ANDERSON'S ORTHOGONALITY CATASTROPHE

DISSERTATION

AN DER

FAKULTÄT FÜR MATHEMATIK, INFORMATIK UND STATISTIK

DER

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

vorgelegt von

Heinrich Küttler

am 2. Juli 2014

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Berichterstatter
Prof. Dr. Peter Müller
Prof. Dr. Werner Kirsch

Tag der Disputation
19. September 2014

1. Gutachter: Prof. Dr. Peter Müller
2. Gutachter: Prof. Dr. Werner Kirsch

Tag der Disputation: 19. September 2014

I know that there is nothing better for people
than to be happy and to do good while they live.
That each of them may eat and drink,
and find satisfaction in all their toil – this is the gift of God.
ECCLESIASTES 3:12-13

ZUSAMMENFASSUNG

Das Thema dieser Arbeit ist die mathematische Behandlung von Andersons Orthogonalitätskatastrophe, einem intrinsischen Effekt in Fermi-Gasen. P. W. Anderson untersuchte das nach ihm benannte Phänomen in den späten 60iger Jahren. In seinem ersten Beitrag zur Katastrophe in [And67a] behandelte Anderson ein System von N nicht-wechselwirkenden Fermionen im dreidimensionalen Raum und stellte fest, dass der Grundzustand asymptotisch orthogonal ist zum Grundzustand des gleichen Systems, gestört durch ein Streupotential mit endlicher Reichweite.

Genauer formuliert: Sei Φ_L^N der N-Teilchen-Grundzustand des Fermionensystems in einer d-dimensionalen Box mit Kantenlänge L, und sei Ψ_L^N der Grundzustand des entsprechenden Systems mit einem zusätzlichen Potential endlicher Reichweite. Dann verursacht die Katastrophe das asymptotische Verschwinden

$$\mathcal{S}_L^N := \langle \Phi_L^N, \Psi_L^N \rangle \sim L^{-\gamma/2} \tag{$*$}$$

des Überlapps $\mathcal{S}_L^N$ der N-Teilchen-Grundzustände Φ_L^N und Ψ_L^N. Die Asymptotik in Gleichung $(*)$ versteht sich im thermodynamischen Limes $L \to \infty$ und $N \to \infty$ mit fester Dichte $N/L^d \to \rho > 0$.

In [GKM14] wurde der Überlapp $\mathcal{S}_L^N$ durch eine asymptotische Schranke der Form

$$|\mathcal{S}_L^N|^2 \lesssim L^{-\tilde{\gamma}} \tag{$**$}$$

nach oben abgeschätzt. Der Abkling-Koeffizient $\tilde{\gamma}$ dort entspricht demjenigen von Anderson in [And67a]. Eine weitere Arbeit von Anderson aus dem selben Jahr, [And67b], enthält die exakte Asymptotik $(*)$ mit einem größeren Koeffizienten γ.

Die vorliegende Arbeit stellt einen Beitrag dar, zur exakten Asymptotik zu gelangen. Es wird $(**)$ mit einem Koeffizienten γ bewiesen, der in gewissem Sinne dem in [And67b] entspricht und den in [GKM14] verbessert. Die verwendete Methode ist die aus [GKM14], es werden aber in einer Reihenentwicklung von $\ln \mathcal{S}_L^N$ sämtliche Terme statt nur des ersten Terms behandelt. Die Behandlung der höheren Terme geht mit der Schwierigkeit einher, dass die auftretenden Spur-Ausdrücke nicht mehr zwingend nicht-negativ sind, was für einige Abschätzungen aus [GKM14] zusätzliche Argumente nötig macht.

Das Hauptresultat der vorliegenden Arbeit wird auch in einer gemeinsamen Veröffentlichung [GKMO] mit Martin Gebert, Peter Müller und Peter Otte erscheinen.

ABSTRACT

The topic of this thesis is a mathematical treatment of Anderson's orthogonality catastrophe. Named after P. W. Anderson, who studied the phenomenon in the late 1960s, the catastrophe is an intrinsic effect in Fermi gases. In his first work on the topic in [And67a], Anderson studied a system of N noninteracting fermions in three space dimensions and found the ground state to be asymptotically orthogonal to the ground state of the same system perturbed by a finite-range scattering potential.

More precisely, let Φ_L^N be the N-body ground state of the fermionic system in a d-dimensional box of length L, and let Ψ_L^N be the ground state of the corresponding system in the presence of the additional finite-range potential. Then the catastrophe brings about the asymptotic vanishing

$$\mathcal{S}_L^N := \langle \Phi_L^N, \Psi_L^N \rangle \sim L^{-\gamma/2} \tag{$*$}$$

of the overlap $\mathcal{S}_L^N$ of the N-body ground states Φ_L^N and Ψ_L^N. The asymptotics in equation ($*$) is in the thermodynamic limit $L \to \infty$ and $N \to \infty$ with fixed density $N/L^d \to \rho > 0$.

In [GKM14], the overlap $\mathcal{S}_L^N$ has been bounded from above with an asymptotic bound of the form

$$|\mathcal{S}_L^N|^2 \lesssim L^{-\tilde{\gamma}}. \tag{$**$}$$

The decay exponent $\tilde{\gamma}$ there corresponds to the one of Anderson in [And67a]. Another publication by Anderson from the same year, [And67b], contains the exact asymptotics ($*$) with a bigger coefficient γ.

This thesis features a step towards the exact asymptotics. We prove ($**$) with a coefficient γ that corresponds in a certain sense to the one in [And67b], and improves upon the one in [GKM14]. We use the methods from [GKM14], but treat every term in a series expansion of $\ln \mathcal{S}_L^N$, instead of only the first one. Treating the higher order terms introduces additional arguments since the trace expressions occurring are no longer necessarily nonnegative, which complicates some of the estimates from [GKM14].

The main contents of this thesis will also be published in a forthcoming article [GKMO] co-authored with Martin Gebert, Peter Müller, and Peter Otte.

CONTENTS

INTRODUCTION

The topic of this thesis is a mathematical treatment of Anderson's orthogonality catastrophe (AOC). Named after P. W. Anderson, who studied the phenomenon in the late 1960s, the AOC is an intrinsic effect in Fermi gases. In his first work on the topic in [And67a], Anderson studied a system of N noninteracting fermions in three space dimensions and found the ground state to be asymptotically orthogonal to the ground state of the same system perturbed by a finite-range scattering potential. The asymptotics here involve the $N \to \infty$ limit, as well as a spatial limit for the box size the fermionic system resides in.

More precisely, let Φ_L^N be the N-body ground state of the fermionic system in a d-dimensional box of length L, and let Ψ_L^N be the ground state of the corresponding system in the presence of the additional finite-range potential. Then the AOC brings about the asymptotic orthogonality

$$\langle \Phi_L^N, \Psi_L^N \rangle \sim L^{-\gamma/2} \tag{I.1}$$

in the thermodynamic limit $N \to \infty$ and $L \to \infty$, where N/L^d converges to some positive constant.

However, the AOC has shown itself to be a more robust phenomenon with implications beyond single-impurity problems, and the physics literature continues to discuss it. Being classically treated in connection to effects in metals, like Fermi-edge singularities in the x-ray edge problem (see [ND69; OT90]), the recent literature considers the AOC in absorption in quantum dots, or in graphene and other mesoscopic systems (see [Hel+05; Tür+11; HK12a; HK12b], as well as [HUB05; HG07; RH10]).

The original derivation of the power law (I.1) was given by [And67a], where a noninteracting Fermi gas in three dimensions is perturbed by a compactly supported spherically symmetric single-particle potential. Anderson's informal computation uses bounds on the Slater determinant of the two ground states and arrives at

$$\langle \Phi_L^N, \Psi_L^N \rangle = \mathrm{O}(L^{-\tilde{\gamma}/2}) \tag{I.2}$$

in the thermodynamic limit, and he writes the decay exponent $\tilde{\gamma}$ using the (single-particle) scattering phases $(\delta_\ell)_{\ell\in\mathbb{N}_0}$ associated with the perturbation, namely

$$\tilde{\gamma} = \frac{1}{\pi^2}\sum_{\ell=0}^{\infty}(2\ell+1)\big(\sin\delta_\ell\big)^2. \tag{I.3}$$

In [And67b] later that same year, Anderson derived the exact asymptotics (I.1) with an exponent γ bigger than the exponent $\tilde{\gamma}$, stating that »[i]t is interesting that the main difference from the previous result is to replace $\sin^2\delta$ by δ^2« [And67b, p. 164].

In the decade after 1967, Anderson's result was the subject of some discussion in the literature, with [RS71] claiming a different result, but [Ham71] correcting their result back to Anderson's original one, and [KY78] confirming Anderson's result using an adiabatic approach.

By now, Anderson's asymptotics (I.1) are well-established in the physics community. Its mathematical treatment, however, was severely lacking until last year. Although [Ott05] found a limit expression for the overlap involving solutions to a Wiener-Hopf equation, this expression could not be controlled in the thermodynamic limit and did therefore not yield any asymptotics – it did, however, shed some light from a mathematical point of view on the discussion between [RS71] and [Ham71] regarding the correctness of interchanging of limits. The first mathematical proof of the orthogonality (I.2) was given in [KOS13], where a rigorous version of the bound in [And67a] was proved for the one-dimensional case. A proof for the asymptotic bound (I.2) valid for any dimension was then given in [GKM14], with a decay exponent $\tilde{\gamma}$ that reduces to (I.3), the one first given by Anderson, in the case Anderson considers. That proof uses the same bounds on Slater determinants that Anderson employed, too: a series expansion for the logarithm of the overlap is truncated after the first term, see Remark 1.3 below.

The aim of this thesis is to consider the full series expansion in order to arrive at a better asymptotic bound. The methods used are the ones from [GKM14], with some modifications made necessary by the character of the trace expressions that occur in the higher terms of the series. In particular, just as in [GKM14], the argument relies on the smoothing of indicator functions and on the Helffer-Sjőstrand formula (§§ 4 and 5 below). This smoothing necessarily provides just an asymptotic bound on the overlap, instead of the exact asymptotics, and for technical reasons, the asymptotics involves subsequences of length scales; see Theorem 10.1 for the rigorous statement. Formally, the result is the asymptotic bound

$$\langle \Phi_L^N, \Psi_L^N \rangle = \mathrm{O}(L^{-\gamma/2}) \tag{1.4}$$

with a decay exponent γ that is given by

$$\gamma = \frac{1}{\pi^2} \left\| \arcsin |T/2| \right\|_{\mathrm{HS}}^2, \tag{1.5}$$

where T is the transition matrix. This is a bigger expression than the decay exponent $\tilde{\gamma}$ from [GKM14], which can be written as

$$\tilde{\gamma} = \frac{1}{\pi^2} \left\| T/2 \right\|_{\mathrm{HS}}^2. \tag{1.6}$$

Note how this compares with the quote from [And67b] given above: while Anderson first gave an expression involving the sine function and then one without, here we move from an expression without a sine function to one with an arcsine function. In fact, we expect the asymptotics (1.1) to hold with the decay exponent γ given by (1.5). The methods employed here, however, only allow for an upper bound on the overlap. See Remark 10.2 below for a further discussion of open questions regarding the AOC.

The main contents of this thesis will also appear in a forthcoming article [GKMO] co-authored with Martin Gebert, Peter Müller, and Peter Otte.

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OVERVIEW. This thesis is divided into ten sections which follow in a linear fashion. The main result is therefore found in § 10, while the preceding sections contain propositions leading up to the main result.

§ 1 contains a description of the model we investigate, defines the overlap as the main quantity we are interested in and states a series expansion of that quantity.

§ 2 contains a method for rewriting the nth term of that series expansion in a different form.

§ 3 contains an integral formula going back to R. P. Feynman and J. S. Schwinger, and its application to the expression of the preceding section.

§ 4 contains the smoothing argument and the application of the Helffer-Sjőstrand formula as mentioned above.

§ 5 contains a proof of the Helffer-Sjőstrand formula, as well as a proof of a technical lemma from the preceding section, which is one of the core elements of the exposition.

§ 6 contains yet another way to rewrite an estimate of the nth term of the series we started with. In particular, the smoothing done in § 4 is undone in a certain way, and the smoothed functions replaced by discontinuous ones again.

§ 7 contains a proof of the asymptotic behavior of the expression from the preceding section. The expression is shown to diverge logarithmically, with a rate given by the trace of a certain operator times a particular integral.

§ 8 contains an evaluation of this integral.

§ 9 contains a formula expressing the trace part of the rate from § 7 via quantities from scattering theory.

§ 10 finally contains the proof of the asymptotic orthogonality (1.4), which follows from combining the statements from the preceding sections.

After the ten sections of the main matter of this thesis, three sections follow in the appendix. The first one states some conditions for the decay exponent γ to be positive, which is necessary for making the asymptotic bound (1.4) nontrivial. The second section provides some additional propositions and their proofs. The third and final section in the appendix gives a proof of the geometric resolvent inequality in the form needed in § 5.

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A WORD ON NOTATION. This thesis tries to follow certain stylistical and notational conventions; a list of commonly used symbols can be found in the appendix. On top of that, certain expressions occur multiple times and give rise to abbreviations or a certain precedence of operations. For instance, »operator functionals« like traces or determinants have a lower precedence than multiplication, and thus $\operatorname{tr} AB = \operatorname{tr}(AB)$ and $\operatorname{tr} A^n = \operatorname{tr}(A^n)$. Terms like »a.e.« (almost every) or »null set« refer to Lebesgue measure on the appropriate measure space, unless specified otherwise. Components of vectors from $\mathbb{R}^n$ are taken cyclically; in particular, $x_0 = x_n$ and $x_{n+1} = x_1$ for a vector $x \in \mathbb{R}^n$. Commonly used functions take $\pm\infty$ as their continuation whenever that is natural, for instance $\ln 0 := -\infty$ and $\operatorname{tr} A := \infty$ for a positive operator A that is not of trace class. Integration is denoted in the physics way, i.e., $\int_{\mathbb{R}} \mathrm{d}x\, f(x)$ is the integral of f on $\mathbb{R}$; if no measure is specified, the appropriate Lebesgue measure is meant. Expressions like $\int_M \mathrm{d}(x,y) f(x,y)$ for $M \subseteq X \times Y$ denote integration with respect to the product measure of appropriate Lebesgue measures on X and Y. The symbol $\cdot$ is used to denote an anonymous function, for instance $f(g(\cdot)) = f \circ g$; the same function could also be written $x \mapsto f(g(x))$; if the domain or codomain needs to be specified, we write $X \ni x \mapsto f(g(x)) \in Y$. The scalar product $\langle \cdot, \cdot \rangle$ on a Hilbert space is linear in the second argument. The universal quantification $\forall$ (for all) is sometimes put after the expression quantified and in parentheses, for instance $g(x) = f(x) \ (x \in M)$; the quantification statement might be read as »where $x \in M$«. Further abbreviations are introduced as we go along.

ACKNOWLEDGMENTS. To say that this thesis would not have been possible without my supervisor, Prof. Dr. Peter Müller, is to state a triviality. It is in my case, though, a truer triviality than most. Peter's relentless attention to detail inspired me, however often I failed to imitate it. But Peter was more than a teacher: he was also my boss for the last four years – a delightful experience, and one which I consider to be a great privilege.

The SFB/TR 12 of the German Research Council (DFG) supported this work, and I am thankful for that.

My colleagues were essential for the completion of this thesis. Martin Gebert has been a great collaborator and friend, listening to all my dubious ideas, and contributing better ones himself. Dr. Peter Otte not only made us aware of the catastrophe, which has proven to be such a fruitful subject, he also was the first to prove it, and his knowledge of the literature provided the key insight for the integral discussed in § 8.

Many more people gave important advice and were available for fruitful discussions. Among them are Dr. Alexander Pushnitski, Prof. Dr. Lars Diening, Prof. Dr. Wolfgang Spitzer, Prof. Dr. Hubert Kalf, Prof. Dr. Peter Stollmann, and others. I would like to thank all of them. Prof. Dr. Jürgen Voigt should also be mentioned: he was the one who taught me mathematics in the first place.

