note that any eigenfunction u of h_L^D corresponding to an eigenvalue μ has to satisfy $u(L) = 0$ due to the Dirichlet boundary condition at L . Thus, using $\rho_u(x) \neq 0$ for all $x \geq 0$, we obtain $\sin(\theta_{\sqrt{\mu}}(L)) = 0$. With (4.65) and (4.67) this implies for the n th eigenvalue μ_n of h_L^D

$$\theta_{\sqrt{\mu_n}}(L) = n\pi. \quad (4.69)$$

Therefore, integrating (4.60) yields

$$\sqrt{\mu_n} = \frac{n\pi}{L} + \frac{1}{L\sqrt{\mu_n}} \int_0^L dt V(t) \sin^2(\theta_{\sqrt{\mu_n}}(t)). \quad (4.70)$$

Now, using $|\sin(x)| \leq |x|$, (4.64), $|\sin(x)| \leq 1$ and (4.25) we obtain

$$\begin{aligned} \frac{1}{\sqrt{\mu_n}} \int_L^\infty dt V(t) \sin^2(\theta_{\sqrt{\mu_n}}(t)) &\leq \int_L^\infty dt V(t) t \\ &\leq \frac{1}{L} \int_L^\infty dt t^2 V(t) = o\left(\frac{1}{L}\right). \end{aligned} \quad (4.71)$$

Then, (4.63) and $\sqrt{\lambda_n} = \frac{n\pi}{L}$ give the claim. \square

Proof of Lemma 4.12. Part (i) follows from (4.63), (4.64) and (4.25).

Concerning (ii), we first note that $\theta_k \in C^1((0, \infty))$ for fixed $k > 0$ because V is assumed to be continuous and $\theta_{(\cdot)}(x) \in C^\infty((0, \infty))$ for fixed $x > 0$ by (4.66). From now on we consider θ as a function of two variables and write, in abuse of notation, the abbreviation f_x for the partial derivative $\frac{\partial}{\partial x} f$ of a function $f \in C^1(\mathbb{R}^2)$. Also we drop the u index of ρ . Then the ODEs (4.60) and (4.61) imply

$$\begin{aligned} \left(\rho^2 \frac{\partial}{\partial k} \theta \right)_x &= 2\rho \rho_x \frac{\partial}{\partial k} \theta + \rho^2 \frac{\partial}{\partial k} \theta_x \\ &= 2\rho \rho_x \frac{\partial}{\partial k} \theta + \rho^2 \frac{\partial}{\partial k} \left(k - \frac{V \sin^2(\theta)}{k} \right) \\ &= 2\rho \rho_x \frac{\partial}{\partial k} \theta + \rho^2 \left(1 + \frac{V \sin^2(\theta)}{k^2} - \frac{V \sin(2\theta)}{k} \frac{\partial}{\partial k} \theta \right) \\ &= \rho^2 \left(1 + \frac{V \sin^2(\theta)}{k^2} \right). \end{aligned} \quad (4.72)$$

Integrating the latter yields

$$\frac{\partial}{\partial k} \theta_k(x) = \int_0^x dt \frac{\rho^2(t)}{\rho^2(x)} \left(1 + \frac{V(t) \sin^2(\theta_k(t))}{k^2} \right). \quad (4.73)$$

The ODE (4.61), (4.64), the elementary inequality $|\sin x| \leq |x|$ and (4.25) imply

$$\left| \frac{\rho(t)}{\rho(x)} \right| \leq \exp \left(\int_t^x ds s V(s) \right) \leq \exp(\|(\cdot)V\|_1) < \infty. \quad (4.74)$$

From this, (4.64) and $|\sin x| \leq |x|$ we infer the existence of a constant c depending on the potential V such that

$$\left| \frac{\partial}{\partial k} \theta_k(x) \right| \leq c(1+x). \quad (4.75)$$

Then, the above, (4.64) and dominated convergence provide $\delta \in C^1((0, \infty))$ and

$$|\delta'(k)| \leq c \int_0^\infty dt V(t)(1+t+t^2). \quad (4.76)$$

The assumptions on the potential give the claim.

For (iii) we compute as above

$$\left(\rho^2 \frac{\partial^2}{\partial k^2} \theta \right)_x = 2\rho^2 V \left(-\frac{\sin^2(\theta)}{k^3} + \frac{\sin(2\theta) \frac{\partial}{\partial k} \theta}{k^2} - \frac{\cos(2\theta) (\frac{\partial}{\partial k} \theta)^2}{k} \right). \quad (4.77)$$

Using (4.64), $|\sin x| \leq |x|$, (4.74) and (4.75), we see

$$\left| \frac{\partial^2}{\partial k^2} \theta_k(x) \right| \leq \frac{\tilde{c}}{k}, \quad (4.78)$$

where \tilde{c} depends on V . Dominated convergence yields $\delta \in C^2((0, \infty))$ and (4.64) and (4.78) provide

$$|\delta''(k)| \leq \frac{C}{k} \int_0^\infty dt V(t)(1+t+t^2) \quad (4.79)$$

for some C depending on the potential V .

To prove (iv) we use Lemma 4.11. Thus,

$$\sqrt{\mu_n} = \sqrt{\lambda_n} + \frac{\delta(\sqrt{\mu_n})}{L} + o\left(\frac{1}{L}\right). \quad (4.80)$$

Since $\delta \in C^2((0, \infty))$, we compute for $x, y \in (0, \infty)$ with $y > x$ and $y = x + \frac{\delta(y)}{L} + o(\frac{1}{L})$

$$\begin{aligned} \left| \delta(y) - \delta(x) + \frac{\delta'(x)\delta(x)}{L} \right| &\leq \left| \int_x^y dt \int_x^t ds \delta''(s) \right| + |\delta'(x)| \left| y - x + \frac{\delta(x)}{L} \right| \\ &\leq \frac{1}{x} |y - x|^2 + \frac{\|\delta\|_\infty}{L} \left(\left| \int_x^y dt \delta'(t) \right| + o\left(\frac{1}{L}\right) \right). \end{aligned} \quad (4.81)$$

Using Lemma 4.12 (ii) and once again the recursion relation we obtain

$$\left| \delta(y) - \delta(x) + \frac{\delta'(x)\delta(x)}{L} \right| \leq \left(\frac{1}{x} + 1 \right) O\left(\frac{1}{L^2}\right). \quad (4.82)$$

The claim follows from setting $x := \lambda_n$ and $y := \mu_n$. \square

CHAPTER 5

Eigenfunction Correlations in the Anderson Model

In this chapter we present two results which are contrary to the previous ones. The first one concerns upper bounds on products of spectral projections for random Schrödinger operators and the second one deals with lower bounds on the correlation determinant for these random operators.

1. Model and Results

Let $d \in \mathbb{N}$ and $\lambda > 0$. We define the Anderson Hamiltonian on $\ell^2(\mathbb{Z}^d)$ by

$$H_\omega := -\Delta + \lambda V_\omega. \quad (5.1)$$

The operator $-\Delta$ denotes the discrete negative Laplacian, i.e. for $u \in \ell^2(\mathbb{Z}^d)$

$$(-\Delta u)(n) = \sum_{|n-m|_1=1} (u(n) - u(m)), \quad (5.2)$$

where $|\cdot|_1$ denotes the 1-norm on \mathbb{Z}^d and V_ω is a random multiplication operator

$$(V_\omega u)(n) = V_\omega(n)u(n). \quad (5.3)$$

Here, $(V_{(\cdot)}(n))_{n \in \mathbb{Z}^d}$ denotes a family of independent identically distributed real-valued random variables on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Moreover, we assume the single-site distribution μ_0 defined by $\mu_0(A) = \mathbb{P}(V_{(\cdot)}(0) \in A)$, $A \in \text{Borel}(\mathbb{R})$, to be bounded and absolutely continuous with respect to Lebesgue measure with a bounded density g . These conditions are too strong in general, but for simplicity we assume them. Moreover, we define the perturbed Hamiltonian

$$H'_\omega := H_\omega + \nu \langle \delta_0, \cdot \rangle \delta_0, \quad (5.4)$$

where $\nu > 0$ and the vector $\delta_0 \in \ell^2(\mathbb{Z}^d)$ is given by $\delta_0(n) := \begin{cases} 1, & n = 0 \\ 0, & n \neq 0 \end{cases}$, for $n \in \mathbb{Z}^d$.

Let $L \in \mathbb{N}$, and we write for the corresponding operators restricted to the box $\Lambda_L := [-L, L]^d \subset \mathbb{Z}^d$

$$H_{\omega, L} \quad \text{and} \quad H'_{\omega, L}, \quad (5.5)$$

where we do not impose any particular boundary condition, i.e. $H_{\omega, L}^{(\prime)} := 1_{\Lambda_L} H_{\omega}^{(\prime)} 1_{\Lambda_L}$ with 1_{Λ_L} being the orthogonal projection on Λ_L . Using our standard notation, we denote by $\lambda_1^L \leq \lambda_2^L \leq \dots$ and $\mu_1^L \leq \mu_2^L \leq \dots$ the non-decreasing sequences of eigenvalues of the operators $H_{\omega, L}$ respectively $H'_{\omega, L}$ counting multiplicities and by $(\varphi_k^L)_{1 \leq k \leq (2L+1)^d}$ and $(\psi_n^L)_{1 \leq k \leq (2L+1)^d}$ the corresponding normalised eigenvectors, where we omit for brevity the index ω .

The family of operators $(H_\omega)_{\omega \in \Omega}$ form an ergodic family of operators with respect to translations. Therefore, standard results about ergodic operators imply that

$$\sigma(H_\omega) = [0, 4d] + \lambda \operatorname{supp} g \quad (5.6)$$

for \mathbb{P} -a.e. $\omega \in \Omega$, see [K08] or [PF92, Chap. 1]. Since H'_ω is a rank-one perturbation of H_ω located at the origin, the ergodicity is broken but nevertheless the perturbation is small and the spectra of both operators are closely related. We have the following elementary lemma.

Lemma 5.1. $\sigma_{\text{ess}}(H_\omega) = \sigma_{\text{ess}}(H'_\omega)$ and $\sigma(H_\omega) \subset \sigma(H'_\omega)$ for \mathbb{P} -a.e. $\omega \in \Omega$. Moreover, assuming $\sigma(H_\omega)$ to be connected for \mathbb{P} -a.e. $\omega \in \Omega$, we obtain that there exists at most one eigenvalue of multiplicity one, which we call μ_ω , of H'_ω with $\mu_\omega \notin \sigma(H_\omega)$, i.e. $\sigma(H'_\omega) = \sigma(H_\omega) \cup \{\mu_\omega\}$ for \mathbb{P} -a.e. $\omega \in \Omega$.

Proof. Following [PF92, Thm. 2.11] we obtain that $\sigma(H_\omega) = \sigma_{\text{ess}}(H_\omega)$ for \mathbb{P} -a.e. $\omega \in \Omega$. Since H'_ω is a rank-one perturbation of H_ω , Weyl's theorem implies that $\sigma_{\text{ess}}(H'_\omega) = \sigma_{\text{ess}}(H_\omega)$. Thus, $\sigma(H_\omega) \subset \sigma(H'_\omega)$. Moreover, since there are no spectral gaps in $\sigma(H_\omega)$, the min-max principle says that there is at most one eigenvalue exceeding the essential spectrum of H'_ω , see [RS78, Sct. XIII.1]. \square

Remarks 5.2. (i) As expected, the above shows that the rank-one perturbation does not change the spectrum a lot. In general this is not true for the spectral decomposition. While the absolutely continuous spectrum is stable under a rank-one perturbation the pure-point spectrum can change to singular continuous spectrum and vice versa, see [Sim05, Sct. 12].

(ii) For general operators with several spectral gaps a rank-one perturbation can push an eigenvalue of multiplicity one in each spectral gap. To illustrate this, we consider the example of the multiplication operator A on $L^2(\mathbb{R})$ with the function $f(x) := x(1_{[0,1]}(x) + 1_{[2,3]}(x))$, $x \in \mathbb{R}$. Then, $\sigma(A) = [0, 1] \cup [2, 3]$. Let $B = A + |\phi\rangle\langle\phi|$ with $\phi := (1_{[0,1]} + 1_{[2,3]})$. Using Krein's formula, [Sim05, Sct. 12] or equation (3.26), we see that B has an eigenvalue $\mu \notin \sigma(A)$ if and only if $\langle\phi, \frac{1}{A-\mu}\phi\rangle = -1$. A computation shows $\langle\phi, \frac{1}{A-\mu}\phi\rangle = \ln \left| \frac{(1-\mu)(3-\mu)}{\mu(2-\mu)} \right|$ and, therefore, $\sigma(B) = [0, 1] \cup \left\{ \frac{2}{1+e^{-1}} \right\} \cup [2, 3] \cup \left\{ \frac{2}{1-e^{-1}} \right\}$. Thus, the rank-one perturbation created two additional eigenvalues. Even though this phenomenon may happen in general, we do not know, if it does happen in the case considered above. However, this is just a side remark and for the rest of the paragraph not important.

1.1. Bounds on the Anderson Integral. In Chapter 2 we obtained upper bounds on the ground-state overlap by deducing logarithmic divergence of the Anderson integral (5.7) in the length scale L . In this section we show that the Anderson model exhibits a substantially different behaviour in the exponentially localised regime: The Anderson integral stays bounded as $L \rightarrow \infty$.

Let $E \in \mathbb{R}$. In the following we are interested in the behaviour of the product of spectral projections

$$I_L(E) := \operatorname{tr} \{ 1_{(-\infty, E)}(H_{\omega, L}) 1_{(E, \infty)}(H'_{\omega, L}) 1_{(-\infty, E)}(H_{\omega, L}) \}, \quad (5.7)$$

as $L \rightarrow \infty$. Although this is not exactly the Anderson integral defined in the introduction, equation (1.10), we refer to (5.7) as the Anderson integral in this section.

Next we define the set of energies for which suitable fractional moment bounds of the resolvents are satisfied.

Definition 5.3. For $0 < s < 1$ we define the set $A_s^{(\prime)} \subset \mathbb{R}$ as the intersection

$$\mathcal{A}_s^{(\prime)} := \mathcal{B}_s^{(\prime)} \cap \mathcal{C}_s^{(\prime)}, \quad (5.8)$$

where

(i) $\mathcal{B}_s^{(\prime)}$ is the set of all energies $E \in \mathbb{R}$ such that there exist constants $c > 0$ and $C > 0$, which may depend on s and E , such that for all $n, m \in \mathbb{Z}^d$ and for all $\epsilon > 0$

$$\mathbb{E} \left[\left| \langle \delta_n, \frac{1}{H^{(\prime)} - E - i\epsilon} \delta_m \rangle \right|^s \right] \leq C \exp(-c|n - m|_1). \quad (5.9)$$

(ii) $\mathcal{C}_s^{(\prime)} := \cap_{L \in \mathbb{N}} \mathcal{C}_{s,L}^{(\prime)}$ and $\mathcal{C}_{s,L}^{(\prime)}$ is the set of all energies $E \in \mathbb{R}$ such that there exist constants $c > 0$ and $C > 0$, which may depend on s and E , but are independent of Λ_L , such that for all $n, m \in \Lambda_L$ and for all $\epsilon > 0$

$$\mathbb{E} \left[\left| \langle \delta_n, \frac{1}{H_L^{(\prime)} - E - i\epsilon} \delta_m \rangle \right|^s \right] \leq C \exp(-c|n - m|_1). \quad (5.10)$$

Moreover, we set

$$\mathcal{A} := \bigcup_{0 < s < 1} \mathcal{A}_s \quad \mathcal{B} := \bigcup_{0 < s < 1} \mathcal{B}_s. \quad (5.11)$$

Remarks 5.4. (i) Standard results imply that whenever $I \subset \mathcal{A}_s^{(\prime)}$ for an interval $I \subset \mathbb{R}$, then we have only pure-point spectrum with exponentially decaying eigenfunctions within this interval. This follows from the Simon-Wolff criterion, see [SW86, AM93] and the references cited therein.

(ii) In the following we are mainly interested in the set \mathcal{A} and we need the sets \mathcal{A}'_s only in the formulation of Theorem 5.17.

The set $\mathcal{A}_s^{(\prime)}$ is not empty and has positive Lebesgue measure as long as $\lambda > 0$. More precisely, we have at least two regimes, where $\mathcal{A}_s^{(\prime)}$ is rather big.

Proposition 5.5. Let $0 < s < 1$. Then, in the model considered here, we have that the Lebesgue measure $|\mathcal{A}_s^{(\prime)}| > 0$ for all coupling constants $\lambda > 0$. More precisely,

(i) (Large disorder regime) there exists a coupling constant $\lambda_0 > 0$ such that for all $\lambda \geq \lambda_0$ we obtain for \mathbb{P} -a.e. $\omega \in \Omega$

$$\mathcal{A}_s^{(\prime)} = \sigma(H_\omega^{(\prime)}), \quad (5.12)$$

see [AM93].

(ii) (Lifschitz tail regime) for all coupling constants $\lambda > 0$ there exists a $\eta_\lambda > 0$ such that for \mathbb{P} -a.e. $\omega \in \Omega$

$$(\inf \sigma(H_\omega), \inf \sigma(H_\omega) + \eta_\lambda) \cup (\sup \sigma(H_\omega) - \eta_\lambda, \sup \sigma(H_\omega)) \subset \mathcal{A}_s, \quad (5.13)$$

see [ASFH01].

Remark 5.6. We remark that the proof of the fractional moment bounds of the resolvents for operators with a random potential in [AM93, Sct. 3] is stated for rather arbitrary kinetic terms. This includes $-\Delta + |\delta_0\rangle\langle\delta_0|$. The proofs of these bounds do not rely on ergodicity. Therefore, the localisation results for the Anderson model also apply to the operator H'_ω .

For energies within the set \mathcal{A} and \mathcal{B} we obtain the following asymptotics.

Theorem 5.7. (i) We have for a.e. $(E, \omega) \in \mathcal{A} \times \Omega$

$$\limsup_{L \rightarrow \infty} \operatorname{tr} \{1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L})\} < \infty. \quad (5.14)$$

(ii) We have for a.e. $(E, \omega) \in \mathcal{B} \times \Omega$

$$\operatorname{tr} \{1_{(-\infty, E)}(H_{\omega})1_{(E, \infty)}(H'_{\omega})1_{(-\infty, E)}(H_{\omega})\} < \infty. \quad (5.15)$$

Throughout, for $C \in \text{Borel}(\mathbb{R})$ the notation for a.e. $(E, \omega) \in C \times \Omega$ refers to the product measure $\lambda \otimes \mathbb{P}$ where λ denotes the Lebesgue measure.

We prove the above theorem in Subsection 2.1 below.

Remarks 5.8. (i) In other words, the above says that for Leb.-a.e. $E \in \mathbb{R}$ within the exponentially localised regime equation (5.14) and (5.15) hold for \mathbb{P} -a.e. $\omega \in \Omega$.

(ii) Since $\|1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L})\| \leq 1$, the above bounds are also valid for traces of the operators $(1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L}))^n$, $n \in \mathbb{N}$.

(iii) We assumed exponential decay of the fractional moments of the resolvents for the proof. Sufficient polynomial decay of the fractional moments is enough.

(iv) Let $\omega \in \Omega$ and $E \in \sigma(H_{\omega})$. Comparing the above with our general results from Chapter 2 we define

$$\gamma_{\omega}(E) := \frac{1}{\pi^2} \lim_{\epsilon \searrow 0} \left\{ \operatorname{Im} \langle \delta_0, \frac{1}{H_{\omega} - E - i\epsilon} \delta_0 \rangle \operatorname{Im} \langle \delta_0, \frac{1}{H'_{\omega} - E - i\epsilon} \delta_0 \rangle \right\}. \quad (5.16)$$

Then, as discussed in Chapter 2, $\gamma_{\omega}(E) = \frac{1}{\pi^2} \|T_E\|_{\text{HS}}^2$, where T_E is the T -matrix of the pair H_{ω} and H'_{ω} and HS denotes the Hilbert-Schmidt norm. Now, Theorem 2.4, which is also valid in our setting, implies that for Leb.-a.e. $E \in \mathbb{R}$

$$\operatorname{tr} \{1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L})\} \geq \gamma_{\omega}(E) \ln L + o(\ln L), \quad (5.17)$$

as $L \rightarrow \infty$. This does not violate Theorem 5.7. To see this we note that for any bounded operator $A \in \text{BL}(\mathcal{H})$ standard results on the Borel transform of measures imply that the imaginary part of the resolvent satisfies

$$\lim_{\epsilon \searrow 0} \frac{1}{\pi} \operatorname{Im} \langle \delta_0, \frac{1}{A - E - i\epsilon} \delta_0 \rangle = \frac{d\mu_{\text{ac}}}{dx} \Big|_{x=E}. \quad (5.18)$$

Here, μ_{ac} denotes the absolutely continuous part of the spectral measure $B \mapsto \langle \delta_0, 1_B(A) \delta_0 \rangle$, $B \in \text{Borel}(\mathbb{R})$, see [Sim05, Chap. 11]. Now, assume that a neighbourhood of the energy E is within the set \mathcal{A} , i.e. the operator H_{ω} admits purely pure-point spectrum in a neighbourhood of E . Then, the Lebesgue density of μ_{ac} is 0 for Leb.-a.e. E in this neighbourhood. Thus, it follows that

$$\gamma_{\omega}(E) = 0 \quad (5.19)$$

for a.e. $(E, \omega) \in \mathcal{A} \times \Omega$. Hence, (5.17) does not contradict Theorem 5.7.

(v) Let $\omega \in \Omega$. Now, we assume that H_{ω} has absolutely continuous spectrum in some interval $\mathcal{I} \subset \sigma(H_{\omega})$, so has H'_{ω} by [Sim05, Chap. 12]. Moreover, assume for Leb.-a.e. $E \in \mathcal{I}$

$$\lim_{\epsilon \searrow 0} \operatorname{Im} \langle \delta_0, \frac{1}{H_{\omega} - E - i\epsilon} \delta_0 \rangle > 0 \quad \text{and} \quad \lim_{\epsilon \searrow 0} \operatorname{Im} \langle \delta_0, \frac{1}{H'_{\omega} - E - i\epsilon} \delta_0 \rangle > 0. \quad (5.20)$$

Thus, in this case $\gamma_\omega(E) > 0$ for Leb.-a.e. $E \in \mathcal{I}$ and (5.17)

$$\liminf_{L \rightarrow \infty} \text{tr} \{1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})\} = \infty, \quad (5.21)$$

where the divergence is at least logarithmic. This implies the following deterministic statement.

Corollary 5.9. *Let P_{δ_0} be the orthogonal projection onto the set $\text{span}\{H_{\omega}^n \delta_0 : n \in \mathbb{N}_0\} \subset \ell^2(\mathbb{Z}^d)$.*

(i) *Assume there exists an interval \mathcal{I} such that for Leb.-a.e. $E \in \mathcal{I}$*

$$\limsup_{L \rightarrow \infty} \text{tr} \{1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L})\} < \infty. \quad (5.22)$$

Then,

$$\sigma_{\text{ac}}(P_{\delta_0} H_{\omega} P_{\delta_0}) \cap \mathcal{I} = \emptyset. \quad (5.23)$$

(ii) *Assume there exists an interval \mathcal{I} such that for Leb.-a.e. $E \in \mathcal{I}$*

$$\text{tr} \{1_{(-\infty, E)}(H_{\omega})1_{(E, \infty)}(H'_{\omega})1_{(-\infty, E)}(H_{\omega})\} < \infty. \quad (5.24)$$

Then,

$$\sigma_{\text{ac}}(P_{\delta_0} H_{\omega} P_{\delta_0}) \cap \mathcal{I} = \emptyset. \quad (5.25)$$

Proof of Corollary 5.9. Assume that $\sigma_{\text{ac}}(P_{\delta_0} H_{\omega} P_{\delta_0}) \cap \mathcal{I} \neq \emptyset$. This implies for a set of positive Lebesgue measure $\mathcal{J} \subset \mathcal{I}$ that (5.20) holds and, therefore, $\gamma_{\omega}(E) > 0$ within the set \mathcal{J} .

Hence, (5.17) gives a contradiction to (5.22). To obtain a contradiction to (5.24) we note that the operator inequality $1_{(E, \infty)}(H'_{\omega}) \geq 1_{(E+\epsilon, \infty)}(H'_{\omega})$ for all $\epsilon > 0$ implies

$$\begin{aligned} & \text{tr} \{1_{(-\infty, E)}(H_{\omega})1_{(E, \infty)}(H'_{\omega})1_{(-\infty, E)}(H_{\omega})\} \\ & \geq \limsup_{\epsilon \searrow 0} \text{tr} \{1_{(-\infty, E)}(H_{\omega})1_{(E+\epsilon, \infty)}(H'_{\omega})1_{(-\infty, E)}(H_{\omega})\} \\ & = \limsup_{\epsilon \searrow 0} \{\gamma_{\omega}(E) |\ln \epsilon| + o(|\ln \epsilon|)\}. \end{aligned} \quad (5.26)$$

The last line follows along the same line as in Lemma 2.21 or see [GKM14, Sct. 3]. Since $\gamma_{\omega}(E) > 0$ for all $E \in \mathcal{J}$, this contradicts (5.24). \square

Remarks 5.10. (i) Under the assumption that δ_0 is cyclic for the operator H_{ω} we obtain in the equations (5.23) and (5.25) that $\sigma_{\text{ac}}(H_{\omega}) \cap \mathcal{I} = \emptyset$. In the Anderson model cyclicity of the vector δ_0 is a delicate issue. In the localised regime [Sim94, KM06] showed that δ_0 is a cyclic vector of the operator $H_{\omega}|_{\mathcal{H}_{pp}}$ for \mathbb{P} -a.e. $\omega \in \Omega$, where \mathcal{H}_{pp} denotes the pure-point spectral subspace. This result was extended in [JL06]. They proved that the vector δ_0 is for \mathbb{P} -a.e. $\omega \in \Omega$ cyclic on the entire singular part of the spectrum. However, it is an open problem to show cyclicity of δ_0 for the entire spectrum independently of the spectral type. It was even suggested that showing non-cyclicity of the vector δ_0 might be a suitable way to prove delocalisation in the Anderson model [JL06].

(ii) The second part of the above corollary is related to the Simon-Wolff criterion because

$$\text{tr} \{1_{(-\infty, E)}(H_{\omega})1_{(E, \infty)}(H'_{\omega})1_{(-\infty, E)}(H_{\omega})\} \leq \langle \delta_0, \left(\frac{1}{H_{\omega} - E} \right)^2 \delta_0 \rangle, \quad (5.27)$$

see Section 2 below. Whenever the Simon-Wolff criterion holds, the right hand side of (5.27) is finite. Since this is the case in the localised regime, this proves (5.15) already. We refer to [SW86] or [Sim05, Chap. 12] for more details about the Simon-Wolff criterion.

(iii) We do not know, whether (5.22) or (5.24) are sufficient to exclude singular-continuous spectrum.

Theorem 5.7 states almost sure results. The next apparent question concerns the expectation value of the latter. In particular, the behaviour of the expectation value of the infinite-volume Anderson integral

$$\mathbb{E} [\operatorname{tr} \{1_{(-\infty, E)}(H)1_{(E, \infty)}(H'_\omega)1_{(-\infty, E)}(H)\}], \quad (5.28)$$

where we omit the subscript ω in the expectation value throughout. We begin with a representation of the Anderson integral.

Lemma 5.11. *For all $E \in \mathbb{R}$ we have the following identity*

$$\mathbb{E} [\operatorname{tr} \{1_{(-\infty, E)}(H)1_{(E, \infty)}(H')1_{(-\infty, E)}(H)\}] = \int_{(-\infty, E) \times (E, \infty)} d\bar{\mu}(x, y) \frac{1}{(y-x)^2}, \quad (5.29)$$

where the measure $\bar{\mu}$ is given by

$$\bar{\mu}(B \times B') := \nu^2 \mathbb{E} [\langle \delta_0, 1_B(H)\delta_0 \rangle \langle \delta_0, 1_{B'}(H')\delta_0 \rangle], \quad (5.30)$$

with $B, B' \in \text{Borel}(\mathbb{R})$.

Proof. By Appendix A, Theorem A.1, we obtain

$$\operatorname{tr} \{1_{(-\infty, E)}(H_\omega)1_{(E, \infty)}(H'_\omega)1_{(-\infty, E)}(H_\omega)\} = \int_{(-\infty, E) \times (E, \infty)} d\mu(x, y) \frac{1}{(y-x)^2}. \quad (5.31)$$

where the measure μ is uniquely defined by $\mu(B \times B') := \langle \delta_0, 1_B(H_\omega)\delta_0 \rangle \langle \delta_0, 1_{B'}(H'_\omega)\delta_0 \rangle$. Moreover, we note that also (5.30) gives rise to a uniquely defined Borel measure on \mathbb{R}^2 using monotone convergence. We have for all $S \in \text{Borel}(\mathbb{R}^2)$ the identity

$$\mathbb{E} \left[\int_{\mathbb{R}^2} d\mu(x, y) 1_S(x, y) \right] = \mathbb{E} [\mu(S)] = \int_{\mathbb{R}^2} d\bar{\mu}(x, y) 1_S(x, y). \quad (5.32)$$

Approximating the function $f(x, y) := (y-x)^{-2} 1_{(-\infty, E) \times (E, \infty)}(x, y)$ by simple functions from below and using the monotone convergence theorem gives the identity (5.29). \square

Remark 5.12. The corresponding representation is also valid for the pair of the finite-volume operators $H_{\omega, L}$ and $H'_{\omega, L}$.

Thus, the behaviour of the left hand side of (5.29) is closely related to the regularity of the spectral-correlation measure (5.30) near the point (E, E) on the diagonal. Using the technics developed in Chapter 2, we obtain.