My office mate Dr. Ingo Wagner routinely answered my often weird and pointless questions about physics and mathematics. More than that, he was always available for weird and pointless dialogues about any subject matter whatsoever. Life would have been duller without his insights into popular culture.

Among my other colleagues, I want to distinguish Andreas Groh, Josef Mehringer, Michael Handrek, Lisa Kraus, and especially Verena von Conta, Dr. Constanza Rojas-Molina, Dr. Parth Soneji and Andrej Nikonov. All of you were important during my time here. So were other friends and acquaintances, among them Kathleen Schmidt, Gleda Golemi, and Gina Lularevic. Special thanks go to Eliane Wolf, who was present when this project was hardest.

Lest this list get too long and strenuous, I will stop here. But not before I thank my parents and siblings for their support, and Dr. Nadine Al-Kaisi, for more than medical supervision.

1 THE SETUP

Let $d \in \mathbb{N}$. Let $\Omega_1 \subseteq \mathbb{R}^d$ be open and bounded with $0 \in \Omega_1$. For $L > 1$, define $\Omega_L := L \cdot \Omega_1$.

Let the negative Laplacian $-\Delta_L$ be supplied with Dirichlet boundary conditions on Ω_L. We define two multiplication operators V_0 and V acting on $L_2(\Omega_L)$, corresponding to real-valued functions on $\mathbb{R}^d$ with the properties

$$\max\{V_0, 0\} \in K_{\text{loc}}(\mathbb{R}^d), \quad \max\{-V_0, 0\} \in K(\mathbb{R}^d) \tag{v$_0$}$$

and

$$V \in L_\infty(\mathbb{R}^d), \quad V \geq 0, \quad \text{spt}\, V \subseteq \Omega_1 \text{ compact.} \tag{v}$$

Here, $K(\mathbb{R}^d)$ and $K_{\text{loc}}(\mathbb{R}^d)$ denote the functions of Kato class and local Kato class, respectively, see [Sim82, §A2]; a list of notations used in this work can be found in the appendix. The *finite-volume one-particle Schrödinger operators* $H_L := -\Delta_L + V_0$ and $H'_L := H_L + V$ are self-adjoint and densely defined in the Hilbert space $L_2(\Omega_L)$. The *infinite-volume operators* $H := -\Delta + V_0$ and $H' := H + V$ are self-adjoint and densely defined in the Hilbert space $L_2(\mathbb{R}^d)$. Birman's theorem (see [BÈ67, Thm. 2] or [RS79, Thm. XI.10]; the assumptions there are satisfied due to [Sim82, Thm. B.9.1]) guarantees the existence and completeness of the wave operators for the pair H, H'. In particular, their absolutely continuous spectra are the same, i.e.,

$$\sigma_{\text{ac}}(H) = \sigma_{\text{ac}}(H'). \tag{1.1}$$

The assumptions (v$_0$) and (v) on V_0 and V, together with [BHL00, Thm. 6.1 and Remark 6.2 iii)], imply that the semigroup operators e^{-tH_L} and $e^{-tH'_L}$ generated by the finite-volume one-particle operators H_L and H'_L are trace class for every $t > 0$, and, a fortiori, compact. In particular, H_L and H'_L are bounded from below and have purely discrete spectra.

Let $\lambda_1^L \leq \lambda_2^L \leq \cdots$ and $\mu_1^L \leq \mu_2^L \leq \cdots$ be the sequences of the eigenvalues of H_L and H'_L, respectively, counting multiplicities. Let $(\varphi_j^L)_{j\in\mathbb{N}}$ and $(\psi_k^L)_{k\in\mathbb{N}}$ be the corresponding normalized eigenfunctions, with an arbitrary choice of basis vectors in any eigenspace of dimension greater than one.

Let $N \in \mathbb{N}$. The *induced (noninteracting) finite-volume N-particle Schrödinger operators* $\hat{H}_L$ and $\hat{H}'_L$ act on the totally antisymmetric subspace $\bigwedge_{j=1}^N L_2(\Omega_L)$ of the N-fold tensor product space and are given by

$$\hat{H}_L^{(\prime)} := \sum_{j=1}^{N} I \otimes \cdots \otimes I \otimes H_L^{(\prime)} \otimes I \otimes \cdots \otimes I, \tag{1.2}$$

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

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

Given $L > 1$ and a *Fermi energy* $E \in \mathbb{R}$, the *number of particles* is defined as

$$N_L(E) := \#\{j \in \mathbb{N};\, \lambda_j^L \le E\} \in \mathbb{N}_0, \tag{1.4}$$

which is the eigenvalue counting function of H_L at E. The main quantity of interest is the *ground-state overlap*

$$\mathcal{S}_L(E) := \big\langle \Phi_L^{N_L(E)}, \Psi_L^{N_L(E)} \big\rangle_{N_L(E)} = \det\Big(\langle \varphi_j^L, \psi_k^L \rangle \Big)_{j,k=1,\ldots,N_L(E)}, \tag{1.5}$$

in particular its asymptotic behavior as $L \to \infty$. In (1.5), $\langle \cdot\,, \cdot \rangle_N$ stands for the scalar product on the N-fermion space $\bigwedge_{j=1}^N L_2(\Omega_L)$, and $\langle \cdot\,, \cdot \rangle$ for the one on the single-particle space $L_2(\Omega_L)$. The equality in (1.5) is a consequence of the Leibniz formula for determinants.

If $N_L(E) = 0$, we set $\mathcal{S}_L(E) := 1$.

1.1 Remark. The particular choice (1.4) of $N_L(E)$ as an eigenvalue counting function turns out to be technically useful when conducting the thermodynamic limit, see Lemma 2.1 below. The *particle density* $\rho(E)$ of the two noninteracting fermion systems in the thermodynamic limit coincides with the integrated density of states

$$\rho(E) = \lim_{L \to \infty} \frac{N_L(E)}{L^d\, |\Omega_1|} \tag{1.6}$$

of the single-particle Schrödinger operator H (which is the same as the integrated density of states of H', see Lemma B.3 on page 57), provided the limit exists. Here, $|\Omega_1|$ denotes the Lebesgue measure of $\Omega_1 \subseteq \mathbb{R}^d$. Situations where the limit (1.6) is known to exist include periodic V_0, or V_0 vanishing at infinity. If the limit (1.6) does not exist, there is more than one accumulation point, since assumption (V_0), together with [Sim82, Thm. C.7.3], imply $\limsup_{L\to\infty} N_L(E)/L^d < \infty$ for every $E \in \mathbb{R}$. We will study the asymptotic behavior of the overlap $\mathcal{S}_L(E)$ as $L \to \infty$ regardless of the existence of the limit (1.6).

In order to expand the ground-state overlap as a series, we introduce the orthogonal projections

$$\mathrm{P}_L^N := \sum_{j=1}^N \langle \varphi_j^L, \cdot \rangle \varphi_j^L \quad \text{and} \quad \Pi_L^N := \sum_{k=1}^N \langle \psi_k^L, \cdot \rangle \psi_k^L \qquad (N \in \mathbb{N}_0). \tag{1.7}$$

Using those, we can prove the following lemma.

1.2 Lemma. Assume that $\mathcal{S}_L(E) \neq 0$. Then

$$|\mathcal{S}_L(E)|^2 = \exp\Big(-\sum_{n=1}^{\infty} \frac{1}{n} \operatorname{tr}\big(\mathrm{P}_L^{N_L(E)}(I - \Pi_L^{N_L(E)})\big)^n\Big), \tag{1.8}$$

where the trace is in the Hilbert space $L_2(\Omega_L)$.

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

$$(MM^*)_{j,\ell} = \sum_{k=1}^{N} \langle \varphi_j^L, \psi_k^L \rangle \langle \psi_k^L, \varphi_\ell^L \rangle = \langle \varphi_j^L, \Pi_L^N \varphi_\ell^L \rangle. \tag{1.9}$$

By assumption, $\mathcal{S}_L(E) \neq 0$, and therefore $M \neq 0$ and $MM^* > 0$. Moreover, MM^* is unitarily equivalent to $\mathrm{P}_L^N \Pi_L^N \mathrm{P}_L^N\big|_{\operatorname{lin}\{\varphi_1^L,\dots,\varphi_N^L\}} : \operatorname{ran} \mathrm{P}_L^N \to \operatorname{ran} \mathrm{P}_L^N$, since

$$\langle \varphi_j^L, \mathrm{P}_L^N \Pi_L^N \mathrm{P}_L^N \varphi_\ell^L \rangle = \langle \varphi_j^L, \Pi_L^N \varphi_\ell^L \rangle = (MM^*)_{j,\ell} \qquad (1 \le j, \ell \le N). \tag{1.10}$$

In particular, since P_L^N and Π_L^N are projections, $0 < MM^* \le 1$; it follows that $0 \le 1 - MM^* < 1$. This allows us to compute

$$\ln\big(MM^*\big) = \ln\big(1 - (1 - MM^*)\big) = -\sum_{n=1}^{\infty} \frac{1}{n}(1 - MM^*)^n, \tag{1.11}$$

since the series $\ln(1-x) = -\sum_{n=1}^{\infty} x^n/n$ converges absolutely for $|x| < 1$. This implies

$$|\mathcal{S}_L(E)|^2 = \det MM^* = \exp\big(\operatorname{tr}\ln(MM^*)\big) = \exp\Big(-\sum_{n=1}^{\infty} \frac{1}{n} \operatorname{tr}(1 - MM^*)^n\Big), \tag{1.12}$$

where the trace is in $\mathbb{C}^{N\times N}$. The matrix $1 - MM^*$ is unitarily equivalent to $(\mathrm{P}_L^N - \mathrm{P}_L^N \Pi_L^N \mathrm{P}_L^N)\big|_{\operatorname{lin}\{\varphi_1^L,\dots,\varphi_N^L\}}$, and therefore

$$\begin{aligned}\operatorname{tr}_{\mathbb{C}^{N\times N}}(1 - MM^*)^n &= \operatorname{tr}_{\operatorname{ran}\mathrm{P}_L^N}(\mathrm{P}_L^N - \mathrm{P}_L^N \Pi_L^N \mathrm{P}_L^N)^n \\ &= \operatorname{tr}_{L_2(\Omega_L)}(\mathrm{P}_L^N(I - \Pi_L^N)\mathrm{P}_L^N)^n.\end{aligned} \tag{1.13}$$

Using the projection property and the cyclicity of the trace, the assertion follows. □

1.3 Remark. Lemma 1.2 will be the starting point of our estimates for $|\mathcal{S}_L(E)|$. Equation (1.8) can be written as

$$-\ln|\mathcal{S}_L(E)| = \frac{1}{2}\sum_{n=1}^{\infty} \frac{1}{n} \operatorname{tr}\big(\mathrm{P}_L^{N_L(E)}(I - \Pi_L^{N_L(E)})\big)^n. \tag{1.14}$$

The trace expressions in (1.14) are nonnegative, so any truncation of the series yields a lower bound on $-\ln|\mathcal{S}_L(E)|$, and therefore an upper bound on the overlap. Keeping only the term for $n = 1$, one recovers the so-called *Anderson integral*, which is the bound used in [GKM14].

In the sequel, we will find an upper bound on $|\mathcal{S}_L(E)|$ by bounding the individual terms of (1.14) from below.

2 TRACE EXPRESSIONS AND SPECTRAL PROJECTIONS

In this section, we rewrite the nth term of (1.14) in a form more susceptible to replacing the finite-volume operators H_L and H'_L with their infinite-volume variants.

We begin by recasting the orthogonal projections (1.7) as functions of H_L and H'_L in the sense of the functional calculus. The projections in (1.7) are not necessarily spectral projections of H_L and H'_L, since the Nth eigenvalues might be of multiplicity higher than one. The choice of $N_L(E)$ in (1.4), together with a convergence result of the spectral shift function, allows us to put them into spectral projection form at the cost of passing to a subsequence of length scales:

2.1 Lemma (Adapted from [GKM14, Lemma 3.9]). Let $n \in \mathbb{N}$. Let $(L_m)_{m\in\mathbb{N}}$ be a sequence in $(0,\infty)$ with $L_m \to \infty$. Then there exists a subsequence $(L_{m_k})_{k\in\mathbb{N}}$ such that

$$\Big|\operatorname{tr}\big(1_{(-\infty,E]}(H_{L_{m_k}})1_{(E,\infty)}(H'_{L_{m_k}})\big)^n - \operatorname{tr}\big(\mathrm{P}_{L_{m_k}}^{N_{L_{m_k}}(E)}(I-\Pi_{L_{m_k}}^{N_{L_{m_k}}(E)})\big)^n\Big| = o(\ln L_{m_k}) \tag{2.1}$$

as $k \to \infty$ for a.e. $E \in \mathbb{R}$.

Proof. For fixed $L > 1$ and $E \in \mathbb{R}$, the definition of $N_L(E)$ in (1.4) implies

$$\lambda^L_{N_L(E)} \le E < \lambda^L_{N_L(E)+1} \le \mu^L_{N_L(E)+1} \tag{2.2}$$

if we set $\lambda^L_0 := -\infty$. This allows us to write

$$\mathrm{P}_L^{N_L(E)} = 1_{(-\infty,E]}(H_L) \tag{2.3}$$

and

$$I - \Pi_L^{N_L(E)} = 1_{(E,\infty)}(H'_L) - \sum_{k=1}^{N_L(E)} 1_{(E,\infty)}(\mu^L_k)\langle\psi^L_k,\cdot\rangle\psi^L_k =: 1_{(E,\infty)}(H'_L) - Q. \tag{2.4}$$

The trace norm of the projection Q is the number of nonzero terms in the sum, i.e.,

$$\operatorname{tr} Q = \#\big\{k \in \{1,\dots,N_L(E)\};\ \mu^L_k > E\big\} = N_L(E) - \#\big\{k \in \mathbb{N};\ \mu^L_k \le E\big\} =: \xi_L(E), \tag{2.5}$$

which is the value of the spectral shift function for the pair H_L, H'_L at E. We write the difference of operator powers on the left-hand side of (2.1) as

$$\begin{aligned}&\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H'_L)\big)^n - \big(\mathrm{P}_L^{N_L(E)}(I-\Pi_L^{N_L(E)})\big)^n\\ &\qquad = \sum_{k=1}^{n}\big(\mathrm{P}_L^{N_L(E)}(I-\Pi_L^{N_L(E)})\big)^{k-1}\mathrm{P}_L^{N_L(E)}\,Q\,\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H'_L)\big)^{n-k}.\end{aligned} \tag{2.6}$$

Equation (2.6) is a consequence of the algebraic identity

$$\prod_{j=1}^{n} A_j - \prod_{j=1}^{n} B_j = \sum_{k=1}^{n} B_1 \cdots B_{k-1}(A_k - B_k)A_{k+1} \cdots A_n \tag{2.7}$$

for bounded operators A_j, B_j for $1 \leq j \leq n$, where $n \in \mathbb{N}$. Estimating the traces of the operators on the right-hand side of (2.6) by bounding the operator norms of all projections except Q by 1, we arrive at $n\xi_L(E)$ as a bound. We now use the weak convergence [HM10, Thm. 1.4]

$$\int_I \mathrm{d}E\, \xi_L(E) \xrightarrow{L\to\infty} \int_I \mathrm{d}E\, \xi(E) \tag{2.8}$$

for every bounded interval $I \subseteq \mathbb{R}$, where $\xi \in L_{1,\mathrm{loc}}(\mathbb{R})$ is the spectral shift function for the pair of infinite-volume operators H, H'. Thus, given a sequence of diverging lengths $(L_m)_{m\in\mathbb{N}}$, the sequence of nonnegative functions $(\xi_{L_m}/\ln L_m)_{m\in\mathbb{N}}$ converges to zero in the norm of $L_1(I)$. By standard arguments, there exists a subsequence $(L_{m_k})_{k\in\mathbb{N}}$ such that $(\xi_{L_{m_k}}/\ln L_{m_k})_{k\in\mathbb{N}}$ converges to zero for Lebesgue-a.e. $E \in I$. Expressing $\mathbb{R}$ as a union of bounded intervals, the claim follows. □

2.2 Remark. (A) In Lemma 2.1, we pass to a subsequence since we don't know any good bounds on the finite-volume spectral shift function ξ_L with respect to the volume. In fact, [Kir87] shows that in the simple situation $\Omega_L = [-L, L]^d$ for $d \geq 2$ and $V_0 = 0$, eigenvalues of arbitrary multiplicity occur, which implies that the set $\{E \in \mathbb{R};\ \sup_{m\in\mathbb{N}} \xi_{L_m}(E) = \infty\}$ is dense in $[0, \infty)$, see [Kir87, Thm. 1].