Theorem 5.13. *For Leb.-a.e. $E \in \mathbb{R}$,*

$$\limsup_{\epsilon \searrow 0} \frac{1}{|\ln \epsilon|} \mathbb{E} [\operatorname{tr} \{1_{(-\infty, E-\epsilon)}(H)1_{(E+\epsilon, \infty)}(H')1_{(-\infty, E-\epsilon)}(H)\}] \geq \bar{\gamma}(E), \quad (5.33)$$

where

$$\bar{\gamma}(E) := \lim_{\epsilon \searrow 0} \frac{1}{\epsilon^2} \bar{\mu}((E-\epsilon/2, E+\epsilon/2) \times (E-\epsilon/2, E+\epsilon/2)). \quad (5.34)$$

Proof. The proof essentially follows from the proof of Theorem 2.2 for the deterministic setting observing that all errors can be controlled by the operator norm of the random potential $\|V_\omega\|_\infty$, see Chapter 2 and [GKM14]. Thus, the error is controlled uniformly in $\omega \in \Omega$. \square

Remarks 5.14. The choice of the approximation of the identity in (5.34) is not important and

$$\bar{\gamma}(E) = \frac{1}{\pi^2} \lim_{\epsilon \searrow 0} \mathbb{E} \left[\text{Im} \langle \delta_0, \frac{1}{H - E - i\epsilon} \delta_0 \rangle \text{Im} \langle \delta_0, \frac{1}{H' - E - i\epsilon} \delta_0 \rangle \right] \quad (5.35)$$

as well.

Now, we turn to the regularity of the measure (5.30). The Cauchy-Schwarz inequality and the Wegner estimate [K08] immediately imply for all $B, B' \in \text{Borel}(\mathbb{R})$

$$\begin{aligned} \mathbb{E} [\langle \delta_0, 1_B(H) \delta_0 \rangle \langle \delta_0, 1_{B'}(H') \delta_0 \rangle] &\leq \mathbb{E} [\langle \delta_0, 1_B(H) \delta_0 \rangle]^{\frac{1}{2}} \mathbb{E} [\langle \delta_0, 1_{B'}(H') \delta_0 \rangle]^{\frac{1}{2}} \\ &\leq |B|^{\frac{1}{2}} |B'|^{\frac{1}{2}}. \end{aligned} \quad (5.36)$$

Thus, the measure (5.30) does not have a pure-point part or a part supported on a Cantor type set. But in general one can not exclude a singular continuous part or even obtain a bounded density. Nevertheless, at a first glance the above computation seems to show that the expectation value of (5.28) is infinite because the expectation value in (5.30) regularises the spectral-correlation measure and we expect the measure (5.30) to have an absolutely continuous part. But in the localised regime we can compute the constant $\bar{\gamma}$ and obtain the following.

Lemma 5.15. *Let $\mathcal{I} \subset \mathbb{R}$ be an interval such that both operators H_ω and H'_ω admit purely pure-point spectrum within \mathcal{I} for \mathbb{P} -a.e. $\omega \in \Omega$. Then, for Leb.-a.e. $E \in \mathcal{I}$*

$$\bar{\gamma}(E) := \frac{1}{\pi^2} \lim_{\epsilon \searrow 0} \mathbb{E} \left[\text{Im} \langle \delta_0, \frac{1}{H - E - i\epsilon} \delta_0 \rangle \text{Im} \langle \delta_0, \frac{1}{H' - E - i\epsilon} \delta_0 \rangle \right] = 0. \quad (5.37)$$

We emphasise, that in the above the resolvents are evaluated at the same energies $E + i\epsilon$.

Remarks 5.16. The value of (5.37) can be considered also in the $\nu = 0$ case. But in this case we believe that the corresponding spectral-correlation measure has a singularity on the diagonal even in the localised regime. Such two-point correlation functions are of certain interest concerning conductivity, see e.g. [KLP03].

Proof. We want to apply the dominated convergence theorem to interchange the limit and the expectation in (5.37). To do so, we use the resolvent equation and obtain Krein's formula

$$\langle \delta_0, \frac{1}{H'_\omega - E - i\epsilon} \delta_0 \rangle = \frac{1}{\nu + \langle \delta_0, \frac{1}{H_\omega - E - i\epsilon} \delta_0 \rangle^{-1}}. \quad (5.38)$$

We set $a + bi := \langle \delta_0, \frac{1}{H_\omega - E - i\epsilon} \delta_0 \rangle$, where $a, b \in \mathbb{R}$. Then, using (5.38)

$$\text{Im} \langle \delta_0, \frac{1}{H_\omega - E - i\epsilon} \delta_0 \rangle \text{Im} \langle \delta_0, \frac{1}{H'_\omega - E - i\epsilon} \delta_0 \rangle = \frac{b^2}{(1 + \nu a)^2 + (\nu b)^2} \leq \frac{1}{\nu^2}. \quad (5.39)$$

Moreover, we assumed that both operators H_ω and H'_ω admit purely pure-point spectrum for a.e. $(E, \omega) \in \mathcal{I} \times \Omega$. Hence,

$$\lim_{\epsilon \searrow 0} \left\{ \operatorname{Im} \langle \delta_0, \frac{1}{H_\omega - E - i\epsilon} \delta_0 \rangle \operatorname{Im} \langle \delta_0, \frac{1}{H'_\omega - E - i\epsilon} \delta_0 \rangle \right\} = 0 \quad (5.40)$$

for a.e. $(E, \omega) \in \mathcal{I} \times \Omega$. Thus, (5.37) follows from (5.39), (5.40) and the dominated convergence theorem. \square

Hence, we gain no information out of Theorem 5.13 in the case of purely pure-point spectrum of the underlying pair of operators. Nevertheless, Lemma 5.15 indicates that the expectation in (5.29) should be finite in the localised regime. We prove the following statement pointing precisely in this direction.

Theorem 5.17. *Let $0 < s < 1$. Then, for all $E \in \mathcal{A}_s \cap \mathcal{A}'_s$*

$$\mathbb{E} [(\operatorname{tr} \{1_{(-\infty, E)}(H)1_{(E, \infty)}(H')1_{(-\infty, E)}(H)\})^s] < \infty. \quad (5.41)$$

We prove this theorem in Subsection 2.1 below. We remark that the above is not entirely satisfying because pushing $s \rightarrow 1$ will shrink the set of all possible energies $E \in \mathcal{A}_s \cap \mathcal{A}'_s$ to the empty set. While completing this thesis it was proved that the expectation is indeed finite for energies within the exponentially localised regime.

Theorem 5.18 ([Die15]). *Let $E \in \mathcal{A}_s \cap \mathcal{A}'_s$. Then,*

$$\mathbb{E} [(\operatorname{tr} \{1_{(-\infty, E)}(H)1_{(E, \infty)}(H')1_{(-\infty, E)}(H)\})] < \infty. \quad (5.42)$$

For a proof see the master thesis [Die15].

1.2. Lower Bounds on the Correlation Determinant. Unlike in the above paragraph, we focus here only on the high disorder case. We remind you that for $L \in \mathbb{N}$ and some Fermi energy $E > 0$ we set

$$\mathcal{S}_L(E) := \det \left(\langle \varphi_j^L, \psi_k^L \rangle \right)_{j, k=1, \dots, N_L(E)}, \quad (5.43)$$

where we choose the particle number for $E \in \mathbb{R}$ to be

$$N \equiv N_L(E) := \#\{j \in \mathbb{N} : \lambda_j^L \leq E\} \in \mathbb{N}_0, \quad (5.44)$$

as in Chapter 2. If $N_L(E) = 0$, we set $\mathcal{S}_L(E) = 1$. The main result of this section is the following non-vanishing of the expectation of the ground-state overlap.

Theorem 5.19. *For any constant $c \in (0, 1)$ there exists a coupling constant λ_0 such that for all $\lambda > \lambda_0$*

$$\liminf_{L \rightarrow \infty} \mathbb{E} [|\mathcal{S}_L(E)|] > c \quad (5.45)$$

for Leb.-a.e. $E \in \mathbb{R}$.

Apparently, the above result is only interesting if E is within the almost-sure spectrum.

Remarks 5.20. (i) The above is contrary to the findings in Chapter 2 and Chapter 3. As a reminder, we proved in these chapters under quite weak assumptions on the pair of Schrödinger operators that

$$\mathcal{S}_L(E) \rightarrow 0 \quad (5.46)$$

if the decay exponent $\gamma_\omega(E) > 0$. For the moment let us assume that $\gamma_\omega(E) > 0$ for a.e. $(E, \omega) \in \mathcal{I} \times \Omega$ for an interval \mathcal{I} . The definition of $\gamma_\omega(E)$ implies that $\mathcal{I} \subset \sigma_{\text{ac}}(H_\omega)$, see definition (5.16). Since the determinant is the scalar product of two normalised ground-states, we obtain that it is bounded by 1 uniformly in $\omega \in \Omega$. Therefore, we use dominated convergence to show that in this case the above expectation value has to vanish, i.e.

$$\lim_{L \rightarrow \infty} \mathbb{E} \left[|\mathcal{S}_L(E)| \right] = \mathbb{E} \left[\lim_{L \rightarrow \infty} |\mathcal{S}_L(E)| \right] = 0. \quad (5.47)$$

for Leb.-a.e. $E \in \mathcal{I}$.

(ii) At least in our proof the rate of disorder depends on the strength of the coupling constant ν in the way that one needs at least

$$|\nu|^2 \lesssim |\lambda|. \quad (5.48)$$

Though the square is probably too much and just due to far too rough estimates, numerics, see Figure 1, suggest that such a condition may be necessary for Theorem 5.19 to hold.

(iii) We use the same deterministic estimates used in [KOS13] to deduce a deterministic lower bound on the determinant. These estimates are too bad to obtain sharp lower bounds on the determinant.

(iv) From Theorem 5.19 above one might think it is possible to show that the determinant is almost surely bounded from below depending on the realisation $\omega \in \Omega$. Looking at some numerics and some heuristics stated in Chapter 6 below, we doubt this. Nevertheless, using $\mathcal{S}_L(E) \leq 1$, we obtain a weak pointwise result for subsequences as an immediate corollary of Theorem 5.19.

Corollary 5.21. *There exists a coupling constant λ_0 such that for all $\lambda > \lambda_0$ and Leb.-a.e. $E \in \sigma(H_\omega)$ there exists some $\mathcal{B} \in \mathcal{F}$ with $\mathbb{P}(\mathcal{B}) > 0$ such that there exists a subsequence L_k^ω such that*

$$\liminf_{k \rightarrow \infty} |\mathcal{S}_{L_k^\omega}(E)| > 0. \quad (5.49)$$

Though the latter is valid for subsequences only, it is contrary to Theorem 2.3 in Chapter 2. We proved there that the determinant will vanish for all subsequences in the discrete setting provided $\gamma_\omega(E) > 0$.

2. An Application of the Fractional Moment Bound

We start with investigating the convergence of the fractional moments of the resolvents of the operators $H_{\omega,L}$ to the ones of the operator H_ω . Later on, we use the results deduced in this section to prove Theorem 5.7, Theorem 5.17 and Theorem 5.19.

We define the following abbreviation to shorten notation where we suppress the index $\omega \in \Omega$.

Definition 5.22. Let $E \in \mathbb{R}$ and $\epsilon > 0$.

(i) For $n, m \in \Lambda_L$, we define

$$G_L^{E,\epsilon}(n, m) := \left\langle \delta_n, \frac{1}{H_{\omega,L} - E - i\epsilon} \delta_m \right\rangle. \quad (5.50)$$

(ii) For $n, m \in \mathbb{Z}^d$, we define

$$G^{E,\epsilon}(n, m) := \left\langle \delta_n, \frac{1}{H_\omega - E - i\epsilon} \delta_m \right\rangle. \quad (5.51)$$

Lemma 5.23. *Let $m, n \in \mathbb{Z}^d$. Then, for all $\omega \in \Omega$ the limit*

$$\lim_{\epsilon \searrow 0} G^{E,\epsilon}(m, n) := G^{E,0}(m, n) \in \mathbb{C} \quad (5.52)$$

exists for Leb.-a.e. $E \in \mathbb{R}$.

Proof. See [PF92, App. A] and the references cited therein on limit values of Borel transforms of complex measures. \square

We continue with a result on L^1 -convergence of fractional moments.

Lemma 5.24. *Let $s < \frac{1}{4}$. Then, for Leb.-a.e. $E \in \mathcal{A}_{4s}$ there exist constants c_1, C_1 and $L_0 \geq 0$ such that for all $L \geq L_0$*

$$\mathbb{E} \left[\left| \sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s} - \sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s} \right| \right] \leq C_1 \exp(-c_1 L). \quad (5.53)$$

Proof. Let $L \in \mathbb{N}$. Note that for a given $\omega \in \Omega$ the union of the spectra $\cup_{L \in \mathbb{N}} \sigma(H_{\omega,L})$ is a Lebesgue nullset as a countable union of finite sets. This and Lemma 5.23 imply that

$$(E, \omega) \mapsto X(E, \omega) := \left| \sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s} - \sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s} \right| \in [0, \infty] \quad (5.54)$$

is well-defined for a.e. $(E, \omega) \in \mathbb{R} \times \Omega$ where the exceptional set can be chosen uniformly in $L \in \mathbb{N}$. Thus, for Leb.-a.e. $E \in \mathbb{R}$ the random variable $\omega \mapsto X(E, \omega)$ is well-defined. We restrict ourselves to one of these $E \in \mathbb{R}$ intersected with \mathcal{A}_{4s} . For $0 < r < 1$ the function $\mathbb{R}_{\geq 0} \ni x \mapsto x^r$ is concave, which implies the elementary inequality

$$| |a|^r - |b|^r | \leq |a - b|^r \quad (5.55)$$

valid for all $a, b \in \mathbb{C}$. We split the sum on the left hand side of (5.53) in two parts and first estimate using (5.55)

$$\begin{aligned} & \mathbb{E} \left[\left| \sum_{n \in \Lambda_L} \left(|G_L^{E,0}(0, n)|^{2s} - |G^{E,0}(0, n)|^{2s} \right) \right| \right] \\ & \leq \sum_{n \in \Lambda_L} \mathbb{E} \left[\left| G_L^{E,0}(0, n) - G^{E,0}(0, n) \right|^{2s} \right] \\ & = \sum_{n \in \Lambda_L} \mathbb{E} \left[\lim_{\epsilon \searrow 0} \left| G_L^{E,\epsilon}(0, n) - G^{E,\epsilon}(0, n) \right|^{2s} \right] \\ & \leq \liminf_{\epsilon \searrow 0} \sum_{n \in \Lambda_L} \mathbb{E} \left[\left| G_L^{E,\epsilon}(0, n) - G^{E,\epsilon}(0, n) \right|^{2s} \right], \end{aligned} \quad (5.56)$$

where in last two lines we used definition (5.52) and Fatou's lemma. The geometric resolvent identity, see [K08, Eq. (5.51)], implies

$$(5.56) \leq \liminf_{\epsilon \searrow 0} \sum_{n \in \Lambda_L} \mathbb{E} \left[\left| \sum_{\substack{(k, k') \in \partial \Lambda_L \\ k' \in \Lambda_L}} G^{E,\epsilon}(0, k) G_L^{E,\epsilon}(k', n) \right|^{2s} \right], \quad (5.57)$$

where $\partial \Lambda_L$ denotes the boundary of Λ_L , i.e.

$$\partial \Lambda_L = \{ (k, k') : |k - k'|_1 = 1 \text{ and } k \in \Lambda_L^c, k' \in \Lambda_L \text{ or } k \in \Lambda_L, k' \in \Lambda_L^c \}, \quad (5.58)$$

where $\Lambda_L^c := \mathbb{Z}^d \setminus \Lambda_L$. Since $2s < 1$, we obtain the elementary inequality

$$\left| \sum_{n=1}^N a_n \right|^{2s} \leq \sum_{n=1}^N |a_n|^{2s} \quad (5.59)$$

for $N \in \mathbb{N}$ and $a_1, \dots, a_N \in \mathbb{C}$. Hence, this and the Cauchy-Schwarz inequality imply

$$(5.57) \leq \liminf_{\epsilon \searrow 0} \sum_{n \in \Lambda_L} \sum_{\substack{(k, k') \in \partial \Lambda_L \\ k' \in \Lambda_L}} \left(\mathbb{E} \left[|G^{E, \epsilon}(0, k)|^{4s} \right] \right)^{1/2} \left(\mathbb{E} \left[|G_L^{E, \epsilon}(k', n)|^{4s} \right] \right)^{1/2}. \quad (5.60)$$

Since $E \in \mathcal{A}_{4s}$, Definition 5.3 yields independently of ϵ

$$(5.60) \leq \sum_{n \in \Lambda_L} \sum_{\substack{(k, k') \in \partial \Lambda_L \\ k' \in \Lambda_L}} C \exp(-c|k|_1/2) \leq (2L+1)^d |\partial \Lambda_L| C \exp(-cL/2). \quad (5.61)$$

Since $|\partial \Lambda_L| \leq C_d L^{d-1}$, where the constant C_d depends only on the dimension d , we obtain for all $c_2 < c$

$$(5.61) \leq C \exp(-c_2 L) \quad (5.62)$$

for all $L \geq L_0(c_2)$ big enough. Moreover, the Definition 5.3 of \mathcal{A}_{4s} implies

$$\begin{aligned} \mathbb{E} \left[\sum_{n \notin \Lambda_L} \left| \lim_{\epsilon \searrow 0} G^{E, \epsilon}(0, n) \right|^{2s} \right] &\leq \liminf_{\epsilon \searrow 0} \sum_{n \notin \Lambda_L} C \exp(-c|n|_1) \\ &\leq C_2 \exp(-cL) \end{aligned} \quad (5.63)$$

for all $E \in \mathcal{A}_{4s}$. Set $C_1 := \max\{C, C_2\}$ and $c_1 := \min\{c, c_2\}$, and the assertion follows. \square

Using a Borel-Cantelli argument, the above can be strengthened to obtain pointwise convergence. We demonstrate it for convenience.

Lemma 5.25. *Let $s < \frac{1}{4}$. Then, we have for a.e. $(E, \omega) \in \mathcal{A}_{4s} \times \Omega$*

$$\lim_{L \rightarrow \infty} \sum_{n \in \Lambda_L} |G_L^{E, 0}(0, n)|^{2s} = \sum_{n \in \mathbb{Z}^d} |G^{E, 0}(0, n)|^{2s}. \quad (5.64)$$

Proof. Since we consider a discrete model, we note that every sequence $(L_n)_{n \in \mathbb{N}}$ is a subsequence of $(n)_{n \in \mathbb{N}}$, i.e. the sequence of the natural numbers. Hence, we restrict ourselves to this sequence $(L)_{L \in \mathbb{N}}$. Let $m \in \mathbb{N}$ and $s < \frac{1}{4}$. Then, the event

$$A_L^m := \left\{ \left| \sum_{n \in \Lambda_L} |G_L^{E, 0}(0, n)|^{2s} - \sum_{n \in \mathbb{Z}^d} |G^{E, 0}(0, n)|^{2s} \right| > \frac{1}{m} \right\} \quad (5.65)$$

is well-defined for Leb.-a.e. $E \in \mathbb{R}$, see (5.54). Then, by the Markov inequality and Lemma 5.24

$$\begin{aligned} \mathbb{P}(A_L^m) &\leq m \mathbb{E} \left[\left| \sum_{n \in \Lambda_L} |G_L^{E, 0}(0, n)|^{2s} - \sum_{n \in \mathbb{Z}^d} |G^{E, 0}(0, n)|^{2s} \right| \right] \\ &\leq m C_1 \exp(-c_1 L). \end{aligned} \quad (5.66)$$

Thus,

$$\sum_{L \in \mathbb{N}} \mathbb{P}(A_L^m) < \infty \quad (5.67)$$

and the Borel-Cantelli Lemma implies

$$\mathbb{P}(A_L^m \text{ happens for infinitely many } L \in \mathbb{N}) = 0. \quad (5.68)$$

Hence, there exists a set $B_m \in \Omega$ with $\mathbb{P}(B_m) = 1$ such that for all $\omega \in B_m$

$$\limsup_{L \rightarrow \infty} \left| \sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s} - \sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s} \right| \leq \frac{1}{m}. \quad (5.69)$$

Now, the assertion holds for all $\omega \in \cap_{m \in \mathbb{N}} B_m$ which still has probability 1. \square

2.1. Proof of Theorem 5.7 and Theorem 5.17.

Proof of Theorem 5.7. We prove (i) only, (ii) follows along the same line. First note that $\mathcal{A}_{s_2} \subset \mathcal{A}_{s_1}$ for $s_1 < s_2$. This follows from Hölder's inequality. Thus, \mathcal{A} is a countable union $\mathcal{A} = \cup_{n \geq 2} \mathcal{A}_{\frac{1}{n}}$ and it suffices to prove (i) only for a.e. $(E, \omega) \in \mathcal{A}_r \times \Omega$ for a fixed $r < 1$ to obtain the assertion for a.e. $(E, \omega) \in \mathcal{A} \times \Omega$.

Let $0 < r < 1$, and set $s := r/4$. Let $(E, \omega) \in \mathcal{A}_{4s} \times \Omega$ such that Lemma 5.25 holds. Using Lemma 2.12 or Appendix A, we rewrite

$$\text{tr} \{1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L})\} = \int_{(-\infty, E) \times (E, \infty)} d\mu_L(x, y) \frac{1}{(y - x)^2}, \quad (5.70)$$

where, as before, μ_L is the spectral-correlation measure defined on Borel sets $B, B' \in \text{Borel}(\mathbb{R})$ by

$$\mu_L(B \times B') := \nu^2 \langle \delta_0, 1_B(H_{\omega, L})\delta_0 \rangle \langle \delta_0, 1_{B'}(H_{\omega, L})\delta_0 \rangle. \quad (5.71)$$

Hence, we estimate

$$\begin{aligned} & \text{tr} \{1_{(-\infty, E)}(H_{\omega, L})1_{(E, \infty)}(H'_{\omega, L})1_{(-\infty, E)}(H_{\omega, L})\} \\ & \leq \int_{(-\infty, E) \times (E, \infty)} d\mu_L(x, y) \frac{1}{(E - x)^2} \\ & \leq \nu^2 \langle \delta_0, \left(\frac{1}{H_{\omega, L} - E} \right)^2 \delta_0 \rangle \langle \delta_0, 1_{(E, \infty)}(H'_{\omega, L})\delta_0 \rangle. \end{aligned} \quad (5.72)$$

We estimate the second part by 1 and insert an identity in the first part of the above product of scalar products. Therefore,

$$\begin{aligned} (5.72) & \leq \nu^2 \sum_{n \in \Lambda_L} \left| \langle \delta_0, \frac{1}{H_{\omega, L} - E} \delta_n \rangle \right|^2 \\ & = \nu^2 \sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^2 \\ & \leq \nu^2 \left(\sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s} \right)^{1/s}, \end{aligned} \quad (5.73)$$

where $0 < s < 1$ and we used the inequality (5.59) in the last line. Now, Lemma 5.25 implies for a.e. $(E, \omega) \in \mathcal{A}_{4s} \times \Omega$

$$\limsup_{L \rightarrow \infty} \sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s} \leq \sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s} \quad (5.74)$$

and Fatou's lemma together with the definition of the set \mathcal{A}_{4s} provide for all $E \in \mathcal{A}_{4s}$ that

$$\sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s} \leq \liminf_{\epsilon \searrow 0} \sum_{n \in \mathbb{Z}^d} |G^{E,\epsilon}(0, n)|^{2s} < \infty, \quad (5.75)$$

for \mathbb{P} -a.e. $\omega \in \Omega$. This and the inequalities (5.73) and (5.74) give the assertion. \square

Proof of Theorem 5.17. We fix $0 < s < 1$ and $E \in \mathcal{A}_s \cap \mathcal{A}'_s$. We begin with the integral representation deduced in Appendix A

$$\text{tr} \{1_{(-\infty, E)}(H_\omega)1_{(E, \infty)}(H'_\omega)1_{(-\infty, E)}(H_\omega)\} = \int_{(-\infty, E) \times (E, \infty)} d\mu(x, y) \frac{1}{(y - x)^2}. \quad (5.76)$$

Then, the inequality

$$\frac{1}{(y - x)^2} 1_{(-\infty, E)}(x)1_{(E, \infty)}(y) \leq \frac{1}{E - x} 1_{(-\infty, E)}(x) \frac{1}{y - E} 1_{(E, \infty)}(y) \quad (5.77)$$

implies the bound

$$\begin{aligned} & \mathbb{E} [\text{tr} \{1_{(-\infty, E)}(H)1_{(E, \infty)}(H')1_{(-\infty, E)}(H)\}^s] \\ & \leq \nu^{2s} \mathbb{E} \left[\left(\langle \delta_0, \frac{1}{E - H} 1_{(-\infty, E)}(H) \delta_0 \rangle \langle \delta_0, \frac{1}{H' - E} 1_{(E, \infty)}(H') \delta_0 \rangle \right)^s \right]. \end{aligned} \quad (5.78)$$

In the above inequality, we do not a priori claim that the right hand side is finite. We continue with the resolvent equation and estimate

$$\begin{aligned} (5.78) & = \nu^s \mathbb{E} \left[\left(\langle 1_{(-\infty, E)}(H) \delta_0, \left(\frac{1}{H' - E} - \frac{1}{H - E} \right) 1_{(E, \infty)}(H') \delta_0 \rangle \right)^s \right] \\ & \leq \nu^s \mathbb{E} \left[\left| \langle 1_{(-\infty, E)}(H) \delta_0, \frac{1}{H' - E} 1_{(E, \infty)}(H') \delta_0 \rangle \right|^s \right] \\ & \quad + \nu^s \mathbb{E} \left[\left| \langle 1_{(-\infty, E)}(H) \delta_0, \frac{1}{H - E} 1_{(E, \infty)}(H') \delta_0 \rangle \right|^s \right], \end{aligned} \quad (5.79)$$

where we used $s < 1$ and (5.59) for the last inequality. Now, the Cauchy-Schwarz inequality implies

$$\begin{aligned} (5.79) & \leq \nu^s \mathbb{E} \left[\left\| \frac{1}{H' - E} \delta_0 \right\|^s \right] + \nu^s \mathbb{E} \left[\left\| \frac{1}{H - E} \delta_0 \right\|^s \right] \\ & \leq \nu^s \mathbb{E} \left[\sum_{n \in \mathbb{Z}^d} \left| \langle \delta_n, \frac{1}{H' - E} \delta_0 \rangle \right|^s \right] + \nu^s \mathbb{E} \left[\sum_{n \in \mathbb{Z}^d} \left| \langle \delta_n, \frac{1}{H - E} \delta_0 \rangle \right|^s \right], \end{aligned} \quad (5.80)$$

where we used once again the elementary inequality (5.59) in the last line. Since we chose $E \in \mathcal{A}_s \cap \mathcal{A}'_s$ the theorem follows from Definition 5.3. \square

2.2. Proof of Theorem 5.19. The key to the proof of Theorem 5.19 is the following asymptotics of the expectation value of the fractional moments.

Lemma 5.26. *Let $0 < 2s < 1$. There exists a coupling constant λ_0 and a constant C_s such that for all $\lambda > \lambda_0$*

$$\mathbb{E} \left[\sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s} \right] \leq C_s \frac{1}{|\lambda|^s} \quad (5.81)$$

for Leb.-a.e. $E \in \mathbb{R}$.

This is a classical result for the Anderson model. For a proof of this lemma see [AM93] or [AG98, App. B] and keep track of all the constants. We note that in the above lemma the constant C_s can be chosen independently of the energy E .

Proof of Theorem 5.19. Let $E \in \mathbb{R}$. Since $|\mathcal{S}_L(E)| \leq 1$ we estimate

$$\mathbb{E} [|\mathcal{S}_L(E)|] \geq \mathbb{E} [|\mathcal{S}_L(E)|^2]. \quad (5.82)$$

Let $c > 0$. Then, the Markov inequality implies

$$\mathbb{E} [|\mathcal{S}_L(E)|^2] \geq e^{-c} \mathbb{P} (|\mathcal{S}_L(E)|^2 > e^{-c}). \quad (5.83)$$

Now, expanding the determinant, as in Lemma 2.9, we obtain

$$|\mathcal{S}_L(E)|^2 = \exp \left(- \sum_{n=1}^{\infty} \frac{1}{n} \text{tr} \left\{ \left(P_L^N (I - \Pi_L^N) P_L^N \right)^n \right\} \right), \quad (5.84)$$

where we write $N \equiv N_L(E)$

$$P_L^N := \sum_{j=1}^N \langle \varphi_j^L, \cdot \rangle \varphi_j^L \quad \text{and} \quad \Pi_L^N := \sum_{k=1}^N \langle \psi_k^L, \cdot \rangle \psi_k^L. \quad (5.85)$$

Hence, we rewrite the right hand side of (5.83) as

$$\mathbb{P} (|\mathcal{S}_L(E)|^2 > e^{-c}) = \mathbb{P} \left(\sum_{n=1}^{\infty} \frac{1}{n} \text{tr} \left\{ \left(P_L^N (I - \Pi_L^N) P_L^N \right)^n \right\} < c \right). \quad (5.86)$$

The inequality $\sum_{k \in \mathbb{N}} |a_k|^n \leq (\sum_{k \in \mathbb{N}} |a_k|)^n$ for $a_k \in \mathbb{C}$, $n \in \mathbb{N}$, implies

$$\text{tr} \left\{ \left(P_L^N (I - \Pi_L^N) P_L^N \right)^n \right\} \leq \left(\text{tr} \left\{ P_L^N (I - \Pi_L^N) P_L^N \right\} \right)^n. \quad (5.87)$$

We define the event

$$\mathcal{K} := \left\{ \omega : \text{tr} \left\{ P_L^N (I - \Pi_L^N) P_L^N \right\} < 1 \right\} \in \mathcal{F}. \quad (5.88)$$