We also note that since $\xi_L(E) \in \mathbb{N}_0$ for all $L > 1$ and $E \in \mathbb{R}$, pointwise convergence of ξ_L a.e. would imply $\xi \in \mathbb{N}_0$ a.e.; a much stronger convergence result than (2.8) is therefore unlikely to be true. Remark 4.7 (D) below mentions another idea that might help to circumvent the lack of known bounds for ξ_L.

In some situations however, better bounds on the spectral shift function are known. For instance in $d = 1$, a Dirichlet-Neumann bracketing argument shows

$$\sup_{L>1} \sup_{E\in\mathbb{R}} \xi_L(E) < \infty. \tag{2.9}$$

The same is true if one considers not $-\Delta$ on $L_2(\Omega_L)$ but the discrete Laplacian on a subspace of $\ell_2(\mathbb{Z}^d)$. Whenever a bound like (2.9) is known, passing to a subsequence is not necessary.

(B) In following sections, we will repeatedly estimate the trace of the difference of products of operators, and the algebraic identity (2.7) will be used at every such step. The proofs of Lemma 4.5 and Lemma 6.7 are examples of this.

Having established (2.1), we will treat the $L \to \infty$ asymptotics of the trace expression $\operatorname{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H_L')\big)^n$, where no restriction to particular length scales will be necessary.

The next lemma will be used to get lower bounds of our trace expressions.

2.3 Lemma. Let $A, B, \tilde{A}, \tilde{B} \geq 0$ be self-adjoint bounded operators in a Hilbert space $\mathcal{H}$, and let $\tilde{A} \leq A$ and $\tilde{B} \leq B$. Assume $\sqrt{A}$ is trace class and let $n \in \mathbb{N}$. Then

$$\operatorname{tr}(AB)^n \geq \operatorname{tr}(\tilde{A}\tilde{B})^n \geq 0. \tag{2.10}$$

Proof. From $\sqrt{A}B\sqrt{A} \geq \sqrt{A}\tilde{B}\sqrt{A}$ we deduce

$$\operatorname{tr}(AB)^n = \operatorname{tr}(\sqrt{A}B\sqrt{A})^n \geq \operatorname{tr}(\sqrt{A}\tilde{B}\sqrt{A})^n = \operatorname{tr}(\tilde{B}A)^n, \tag{2.11}$$

since the eigenvalues of the positive operator $\sqrt{A}B\sqrt{A}$ are larger than those of $\sqrt{A}\tilde{B}\sqrt{A}$, and so are their respective nth powers. In the same manner,

$$\operatorname{tr}(\tilde{B}A)^n = \operatorname{tr}(\sqrt{\tilde{B}}A\sqrt{\tilde{B}})^n \geq \operatorname{tr}(\sqrt{\tilde{B}}\tilde{A}\sqrt{\tilde{B}})^n = \operatorname{tr}(\tilde{A}\tilde{B})^n. \tag{2.12}$$

□

As the final step in this section, we write the trace expression $\operatorname{tr}\big(f(H_L)g(H_L')\big)^n$ in a different form.

2.4 Lemma. Let $n \in \mathbb{N}$. Let $L > 1$ and $E \in \mathbb{R}$. Let $f, g : \mathbb{R} \to [0,1]$ be measurable functions with compact supports $\operatorname{spt} f \subseteq (-\infty, E]$ and $\operatorname{spt} g \subseteq (E, \infty)$. Then

$$\operatorname{tr}\big(f(H_L)g(H_L')\big)^n = \sum_{\alpha,\beta\in\mathbb{N}^n} \prod_{j=1}^{n} \left(f(\lambda_{\alpha_j}^L) g(\mu_{\beta_j}^L) \frac{\langle \varphi_{\alpha_j}^L, V\psi_{\beta_j}^L\rangle \langle \psi_{\beta_j}^L, V\varphi_{\alpha_{j+1}}^L\rangle}{(\mu_{\beta_j}^L - \lambda_{\alpha_j}^L)(\mu_{\beta_j}^L - \lambda_{\alpha_{j+1}}^L)} \right) \tag{2.13}$$

with the convention $\alpha_{n+1} := \alpha_1$ for multi-indices $\alpha \in \mathbb{N}^n$.

Proof. We begin by noting that

$$f(H_L) = \sum_{j\in\mathbb{N}} f(\lambda_j^L)\, \langle \varphi_j^L, \cdot\rangle \varphi_j^L, \qquad g(H_L') = \sum_{k\in\mathbb{N}} g(\mu_k^L)\, \langle \psi_k^L, \cdot\rangle \psi_k^L. \tag{2.14}$$

To ease notation, we employ *bra-ket* notation, writing $\langle \varphi, \cdot\rangle\varphi = |\varphi\rangle\langle\varphi|$ for $\varphi \in L_2(\Omega_L)$. Then (2.14) implies

$$\big(f(H_L)g(H_L')\big)^n = \sum_{\alpha,\beta\in\mathbb{N}^n} \Big(\prod_{j=1}^{n} f(\lambda_{\alpha_j}^L) g(\mu_{\beta_j}^L) \Big) \prod_{j=1}^{n} |\varphi_{\alpha_j}^L\rangle\langle\varphi_{\alpha_j}^L|\psi_{\beta_j}^L\rangle\langle\psi_{\beta_j}^L|, \tag{2.15}$$

and

$$\operatorname{tr}\big(f(H_L)g(H_L')\big)^n = \sum_{\alpha,\beta\in\mathbb{N}^n} \Big(\prod_{j=1}^{n} f(\lambda_{\alpha_j}^L) g(\mu_{\beta_j}^L) \Big) \prod_{j=1}^{n} \langle\varphi_{\alpha_j}^L|\psi_{\beta_j}^L\rangle\langle\psi_{\beta_j}^L|\varphi_{\alpha_{j+1}}^L\rangle, \tag{2.16}$$

where we used the convention $\alpha_{n+1} := \alpha_1$ for $\alpha \in \mathbb{N}^n$.

Now, we note that the eigenvalue equations imply

$$\lambda_j^L \langle \varphi_j^L, \psi_k^L \rangle = \langle H_L \varphi_j^L, \psi_k^L \rangle = \mu_k^L \langle \varphi_j^L, \psi_k^L \rangle - \langle \varphi_j^L, V\psi_k^L \rangle \tag{2.17}$$

for $j, k \in \mathbb{N}$, and therefore

$$\langle \varphi_j^L, \psi_k^L \rangle = \frac{\langle \varphi_j^L, V\psi_k^L \rangle}{\mu_k^L - \lambda_j^L} \tag{2.18}$$

whenever $\lambda_j^L \neq \mu_k^L$. Using this, (2.16) reads

$$\operatorname{tr}\big(f(H_L)g(H_L')\big)^n = \sum_{\alpha,\beta \in \mathbb{N}^n} \Big(\prod_{j=1}^n f(\lambda_{\alpha_j}^L) g(\mu_{\beta_j}^L) \Big) \prod_{j=1}^n \frac{\langle \varphi_{\alpha_j}^L, V\psi_{\beta_j}^L \rangle \langle \psi_{\beta_j}^L, V\varphi_{\alpha_{j+1}}^L \rangle}{(\mu_{\beta_j}^L - \lambda_{\alpha_j}^L)(\mu_{\beta_j}^L - \lambda_{\alpha_{j+1}}^L)}. \tag{2.19}$$

□

2.5 Remark. In [GKM14], the role of Lemma 2.4 here is played by Lemma 3.11, where a special (finite-volume) spectral correlation measure occurs. It would be possible to do something similar in our case, for instance by defining

$$\mu_L^{2n}(A_1 \times \cdots \times A_n \times B_1 \times \cdots \times B_n) \\ := \operatorname{tr}(1_{A_1}(H_L)V1_{B_1}(H_L')V \cdots 1_{A_n}(H_L)V1_{B_n}(H_L')V) \tag{2.20}$$

for $n \in \mathbb{N}$, $L > 1$ and bounded $A_1, \ldots, A_n, B_1, \ldots, B_n \in \operatorname{Borel}(\mathbb{R})$. Lemma 2.4 would then read

$$\operatorname{tr}\big(f(H_L)g(H_L')\big)^n = \int_{\mathbb{R}^n \times \mathbb{R}^n} d\mu_L^{2n}(x, y) \prod_{j=1}^n \frac{f(x_j)g(y_j)}{(y_j - x_j)(y_j - x_{j+1})}. \tag{2.21}$$

However, for $n \geq 2$ the expression (2.20) is not necessarily nonnegative, and defining μ_L^{2n} as a signed measure on $\operatorname{Borel}(\mathbb{R}^{2n})$ might not be possible due to the missing vector space structure of the two-point compactification $[-\infty, \infty]$ of $\mathbb{R}$. Since writing the trace expressions using spectral correlation measures is merely a question of convenient notation, we choose not to do so in our present case.

3 FEYNMAN-SCHWINGER PARAMETRIZATION

In this section, we rewrite the right-hand side of (2.13) using an integral formula that goes back to Feynman and Schwinger.

We start with a well-known theorem from integration theory, which we state for the convenience of the reader. In the whole section, let $n \in \mathbb{N}$.

3.1 Theorem (Coarea formula)**.** Let $\Omega \subseteq \mathbb{R}^n$ be open, $g : \Omega \to \mathbb{R}$ continuously differentiable, and $\operatorname{grad} g(x) \neq 0$ for all $x \in \Omega$. Then the level set $M_r := \{x \in \Omega;\ g(x) = r\}$ is a hyper-surface for all $r \in \mathbb{R}$. Let $f \in C(\Omega)$, and either $f \in L_1(\Omega)$ or $f \geq 0$. Then

$$\int_\Omega \mathrm{d}x\, f(x) = \int_{\mathbb{R}} \mathrm{d}r \int_{M_r} \mathrm{d}S(\xi) f(\xi) \frac{1}{|\operatorname{grad} g(\xi)|}, \tag{3.1}$$

where $\mathrm{d}S$ stands for integration with respect to the surface measure on M_r.

In more specialized situations, Theorem 3.1 can be refined further.

3.2 Corollary. In the situation of Theorem 3.1, suppose g is positive and positive homogeneous, i.e., $g(x) \geq 0$ and $g(rx) = rg(x)$ for $x \in \Omega$ and $r \geq 0$. Then

$$\int_\Omega \mathrm{d}x\, f(x) = \int_0^\infty \mathrm{d}r \int_{M_1} \frac{\mathrm{d}S(\xi)}{|\operatorname{grad} g(r\xi)|} r^{n-1} f(r\xi). \tag{3.2}$$

3.3 Remarks. (A) In the physics literature, the integration with respect to the surface measure on M_r is often written using the one-dimensional Dirac distribution, namely

$$\int_\Omega \mathrm{d}\xi\, \delta(r - g(\xi)) f(\xi) := \int_{M_r} \frac{\mathrm{d}S(\xi)}{|\operatorname{grad} g(\xi)|} f(\xi). \tag{3.3}$$

We will employ this notation where it is convenient.

(B) We will use Corollary 3.2 in the situation $\Omega = (0, \infty)^n$ and $g(x) = |x|_1 := x_1 + \cdots + x_n$. Then $|\operatorname{grad} g(x)| = \sqrt{n}$ and

$$\int_{(0,\infty)^n} \mathrm{d}x\, f(x) = \int_0^\infty \mathrm{d}r \int_{\{\xi \in \Omega;\, |\xi|_1 = 1\}} \frac{\mathrm{d}S(\xi)}{\sqrt{n}} r^{n-1} f(r\xi). \tag{3.4}$$

Notice that

$$\int_{|\xi|_1 = 1} \frac{\mathrm{d}S(\xi)}{\sqrt{n}} = \int_{\Delta_{n-1}} \mathrm{d}x = \frac{1}{(n-1)!}, \tag{3.5}$$

where $\Delta_{n-1} := \{x \in [0,1]^{n-1};\, x_1 + \cdots + x_{n-1} \le 1\}$ is the $(n-1)$-dimensional standard simplex; (3.5) can be seen by parameterizing $\{\xi \in (0,\infty)^n;\, |\xi|_1 = 1\}$ via $\Delta_{n-1} \ni x \mapsto (x, 1-|x|_1) \in \mathbb{R}^n$. This implies, using the physics notation,

$$\int_{[0,1]^n} \mathrm{d}\xi\, \delta(1-|\xi|_1) f(\xi) = \int_{\Delta_{n-1}} \mathrm{d}x\, f(x_1,\ldots,x_{n-1},1-x_1-\cdots-x_{n-1}). \tag{3.6}$$

We now prove the Feynman-Schwinger parametrization formula in a well-known generalization.

3.4 Corollary (Generalized Feynman-Schwinger parametrization)**.** Let $x_1,\ldots,x_n \in \mathbb{C}$ and $\alpha_1,\ldots,\alpha_n \in \mathbb{C}$ with $\operatorname{Re} x_j > 0$ and $\operatorname{Re}\alpha_j > 0$ for $1 \le j \le n$. Then

$$\frac{1}{x_1^{\alpha_1}\cdots x_n^{\alpha_n}} = \frac{\Gamma(\alpha_1+\cdots+\alpha_n)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_n)} \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \frac{u_1^{\alpha_1-1}\cdots u_n^{\alpha_n-1}}{(u_1x_1+\cdots+u_nx_n)^{\alpha_1+\cdots+\alpha_n}}. \tag{3.7}$$

Proof. The definition of the Gamma function implies

$$\int_0^\infty \mathrm{d}t\, t^{\gamma-1}e^{-tx} = \frac{\Gamma(\gamma)}{x^\gamma} \tag{3.8}$$

for $x,\gamma \in \mathbb{C}$ with $\operatorname{Re} x > 0$ and $\operatorname{Re}\gamma > 0$. Using (3.8) for each $x_j^{-\alpha_j}$ yields

$$\frac{\Gamma(\alpha_1)\cdots\Gamma(\alpha_n)}{x_1^{\alpha_1}\cdots x_n^{\alpha_n}} = \int_{(0,\infty)^n} \mathrm{d}u\, u_1^{\alpha_1-1}\cdots u_n^{\alpha_n-1} e^{-\sum_{j=1}^n u_jx_j}$$

the coarea formula gives

$$= \int_0^\infty \mathrm{d}r \int_{|u|_1=1} \frac{\mathrm{d}S(u)}{\sqrt{n}} r^{n-1} r^{\sum_{j=1}^n \alpha_j - n} u_1^{\alpha_1-1}\cdots u_n^{\alpha_n-1} e^{-r\sum_{j=1}^n u_jx_j}$$

$$= \int_{|u|_1=1} \frac{\mathrm{d}S(u)}{\sqrt{n}} u_1^{\alpha_1-1}\cdots u_n^{\alpha_n-1} \int_0^\infty \mathrm{d}r\, r^{\sum_{j=1}^n \alpha_j - 1} e^{-r\sum_{j=1}^n u_jx_j}$$

using (3.8) with $\gamma = \sum_{j=1}^n \alpha_j$ yields

$$= \int_{|u|_1=1} \frac{\mathrm{d}S(u)}{\sqrt{n}} u_1^{\alpha_1-1}\cdots u_n^{\alpha_n-1} \frac{\Gamma(\sum_{j=1}^n \alpha_j)}{\left(\sum_{j=1}^n u_jx_j\right)^{\sum_{j=1}^n \alpha_j}}. \tag{3.9}$$

□

3.5 Remark. Corollary 3.4 for $\alpha_1 = \cdots = \alpha_n = 1$ implies

$$\begin{aligned} \frac{1}{x_1\cdots x_n} &= \Gamma(n) \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \frac{1}{(u\cdot x)^n} \\ &= \int_0^\infty \mathrm{d}t\, t^{n-1} \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) e^{-tu\cdot x} \qquad (x \in (0,\infty)^n), \end{aligned} \tag{3.10}$$

where $u \cdot x = \sum_{j=1}^{n} u_j x_j$ is the Euclidean scalar product. For $n = 2$, this reads

$$\frac{1}{ab} = \int_0^\infty \mathrm{d}t \, \frac{e^{-ta} - e^{-tb}}{b - a} \qquad (a, b > 0, \ a \neq b). \tag{3.11}$$

We also mention that the right-hand side of (3.10) can be written as

$$\int_0^\infty \mathrm{d}t \, t^{n-1} \int_{(0,\infty)^n} \mathrm{d}u \, |u|_1 e^{-|u|_1} e^{-tu \cdot x}, \tag{3.12}$$

cf. Lemma 8.3; this variant of the Feynman-Schwinger parametrization formula will be used in the upcoming publication [GKMO] and has the advantage that it needs no Dirac distribution or surface integration.