For all $\omega \in \mathcal{K}$ we compute using the inequality (5.87) and the geometric series

$$\sum_{n=1}^{\infty} \frac{1}{n} \text{tr} \left\{ \left(P_L^N (I - \Pi_L^N) P_L^N \right)^n \right\} \leq \frac{\text{tr} \left\{ P_L^N (I - \Pi_L^N) P_L^N \right\}}{1 - \text{tr} \left\{ P_L^N (I - \Pi_L^N) P_L^N \right\}}. \quad (5.89)$$

This implies that

$$\begin{aligned} \text{r.h.s. (5.86)} &\geq \mathbb{P}\left(\left\{\frac{\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\}}{1 - \text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\}} < c\right\} \cap \mathcal{K}\right) \\ &= \mathbb{P}\left(\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\} < \frac{c}{1+c}\right), \end{aligned} \quad (5.90)$$

where we used $\frac{c}{1+c} < 1$ for $c > 0$. Smuggling in a $0 < s < \frac{1}{4}$ and another application of the Markov inequality provide

$$\begin{aligned} (5.90) &= 1 - \mathbb{P}\left(\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\} \geq \frac{c}{1+c}\right) \\ &= 1 - \mathbb{P}\left(\left(\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\}\right)^s \geq \left(\frac{c}{1+c}\right)^s\right) \\ &\geq 1 - \left(\frac{1+c}{c}\right)^s \mathbb{E}\left[\left(\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\}\right)^s\right]. \end{aligned} \quad (5.91)$$

Moreover, the special choice of $N = N_L(E)$, see (5.44) implies $\lambda_N^L \leq E < \mu_{N+1}^L$. Hence,

$$\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\} \leq \text{tr}\{1_{(-\infty, E)}(H_L)1_{[E, \infty)}(H_L')1_{(-\infty, E)}(H_L)\} \quad (5.92)$$

and we use once again the integral representation deduced in Appendix A to compute

$$\begin{aligned} \left(\text{tr}\{P_L^N(I - \Pi_L^N)P_L^N\}\right)^s &\leq \left(\int_{(-\infty, E) \times [E, \infty)} d\mu_L(x, y) \frac{1}{(y-x)^2}\right)^s \\ &\leq \nu^{2s} \left(\langle \delta_0, \left(\frac{1}{H_L - E}\right)^2 \delta_0 \rangle\right)^s \\ &\leq \nu^{2s} \sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s}, \end{aligned} \quad (5.93)$$

where the latter inequalities follow along the same line as in (5.72) and (5.73). Now, Lemma 5.24 provides for Leb.-a.e. $E \in \mathbb{R}$

$$\mathbb{E}\left[\sum_{n \in \Lambda_L} |G_L^{E,0}(0, n)|^{2s}\right] \rightarrow \mathbb{E}\left[\sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s}\right] \quad (5.94)$$

as $L \rightarrow \infty$. Therefore, the above and the equations (5.83) and (5.91) imply

$$\liminf_{L \rightarrow \infty} \mathbb{E}[|\mathcal{S}_L(E)|^2] \geq e^{-c} \left(1 - \left(\frac{1+c}{c}\right)^s \nu^{2s} \mathbb{E}\left[\sum_{n \in \mathbb{Z}^d} |G^{E,0}(0, n)|^{2s}\right]\right). \quad (5.95)$$

Lemma 5.26 gives

$$(5.95) \geq e^{-c} \left(1 - \left(\frac{1+c}{c}\right)^s \nu^{2s} \frac{C_s}{|\lambda|^s}\right) \quad (5.96)$$

and increasing the disorder strength λ sufficiently far, provides the assertion. \square

CHAPTER 6

Outlook

In this chapter we begin with some numerics on the ground-state overlap. Later on, motivated by these numerics, we formulate some open questions and conjectures concerning the ground-state overlap.

1. Let the Computer Compute

In this section we present some numerics on the ground-state overlap. We visualise and illustrate the behaviour of the ground-state overlap for different Fermi energies or magnitudes of the perturbation. In particular, since the pointwise results for the Anderson model in Chapter 5 are not entirely satisfying, numerics will help to get a feeling for the behaviour of the ground-state overlap. Throughout we consider the discrete setting on the half line, i.e. $\mathcal{H} = \ell^2(\mathbb{N})$ and for $u \in \ell^2(\mathbb{N})$

$$(-\Delta u)(n) := \begin{cases} 2u(n) - u(n-1) - u(n+1) & n > 1 \\ u(1) - u(2) & n = 1 \end{cases} \quad (6.1)$$

and we define the pair of operators

$$H := -\Delta + bV_0 \quad \text{and} \quad H' := H + bV_0 + aV, \quad (6.2)$$

where $a, b \in \mathbb{R}$. Here, V_0 denotes some background potential, which is in the following either zero or a random multiplication operator. Moreover, V is some multiplication operator with compact support, which will be a rank-one up to a rank-four perturbation. Let $L \in \mathbb{N}$. Then, we denote by H_L and H'_L the restrictions of H and H' to the interval $[1, L] \subset \mathbb{N}$. Thus, H_L and H'_L are just $L \times L$ matrices. Moreover, we introduce the energy $E \in (0, 1)$ to parametrise the Fermi energy, i.e. for a given $E \in (0, 1)$ and a length $L \in \mathbb{N}$ we choose the particle number $N_L \in \mathbb{N}$ according to

$$N_L := \lfloor EL \rfloor \quad \text{which implies} \quad \lim_{L \rightarrow \infty} \frac{N_L}{L} = E, \quad (6.3)$$

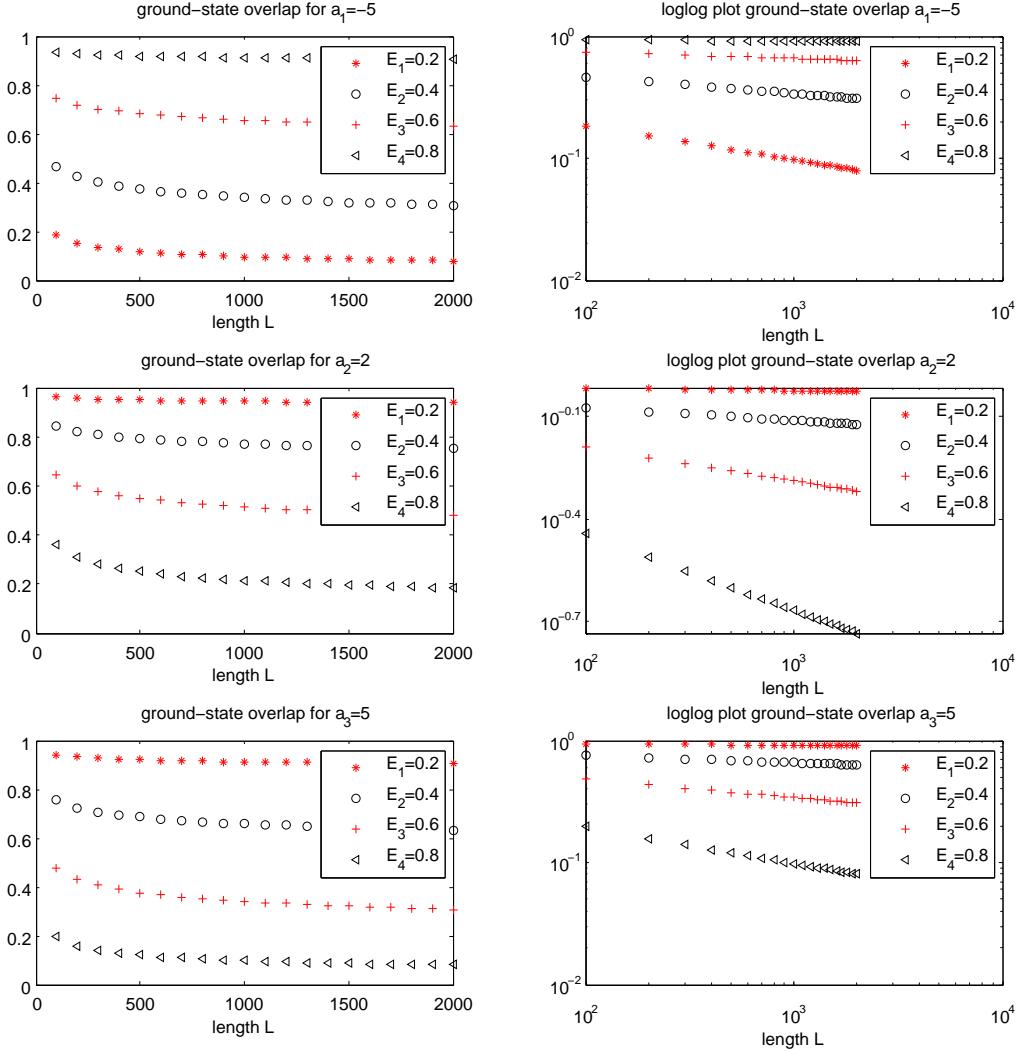
where $\lfloor x \rfloor := \max\{n \in \mathbb{N} : n \leq x\}$. We slightly changed our notation in this section. In the previous chapters we choose the thermodynamic limit as $N_L/L \rightarrow \rho(E)$ for $L \rightarrow \infty$, where ρ is the integrated density of states of the unperturbed operator. Here, for brevity we don't introduce ρ and $E = \rho(\tilde{E})$ for some $\tilde{E} \in \sigma(H)$.

In the following we write $\mathcal{S}_L(E)$ for the ground-state overlap corresponding to H_L and H'_L defined in (2.5) with N_L chosen as in (6.3) above.

The Deterministic Case. We start with the case $V_0 = 0$ and $V = |\delta_1\rangle\langle\delta_1|$ a rank-one perturbation. Thus, we are in position to use the product formula deduced in Chapter 3, Theorem 3.3, to compute the values of the ground-state overlap $\mathcal{S}_L(E)$. We do this for three different coupling constants $a_1 = -5$, $a_2 = 1$ and $a_3 = 5$ and various Fermi energies

E and obtain Figure 1. We remind you that the analytic proof of Chapter 3 extends to the discrete setting considered here.

Figure 1. The ground-state overlap $\mathcal{S}_L(E)$ for various parameters

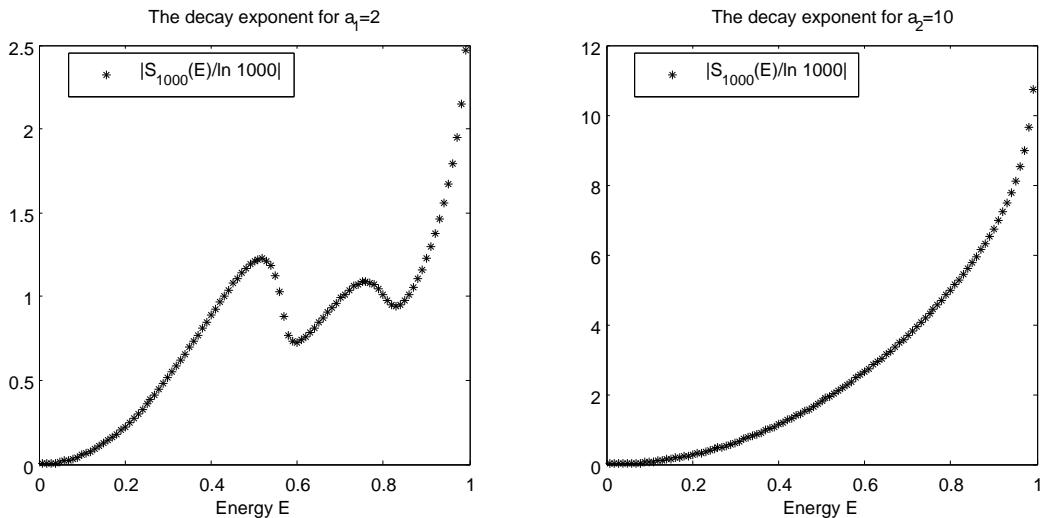


Even though the determinant behaves in Figure 1 perfectly as proven in Theorem 3.17 and Theorem 3.20, let us comment on two things. We can not create arbitrary decay of the ground-state overlap with a rank-one perturbation. This is due to the interlacing of the eigenvalues, which implies that the scattering phase shift is uniformly bounded independent of the precise strength of the rank-one perturbation. Let us also note that the ground-state overlap behaves in the same way for a negative perturbation and small energies as for a positive perturbation and high energies. This can be observed well in the figure. Therefore, we believe that in the case of an absent background potential there is a duality of the form $\mathcal{S}_L(E, a) \sim \mathcal{S}_L(1 - E, -a)$, as $L \rightarrow \infty$, at least for energies $E \in (0, 1) \setminus \{0.5\}$. In the above, we included the index a which refers to the coupling constant in front of the perturbation. This is an effect of the discrete setting and the symmetric bounded spectrum

of the discrete negative Laplacian. Since we considered so far models in the continuum only, we will not discuss this discrete ambiguity.

We proceed with a plot of the decay exponent $\zeta(E)$ for various energies in the interval $E \in (0, 1)$. In this case we consider a rank-four perturbation $V := |\delta_1\rangle\langle\delta_1| + |\delta_2\rangle\langle\delta_2| + |\delta_3\rangle\langle\delta_3| + |\delta_4\rangle\langle\delta_4|$. Though we didn't prove $|\ln S_L(E)/\ln L| \rightarrow \zeta(E)$ as $L \rightarrow \infty$ in the case of a rank-four perturbation, we approximate the decay exponent $\zeta(E)$ by $|\ln S_{1000}(E)/\ln 1000|$ and plot this value for a variety of energies E in Figure 2. Qualitatively, this should be a good approximation of the behaviour of the decay exponent when changing the energy E .

Figure 2. The decay exponent $\zeta(E)$ of the ground-state overlap $S_L(E)$ depending on the energy E

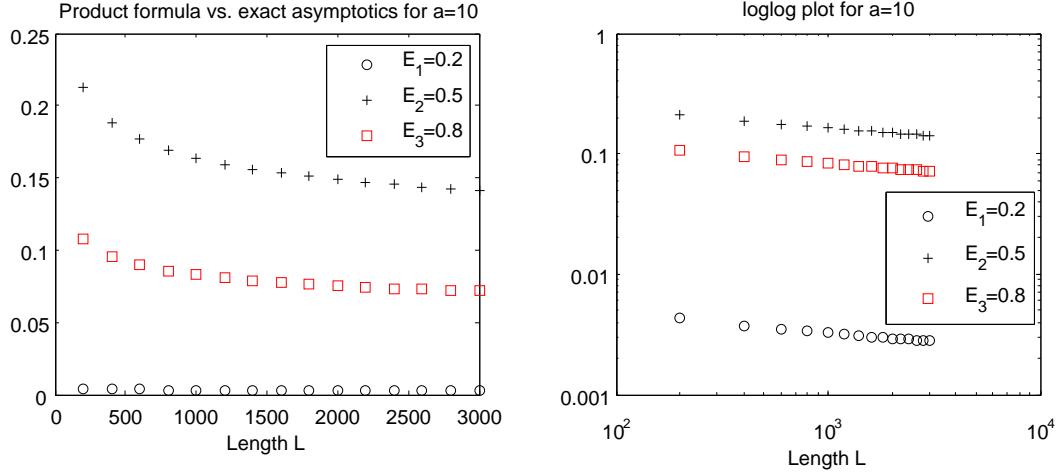


We comment on one thing concerning Figure 2. The behaviour of the decay exponent ζ at the right spectral edge is related, up to a factor of π , to the number of the eigenvalues which are pushed over the spectral edge by the non-negative perturbation V . In our case this number is at most 4π due to the rank-four perturbation. One can see this number in the second picture of Figure 2 at the right spectral edge. Such theorems go under the name Levinson's theorem in the theory of ODEs, see e.g. [RS79].