We use (3.10) to rewrite the right-hand side of (2.13).

3.6 Lemma. Let $L > 1$ and $E \in \mathbb{R}$. Let $f, g : \mathbb{R} \to [0,1]$ be measurable functions with compact supports $\operatorname{spt} f \subseteq (-\infty, E]$ and $\operatorname{spt} g \subseteq (E, \infty)$. Then

$$\operatorname{tr}\big(f(H_L)g(H'_L)\big)^n = \int_0^\infty \mathrm{d}t \, t^{2n-1} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v) \, \delta(1 - |u|_1 - |v|_1) \\ \times \operatorname{tr} \prod_{j=1}^{n} \sqrt{V} f(H_L) e^{(u_j + v_{j-1})t(H_L - E)} V g(H'_L) e^{-(u_j+v_j)t(H'_L - E)} \sqrt{V}, \tag{3.13}$$

with the convention $v_0 := v_n$ for $v \in \mathbb{R}^n$.

Proof. Let $x \in (-\infty, 0]^n$ and $y \in (0, \infty)^n$. Then, by (3.10),

$$\frac{1}{\prod_{j=1}^{n}(y_j - x_j)(y_j - x_{j+1})} = \int_0^\infty \mathrm{d}t \, t^{2n-1} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v) \, \delta(1 - |u|_1 - |v|_1) \\ \times \exp\big(-t(\textstyle\sum_{j=1}^{n} u_j(y_j - x_j) + \sum_{j=1}^{n} v_j(y_j - x_{j+1}))\big), \tag{3.14}$$

where $x_{n+1} := x_1$ and

$$\sum_{j=1}^{n} u_j(y_j - x_j) + \sum_{j=1}^{n} v_j(y_j - x_{j+1}) = \sum_{j=1}^{n}\big((u_j + v_j)y_j - (u_j + v_{j-1})x_j\big) \tag{3.15}$$

for $u, v \in [0,1]^n$. Now, let $\alpha, \beta \in \mathbb{N}^n$. Using $x_j = \lambda^L_{\alpha_j} - E$ and $y_j = \mu^L_{\beta_j} - E$, we can write the denominator in (2.13) as

$$\frac{1}{\prod_{j=1}^{n}(\mu^L_{\beta_j} - \lambda^L_{\alpha_j})(\mu^L_{\beta_j} - \lambda^L_{\alpha_{j+1}})} = \int_0^\infty \mathrm{d}t \, t^{2n-1} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v) \, \delta(1 - |u|_1 - |v|_1) \\ \times \prod_{j=1}^{n} e^{-(u_j+v_j)t(\mu^L_{\beta_j} - E)} e^{(u_j + v_{j-1})t(\lambda^L_{\alpha_j} - E)}. \tag{3.16}$$

Looking at (2.13), the sum is finite thanks to the compact supports of f and g, and therefore the summation can be interchanged with the integrals from (3.16), resulting in

$$\operatorname{tr}\big(f(H_L)g(H_L')\big)^n = \int_0^\infty \mathrm{d}t\, t^{2n-1} \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\, \delta(1-|u|_1-|v|_1) \\ \times \sum_{\alpha,\beta\in\mathbb{N}^n} \prod_{j=1}^n \Big(f(\lambda^L_{\alpha_j}) e^{(u_j+v_{j-1})t(\lambda^L_{\alpha_j}-E)} g(\mu^L_{\beta_j}) e^{-(u_j+v_j)t(\mu^L_{\beta_j}-E)} \\ \times \langle \varphi^L_{\alpha_j}, V\psi^L_{\beta_j}\rangle \langle \psi^L_{\beta_j}, V\varphi^L_{\alpha_{j+1}}\rangle \Big), \quad (3.17)$$

from which the assertion follows. □

4 SMOOTHING AND INFINITE-VOLUME OPERATORS

In this section, we apply Lemma 3.6 using suitable functions f and g and rewrite the right-hand side of (3.13) as a trace expression of the infinite-volume operators H and H'.

Switching from finite-volume to infinite-volume operators constitutes the core of the argument. The technical tool to implement this switch to infinite-volume objects is the Helffer-Sjőstrand formula (see Theorem 5.1 below). Since it is applicable to smooth functions only, we define appropriately smoothed versions of our indicator functions.

In the whole section, let $a \in (0,1)$ be fixed.

4.1 Definition (Adapted from [GKM14, Def. 3.13])**.** Given a length $L > 1$, a cut-off energy $E_0 \geq 1$, and a Fermi energy $E \in [-E_0+1, E_0-1]$, we say that $\chi_L^\pm \in C_c^\infty(\mathbb{R})$ are *smooth cut-off functions* if they obey

$$1_{[E+2L^{-a},E_0]} \leq \chi_L^+ \leq 1_{(E+L^{-a},E_0+1)} \quad \text{and} \quad 1_{[-E_0,E-2L^{-a}]} \leq \chi_L^- \leq 1_{(-E_0-1,E-L^{-a})}, \tag{4.1}$$

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

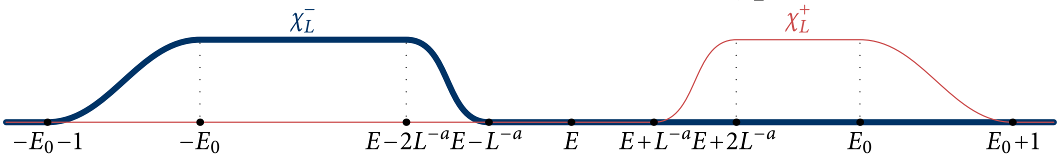
$$\chi_L^\pm(E \pm L^{-a} \pm x) \leq c_0 L^a x \tag{4.2}$$

for all $x \in [0, L^{-a})$, and

$$\left|\frac{\partial^k}{\partial x^k}\chi_L^\pm(E \pm L^{-a} \pm x)\right| \leq \begin{cases} c_k L^{ak} & \text{if } 0 \leq x < L^{-a}, \\ c_k & \text{otherwise} \end{cases} \tag{4.3}$$

for every $k \in \mathbb{N}$ and $x \in \mathbb{R}$. To ease estimates, choose $c_0 \geq 1$, then (4.3) holds for $k = 0$ as well.

Thus, χ_L^+ equals one inside $[E+2L^{-a}, E_0]$ and zero in $(-\infty, E] \cup [E_0+1, \infty)$. Whereas its smooth growth in $[E+L^{-a}, E+2L^{-a}]$ gets steeper with increasing L, we choose its smooth decay in $[E_0, E_0+1]$ independently of L. The properties of χ_L^- are analogous. The following figure illustrates the behavior of $\chi_L^\pm$.



4.2 Remark. We are interested in lower bounds on the terms of (1.14) (plus a sublogarithmic error). Using Lemma 2.1, this is equivalent to bounding $\operatorname{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H_L')\big)^n$ from below. For this bound, we use the inequalities

$$1_{(-\infty,E]} \geq \chi_L^- \quad \text{and} \quad 1_{(E,\infty)} \geq \chi_L^+. \tag{4.4}$$

Looking at Lemma 2.3, Lemma 2.4, and Lemma 3.6, this yields

$$\operatorname{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H'_L)\big)^n \geq \int_0^\infty \mathrm{d}t\, t^{2n-1} \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\,\delta(1-|u|_1-|v|_1)$$
$$\times \operatorname{tr}\prod_{j=1}^n \sqrt{V}\chi_L^-(H_L)e^{(u_j+v_{j-1})t(H_L-E)}V\chi_L^+(H'_L)e^{-(u_j+v_j)t(H'_L-E)}\sqrt{V}. \quad (4.5)$$

The inequality in (4.5) is in fact the only place in this thesis where we actually bound the nth term of (1.14) instead of computing its exact asymptotics. We know of no way to bound the error introduced in this step in the general case. In $d=1$, the following approach might yield a bound on this error and therefore the exact asymptotics of the nth term: Define the smoothed functions $\chi_L^\pm$ with $(1-a)L^{-a}$ in place of where L^{-a} is in the definition above, and bound the error introduced by χ_L^+ via an estimate on the number of eigenvalues in the interval $[E, E+(1-a)L^{-a}]$, and analogously for χ_L^-; then perform a coupled $a\to 1$, $L\to\infty$ limit. Since exact first-order asymptotics of the nth term by themselves don't yield the exact asymptotics of the overlap $\mathcal{S}_L(E)$, and this approach only seems promising for $d=1$, we will not follow it in this thesis.

The following technical lemma is at the core of the arguments in the present section. Its proof will be given in the next section.

4.3 Lemma ([GKM14, Lemma 3.14])**.** For $L>1$, $t\geq 0$ and $x\in\mathbb{R}$, define

$$f_L^t(x) := \chi_L^-(x)e^{t(x-E)} \quad \text{and} \quad g_L^t(x) := \chi_L^+(x)e^{-t(x-E)} \quad (4.6)$$

and let h_L^t stand for either f_L^t or g_L^t. Let $\varepsilon\in(0,1-a)$. Let $M\in\mathbb{N}$ with $M\geq 2$.

Then there is a constant $c>0$ and $L_0>1$ and a polynomial Q_M of degree $M+1$ with nonnegative coefficients, with c, L_0, and Q_M all independent of t, L, and ε, such that

$$\big\|\sqrt{V}\big(h_L^t(H_L^{(\prime)}) - h_L^t(H^{(\prime)})\big)\sqrt{V}\big\| \leq Q_M(t/L^a)\big(L^{a-M(1-a-\varepsilon)} + L^{d+a(M+1)}e^{-cL^\varepsilon}\big) \quad (4.7)$$

for $t\geq 0$ and $L>L_0$.

Before we prove the main assertion of this section, we need one more technical lemma that takes the form of a spectral gap estimate.

4.4 Lemma. There is a constant $C>0$ such that

$$\operatorname{tr}\big(\sqrt{V}h_L^t(H_{(L)}^{(\prime)})\sqrt{V}\big) \leq Ce^{-tL^{-a}} \qquad (L>1, t\geq 0), \quad (4.8)$$

where $h_L^t\in C_c^\infty(\mathbb{R})$ is as in Lemma 4.3.

Proof. There is a bounded interval $I \subseteq \mathbb{R}$ such that $h_L^t \le 1_I e^{-tL^{-a}}$ for all $t \ge 0$ and $L > 1$. Thus,

$$\begin{aligned}\operatorname{tr}\big(\sqrt{V} h_L^t(H_{(L)}^{(\prime)})\sqrt{V}\big) &\le e^{-tL^{-a}} \operatorname{tr}\big(\sqrt{V} 1_I(H_{(L)}^{(\prime)})\sqrt{V}\big) \\ &\le e^{-tL^{-a}} e^{\sup I} \operatorname{tr}\big(\sqrt{V} e^{-H_{(L)}^{(\prime)}}\sqrt{V}\big) \\ &\le e^{-tL^{-a}} e^{\sup I} \operatorname{tr}\big(\sqrt{V} e^{-H^{(\prime)}}\sqrt{V}\big) \end{aligned} \tag{4.9}$$

for $t \ge 0$ and $L > 1$. The last inequality and the finiteness of $\operatorname{tr}\big(\sqrt{V}e^{-H^{(\prime)}}\sqrt{V}\big)$ can be seen from [BHL00, Thm. 6.1]. □

The next lemma accomplishes the transition from finite-volume to infinite-volume expressions.

4.5 Lemma. For $L > 1$ and $t \ge 0$, let $f_L^t, g_L^t \in C_c^\infty(\mathbb{R})$ as in Lemma 4.3. Let $n \in \mathbb{N}$ and $m \in \mathbb{N}$. Then

$$\sup_{\substack{u,v\in[0,1]^n \\ |u|_1+|v|_1=1}} \int_0^\infty \mathrm{d}t\; t^m \operatorname{tr}\Big|\prod_{j=1}^n \sqrt{V} f_L^{(u_j+v_{j-1})t}(H_L) V g_L^{(u_j+v_j)t}(H_L')\sqrt{V} - \prod_{j=1}^n \sqrt{V} f_L^{(u_j+v_{j-1})t}(H) V g_L^{(u_j+v_j)t}(H')\sqrt{V}\Big| \to 0 \tag{4.10}$$

as $L \to \infty$.

Proof. Let $u, v \in [0,1]^n$ with $|u|_1 + |v|_1 = 1$. To shorten formulas, we introduce a vector $\alpha \in (0,\infty)^{2n}$ via

$$\alpha_{2j-1} := u_j + v_{j-1} \quad \text{and} \quad \alpha_{2j} := u_j + v_j \tag{4.11}$$

for $1 \le j \le n$, and operators

$$A_k^{(L)} := \begin{cases} \sqrt{V} f_L^{\alpha_k t}(H_{(L)})\sqrt{V} & \text{for } k \text{ odd,} \\ \sqrt{V} g_L^{\alpha_k t}(H_{(L)}')\sqrt{V} & \text{for } k \text{ even} \end{cases} \tag{4.12}$$

for $1 \le k \le 2n$. The difference of operator products in (4.10) is then

$$\prod_{j=1}^{2n} A_j^L - \prod_{j=1}^{2n} A_j = \sum_{k=1}^{2n} A_1 \cdots A_{k-1}(A_k^L - A_k)A_{k+1}^L \cdots A_{2n}^L. \tag{4.13}$$

The trace norm of this difference can be estimated via Lemma 4.4: There is a constant $C > 0$ such that

$$\operatorname{tr}\Big|\prod_{j=1}^{2n} A_j^L - \prod_{j=1}^{2n} A_j\Big| \le \sum_{k=1}^{2n} \|A_k^L - A_k\| \Big(\prod_{j=1}^{k-1} \operatorname{tr}|A_j|\Big)\Big(\prod_{j=k+1}^{2n} \operatorname{tr}|A_j^L|\Big)$$
$$\le C^{2n-1} \sum_{k=1}^{2n} \|A_k^L - A_k\| e^{-(|\alpha|_1-\alpha_k)tL^{-a}}, \tag{4.14}$$

where $|\alpha|_1 = \alpha_1 + \dots + \alpha_{2n}$ denotes the 1-norm of $\alpha \in (0,\infty)^{2n}$, and the definition of α implies $|\alpha|_1 = 2$. We estimate the kth term in this sum. Notice that $|\alpha|_1 - \alpha_k \ge 1 \ge \alpha_k$. Let $\varepsilon \in (0, 1-a)$ and $M \in \mathbb{N}$. For L sufficiently large, Lemma 4.3 yields

$$\|A_k^L - A_k\| e^{-(|\alpha|_1-\alpha_k)tL^{-a}} \le \|A_k^L - A_k\| e^{-tL^{-a}}$$
$$\le Q_M(\alpha_k t/L^a)\big(L^{a-M(1-a-\varepsilon)} + L^{d+a(M+1)} e^{-cL^\varepsilon}\big) e^{-tL^{-a}}, \tag{4.15}$$

where $Q_M(x) = \sum_{\ell=0}^{M+1} q_\ell x^\ell$ is the polynomial in Lemma 4.3 with nonnegative coefficients q_ℓ. Integrating (4.15) yields

$$\int_0^\infty \mathrm{d}t\, t^m \|A_k^L - A_k\| e^{-(|\alpha|_1-\alpha_k)tL^{-a}}$$
$$\le \big(L^{a-M(1-a-\varepsilon)} + L^{d+a(M+1)} e^{-cL^\varepsilon}\big) \sum_{\ell=0}^{M+1} q_\ell \int_0^\infty \mathrm{d}t\, t^m e^{-tL^{-a}} \frac{t^\ell}{L^{a\ell}}$$
$$= \big(L^{a-M(1-a-\varepsilon)} + L^{d+a(M+1)} e^{-cL^\varepsilon}\big) \sum_{\ell=0}^{M+1} \frac{q_\ell \Gamma(2n+\ell) L^{a(m+\ell+1)}}{L^{a\ell}}$$
$$\le C_M L^{a(m+1)}\big(L^{a-M(1-a-\varepsilon)} + L^{d+a(M+1)} e^{-cL^\varepsilon}\big), \tag{4.16}$$

with a constant $C_M > 0$ depending on Q_M and n. For given $\varepsilon < 1-a$, we can choose M large enough for the L-terms to vanish as $L \to \infty$. □

Using Lemma 4.5, we can rewrite the right-hand side of (4.5).