In Figure 3 we focus again on the product formula deduced for rank-one perturbations in Chapter 3, Theorem 3.3. One can ask, whether this formula is a good approximation of the actual asymptotics of $S_L(E)$ for more general perturbations than a rank-one perturbation. This is in particular interesting if we remember that the main ingredient to obtain the asymptotics out of the product formula was Lemma 3.15. This lemma relates the eigenvalues of the perturbed operator H'_L with the eigenvalues of the unperturbed operator H_L in terms of the scattering phase shift. Later on, we saw that this relation does not rely on the rank-one perturbation and we proved a corresponding lemma also for more general perturbations, see Lemma 4.11.

We consider a rank-two perturbation V and compare the decay exponent of the actual value of $S_L(E)$ with the value of the decay exponent given by the product formula in this situation. More precisely, let us call $Q_L(E)$ the value of the overlap resulting from the

Figure 3. The difference of the decay exponents of the ground-state overlap $\mathcal{S}_L(E)$ and the product formula $Q_L(E)$ for rank-two perturbations



product formula in Theorem 3.3. Then, we plot in Figure 3 the difference $|\ln \mathcal{S}_L(E) - \ln Q_L(E)| / \ln L$ for increasing length scales L . Figure 3 suggests that the product formula might be a good approximation of the asymptotics. Moreover, the loglog plot indicates that the difference of the decay exponents may converge algebraically to 0 as $L \rightarrow \infty$.

Conjecture: We have the following behaviour $|\frac{\ln \mathcal{S}_L(E)}{\ln L} - \frac{\ln Q_L(E)}{\ln L}| = O\left(\frac{1}{L^\alpha}\right)$ for some $\alpha > 0$ as $L \rightarrow \infty$, i.e. the asymptotic behaviour of the product formula gives the asymptotics of the ground-state overlap also for more general perturbations than rank-one perturbations.

The Case including a Random Background Potential. In this subsection let V_0 be the multiplication operator given by a family of random variables $(V_\omega(n))_{n \in \mathbb{N}}$, which are independent and identically uniformly distributed on the interval $[0, 1]$.

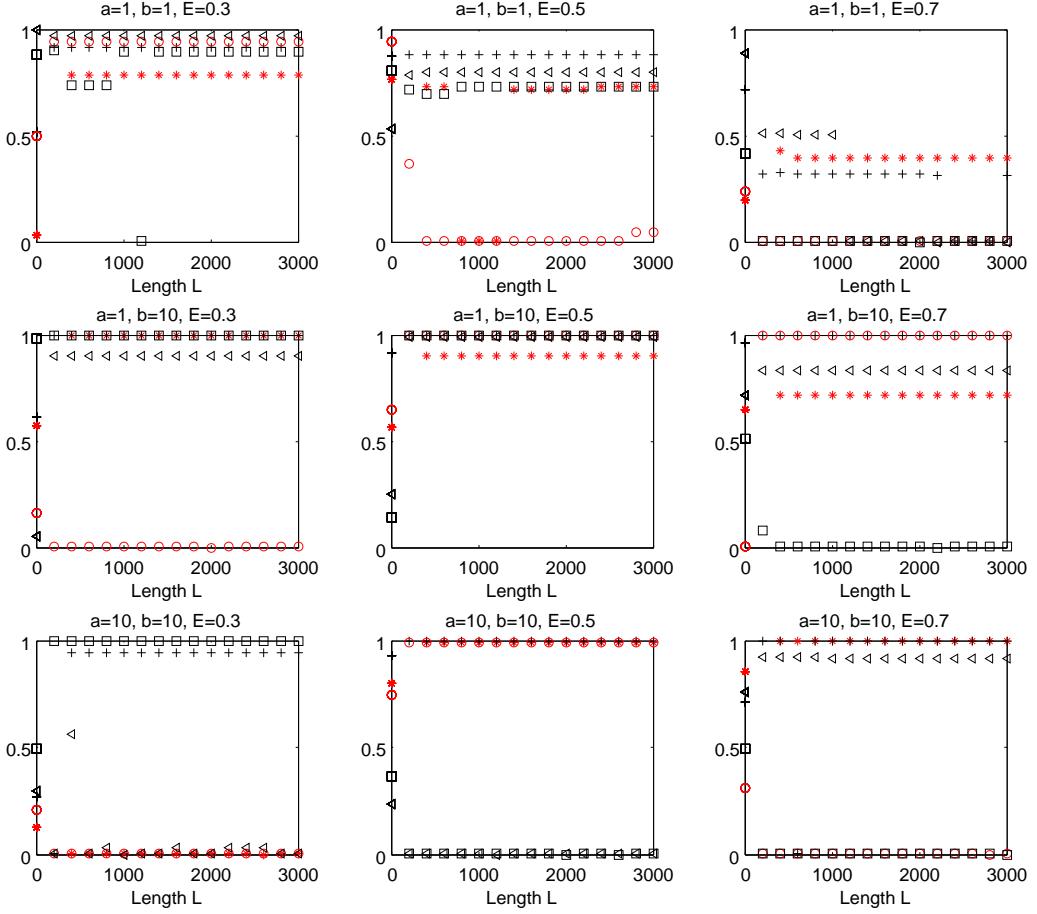
Morally, this setting is the same as in Chapter 5, just on the half-axis. We proved in Chapter 5 that the expectation value of the ground-state overlap stays bounded away from 0 at least for high disorder. But we were not able to obtain almost sure results or even results concerning a single realisation of the random potential.

Therefore, we start with Figure 4 which illustrates the behaviour of the ground-state overlap for various coupling constants a and various magnitudes of the random potential b . Here, the perturbation is the rank-one perturbation $V = |\delta_1\rangle\langle\delta_1|$ as considered in Chapter 5. We point out that we chose in any of the subplots in Figure 4 five realisations of the random potential. Moreover, the realisations in different subplots are independently chosen.

Throughout, one sees in Figure 4 that the ground-state overlap has a tendency to be either near one or near 0. Heuristically, this is reminiscent of the following. If one eigenvalue of H_L , which lies near the Fermi energy, is localised at δ_1 this eigenvalue jumps over the Fermi energy when turning on the perturbation. This implies a quite small ground-state overlap. If this does not happen, i.e. no relevant eigenvalue is localised near δ_1 the ground-state overlap stays near 1.

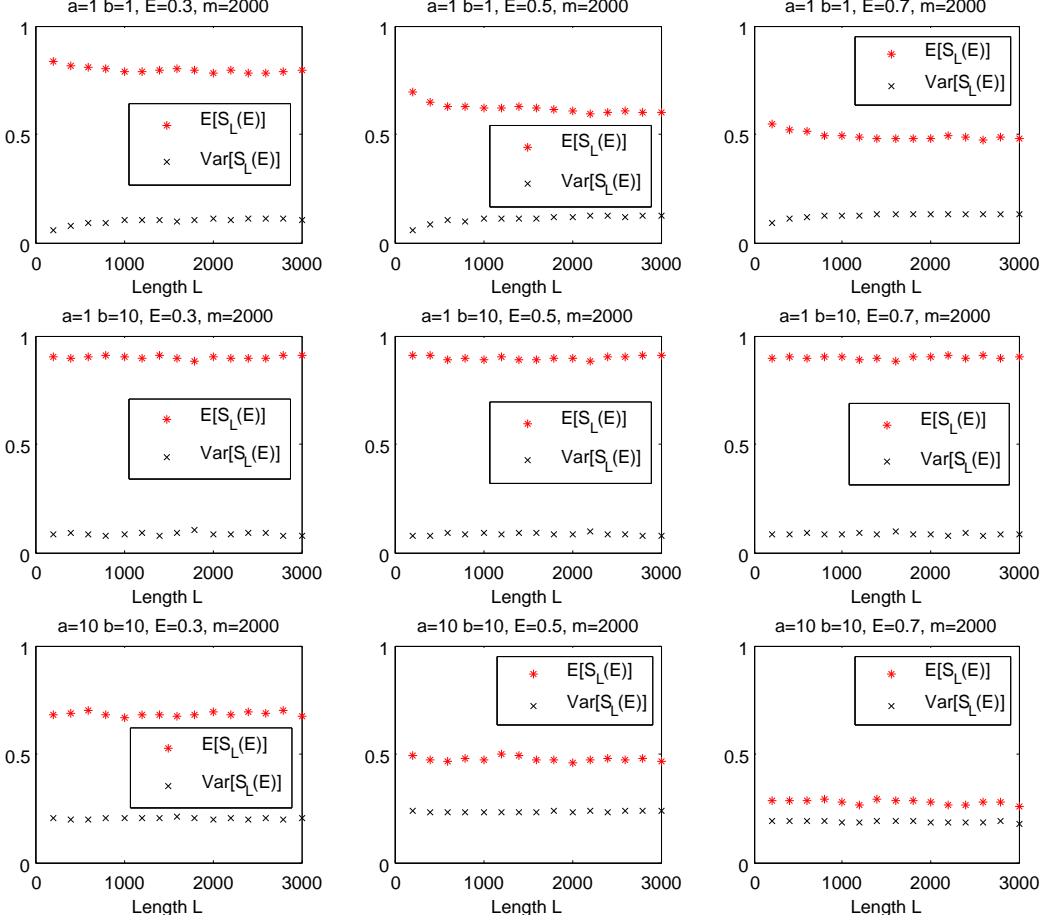
In general, we expect no non-trivial lower bounds on the ground-state overlap to hold at least for almost all realisations. Moreover, we expect the deviations from the mean to be quite big. Thus, we continue with a plot of the expectation value and the variance of

Figure 4. The ground-state overlap $\mathcal{S}_L(E)$ for various realisations of the random potential



the ground-state overlap. We computed in Figure 5 the value of the ground-state overlap for $m = 2000$ realisations of the random potential and plotted the mean and the variance of this vector. We did this for the same coupling constants and parameters as in Figure 4.

The first observation from Figure 5 is the large variance of $\mathcal{S}_L(E)$. Since $|\mathcal{S}_L(E)| \leq 1$, a variance of approximately 0.2, which implies a standard deviation of more than 0.4, is enormous compared to the value of $\mathcal{S}_L(E)$. Thus, we have large fluctuations of the ground-state overlap. Moreover, from the picture one sees that in the high disorder regime the expectation stays bounded away from 0. This is proven in Theorem 5.19. On the other hand in the case of moderate disorder, i.e. $b = 1$, it is not entirely clear what to expect by investigating our numerics only. Somehow it rather looks like the non-random picture, see Figure 1, but this could be reminiscent to considering too small length scales.

Figure 5. The expectation and the variance of the ground-state overlap $S_L(E)$ 

2. What is the Asymptotics of the Ground-State Overlap?

In this section we comment on the correct asymptotics of the ground-state overlap. As already pointed out earlier on, the upper bound found in [GKMO14]

$$\limsup_{k \rightarrow \infty} \frac{\ln |\mathcal{S}_{L_{n_k}}(E)|}{\ln L_{n_k}} \leq -\frac{\gamma(E)}{2}, \quad \text{with} \quad \gamma(E) := \frac{1}{\pi^2} \|\arcsin |T_E/2|\|_{\text{HS}}^2 \quad (6.4)$$

does not provide a sharp upper bound on the decay of the ground-state overlap in general. Therefore, the most striking question is to find larger decay exponents than γ or even optimal ones in more general situations than Dirac- δ perturbations.

The results of Chapter 3, deduced for a Dirac- δ perturbation, suggest that bound states prevent the result of [GKMO14] from being sharp. Here, we want to emphasise that this is not the case. To be more precise, we are not missing a correction in terms of the bound states in the exponent γ . We are rather missing a term depending on the finite-volume spectral-shift function at the Fermi energy E . Let us vaguely sketch this. We consider two systems on the half-axis which differ by a multiplication operator V , which creates one additional exponentially localised bound state ψ_1^L whereas the finite-volume spectral-shift

function $\xi_L(E) = 0$. We introduce the ground-state overlap using the notation of Chapter 2

$$\mathcal{S}_L(E) := \det \begin{pmatrix} \langle \varphi_1^L, \psi_1^L \rangle & \cdots & \langle \varphi_1^L, \psi_N^L \rangle \\ \vdots & & \vdots \\ \langle \varphi_N^L, \psi_1^L \rangle & \cdots & \langle \varphi_N^L, \psi_N^L \rangle \end{pmatrix}. \quad (6.5)$$

The following is not a rigorous argument but we think one can make it precise. Consider the k th column with $k > 1$. Then, the entry with the maximal absolute value of this vector is at the scalar product $\langle \varphi_{j_0(k)}^L, \psi_k^L \rangle$ where

$$\lambda_{j_0(k)}^L := \min \{ |\mu_k^L - \lambda_j^L| : 1 \leq j \leq N \} \quad (6.6)$$

and each column has some decay away from its maximum. This maximum is morally at the $k+1$ -entry of the vector. At a first glance the $k=1$ row which includes the exponentially localised ψ_1^L seems to behave differently. Due to the exponential fall-off, the matrix elements near the diagonal, e.g. $\langle \varphi_1^L, \psi_1^L \rangle$, are of lower order than $\langle \varphi_k^L, \psi_{j_0(k)}^L \rangle$ for $k > 1$. One might guess that this causes additional decay of the determinant. This intuition is wrong because the maximal entry of the $k=1$ column lies at the very end of this column, i.e. at $\langle \varphi_N^L, \psi_1^L \rangle$, and this scalar product is of the same order as $\langle \varphi_{j_0(k)}^L, \psi_k^L \rangle$ for $k > 1$. Heuristically, after shifting each column to the left, the maximum of each row lies on the diagonal of the matrix. Therefore, after this reordering one sees that there is no additional decay caused by the bound state. We have to admit that the above is very vague and of course the question is now: Where does the additional decay emerge? It comes from the states near the Fermi energy E . To illustrate this, we assume that the finite-volume spectral-shift function satisfies $\xi_L(E) = 2$, which means that the perturbation V pushes two eigenvalues over the Fermi energy E . Moreover, we suppose that $\lambda_{j_0(N)}^L = \lambda_{N+1}^L$. Now, consider the last row of the matrix in (6.5). Due to the above assumption, the natural partner of the eigenvalue μ_N^L in the sense of (6.6) is missing in the N th row. Therefore, the maximal entry of the row is abnormally small compared to the others. This effect will cause additional decay of the determinant not measured by γ .

The heuristics indicate that we are not missing a factor proportional to the number of bound states created by the perturbation but rather to the eigenvalues pushed over the Fermi energy by the perturbation. With these heuristics in mind, we consider a 3-dimensional spherically symmetric model and a spherically symmetric perturbation V . Then, we define

$$\theta(E) := \frac{1}{\pi^2} \sum_{\ell \in \mathbb{N}} (2\ell + 1) (\delta_\ell(\sqrt{E}))^2, \quad (6.7)$$

where δ_ℓ denotes the scattering-phase shift in the ℓ th angular momentum channel. Since δ_ℓ is a priori just defined up to a multiple of π , one has to find the right choice of δ_ℓ . It is convenient to take the δ_ℓ to be continuous with $\lim_{E \rightarrow \infty} \delta_\ell(\sqrt{E}) = 0$. This seems to be consistent with the above heuristics and Remark 4.6(iv), which says that the spectral-shift function corresponds to the scattering phase shift, normalised in the above way, at least for models on the half-axis. Moreover, we remark that this choice ensures that Levinson's theorem holds, see [RS79, Sct. XI]. In scattering theory the choice $|\tilde{\delta}_\ell| \in [0, \pi/2]$ is more common because one is interested in the behaviour of the generalised eigenvalues far away from the origin only. However, when $\tilde{\delta}_\ell$ crosses $\pi/2$ we pick up a winding number in the phase space of the Prüfer variables. Considering again the exponent γ , we rewrite using

the above definitions

$$\begin{aligned}\gamma(E) &= \frac{1}{\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1) (\arcsin(\sin(\delta_\ell(\sqrt{E}))))^2 \\ &= \frac{1}{\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1) (\tilde{\delta}_\ell(\sqrt{E}))^2,\end{aligned}\tag{6.8}$$

where $\tilde{\delta}_\ell$ is normalised according to $\tilde{\delta}_\ell \in [-\pi/2, \pi/2]$. Therefore, the crucial point, which we missed in the proof of [GKMO14], is the winding number of the scattering phase shifts.

We included in (6.7) the scattering phase shifts of the infinite volume. However, we obtain in the heuristics rather the phase shifts in the finite volume. Unfortunately, in higher dimensions we don't know if the infinite sum of the finite-volume scattering phase shifts converges to (6.7). Such convergence issues related to the finite-volume spectral-shift function are a quite delicate thing in higher dimensions, see [Kir87] and [HM10]. Therefore, one might generate faster decay than given by (6.7) for some choices of the thermodynamic limit. Nevertheless, we conjecture:

Conjecture: Let θ be the exponent defined in (6.7). Then,

$$\lim_{L \rightarrow \infty} \frac{S_L(E)}{\ln L} \leq \frac{\theta(E)}{2}.\tag{6.9}$$

We emphasise that the \leq sign is due to possible finite-size effects. To overcome such finite-size effects concerning the finite-volume spectral-shift function, one can consider related problems in the infinite volume. Recalling Lemma 2.9, we have the following identity of Fredholm determinants

$$|\mathcal{S}_L(E)|^2 = \det \left(I - 1_{(-\infty, \lambda_N^L]}(H_L) 1_{[\mu_{N+1}^L, \infty)}(H'_L) 1_{(-\infty, \lambda_N^L]}(H_L) \right)\tag{6.10}$$

up to a question of multiplicity of the eigenvalue μ_{N+1}^L . The above determinant is understood as a Fredholm determinant. There are at least two ways to generalise this to the infinite volume.

One is to consider the asymptotics of the Fredholm determinant

$$\det(I - 1_{\Lambda_L} Q(E) 1_{\Lambda_L}),\tag{6.11}$$

where 1_{Λ_L} is the projection on $\Lambda_L := [L/2, L/2]^d$ and

$$Q(E) := 1_{(-\infty, E)}(H) 1_{(E, \infty)}(H') 1_{(-\infty, E)}(H).\tag{6.12}$$

We conjecture that in the $d = 1$ case the following is true

$$\lim_{L \rightarrow \infty} \frac{\ln \det(I - 1_{\Lambda_L} Q(E) 1_{\Lambda_L})}{\ln L} = \theta(E)\tag{6.13}$$

for Leb.-a.e. $E \in \mathbb{R}$. Here, $\theta(E)$ is the one-dimensional analogue to (6.7).

Another one is introducing for $\epsilon > 0$ the operators

$$Q_\epsilon(E) := 1_{(-\infty, E-\epsilon]}(H) 1_{[E+\epsilon, \infty)}(H') 1_{(-\infty, E-\epsilon]}(H).\tag{6.14}$$

Products of traces of such operators are investigated in [FP15]. However, here we are interested in the exact asymptotics of the entire Fredholm determinant

$$\det(I - Q_\epsilon(E)).\tag{6.15}$$

in the limit $\epsilon \searrow 0$. We conjecture:

Conjecture: The decay exponent θ given in (6.7) provides precisely the right asymptotic behaviour of the Fredholm determinant Q_ϵ , i.e.

$$\lim_{\epsilon \searrow 0} \frac{\ln \det(I - Q_\epsilon(E))}{|\ln \epsilon|} = \theta(E). \quad (6.16)$$

APPENDIX A

An Integral Representation for Products of Spectral Projections

In this chapter we give a more detailed analysis on the spectral-correlation measures defined in Chapter 2, equation (2.22), and used throughout this thesis. Let again be

$$H = -\Delta + V_0 \quad \text{and} \quad H' = H + V, \quad (\text{A.1})$$

where

$$\begin{aligned} \max\{V_0, 0\} &\in K_{\text{loc}}^d(\mathbb{R}^d), \quad \max\{-V_0, 0\} \in K^d(\mathbb{R}^d), \\ V &\in L^1(\mathbb{R}^d), \quad V \geq 0. \end{aligned} \quad (\text{B})$$

Theorem A.1. *Assume conditions (B). Then, the mapping μ defined for all product sets by*

$$\mu(B \times B') := \text{tr} \left\{ \sqrt{V} 1_B(H) V 1_{B'}(H') \sqrt{V} \right\}, \quad B, B' \in \text{Borel}(\mathbb{R}), \quad (\text{A.2})$$

gives rise to a well-defined locally finite Borel measure on \mathbb{R}^2 . Moreover, for two disjoint open intervals A and B , which might touch, we have the identity

$$\text{tr} \left\{ 1_A(H) 1_B(H') 1_A(H) \right\} = \int_{A \times B} d\mu(x, y) \frac{1}{(y - x)^2}. \quad (\text{A.3})$$

Remarks A.2. (i) We point out that if $1_A(H) 1_B(H') 1_A(H)$ is not trace class the identity (A.3) still makes sense. In this case both sides of (A.3) are infinite. This may happen, if the intervals A and B touch.

(ii) The identity (A.1) also holds for the finite-volume restrictions of H and H' . In this case, the proof follows either along the same line as below or one uses the pure-point spectrum of the finite-volume operators, which was done in Lemma 2.12. Of course, one can use the representation for finite-volume operators to lift (A.3) to the infinite-volume operators by proving convergence of both sides in (A.3). Here, we will not do this but prove the above identity directly.

(iii) For a corresponding integral representation of higher powers of the operator $1_A(H) 1_B(H') 1_A(H)$, we run into the problem that for Borel sets $A_1, B_1, A_2, B_2, \dots, A_n, B_n$ traces of the form

$$\text{tr} \left\{ \sqrt{V} 1_{A_1}(H) V 1_{B_1}(H') V 1_{A_2}(H) V 1_{B_2}(H') \cdots 1_{A_n}(H) V 1_{B_n}(H') \sqrt{V} \right\} \quad (\text{A.4})$$

need not to be non-negative or real-valued, see [GKMO14] and [Küt14]. Nevertheless, viewed as a complex measure a corresponding formula to (A.3) holds at least for bounded Borel sets, see [Küt14].

From (A.3) we obtain the corollary.

Corollary A.3. *Let A, B be two intervals with $\text{dist}(A, B) > 0$. Then,*

$$\text{tr} \{1_A(H)1_B(H')1_A(H)\} \leq \frac{\text{tr} \left\{ \sqrt{V}1_A(H)V1_B(H')\sqrt{V} \right\}}{\text{dist}(A, B)^2}. \quad (\text{A.5})$$

In some cases the measure μ is absolutely continuous with a continuous density, see Lemma 2.19, and we obtain the sharper bound.

Corollary A.4. *Assume the measure μ has a density $\gamma \in L_{loc}^\infty(\mathbb{R}^2)$ and let $K \subset \mathbb{R}^2$ be compact. Then, for all intervals A, B within $K \subset \mathbb{R}^2$ and $\text{dist}(A, B) > 0$ there exists a constant $C(K)$ depending on K such that*

$$\text{tr} \{1_A(H)1_B(H')1_A(H)\} \leq C(K) |\ln(\text{dist}(A, B))|. \quad (\text{A.6})$$

Remarks A.5. (i) In the case of $V_0 = 0$, $0 \leq V \in L^\infty(\mathbb{R}^d)$ with $\text{supp } V$ compact, the measure μ is absolutely continuous with a continuous density within \mathbb{R}_+^2 , see Lemma 2.19. Thus, Corollary A.4 holds.

(ii) Apparently, this logarithmic divergence is the key to the findings in Chapter 2 and in [FP15].

Proof of Corollary A.4. Since the measure μ is absolutely continuous with a locally bounded density, we estimate

$$\text{tr} \{1_A(H)1_B(H')1_A(H)\} \leq \|\gamma\|_{L^\infty(K)} \int_{A \times B} dx dy \frac{1}{(y-x)^2}. \quad (\text{A.7})$$

Integrating the latter yields the corollary. \square

Though we allowed both sides in (A.3) to be infinite, in the case of $\text{dist}(A, B) > 0$ they are not.

Lemma A.6 (Lemma 3.2 [FP15]). *Let $A, B \in \text{Borel}(\mathbb{R})$ be two disjoint bounded intervals with $\text{dist}(A, B) > 0$. Then,*

$$1_A(H)1_B(H') \in \mathcal{S}_2 \quad \text{and} \quad 1_B(H')1_A(H) \in \mathcal{S}_2, \quad (\text{A.8})$$

where we denote by \mathcal{S}_2 the set of all Hilbert-Schmidt operators.

Proof. Note that the assumption on the perturbation provides $\sqrt{V} \in L^2(\mathbb{R}^d)$. Then, [Sim82, Thm. B.9.1] implies

$$\sqrt{V}1_A(H) \in \mathcal{S}_2 \quad \text{and} \quad \sqrt{V}1_B(H') \in \mathcal{S}_2. \quad (\text{A.9})$$

The rest follows along the very same line as in [FP15, Pf. of Lem. 3.2]. \square

Remark A.7. For two disjoint bounded intervals A and B , the assumption $V \in L^1(\mathbb{R}^d)$ does not imply that the operator $1_A(H)1_B(H')$ is trace class. Thus, we can not justify

$$\text{tr} \{1_A(H)1_B(H')1_A(H)\} = \text{tr} \{1_A(H)1_B(H')\}. \quad (\text{A.10})$$

To obtain that $1_A(H)1_B(H')$ is trace class, it suffices to assume $V \in \ell^1(L^1(\mathbb{R}))$, where the latter is some Birman-Solomjak space, see [Sim82, Sct. B.9]. Throughout this thesis, the perturbations V are nice enough to provide (A.10).

Proof of Theorem A.1. Let $B, B' \in \text{Borel}(\mathbb{R})$ be bounded. Then, by Lemma A.6 we may use cyclicity of the trace to see

$$\text{tr} \left\{ \sqrt{V} 1_B(H) V 1_{B'}(H') \sqrt{V} \right\} = \text{tr} \left\{ 1_B(H) V 1_{B'}(H') V 1_B(H) \right\} \geq 0. \quad (\text{A.11})$$

Moreover, Hölder's inequality and the norm inequality $\|\cdot\|_{\ell^2} \leq \|\cdot\|_{\ell^1}$ imply

$$\text{tr} \left\{ \sqrt{V} 1_B(H) V 1_{B'}(H') \sqrt{V} \right\} \leq \text{tr} \left\{ \sqrt{V} 1_B(H) \sqrt{V} \right\} \text{tr} \left\{ \sqrt{V} 1_{B'}(H') \sqrt{V} \right\}. \quad (\text{A.12})$$

The latter is finite due to Lemma A.6. Thus, results for bimeasures, see [Hor77], provide that the expression A.2 gives rise to uniquely defined locally finite Borel measures on \mathbb{R}^2 . Let $-\infty < a_1 < a_2 \leq b_1 < b_2 < \infty$ and $A := (a_1, a_2)$ and $B := (b_1, b_2)$ be two disjoint bounded intervals. If the intervals touch $a_2 = b_1$, consider A and $B_\epsilon := [b_1 + \epsilon, b_2]$ for $\epsilon > 0$ and use monotone convergence. Thus, we assume $a_2 < b_1$ and consider the function $F : \mathbb{R}_+ \rightarrow \mathbb{R}_+$

$$F : t \mapsto \text{tr} \left\{ 1_A(H) e^{tH} e^{-tH'} 1_B(H') 1_A(H) \right\}, \quad (\text{A.13})$$

which is well-defined by Lemma A.6. The idea of considering this function appears in [Pus08] and was also used in [FP15]. Now, F is twice differentiable with

$$F'(t) = - \text{tr} \left\{ 1_A(H) e^{tH} V e^{-tH'} 1_B(H') 1_A(H) \right\} \quad (\text{A.14})$$

$$F''(t) = \text{tr} \left\{ \sqrt{V} 1_A(H) e^{tH} V 1_B(H') e^{-tH'} \sqrt{V} \right\}, \quad (\text{A.15})$$

which we prove in Lemma A.8 below. Moreover, $F(0) = \text{tr} \{ 1_A(H) 1_B(H') 1_A(H) \}$, $\lim_{t \rightarrow \infty} F(t) = 0$, $\lim_{t \rightarrow 0} tF'(t) = 0$ and $\lim_{t \rightarrow \infty} tF'(t) = 0$. This follows from $a_2 < b_1$ and the estimate of the operator norm $\|e^{t(H-E)} 1_A(H)\| \leq e^{-t(E-a_2)}$, with $E := (b_1 + a_2)/2$, which implies $E - a_2 > 0$. Hence, the fundamental theorem of calculus and integration by parts imply

$$\begin{aligned} \text{tr} \{ 1_A(H) 1_B(H') 1_A(H) \} &= - \int_0^\infty dt F'(t) 1 \\ &= \int_0^\infty dt t \text{tr} \left\{ \sqrt{V} 1_A(H) e^{tH} V 1_B(H') e^{-tH'} \sqrt{V} \right\}. \end{aligned} \quad (\text{A.16})$$

On the other hand, since $a_2 < b_1$, we use the identity $\int_0^\infty dt t e^{-tx} = 1/x^2$, which is valid for $x \geq 0$, and Fubini's theorem to obtain

$$\begin{aligned} \int_{A \times B} d\mu(x, y) \frac{1}{(y-x)^2} &= \int_0^\infty dt t \int_{\mathbb{R}^2} d\mu(x, y) 1_A(x) e^{tx} 1_B(y) e^{-ty} \\ &= \int_0^\infty dt t \text{tr} \left\{ \sqrt{V} 1_A(H) e^{tH} V 1_B(H') e^{-tH'} \sqrt{V} \right\}. \end{aligned} \quad (\text{A.17})$$