4.6 Corollary. Let $n \in \mathbb{N}$. Then

$$\int_0^\infty \mathrm{d}t\, t^{2n-1} \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\, \delta(1-|u|_1-|v|_1)$$
$$\times \Big(\operatorname{tr}\prod_{j=1}^{n} \sqrt{V} f_L^{(u_j+v_{j-1})t}(H_L) V g_L^{(u_j+v_j)t}(H_L')\sqrt{V}$$
$$- \operatorname{tr}\prod_{j=1}^{n} \sqrt{V} f_L^{(u_j+v_{j-1})t}(H) V g_L^{(u_j+v_j)t}(H')\sqrt{V}\Big) = \mathrm{o}(1) \tag{4.17}$$

as $L \to \infty$.

Proof. After interchanging the integrations with respect to t and (u, v), the claim follows from Lemma 4.5 and the uniform convergence therein. □

4.7 Remarks. (A) From Remark 4.2 and Corollary 4.6, we conclude

$$\operatorname{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H'_L)\big)^n \geq \int_0^\infty \mathrm{d}t\, t^{2n-1} \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\, \delta(1-|u|_1-|v|_1) \times \operatorname{tr}\prod_{j=1}^n \sqrt{V}\chi_L^-(H)e^{(u_j+v_{j-1})t(H-E)}V\chi_L^+(H')e^{-(u_j+v_j)t(H'-E)}\sqrt{V} + \mathrm{o}(1) \quad (4.18)$$

as $L \to \infty$.

It is possible to rewrite the right-hand side of (4.18) as $\operatorname{tr}\big(\chi_L^-(H)\chi_L^+(H')\big)^n$. This form is useful for lower bounds, e.g., for the bound $\operatorname{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H'_L)\big)^n \geq \operatorname{tr}\big(1_{[-E_0,E-L^{-a}]}(H)1_{[E+L^{-a},E_0]}(H')\big)^n$. However, we will not use this form and therefore omit the proof of this representation.

(B) When comparing the smooth cut-off functions $\chi_L^\pm$ with the ones in [GKM14, Def. 3.13], the difference is that the cut-off functions there have E as the boundary of their support, while the ones here have distance L^{-a} between E and their support. To compensate, the t-integral has been cut off at $t = L^{-a}$ in [GKM14, Lemma 3.11], which yields a lower bound for $n = 1$. For $n \geq 2$, it is not immediately clear if the integrand in (4.18) is positive, so cutting off the integration might not result in a lower bound; this is the reason we chose the cut-off functions differently than in [GKM14].

(C) In this connection, we mention the Bessis-Moussa-Villani conjecture [BMV75], recently proven by Stahl [Sta11]: For two self-adjoint matrices A and B, the function $\lambda \mapsto \operatorname{tr}\exp(A-\lambda B)$ is the Laplace transform of a positive measure. One consequence of this is that

$$\int_{[0,1]^{k+1}} \mathrm{d}u\, \delta(1-|u|_1)\operatorname{tr}\big(e^{u_1A}Be^{u_2A}B\cdots e^{u_kA}Be^{u_{k+1}A}\big) \geq 0 \quad (4.19)$$

for $k \in \mathbb{N}$, see [LS12, Thm. 4]. The expression in (4.19) is similar to the one in (4.18), where we also expect the integration with respect to (u, v) to yield a positive expression for any t. If that was the case, we could adopt the same method as in [GKM14]. However, it is not clear if (4.19) implies positivity in the context of (4.18), where more than one operator occurs as exponent.

(D) As a final remark in this section, we mention that the distance L^{-a} between E and the support of $\chi_L^\pm$ might give a way of circumventing the lack of known bounds on the spectral shift function that resulted in the introduction of a subsequence in Lemma 2.1, see also Remark 2.2: A bound like

$$\mu^L_{N_L(E)+1} - \lambda^L_{N_L(E)} = \mathrm{O}(L^{-1}) \qquad (L \to \infty) \quad (4.20)$$

on the distance between eigenvalues of H_L and H'_L would imply a version of Lemma 2.1 for the operators $\chi_L^-(H)$ and $\chi_L^+(H')$ that does not require a subsequence. However, we did not find a bound like (4.20) in the literature and will therefore prove a result involving subsequences in the sequel.

5 Proof of Lemma 4.3: A Formula of Helffer and Sjőstrand

In this section, we prove Lemma 4.3. The main technical tool to do so is a functional calculus formula due to Helffer and Sjőstrand [HS89]. We state it here in the formulation of [HS00], see also [Dav95].

5.1 Theorem (Helffer-Sjőstrand formula [HS00, Section IX])**.** Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Let $n \in \mathbb{N}$ and $f \in C_c^{n+1}(\mathbb{R})$. Let $\xi \in C_c^\infty(\mathbb{C})$ with the identification $\mathbb{C} \cong \mathbb{R}^2$ and $\xi(z) = 1$ in some complex neighborhood U of $\operatorname{spt} f$. Define an *almost analytic extension* $\tilde{f} \in C_c^2(\mathbb{C})$ of f via

$$\tilde{f}(x+iy) := \xi(x+iy) \sum_{k=0}^{n} f^{(k)}(x) \frac{(iy)^k}{k!} \qquad (x, y \in \mathbb{R}). \tag{5.1}$$

Then

$$f(A) = -\frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \, (x+iy-A)^{-1} \partial_{\bar{z}} \tilde{f}(x+iy), \tag{5.2}$$

where $\partial_{\bar{z}} := \partial_x + i\partial_y$.

Proof. We prove that the integrand in (5.2) is absolutely (Bochner) integrable. First notice that it has compact support. Moreover, $\partial_{\bar{z}}\tilde{f}(z) = f^{(n+1)}(x)(iy)^n/n!$ for $z = x+iy \in U$, and thus there is $C > 0$ such that $|\partial_{\bar{z}}\tilde{f}(x+iy)| \le C|y|^n$ for $x, y \in \mathbb{R}$. Since $\|(z-A)^{-1}\| \le |\operatorname{Im} z|^{-1}$ for $z \in \mathbb{C} \setminus \sigma(A)$, the integrand in (5.2) has no singularities and therefore exists. It remains to show the equality in (5.2). For $t \in \mathbb{R}$ and $\varepsilon > 0$, define

$$f_\varepsilon(t) := -\frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \int_{|y|>\varepsilon} \mathrm{d}y \, (x+iy-t)^{-1} \partial_{\bar{z}} \tilde{f}(x+iy). \tag{5.3}$$

The assertion follows once we have established $f_\varepsilon(t) \to f(t)$ for $t \in \mathbb{R}$ as $\varepsilon \to 0$. Integrating by parts yields

$$\begin{aligned} f_\varepsilon(t) = {} & \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \int_{|y|>\varepsilon} \mathrm{d}y \, \partial_{\bar{z}} \frac{1}{x+iy-t} \tilde{f}(x+iy) \\ & + \frac{i}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \Big(\frac{1}{x+i\varepsilon-t} \tilde{f}(x+i\varepsilon) - \frac{1}{x-i\varepsilon-t} \tilde{f}(x-i\varepsilon) \Big). \end{aligned} \tag{5.4}$$

The first term is zero due to holomorphy. The second term is, for ε small enough,

$$\sum_{k=0}^{n} \frac{(i\varepsilon)^k}{k!} \frac{i}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \, f^{(k)}(x) \Big(\frac{1}{x+i\varepsilon-t} - \frac{(-1)^k}{x-i\varepsilon-t} \Big). \tag{5.5}$$

The integral in (5.5) converges for all k due to the Sokhotski-Plemelj formula, see below. Thus only the $k = 0$ term of the sum remains in the limit and yields $f(t)$. □

In the proof of Theorem 5.1, we used the Sokhotski-Plemelj formula, which we state and prove as a convenience for the reader.

5.2 Theorem (Sokhotski-Plemelj formula)**.** Let $a < x_0 < b$ and $\varphi\colon[a,b] \to \mathbb{C}$ be continuous, and differentiable at x_0. Then

$$\lim_{\varepsilon\downarrow 0} \int_a^b \mathrm{d}x \, \frac{\varphi(x)}{x - x_0 \pm i\varepsilon} = \mp i\pi\varphi(x_0) + \mathrm{PV}\!\int_a^b \mathrm{d}x \, \frac{\varphi(x)}{x - x_0}, \tag{5.6}$$

where $\mathrm{PV}\!\int_a^b \mathrm{d}x$ stands for the Cauchy principal value.

Proof. By extending φ continuously, it suffices to treat the case $x_0 = (a+b)/2$. Then

$$\begin{aligned}\int_a^b \mathrm{d}x \, \frac{\varphi(x)}{x - x_0 \pm i\varepsilon} &= \int_a^b \mathrm{d}x \, \varphi(x) \frac{x - x_0 \mp i\varepsilon}{(x-x_0)^2 + \varepsilon^2} \\ &= \varphi(x_0) \int_a^b \mathrm{d}x \, \frac{x - x_0 \mp i\varepsilon}{(x-x_0)^2 + \varepsilon^2} + \int_a^b \mathrm{d}x \, \frac{\varphi(x) - \varphi(x_0)}{x - x_0 \pm i\varepsilon}. \end{aligned} \tag{5.7}$$

The first integral has two parts: Its real part is zero by cancellation, while the integrand of its imaginary part has $x \mapsto \mp i \arctan \frac{x - x_0}{\varepsilon}$ as an antiderivative. The second integral has a pointwise convergent integrand that is dominated by

$$\left| \frac{\varphi(x) - \varphi(x_0)}{x - x_0} \right| \le C \qquad (a \le x \le b) \tag{5.8}$$

for some $C > 0$. Therefore,

$$\lim_{\varepsilon\to\infty} \int_a^b \mathrm{d}x \, \frac{\varphi(x)}{x - x_0 \pm i\varepsilon} = \mp i\pi\varphi(x_0) + \int_a^b \mathrm{d}x \, \frac{\varphi(x) - \varphi(x_0)}{x - x_0}. \tag{5.9}$$

The second term is the principal value $\mathrm{PV}\!\int \frac{\varphi(x)}{x - x_0} \mathrm{d}x$, since

$$\begin{aligned}\Big(\int_a^{x_0 - \varepsilon} \mathrm{d}x + \int_{x_0+\varepsilon}^b \mathrm{d}x \Big) \frac{\varphi(x)}{x - x_0} &= \Big(\int_a^{x_0 - \varepsilon} \mathrm{d}x + \int_{x_0+\varepsilon}^b \mathrm{d}x \Big) \frac{\varphi(x) - \varphi(x_0)}{x - x_0} \\ &\quad + \varphi(x_0) \Big(\int_a^{x_0 - \varepsilon} \mathrm{d}x + \int_{x_0+\varepsilon}^b \mathrm{d}x \Big) \frac{1}{x - x_0} \end{aligned} \tag{5.10}$$

for $\varepsilon > 0$, where the second term is zero due to cancellation. □

Before we can prove Lemma 4.3, we need one additional technical result, which is a consequence of the geometric resolvent inequality. We state it here in a formulation suited for our application and give a proof in Theorem C.2 in the Appendix for a more general formulation. The proof is an adaptation of the one in [Sto01].

5.3 Lemma. Let $L > 1$ and let $A \subseteq \Omega_{L-1}$ be closed. Take $\varphi \in C_c^1(\Omega_L)$ with $\varphi(x) = 1$ for $x \in \Omega_{L-1}$. Then $U_L := \Omega_L \setminus \overline{\Omega_{L-1}}$ is an open neighborhood of $\operatorname{spt} \nabla\varphi$ and $\delta := \operatorname{dist}(\partial U_L, \operatorname{spt} \nabla\varphi) > 0$. Let $K \subseteq \mathbb{C}$ be compact. Then there exists $C_{\mathrm{GR}} > 0$ depending on δ, $\|\nabla\varphi\|_\infty$, V, and K such that for all $z \in \rho(H_L^{(\prime)}) \cap \rho(H^{(\prime)}) \cap K$ the operator norm estimate

$$\left\|1_A\left((z-H^{(\prime)})^{-1}-(z-H_L^{(\prime)})^{-1}\right)1_A\right\| \le C_{\mathrm{GR}}\|1_A(z-H_L^{(\prime)})^{-1}1_{U_L}\|\|1_{U_L}(z-H^{(\prime)})^{-1}1_A\| \tag{5.11}$$

holds, where the indicator functions are understood as their associated multiplication operators.

Proof of Lemma 4.3. The proof is an adaptation of [GKM14, Proof of Lemma 3.14]. We use the identification $\mathbb{R}^2 \cong \mathbb{C}$ and choose $\xi \in C_c^\infty(\mathbb{C})$ with $\xi(z) = 1$ for $z \in \operatorname{spt} h_L^t \times [-1,1]$ and $\xi(z) = 0$ for z with $\operatorname{dist}_{\mathbb{C}}(z, \operatorname{spt} h_L^t) \ge 3$ for all $t \ge 0$ and $L > 1$. Since $\operatorname{spt} h_L^t \subseteq [E, E_0 + 1]$, the function ξ can be chosen independently of L and t, with $\|\xi\|_\infty = 1$ and $\|\xi'\|_\infty \le 1$. For $n \in \mathbb{N}$, define an almost analytic extension $\tilde{h}_L^t$ of h_L^t as in Theorem 5.1, i.e.,

$$\tilde{h}_L^t(z) := \xi(z)\sum_{k=0}^{n}\frac{(iy)^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}x^k}h_L^t(x) \qquad (z = x + iy \in \mathbb{C}). \tag{5.12}$$

Let T_L and T stand for either H_L and H or H_L' and H'. By Theorem 5.1,

$$h_L^t(T_L) - h_L^t(T) = \frac{1}{2\pi}\int_{\mathbb{C}}\mathrm{d}z\left((z-T)^{-1}-(z-T_L)^{-1}\right)\partial_{\bar{z}}\tilde{h}_L^t(z). \tag{5.13}$$

In (5.13), we consider the bounded operators occurring there as mapping from $L_2(\Omega_L)$ to $L_2(\mathbb{R}^d)$ by restricting and embedding canonically.

Now, note that there is a constant $C > 0$, independent of L and t, such that

$$|\partial_{\bar{z}}\tilde{h}_L^t(z)| \le C|y|^n\sum_{k=0}^{n+1}\left|\frac{\mathrm{d}^k}{\mathrm{d}x^k}h_L^t(x)\right| \qquad (z = x + iy \in \mathbb{C}) \tag{5.14}$$

and the bounds (4.2) and (4.3) imply, by the Leibniz rule,

$$\left|\frac{\mathrm{d}^k}{\mathrm{d}x^k}h_L^t(x)\right| \le L^{bk}\sum_{j=0}^{k}\binom{k}{j}\left(\frac{t}{L^a}\right)^j c_{k-j}1_{[-E_0-1,E_0+1]}(x) \tag{5.15}$$

for $t \ge 0$, $L > 1$, and $x \in \mathbb{R}$. Notice that (5.15) is true for both f_L^t and g_L^t, since the exponential part of both functions is bounded by one and their supports are subsets of $[-E_0-1,E_0+1]$. From (5.15), we conclude that there is a polynomial Q_n over $\mathbb{R}$ of degree $n+1$ with nonnegative coefficients such that

$$0 \le \sum_{k=0}^{n+1}\Big|\frac{\mathrm{d}^k}{\mathrm{d}x^k} h_L^t(x)\Big| \le Q_n(t/L^a)L^{a(n+1)}1_{[-E_0-1,E_0+1]}(x) \tag{5.16}$$

for all $t \ge 0$, $L > 1$, and $x \in \mathbb{R}$. We are looking for a bound on $\|\sqrt{V}\big(h_L^t(T_L) - h_L^t(T)\big)\sqrt{V}\|$, which we can express using (5.13). We split the integration in two parts and define

$$\begin{aligned} D_L^<(t) &:= \frac{1}{2\pi}\int_{|y|\le L^{-1+\varepsilon}} \mathrm{d}z\,\sqrt{V}\Big((z-T)^{-1}-(z-T_L)^{-1}\Big)\sqrt{V}\,\partial_{\bar z}\tilde h_L^t(z),\\ D_L^>(t) &:= \frac{1}{2\pi}\int_{|y|> L^{-1+\varepsilon}} \mathrm{d}z\,\sqrt{V}\Big((z-T)^{-1}-(z-T_L)^{-1}\Big)\sqrt{V}\,\partial_{\bar z}\tilde h_L^t(z). \end{aligned} \tag{5.17}$$

Then $\sqrt{V}\big(h_L^t(T_L) - h_L^t(T)\big)\sqrt{V} = D_L^<(t) + D_L^>(t)$, and we can bound $D_L^<(t)$ using the boundedness of $\sqrt{V}$ and estimates (5.14) and (5.16) and the norm bounds of the resolvents:

$$\begin{aligned} \|D_L^<(t)\| &\le \frac{1}{2\pi}\int_{|y|\le L^{-1+\varepsilon}} \mathrm{d}z\,\frac{2}{|y|}\|\sqrt{V}\|^2|\partial_{\bar z}\tilde h_L^t(z)|\\ &\le \frac{C}{\pi}\|V\|_\infty \int_{|y|\le L^{-1+\varepsilon}} \mathrm{d}z\,|y|^{n-1}\sum_{k=0}^{n+1}\Big|\frac{\mathrm{d}^k}{\mathrm{d}x^k}h_L^t(x)\Big|\\ &= \frac{2C}{\pi n}\|V\|_\infty L^{n(-1+\varepsilon)}\int_{\mathbb{R}} \mathrm{d}x\,\sum_{k=0}^{n+1}\Big|\frac{\mathrm{d}^k}{\mathrm{d}x^k}h_L^t(x)\Big|\\ &\le C_< Q_n(t/L^a)L^{a+n(-1+\varepsilon+a)} \qquad (t\ge 0, L>1), \end{aligned} \tag{5.18}$$

with $C_< := (4C/\pi n)(E_0+1)\|V\|_\infty < \infty$ and the convention $z = x+iy \in \mathbb{C}$.

We turn now to $D_L^>(t)$, which we bound using Lemma 5.3, estimate (5.14), the properties of ξ, and the norm bound for one of the resolvents:

$$\begin{aligned} \|D_L^>(t)\| &\le \frac{C_{\mathrm{GR}}}{2\pi}\|V\|_\infty\int_{|y|>L^{-1+\varepsilon}} \mathrm{d}z\,\|1_{\operatorname{spt}V}(z-T_L)^{-1}1_{U_L}\|\|1_{U_L}(z-T)^{-1}1_{\operatorname{spt}V}\||\partial_{\bar z}\tilde h_L^t(z)|\\ &\le \frac{CC_{\mathrm{GR}}}{2\pi}\|V\|_\infty\int_{L^{-1+\varepsilon}<|y|\le 3} \mathrm{d}z\,|y|^{n-1}\|1_{U_L}(z-T)^{-1}1_{\operatorname{spt}V}\|\sum_{k=0}^{n+1}\Big|\frac{\mathrm{d}^k}{\mathrm{d}x^k}h_L^t(x)\Big| \end{aligned} \tag{5.19}$$

for $t \ge 0$ and $L > 3$, where $U_L := \Omega_L \setminus \overline{\Omega_{L-1}}$, and the constant C_{GR} depends only on E_0, ξ, and the potentials V_0 and V. To bound the operator norm in (5.19), we employ a Combes-Thomas estimate for operator kernels of resolvents of Schrödinger operators, which implies

$$\left\|1_\Lambda(x+iy-T)^{-1}1_{\Lambda'}\right\| \le \frac{C_{\mathrm{CT}}}{|y|}e^{-c_{\mathrm{CT}}\,\mathrm{dist}(\Lambda,\Lambda')|y|} \qquad (|x|\le E_0+1, |y|\le 3), \tag{5.20}$$

where Λ and Λ' are cubes of side length 1, see [GK03, Thm. 1] or [Sto01, Thm. 2.4.1 and Rem. 2.4.3]. The constants C_{CT} and c_{CT} in (5.20) depend only on E_0, the space dimension d, and the potentials V and V_0. Thus, by covering spt V and U_L with cubes of side length 1, we can find a constant $\tilde{C}>0$, independent of L and t, such that

$$\frac{CC_{\mathrm{GR}}}{\pi}\|V\|_\infty \|1_{U_L}(z-T)^{-1}1_{\mathrm{spt}\,V}\| \le \tilde{C}L^d|y|^{-1}e^{-c_{\mathrm{CT}}|y|L/2} \tag{5.21}$$

for $L>L_0$, where L_0 depends on spt V and Ω_1. Let $n\ge 2$. Applying (5.21) and (5.16) to (5.19) gives

$$\begin{aligned}\|D_L^>(t)\| &\le \tilde{C}(E_0+1)Q_n(t/L^a)L^{d+a(n+1)}\int_{L^{-1+\varepsilon}<|y|\le 3}\mathrm{d}y\,|y|^{n-2}e^{-c_{\mathrm{CT}}|y|L/2}\\ &\le C_> Q_n(t/L^a)L^{d+a(n+1)}e^{-c_{\mathrm{CT}}L^{\varepsilon}/2}\end{aligned} \tag{5.22}$$

for $t\ge 0$ and $L>L_0$, with $C_> := 2\cdot 3^{n-1}/(n-1)\tilde{C}(E_0+1)$.

Combining the estimates (5.18) and (5.22), we arrive at

$$\begin{aligned}\left\|\sqrt{V}\big(h_L^t(T_L)-h_L^t(T)\big)\sqrt{V}\right\| &\le \|D_L^<(t)\| + \|D_L^>(t)\|\\ &\le (C_< + C_>)Q_n(t/L^a)\Big(L^{a+n(-1+\varepsilon+a)} + L^{d+a(n+1)}e^{-c_{\mathrm{CT}}L^{\varepsilon}/2}\Big),\end{aligned} \tag{5.23}$$

which implies the assertion for $n=M$. □

6 INFINITE-VOLUME TRACE EXPRESSIONS

Let $n \in \mathbb{N}$. In (4.18), we gave a lower bound on the nth term of (1.14) in which only infinite-volume objects occur. In order to control the errors in that step, it was necessary to introduce smoothed versions of indicator functions in (4.4). In the present section, our aim is to replace these smoothed functions with discontinuous ones, which will allow us to determine the asymptotics of the resulting expression.

We introduce the measures $\mu^1, \nu^1 : \mathrm{Borel}(\mathbb{R}) \to [0, \infty]$ defined via

$$\mu^1(A) := \operatorname{tr}\big(\sqrt{V} 1_A(H)\sqrt{V}\big) \quad \text{and} \quad \nu^1(B) := \operatorname{tr}\big(\sqrt{V} 1_B(H')\sqrt{V}\big) \tag{6.1}$$

for $A, B \in \mathrm{Borel}(\mathbb{R})$. The expressions in (6.1) are finite for bounded Borel sets as a consequence of [Sim82, Thm. B.9.2].

The absolutely continuous parts of the measures μ^1 and ν^1 will turn out to be important. To define their densities in an applicable manner, we use a convergence result due to Birman and Èntina. This statement is known as the *limiting absorption principle* [Yaf10a, Chap. 6].

6.1 Proposition ([BÈ67, Lemma 4.3])**.** There exists a Lebesgue null set $\mathcal{N}_0 \subset \mathbb{R}$ such that the limits

$$\begin{aligned} A(E) &:= \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon} \sqrt{V} 1_{(E-\varepsilon, E+\varepsilon)}(H)\sqrt{V}, \\ B(E) &:= \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon} \sqrt{V} 1_{(E-\varepsilon, E+\varepsilon)}(H')\sqrt{V} \end{aligned} \tag{6.2}$$

exist in trace class for all $E \in \mathbb{R} \setminus \mathcal{N}_0$ and define nonnegative trace class operators $A(E)$ and $B(E)$.

We state a simple consequence of Proposition 6.1 that follows directly from the definitions.

6.2 Corollary. The functions $E \mapsto \operatorname{tr} A(E)$, respectively $E \mapsto \operatorname{tr} B(E)$, are locally integrable Lebesgue densities of the absolutely continuous parts of μ^1, respectively ν^1.

We will need two auxiliary propositions.

6.3 Lemma. Let μ be a locally finite Borel measure on $\mathbb{R}$. Let $c_0 > 0$ and $0 < \delta < c_0$. Then for a.e. $x_0 \in \mathbb{R}$ there is a constant C, depending on x_0, c_0, and μ, such that

$$\int_{(x_0, x_0+\delta)} \mathrm{d}\mu(x)\, e^{-t(x-x_0)} \le C \frac{1 - e^{-t\delta}}{t} \qquad (t > 0). \tag{6.3}$$

The exceptional set of values of x_0 for which the assertion does not hold does not depend on c_0 or δ.

Proof. The constant defined by

$$C := \sup_{\varepsilon\in(0,c_0)} \frac{1}{\varepsilon}\mu([x_0, x_0+\varepsilon]) \tag{6.4}$$

is finite for a.e. $x_0 \in \mathbb{R}$. We compute using Tonelli's theorem

$$\begin{aligned}
\int_{[x_0,x_0+\delta]} \mathrm{d}\mu(x)\, e^{-t(x-x_0)} \\
&= \int_{[x_0,x_0+\delta]} \mathrm{d}\mu(x)\Big(e^{-t\delta} + t\int_x^{x_0+\delta} \mathrm{d}\xi e^{-t(\xi-x_0)}\Big) \\
&= \delta e^{-t\delta}\frac{1}{\delta}\mu([x_0, x_0+\delta]) + t\int_{x_0}^{x_0+\delta} \mathrm{d}\xi \int_{[x_0,\xi]} \mathrm{d}\mu(x)\, e^{-t(\xi-x_0)} \\
&\le C\delta e^{-t\delta} + t\int_{x_0}^{x_0+\delta} \mathrm{d}\xi\, e^{-t(\xi-x_0)}\frac{\xi-x_0}{\xi-x_0}\mu([x_0,\xi]) \\
&\le C\delta e^{-t\delta} + Ct\int_0^{\delta} \mathrm{d}\xi\, \xi e^{-t\xi} = C\frac{1-e^{-t\delta}}{t}.
\end{aligned} \tag{6.5}$$

□

6.4 Corollary. In the situation of Lemma 6.3, let $0 < \varepsilon < \delta$. Then for a.e. $x_0 \in \mathbb{R}$ the bound

$$\int_{(x_0+\varepsilon,x_0+\delta)} \mathrm{d}\mu(x)\, e^{-t(x-x_0)} \le Ce^{-t\varepsilon/2}\frac{1-e^{-t\delta/2}}{t/2} \le C\frac{e^{-t\varepsilon/2}}{t/2} \qquad (t>0) \tag{6.6}$$

holds, with $C > 0$ from Lemma 6.3. The exceptional set of measure zero does not depend on c_0, ε, or δ.

Proof. The assertion follows from $e^{-t(x-x_0)} \le e^{-t\varepsilon/2}e^{-t(x-x_0)/2}$ for $\varepsilon \le x - x_0 \le \delta$ and Lemma 6.3. □

6.5 Definition. (A) For $n \in \mathbb{N}$, we define

$$I_n := \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1)\frac{1}{\prod_{j=1}^n (u_j + u_{j+1})}, \tag{6.7}$$

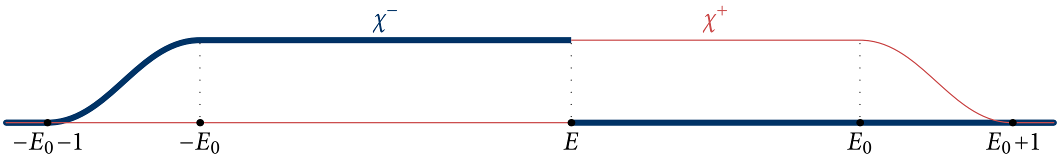
where $u_{n+1} := u_1$ for $u \in \mathbb{R}^n$.

(B) We define discontinuous L-independent functions $\chi^\pm : \mathbb{R} \to [0,1]$ by

$$\chi^- := \max\{\chi_L^-, 1_{[-E_0,E)}\} \quad \text{and} \quad \chi^+ := \max\{\chi_L^+, 1_{(E,E_0]}\}. \tag{6.8}$$

6.6 Remarks. (A) The integral I_n will be discussed further in § 8; in particular, I_n is finite for every $n \in \mathbb{N}$.

(B) The functions $\chi_L^\pm$ converge pointwise to $\chi^\pm$ as $L \to \infty$. They are obtained from replacing the smooth L-dependent part by a discontinuous step at E. The following figure illustrates the behavior of $\chi^\pm$.



The next lemma is the main result of the present section.

6.7 Lemma. There is a null set $\mathcal{N} \subseteq \mathbb{R}$ such that for $E \in \mathbb{R} \setminus \mathcal{N}$,

$$\begin{aligned} &\int_0^\infty \mathrm{d}t\, t^{2n-1} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v)\, \delta(1 - |u|_1 - |v|_1) \\ &\quad \times \Big(\operatorname{tr} \prod_{j=1}^n \sqrt{V} \chi_L^-(H) e^{(u_j + v_{j-1})t(H-E)} V \chi_L^+(H') e^{-(u_j+v_j)t(H'-E)} \sqrt{V} \\ &\quad - e^{-tL^{-a}} \operatorname{tr} \prod_{j=1}^n \sqrt{V} \chi^-(H) e^{(u_j + v_{j-1})t(H-E)} V \chi^+(H') e^{-(u_j+v_j)t(H'-E)} \sqrt{V} \Big) = \mathrm{O}(1) \end{aligned} \tag{6.9}$$

as $L \to \infty$.