Thus, (A.16) and (A.17) give the claim for intervals $[a_1, a_2]$ and $[b_1, b_2]$ with $-\infty < a_1 < a_2 \leq b_1 < b_2 < \infty$. For intervals with $-\infty < b_1 < b_2 \leq a_1 < a_2 < \infty$ consider the function

$$G : t \mapsto \text{tr} \left\{ 1_A(H) e^{-tH} e^{tH'} 1_B(H') 1_A(H) \right\}, \quad (\text{A.18})$$

and the same as above holds. \square

Lemma A.8. *Let $-\infty < a_1 \leq a_2 < b_1 \leq b_2 < \infty$ and $A := (a_1, a_2)$ and $B := (b_1, b_2)$. Define the function $F : \mathbb{R}_+ \rightarrow \mathbb{R}_+$*

$$F : t \mapsto \text{tr} \left\{ 1_A(H) e^{tH} e^{-tH'} 1_B(H') 1_A(H) \right\}. \quad (\text{A.19})$$

Then, F is twice differentiable with

$$F'(t) = -\operatorname{tr} \left\{ 1_A(H) e^{tH} V e^{-tH'} 1_B(H') 1_A(H) \right\} \quad (\text{A.20})$$

$$F''(t) = \operatorname{tr} \left\{ \sqrt{V} 1_A(H) e^{tH} V 1_B(H') e^{-tH'} \sqrt{V} \right\}. \quad (\text{A.21})$$

Proof. First, note that the spectral theorem implies

$$F(t) = \operatorname{tr} \left\{ e^{t\tilde{H}} 1_A(H) 1_B(H') e^{-t\tilde{H}'} 1_B(H') 1_A(H) \right\}, \quad (\text{A.22})$$

where $\tilde{H} := H 1_A(H)$ and $\tilde{H}' := H' 1_B(H')$ are bounded operators. Thus, we can expand $e^{t\tilde{H}}$ and $e^{-t\tilde{H}'}$ in norm-convergent power series and we obtain

$$\begin{aligned} & \frac{1}{h} \left(e^{h\tilde{H}} 1_A(H) 1_B(H') e^{-h\tilde{H}'} - 1_A(H) 1_B(H') \right) + 1_A(H) V 1_B(H') \\ &= h \sum_{j=1}^5 f_j(H) 1_A(H) 1_B(H') g_j(H'), \end{aligned} \quad (\text{A.23})$$

where the f'_j s and g'_j s are some bounded functions. Since $1_A(H) 1_B(H')$ is Hilbert-Schmidt by Lemma A.6, (A.20) follows from (A.23). Moreover, the proof of Lemma A.6 provides that $1_A(H) V 1_B(H')$ is trace class. Hence, we use the cyclicity of the trace to obtain

$$F'(t) = -\operatorname{tr} \left\{ 1_A(H) V 1_B(H') e^{-tH'} e^{tH} 1_A(H) \right\}. \quad (\text{A.24})$$

Now, the second assertion (A.21) follows along the same line as above. \square

APPENDIX B

The Cauchy determinant

In this chapter we compute the determinant of the Cauchy matrix. We use this in Theorem 3.3 to obtain a product representation of the ground-state overlap. We do this only for convenience and completeness. One can find a proof e.g. in [Wey13, Lem. 7.6.A].

Theorem B.1. *Let $N \in \mathbb{N}$ and $\alpha_1, \dots, \alpha_N, \beta_1, \dots, \beta_N \in \mathbb{R}$ be two sequences such that $(\beta_k - \alpha_j) \neq 0$ for all $1 \leq j, k \leq N$. Then,*

$$\left| \det \left(\frac{1}{\beta_k - \alpha_j} \right)_{1 \leq j, k \leq N} \right|^2 = \frac{\prod_{j,k=1, j \neq k}^N |\beta_k - \beta_j| |\alpha_j - \alpha_k|}{\prod_{j,k=1}^N |\beta_k - \alpha_j|^2}. \quad (\text{B.1})$$

Remark B.2. For the particular choice $\beta_k := k$ and $\alpha_j := j - 1$, the latter matrix is the Hilbert matrix.

Proof. We prove the above by induction. For $N = 1$, (B.1) is satisfied. Let $N \in \mathbb{N}$. We call v_1, \dots, v_N the columns of the matrix on the l.h.s. of (B.1), i.e. for $1 \leq i \leq N$

$$v_i^T := \left(\frac{1}{\beta_1 - \alpha_i} \quad \cdots \quad \frac{1}{\beta_N - \alpha_i} \right). \quad (\text{B.2})$$

Since the determinant is linear in the columns and is equal to 0, if two columns coincide, we manipulate

$$\begin{aligned} \det(v_1 \cdots v_N) &= \det(v_1, v_2 - v_1, v_3, \dots, v_N) \\ &= \det(v_1, v_2 - v_1, \dots, v_N - v_1) \\ &= \det \begin{pmatrix} \frac{1}{\beta_1 - \alpha_1} & \frac{\alpha_1 - \alpha_2}{(\beta_1 - \alpha_2)(\beta_1 - \alpha_1)} & \cdots & \frac{\alpha_1 - \alpha_N}{(\beta_1 - \alpha_N)(\beta_1 - \alpha_1)} \\ \vdots & & & \vdots \\ \frac{1}{\beta_N - \alpha_1} & \frac{\alpha_1 - \alpha_2}{(\beta_N - \alpha_2)(\beta_N - \alpha_1)} & \cdots & \frac{\alpha_1 - \alpha_N}{(\beta_N - \alpha_N)(\beta_N - \alpha_1)} \end{pmatrix}. \end{aligned} \quad (\text{B.3})$$

The multi-linearity of the determinant gives

$$(\text{B.3}) = \prod_{k=1}^N \frac{1}{(\beta_k - \alpha_1)} \prod_{j=2}^N (\alpha_1 - \alpha_N) \det \begin{pmatrix} 1 & \frac{1}{\beta_1 - \alpha_2} & \cdots & \frac{1}{\beta_1 - \alpha_N} \\ \vdots & & & \vdots \\ 1 & \frac{1}{\beta_N - \alpha_2} & \cdots & \frac{1}{\beta_N - \alpha_N} \end{pmatrix}. \quad (\text{B.4})$$

We call rows of the matrix on the r.h.s. of (B.4) w_1, \dots, w_N , i.e. for $1 \leq j \leq N$

$$w_j := \left(1 \quad \frac{1}{\beta_j - \alpha_2} \quad \cdots \quad \frac{1}{\beta_j - \alpha_N} \right). \quad (\text{B.5})$$

As before, we subtract the row w_1 from w_2, \dots, w_N and end up with

$$\begin{aligned} \det \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{pmatrix} &= \det \begin{pmatrix} w_1 \\ w_2 - w_1 \\ \vdots \\ w_N - w_1 \end{pmatrix} \\ &= \det \begin{pmatrix} 1 & \frac{1}{\beta_1 - \alpha_2} & \cdots & \frac{1}{\beta_1 - \alpha_N} \\ 0 & \frac{1}{(\beta_2 - \alpha_2)(\beta_1 - \alpha_2)} & \cdots & \frac{1}{(\beta_2 - \alpha_N)(\beta_1 - \alpha_N)} \\ \vdots & \vdots & & \vdots \\ 0 & \frac{1}{(\beta_N - \alpha_2)(\beta_1 - \alpha_2)} & \cdots & \frac{1}{(\beta_N - \alpha_N)(\beta_1 - \alpha_N)} \end{pmatrix}. \end{aligned} \quad (\text{B.6})$$

Now the multi-linearity and the Leibniz formula imply

$$\begin{aligned} (\text{B.6}) &= \prod_{j=2}^N \frac{1}{(\beta_1 - \alpha_j)} \prod_{k=2}^N (\beta_1 - \beta_k) \det \begin{pmatrix} 1 & \frac{1}{\beta_2 - \alpha_2} & \cdots & \frac{1}{\beta_2 - \alpha_N} \\ 0 & \frac{1}{\beta_3 - \alpha_2} & \cdots & \frac{1}{\beta_3 - \alpha_N} \\ \vdots & \vdots & & \vdots \\ 0 & \frac{1}{\beta_N - \alpha_2} & \cdots & \frac{1}{\beta_N - \alpha_N} \end{pmatrix} \\ &= \prod_{j=2}^N \frac{1}{(\beta_1 - \alpha_j)} \prod_{k=2}^N (\beta_1 - \beta_k) \det \begin{pmatrix} \frac{1}{\beta_2 - \alpha_2} & \cdots & \frac{1}{\beta_2 - \alpha_N} \\ \vdots & & \vdots \\ \frac{1}{\beta_N - \alpha_2} & \cdots & \frac{1}{\beta_N - \alpha_N} \end{pmatrix}, \end{aligned} \quad (\text{B.7})$$

The induction hypothesis, equation (B.4) and equation (B.7) give

$$\begin{aligned} &\left| \det \left(\frac{1}{\beta_k - \alpha_j} \right)_{1 \leq j, k \leq N} \right|^2 \\ &= \prod_{k=2}^N \frac{(\beta_1 - \beta_k)^2}{(\beta_k - \alpha_1)^2} \prod_{j=2}^N \frac{(\alpha_1 - \alpha_N)^2}{(\beta_1 - \alpha_j)^2} \frac{1}{(\beta_1 - \alpha_1)^2} \frac{\prod_{j,k=2, j \neq k}^N |\beta_k - \beta_j| |\alpha_j - \alpha_k|}{\prod_{j,k=2}^N |\beta_k - \alpha_j|^2} \\ &= \frac{\prod_{j,k=1, j \neq k}^N |\beta_k - \beta_j| |\alpha_j - \alpha_k|}{\prod_{j,k=1}^N |\beta_k - \alpha_j|^2}. \end{aligned} \quad (\text{B.8})$$

□

List of symbols

| | |
|-------------------------------|---|
| $H := -\Delta + V_0$ | infinite-volume Schrödinger operator |
| $H' := H + V$ | infinite-volume perturbed Schrödinger operator |
| $-\Delta$ | negative Laplacian |
| V, V_0 | perturbation of H , background potential |
| H_α | negative Laplacian with a Dirac- δ perturbation, see Chaper 3, Section 2 |
| h^l, h^0, h_α^0 | Schrödinger operators on the half-axis, see Chaper 3, Section 2 |
| L | length parameter |
| Λ_L | finite volume of diameter $L > 0$ with $0 \in \Lambda_L$ |
| $B_L(0)$ | Euclidean ball of radius L around the origin |
| H_L, H'_L | restrictions of H and H' to the finite volume Λ_L |
| $H_{\alpha,L}$ | restriction of H_α to $B_L(0)$, see Chaper 3, Section 2 |
| $h_L^\ell, h_{\alpha,L}^\ell$ | restrictions of h^ℓ and h_α^ℓ to the interval $(0, L)$, see Chaper 3, Section 2 |
| H_ω | random Schrödinger operator of the Anderson model, see Equation (5.1) |
| H'_ω | rank-one perturbation of H_ω , see Equation (5.4) |
| λ_j^L, μ_k^L | eigenvalues of the finite-volume restrictions counted from below |
| φ_j^L, ψ_k^L | eigenfunctions corresponding to λ_j^L and μ_k^L |
| N | particle number |
| $N_L(E)$ | particle number corresponding to a Fermi energy E and a lenth scale L |
| $N_L^\ell(E)$ | relative particle number corresponding to the ℓ th angular momentum channel, see Equation (3.85) |
| ρ | integrated density of states of the unperturbed operator |
| S_L^N | ground-state overlap corresponding to some $N \in \mathbb{N}$ and $L > 0$ defined in (1.5) |
| $S_L(E)$ | ground-state overlap S_L^N for a special choice of N depending on E , see Equation (2.5) |
| Ξ_L^N | difference of the ground-state energies, see Equation (1.13) |
| $\tilde{\gamma}(E)$ | decay exponent found in [GKM14], see Theorem 2.2 |
| $\gamma(E)$ | decay exponent found in [GKMO14], see Theorem 2.2 |
| $\zeta(E)$ | decay exponent of Theorem 3.17 |

| | |
|---|---|
| μ_L, μ | spectral-correlation measures, see Lemma 2.12 and Appendix A |
| $\gamma(E, E')$ | density of the absolutely continuous part of the measure μ |
| $\bar{\mu}$ | expectation value of the spectral-correlation measure μ , see Lemma 5.11 |
| $\bar{\gamma}(E)$ | expectation value of the decay exponent $\bar{\gamma}(E)$, see Theorem 5.34 |
| T_E, S_E | T-matrix and S-matrix corresponding to the pair H and H' |
| $\delta(\sqrt{E})$ | scattering phase shift, see Definition 4.5 |
| $\delta_\ell(\sqrt{E})$ | scattering phase shift in the ℓ th angular momentum channel |
| $\delta_\alpha(\sqrt{E})$ | scattering phase shift corresponding to the pair H and H_α , see Definition 3.11 |
| ξ | infinite-volume spectral-shift function, see Remark 4.1(i) |
| ξ_L | finite-volume spectral-shift function, see Equation (4.10) |
| χ_L^+, χ_L^- | smooth cut-off functions, see Definition 2.14 |
| α_j, β_k | eigenvalues of a pair of compact operators A and B , see Equation (3.1) |
| θ_k, ρ_u | Prüfer variables, see Equation (4.59) |
| $A_s^{(\cdot)}, A_s'$ | see Definition 5.3 |
| $G^{E, \epsilon}_{(\cdot)}$ | resolvent at the energy $E + i\epsilon$, see Definition 5.22 |
| ν | coupling constant in front of the perturbation, see Equation (5.4) |
| λ | strength of the disorder, see Equation (5.1) |
| $\langle \cdot, \cdot \rangle$ | scalar product, anti-linear in the first and linear in the second argument |
| $\ \cdot\ _{\text{HS}}$ | Hilbert-Schmidt norm |
| $\ \cdot\ $ | operator norm |
| $ \cdot _1, \cdot _2$ | 1-norm, respectively, 2-norm on \mathbb{R}^d or \mathbb{Z}^d |
| $\mathcal{S}_1, \mathcal{S}_2$ | set of all trace-class, respectively all Hilbert-Schmidt operators on the appropriate Hilbert space |
| $\text{Borel}(X)$ | σ -algebra generated by all open subset of the topological space X |
| $L^2(X), L^\infty(X)$ | set of all square integrable, respectively all essentially bounded, functions on $X \in \text{Borel}(\mathbb{R}^d)$ w.r.t. the Lebesgue measure |
| 1_A | indicator function of a Borel set $A \in \text{Borel}(X)$ |
| $\sigma(T)$ | spectrum of the linear operator T |
| $\sigma_{\text{pp}}(T), \sigma_{\text{sc}}(T),$ | spectral subsets of the linear operator T |
| $\sigma_{\text{ac}}(T)$ | |
| $\varrho(T)$ | resolvent set of the linear operator T |
| $\text{dom}(T)$ | domain of the linear operator T |

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(Siehe Promotionsordnung vom 12. 7. 2011, § 8, Abs. 2 Pkt. 5)

Hiermit erkläre ich an Eides statt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt wurde.

Martin Gebert

Ort, Datum

Unterschrift Doktorand