Proof. First notice that if f_j, g_j are bounded measurable functions of compact support for $1 \le j \le n$, then

$$\begin{aligned} \operatorname{tr} \prod_{j=1}^n \Big| \sqrt{V} f_j(H) V g_j(H') \sqrt{V} \Big| &\le \prod_{j=1}^n \operatorname{tr}\big(\sqrt{V} f_j(H) \sqrt{V}\big) \operatorname{tr}\big(\sqrt{V} g_j(H') \sqrt{V}\big) \\ &= \int_{\mathbb{R}^n} \mathrm{d}\mu^n(x) \int_{\mathbb{R}^n} \mathrm{d}\nu^n(y) \prod_{j=1}^n f_j(x_j) g_j(y_j), \end{aligned} \tag{6.10}$$

where we wrote μ^n and ν^n for the n-fold product measure of μ^1 and ν^1, respectively.

For brevity, set $\delta := L^{-a}$. We introduce a vector $\alpha \in (0, \infty)^{2n}$ via

$$\alpha_{2j-1} := u_j + v_{j-1} \quad \text{and} \quad \alpha_{2j} := u_j + v_j \tag{6.11}$$

for $1 \le j \le n$, and operators

$$A_k^{(L)} := \begin{cases} \sqrt{V} \chi_{(L)}^-(H) e^{\alpha_k t(H-E)} \sqrt{V} & \text{for } k \text{ odd}, \\ \sqrt{V} \chi_{(L)}^+(H') e^{-\alpha_k t(H'-E)} \sqrt{V} & \text{for } k \text{ even} \end{cases} \tag{6.12}$$

for $1 \le k \le 2n$. The difference of operator products in (6.9) is then

$$\prod_{j=1}^{2n} A_j^L - e^{-t\delta} \prod_{j=1}^{2n} A_j = e^{-t\delta}\Big(\prod_{j=1}^{2n} A_j^L - \prod_{j=1}^{2n} A_j\Big) + (1 - e^{-t\delta}) \prod_{j=1}^{2n} A_j^L, \tag{6.13}$$

where as in (4.13),

$$\prod_{j=1}^{2n} A_j^L - \prod_{j=1}^{2n} A_j = \sum_{k=1}^{2n} A_1 \cdots A_{k-1}(A_k^L - A_k) A_{k+1}^L \cdots A_{2n}^L. \tag{6.14}$$

We will treat the two terms on the right-hand side of (6.13) individually. For the first term, we estimate the kth term in (6.14). We will carry out the argument in the case where k is even. The argument is similar for odd k. Since $0 \le \chi^+ - \chi_L^+ \le 1_{[E,E+2\delta]}$, (6.10) implies

$$\begin{aligned}
&\operatorname{tr}\Big|A_1 \cdots A_{k-1}(A_k^L - A_k) A_{k+1}^L \cdots A_{2n}^L\Big| \\
&\le \int_{[-E_0-1,E]^n} \mathrm{d}\mu^n(x) \int_{[E,E_0+1]^n} \mathrm{d}\nu^n(y)\, 1_{[E,E+2\delta]}(y_k) \\
&\qquad \times \exp\Big(-t \sum_{j=1}^{n} \big((u_j + v_j)(y_j - E) - (u_j + v_{j-1})(x_j - E)\big)\Big) \\
&\le C^{2n} \frac{1 - e^{-2t\delta}}{t} \Big(\frac{1 - e^{-2t(E_0+1)}}{t}\Big)^{2n-1} \frac{1}{\prod_{j=1}^{n}(u_j + v_j)(u_j + v_{j-1})},
\end{aligned} \tag{6.15}$$

where the last inequality follows from applying Lemma 6.3. The classical formula

$$\int_0^\infty \mathrm{d}t\, e^{-\delta t} \frac{1 - e^{-\varepsilon t}}{t} = \ln(1 + \varepsilon/\delta) \qquad (\delta, \varepsilon > 0) \tag{6.16}$$

now implies

$$\begin{aligned}
&\int_0^\infty \mathrm{d}t\, t^{2n-1} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v)\, \delta(1 - |u|_1 - |v|_1)\, e^{-t\delta} \operatorname{tr}\Big|\prod_{j=1}^{2n} A_j^L - \prod_{j=1}^{2n} A_j\Big| \\
&\le 2nC^{2n} \int_0^\infty \mathrm{d}t\, e^{-t\delta} \frac{1 - e^{-2t\delta}}{t} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v)\, \frac{\delta(1 - |u|_1 - |v|_1)}{\prod_{j=1}^{n}(u_j + v_j)(u_j + v_{j-1})} \\
&= 2nC^{2n} I_{2n} \ln 3,
\end{aligned} \tag{6.17}$$

with $I_{2n} < \infty$ from (6.7).

The trace norm of the second term on the right-hand side of (6.13) is

$$\begin{aligned}(1-e^{-t\delta})\,\mathrm{tr}\Big|\prod_{j=1}^{2n} A_j^L\Big| &\le (1-e^{-t\delta})\int_{[-E_0-1,E-\delta]^n} \mathrm{d}\mu^n(x)\int_{[E+\delta,E_0+1]^n}\mathrm{d}\nu^n(y)\\ &\quad\times \exp\Big(-t\sum_{j=1}^{n}\big((u_j+v_j)(y_j-E)-(u_j+v_{j-1})(x_j-E)\big)\Big)\\ &\le C^{2n}(1-e^{-t\delta})\prod_{j=1}^{n}\frac{e^{-(u_j+v_{j-1})t\delta/2}e^{-(u_j+v_j)t\delta/2}}{(u_j+v_{j-1})(u_j+v_j)(t/2)^2} = \frac{(2C)^{2n}(1-e^{-t\delta})e^{-t\delta}t^{-2n}}{\prod_{j=1}^n (u_j+v_j)(u_j+v_{j-1})},\end{aligned} \tag{6.18}$$

where the second inequality is a consequence of Corollary 6.4. Integration yields

$$\int_0^\infty \mathrm{d}t\, t^{2n-1}\int_{[0,1]^n\times[0,1]^n}\mathrm{d}(u,v)\,\delta(1-|u|_1-|v|_1)\frac{(1-e^{-t\delta})e^{-t\delta}t^{-2n}}{\prod_{j=1}^n (u_j+v_j)(u_j+v_{j-1})} = I_{2n}\ln 2, \tag{6.19}$$

where we used formula (6.16) again. □

6.8 Remark. From Equation (4.18) in Remark 4.7 (A) and Lemma 6.7, we conclude

$$\begin{aligned}&\mathrm{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H_L')\big)^n\\ &\quad\ge \int_0^\infty \mathrm{d}t\, t^{2n-1}e^{-tL^{-a}}\int_{[0,1]^n\times[0,1]^n}\mathrm{d}(u,v)\,\delta(1-|u|_1-|v|_1)\\ &\quad\times \mathrm{tr}\prod_{j=1}^{n}\sqrt{V}\chi^-(H)e^{(u_j+v_{j-1})t(H-E)}V\chi^+(H')e^{-(u_j+v_j)t(H'-E)}\sqrt{V} + \mathrm{O}(1)\end{aligned} \tag{6.20}$$

as $L\to\infty$, for a.e. $E\in[-E_0,E_0]$, with the exceptional set not depending on a, n, and E_0. In the next section, we determine the asymptotics of the right-hand side of (6.20).

7 THE LOGARITHMIC DIVERGENCE

Let $n \in \mathbb{N}$. In this section, we determine the asymptotics of

$$\int_0^\infty \mathrm{d}t\, t^{2n-1} e^{-tL^{-a}} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v)\, \delta(1 - |u|_1 - |v|_1) \\ \times \operatorname{tr} \prod_{j=1}^n \sqrt{V} \chi^-(H) e^{(u_j+v_{j-1})t(H-E)} V \chi^+(H') e^{-(u_j+v_j)t(H'-E)} \sqrt{V}, \quad (7.1)$$

and therefore the asymptotics of a lower bound of the nth term of (1.14), when taking an appropriate subsequence of length scales – see Remark 6.8 and Lemma 2.1.

We start with a lemma.

7.1 Lemma. For a.e. $E \in [-E_0, E_0]$, the limits

$$\begin{aligned} A_t(E) &:= \sqrt{V} t e^{t(H-E)} \chi^-(H) \sqrt{V} \to A(E) \qquad (t \to \infty), \\ B_t(E) &:= \sqrt{V} t e^{-t(H'-E)} \chi^+(H') \sqrt{V} \to B(E) \qquad (t \to \infty) \end{aligned} \quad (7.2)$$

exist in trace class. Moreover,

$$\begin{aligned} \sup_{t \geq 0} \| A_t(E) \| &\leq \sup_{t\geq 0} \operatorname{tr} A_t(E) < \infty, \\ \sup_{t \geq 0} \| B_t(E) \| &\leq \sup_{t\geq 0} \operatorname{tr} B_t(E) < \infty. \end{aligned} \quad (7.3)$$

Proof. We follow [GKM14, Lemma 3.16] and treat the operator $B_t(E)$; the assertions for $A_t(E)$ can be proved using analogous arguments. Recall that $B_t(E)$ is nonnegative. For (7.2), we show (1) convergence of the trace norms and (2) weak convergence of the operators. Together, this implies convergence in trace class via [Sim05, Addendum H].

For the trace norms, we compute

$$\operatorname{tr} B_t(E) = \operatorname{tr}\big(\sqrt{V} t e^{-t(H'-E)} \chi^+(H') \sqrt{V}\big) \\ = \int_{[E,E_0]} \mathrm{d}\nu^1(y)\, t e^{-t(y-E)} + \int_{[E_0,E_0+1]} \mathrm{d}\nu^1(y)\, \chi^+(y) t e^{-t(y-E)}, \quad (7.4)$$

where the second term converges to zero as $t \to \infty$ for $E < E_0$, while the first term can be written as

$$\int_{[E,E_0]} \mathrm{d}\nu^1(y)\, t e^{-t(y-E)} = (\nu^1_{E_0} * \rho_t)(E), \quad (7.5)$$

where we introduced the finite measure $\nu^1_{E_0}(M) := \nu^1(M \cap [-E_0, E_0])$ for $M \in \mathrm{Borel}(\mathbb{R})$ and the approximation of the identity $x \mapsto \rho_t(x) := t e^{tx} 1_{(-\infty,0)}(x)$. As $t \to \infty$, the convolution in (7.5) converges for a.e. $E \in [-E_0, E_0]$ to $\frac{\mathrm{d}\nu^1_{\mathrm{ac}}}{\mathrm{d}E} = \operatorname{tr} B(E)$, see e.g. [MS13, Subsec. 2.4.1]. Thus, the trace norm of $B_t(E)$ converges to that of $B(E)$ as $t \to \infty$. This, together with the continuity of $[0,\infty) \ni t \mapsto \operatorname{tr} B_t(E)$, which can be seen from (7.4), implies (7.3).

For the weak convergence, take some dense countable set $\mathcal{D} \subseteq L^2(\mathbb{R}^d)$. Then by a similar delta-argument as above,

$$\lim_{t\to\infty} \langle \varphi, B_t(E)\psi \rangle = \langle \varphi, B(E)\psi \rangle \tag{7.6}$$

for all $\varphi, \psi \in \mathcal{D}$ and all $E \in [-E_0, E_0]$ outside a null set depending on $\mathcal{D}$. Together with (7.3), this proves weak convergence to $B(E)$ for a.e. $E \in [-E_0, E_0]$, see [Wei80, Thm. 4.26]. □

The following quantity will enter the asymptotics we set out to prove.

7.2 Definition. For $E_1, \dots, E_{2n} \in \mathbb{R}$, define

$$\eta^{2n}(E_1, \dots, E_{2n}) := \operatorname{tr}\big(A(E_1)B(E_2) \cdots A(E_{2n-1})B(E_{2n})\big) \tag{7.7}$$

if the operators exist, and zero otherwise. In addition to the function $\eta^{2n} : \mathbb{R}^{2n} \to \mathbb{C}$ defined via (7.7), define $\eta^{2n} : \mathbb{R} \to [0,\infty)$ via the diagonal values

$$\eta^{2n}(E) := \eta^{2n}(E, \dots, E) = \operatorname{tr}\big(A(E)B(E)\big)^n \tag{7.8}$$

if the operators exist, and zero otherwise. The nonnegativity of (7.8) can be seen by the cyclicity of the trace, cf. Lemma 2.3.

7.3 Remark. The function $\eta^{2n} : \mathbb{R}^{2n} \to \mathbb{C}$ can be viewed as the density of the (infinite-volume) spectral correlation expression

$$\mu^{2n}(A_1 \times \cdots \times A_n \times B_1 \times \cdots \times B_n) := \operatorname{tr}\big(1_{A_1}(H)V1_{B_1}(H)V \cdots 1_{A_n}(H)V1_{B_n}(H)V\big) \tag{7.9}$$

for $n \in \mathbb{N}$ and bounded $A_1, \dots, A_n, B_1, \dots, B_n \in \operatorname{Borel}(\mathbb{R})$, which can be thought of as the limit measure of the measures μ_L^{2n} mentioned in Remark 2.5. However, it is not immediately clear if (7.9) in fact defines a measure, and if so, it is not necessarily nonnegative for $n \geq 2$. However, its density η^{2n} is defined on the diagonal $(E, \dots, E) \in \mathbb{R}^{2n}$ for a.e. $E \in \mathbb{R}$ and is nonnegative there.

The next corollary will show that the trace expression in (7.1), times an appropriate power of t, converges to $\eta^{2n}(E)$.

7.4 Corollary. Let $\alpha_1, \dots, \alpha_n, \beta_1, \dots, \beta_n > 0$. Then

$$t^{2n} \operatorname{tr} \prod_{j=1}^{n} \sqrt{V}\chi^-(H)\alpha_j e^{\alpha_j t(H-E)} V \chi^+(H')\beta_j e^{-\beta_j t(H'-E)}\sqrt{V} \to \eta^{2n}(E) \tag{7.10}$$

as $t \to \infty$.

Proof. By Lemma 7.1, $\operatorname{tr}|A_{\alpha_j t}(E) - A(E)| \to 0$ and $\operatorname{tr}|B_{\beta_j t}(E) - B(E)| \to 0$ as $t \to \infty$, while $\sup_{t\geq 0}\|A_t(E)\|$ and $\sup_{t\geq 0}\|B_t(E)\|$ are finite. Writing the difference of operator products in (7.10) as in (4.13), this proves the corollary. □

7.5 Remark. Using similar arguments as in Lemma 7.1 and Corollary 7.4, one can show that $t \mapsto A_t(E)$, $t \mapsto B_t(E)$, and

$$t \mapsto t^{2n} \operatorname{tr} \prod_{j=1}^{n} \sqrt{V} \chi^-(H) \alpha_j e^{\alpha_j t(H-E)} V \chi^+(H') \beta_j e^{-\beta_j t(H'-E)} \sqrt{V} \tag{7.11}$$

are continuous maps from $[0, \infty)$ into the space of trace class operators.

We will need the following classical result, which is known as the »final value theorem« in control theory. As a convenience for the reader, we give a proof. The statement and proof can also be found in [Doe74, Thm. 34.3].

7.6 Lemma. Let $f \in L_{1,\mathrm{loc}}(\mathbb{R})$ and suppose $\lim_{t\to\infty} f(t)$ exists. Then

$$\lim_{t\to\infty} f(t) = \lim_{s\downarrow 0} s \int_0^\infty \mathrm{d}t\, e^{-st} f(t). \tag{7.12}$$

Proof. Let $\varepsilon > 0$. Set $y := \lim_{t\to\infty} f(t)$ and write $h(t) := f(t) - y$. Choose $T \geq 1$ such that $|h(t)| < \varepsilon/2$ for $t \geq T$. Then

$$\begin{aligned} F(s) &:= \int_0^\infty \mathrm{d}t\, e^{-st} f(t) \\ &= y \int_0^\infty \mathrm{d}t\, e^{-st} + \int_0^T \mathrm{d}t\, e^{-st}(f(t) - y) + \int_T^\infty \mathrm{d}t\, e^{-st} h(t) \end{aligned} \tag{7.13}$$

for $s > 0$. The first term on the right-hand side of (7.13) is y/s. The others are

$$\left| \int_T^\infty \mathrm{d}t\, e^{-st} h(t) \right| \leq \frac{\varepsilon}{2s} \tag{7.14}$$

and

$$\left| \int_0^T \mathrm{d}t\, e^{-st}(f(t) - y) \right| \leq \int_0^T \mathrm{d}t\, |f(t)| + T|y| =: C \tag{7.15}$$

for $s > 0$, with C independent of s. Thus

$$\left| F(s) - \frac{y}{s} \right| \leq C + \frac{\varepsilon}{2s} \qquad (s > 0), \tag{7.16}$$

and therefore

$$\left| sF(s) - y \right| \leq sC + \frac{\varepsilon}{2} \qquad (s > 0). \tag{7.17}$$

For $s \leq \varepsilon/(2C)$, this is smaller than ε. □

7.7 Corollary. Let $f \in L_{1,\mathrm{loc}}(\mathbb{R})$ and suppose $\lim_{t\to\infty} f(t)$ exists. Then

$$\lim_{t\to\infty} f(t) = -\lim_{s\downarrow 0} \frac{1}{\ln s} \int_1^\infty \mathrm{d}t\, t^{-1} e^{-st} f(t). \tag{7.18}$$

Proof. Take a compact interval $[s_0, c] \subseteq (0, \infty)$. Then

$$\frac{\mathrm{d}}{\mathrm{d}s} \int_1^\infty \mathrm{d}t\, t^{-1} e^{-st} f(t) = -\int_1^\infty \mathrm{d}t\, e^{-st} f(t) \tag{7.19}$$

for $s \in [s_0, c]$, since $\left|\frac{\mathrm{d}}{\mathrm{d}s} t^{-1} e^{-st} f(t)\right| \le e^{-s_0 t} |f(t)|$, which is integrable on $[1, \infty)$. Therefore (7.19) holds for all $s > 0$. Set $y := \lim_{t\to\infty} f(t)$. If $\lim_{s\downarrow 0} \int_1^\infty \mathrm{d}t\, t^{-1} e^{-st} f(t)$ exists, then $y = 0$ and the assertion holds. Otherwise,

$$\begin{aligned} -\lim_{s\downarrow 0} \frac{1}{\ln s} \int_1^\infty \mathrm{d}t\, t^{-1} e^{-st} f(t) &= \lim_{s\downarrow 0} \frac{1}{1/s} \int_1^\infty \mathrm{d}t\, e^{-st} f(t) \\ &= \lim_{s\downarrow 0} s \int_0^\infty \mathrm{d}t\, e^{-st} f(t) \\ &= \lim_{t\to\infty} f(t) \end{aligned} \tag{7.20}$$

by Lemma 7.6. □

We are now ready to compute the asymptotics of (7.1).

7.8 Theorem. For a.e. $E \in [-E_0, E_0]$,

$$\begin{aligned} \lim_{L\to\infty} \frac{1}{a \ln L} \int_0^\infty \mathrm{d}t\, t^{2n-1} e^{-tL^{-a}} \int_{[0,1]^n \times [0,1]^n} \mathrm{d}(u,v)\, \delta(1 - |u|_1 - |v|_1) \\ \times \operatorname{tr} \prod_{j=1}^n \sqrt{V} \chi^-(H) e^{(u_j + v_{j-1}) t (H-E)} V \chi^+(H') e^{-(u_j+v_j) t (H'-E)} \sqrt{V} = I_{2n} \eta^{2n}(E). \end{aligned} \tag{7.21}$$

Proof. Let $u, v \in [0,1]^n$ and define

$$Z(u,v) := \prod_{j=1}^n (u_j + v_{j-1})(u_j + v_j). \tag{7.22}$$

Using the notation of Lemma 7.1,

$$\begin{aligned} Z(u,v) t^{2n} \operatorname{tr} \prod_{j=1}^n \sqrt{V} \chi^-(H) e^{(u_j+v_{j-1}) t (H-E)} V \chi^+(H') e^{-(u_j+v_j) t (H'-E)} \sqrt{V} \\ = \operatorname{tr} \prod_{j=1}^n A_{(u_j+v_{j-1})t}(E) B_{(u_j+v_j)t}(E), \end{aligned} \tag{7.23}$$

where

$$\left|\operatorname{tr}\prod_{j=1}^{n} A_{(u_j+v_{j-1})t}(E)B_{(u_j+v_j)t}(E)\right| \le \Big(\sup_{t\ge0}\operatorname{tr}A_t(E)\sup_{t\ge0}\operatorname{tr}B_t(E)\Big)^n < \infty. \tag{7.24}$$

By Corollary 7.4,

$$\lim_{t\to\infty}\operatorname{tr}\prod_{j=1}^{n} A_{(u_j+v_{j-1})t}(E)B_{(u_j+v_j)t}(E) = \eta^{2n}(E) \tag{7.25}$$

for all $u, v \in (0,1]^n$. By Remark 6.6,

$$I_{2n} = \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\,\delta(1-|u|_1-|v|_1)\,\frac{1}{Z(u,v)} < \infty. \tag{7.26}$$

Equations (7.24) to (7.26) supply the assumptions of the dominated convergence theorem, which yields the convergence

$$\lim_{t\to\infty} f(t) = I_{2n}\eta^{2n}(E) \tag{7.27}$$

for

$$\begin{aligned} f(t) &:= \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\,\delta(1-|u|_1-|v|_1) \\ &\quad\times t^{2n}\operatorname{tr}\prod_{j=1}^{n}\sqrt{V}\chi^-(H)e^{(u_j+v_{j-1})t(H-E)}V\chi^+(H')e^{-(u_j+v_j)t(H'-E)}\sqrt{V} \\ &= \int_{[0,1]^n\times[0,1]^n} \mathrm{d}(u,v)\,\frac{\delta(1-|u|_1-|v|_1)}{Z(u,v)}\operatorname{tr}\prod_{j=1}^{n} A_{(u_j+v_{j-1})t}(E)B_{(u_j+v_j)t}(E) \quad (t>0). \end{aligned} \tag{7.28}$$

The assertion (7.21) then follows from

$$-\lim_{L\to\infty}\frac{1}{\ln(L^{-a})}\int_0^\infty \mathrm{d}t\,t^{-1}e^{-tL^{-a}}f(t) = \lim_{t\to\infty} f(t), \tag{7.29}$$

which is a consequence of Corollary 7.7 and

$$\sup_{L\ge1}\int_0^1 \mathrm{d}t\,t^{-1}e^{-tL^{-a}}f(t) < \infty. \tag{7.30}$$

7.9 Remark. Continuing from Remark 6.8, we have proved the asymptotic bound

$$\operatorname{tr}\big(1_{(-\infty,E]}(H_L)1_{(E,\infty)}(H_L')\big)^n \ge aI_{2n}\eta^{2n}(E)\ln L + \mathrm{o}(\ln L) \tag{7.31}$$

as $L\to\infty$ for every $0<a<1$, with an a-dependent error term. From this, one can infer that (7.31) holds with $a=1$ as well. We will defer this argument to the proof of the asymptotic bound on the full ground-state overlap $|S_L(E)|$ in Theorem 10.1.

8 THE INTEGRAL $\int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \prod_{j=1}^n (u_j + u_{j+1})^{-1}$

In this section[1] we compute the coefficient of $\eta^{2n}(E)$ in the asymptotics in Theorem 7.8, i.e.,

$$I_n = \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \frac{1}{\prod_{j=1}^n (u_j + u_{j+1})} \tag{8.1}$$

from Definition 6.5. We will prove the following theorem.

8.1 Theorem. Let $n \in \mathbb{N}_{\geq 2}$. Then

$$I_n = (2\pi)^{n-2} \frac{\left(\Gamma(\frac{n}{2})\right)^2}{\Gamma(n)}. \tag{8.2}$$

In particular, Theorem 8.1 implies the finiteness of I_n. We begin with two elementary lemmas.

8.2 Lemma. For $n \in \mathbb{N}_{\geq 2}$, define

$$J_n := \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \frac{1}{\prod_{j=1}^{n-1} (u_j + u_{j+1})}. \tag{8.3}$$

Then

$$I_n = \frac{n}{2} J_n. \tag{8.4}$$

Proof.

$$\begin{aligned} I_n &= \frac{1}{2} \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \frac{2|u|_1}{\prod_{j=1}^n (u_j + u_{j+1})} \\ &= \frac{1}{2} \sum_{k=1}^n \int_{[0,1]^n} \mathrm{d}u\, \delta(1-|u|_1) \frac{u_k + u_{k+1}}{\prod_{j=1}^n (u_j + u_{j+1})} \\ &= \frac{n}{2} \int_{[0,1]^n} \mathrm{d}u\, \frac{\delta(1-|u|_1)}{(u_1+u_2)\cdots(u_{n-1}+u_n)} = \frac{n}{2} J_n. \end{aligned} \tag{8.5}$$

□

8.3 Lemma. Let $n \in \mathbb{N}_{\geq 2}$ and let $f \in L_1(0,\infty)$ with $\int_0^\infty \mathrm{d}t\, f(t) \neq 0$. Then

$$J_n = \int_{(0,\infty)^n} \mathrm{d}u\, \frac{f(|u|_1)}{\prod_{j=1}^{n-1} (u_j + u_{j+1})} \Big/ \int_0^\infty \mathrm{d}t\, f(t). \tag{8.6}$$

1 The main results of this section, which lead to the proof of (8.2), were communicated to me by Dr. Peter Otte of Bochum University.

In particular,

$$J_n = \int_{\Delta_n} \frac{\mathrm{d}u}{\prod_{j=1}^{n-1}(u_j + u_{j+1})} = \int_{(0,\infty)^n} \mathrm{d}u \, \frac{e^{-|u|_1}}{\prod_{j=1}^{n-1}(u_j + u_{j+1})}, \tag{8.7}$$

where Δ_n is the n-dimensional standard simplex.

Proof. For $t > 0$, define

$$J_n(t) := \int_{(0,\infty)^n} \mathrm{d}u \, \frac{\delta(t - |u|_1)}{\prod_{j=1}^{n-1}(u_j + u_{j+1})}. \tag{8.8}$$

Then $J_n = J_n(1) = J_n(t)$, where the last equality follows using the substitution $u \rightsquigarrow tu$ and the scaling property of the Dirac distribution. Therefore,

$$\begin{aligned} J_n \int_0^\infty \mathrm{d}t \, f(t) &= \int_{(0,\infty)^n} \mathrm{d}u \int_0^\infty \mathrm{d}t \, \frac{\delta(t - |u|_1) f(t)}{\prod_{j=1}^{n-1}(u_j + u_{j+1})} \\ &= \int_{(0,\infty)^n} \mathrm{d}u \, \frac{f(|u|_1)}{\prod_{j=1}^{n-1}(u_j + u_{j+1})}. \end{aligned} \tag{8.9}$$

□

In the sequel, we will need the Rosenblum-Rovnyak integral operator $T : L_2(0,\infty) \to L_2(0,\infty)$, see [Ros58] and [Rov70], defined via

$$(Tf)(x) := \int_0^\infty \mathrm{d}y \, \frac{e^{-(x+y)/2}}{x+y} f(y) \qquad (x \in (0,\infty), f \in L_2(0,\infty)). \tag{8.10}$$

This operator can be explicitly diagonalized: Following [Yaf10b, Sec. 4.2], we define the unitary operator $U : L_2(0,\infty) \to L_2(0,\infty)$ via

$$(Uf)(k) = \pi^{-1}\sqrt{k \sinh(2\pi k)} \, |\Gamma(1/2 - ik)| \int_0^\infty \mathrm{d}x \, x^{-1} W_{0,ik}(x) f(x) \tag{8.11}$$

for $f \in L_2(0,\infty)$ and $k \in (0,\infty)$, where $W_{0,ik}$ denotes the Whittaker functions, see [DLMF, Sec. 13.14]. The spectral representation of T due to Rosenblum reads

$$(UTf)(k) = \frac{\pi}{\cosh(k\pi)} (Uf)(k) \qquad (k \in (0,\infty), f \in L_2(0,\infty)), \tag{8.12}$$

see [Yaf10b, Prop. 4.1].

Proof of Theorem 8.1. Let $n \in \mathbb{N}_{\geq 2}$. From (8.10) and the second form in (8.7), we see that

$$J_n = \langle \varphi_0, T^{n-1} \varphi_0 \rangle, \tag{8.13}$$

with $\varphi_0(x) := e^{-x/2}$. From (8.13) and (8.12), we obtain

$$J_n = \langle U\varphi_0, UT^{n-1}\varphi_0\rangle = \int_0^\infty \mathrm{d}k\, |\hat{\varphi}_0(k)|^2 \Big(\frac{\pi}{\cosh(k\pi)}\Big)^{n-1}, \tag{8.14}$$

where $\hat{\varphi}_0 := U\varphi_0$. In order to compute $\hat{\varphi}_0$, we employ the classical formula

$$|\Gamma(1/2 - ik)|^2 = \frac{\pi}{\cosh(k\pi)} \qquad (k \in \mathbb{R}), \tag{8.15}$$

which is a consequence of the reflection formula for the Gamma function, and

$$\int_0^\infty \mathrm{d}x\, x^{-1} W_{0,ik}(x) e^{-x/2} = \frac{\pi}{\cosh(k\pi)} \qquad (k > 0), \tag{8.16}$$

which follows from the special case $z = 1/2$ and $\nu = \kappa = 0$ in [DLMF, eq. 13.23.4]. From (8.11), (8.15), and (8.16), we deduce

$$|\hat{\varphi}_0(k)|^2 = 2\pi k \frac{\sinh(k\pi)}{\cosh(k\pi)^2} \qquad (k > 0). \tag{8.17}$$

In (8.14), this yields

$$J_n = 2\pi^{n-2} \int_0^\infty \mathrm{d}k\, k \frac{\sinh(k)}{\cosh(k)^{n+1}} = \frac{2\pi^{n-2}}{n} \int_0^\infty \mathrm{d}k\, \frac{1}{\cosh(k)^n}, \tag{8.18}$$

where we applied the substitution $k \rightsquigarrow k/\pi$ and integrated by parts. This integral can be evaluated using the substitutions $y = \cosh(k)^{-1}$ and $x = y^2$, one after the other:

$$J_n = \frac{2\pi^{n-2}}{n} \int_0^1 \mathrm{d}y\, \frac{y^{n-1}}{\sqrt{1-y^2}} = \frac{\pi^{n-2}}{n} \int_0^1 \mathrm{d}x\, x^{n/2-1}(1-x)^{-1/2} = \frac{\pi^{n-2}}{n} \mathrm{B}(n/2, 1/2), \tag{8.19}$$

since $k'(y) = -y^{-1}(1-y^2)^{-1/2}$, where $\mathrm{B}(x,y) = \int_0^1 \mathrm{d}t\, t^{x-1}(1-t)^{y-1}$ denotes the Beta function. The claim then follows by expressing the Beta function via the Gamma function and then applying the classical duplication formula. □

8.4 Remark. (A) The Rosenblum-Rovnyak operator is the special case $T = \mathcal{H}_0$ in [Ros58, eq. (2.3)] and is unitarily equivalent to the *Hilbert matrix* $H : \ell_2(\mathbb{N}) \to \ell_2(\mathbb{N})$,

$$(Hx)_j := \sum_{k=0}^{\infty} \frac{x_k}{j+k-1} \qquad (j \in \mathbb{N}, x \in \ell_2(\mathbb{N})). \tag{8.20}$$

In analogy to (8.13), the representation

$$I_n = \frac{n}{2}\langle e_1, H^{n-1} e_1\rangle \tag{8.21}$$

holds, where $e_1 := (1, 0, \dots) \in \ell_2(\mathbb{N})$.

(B) Equation (8.2) implies other nontrivial integral identities. For instance, from $I_6 = 3J_6 = \frac{8}{16}\pi^4$ one can deduce

$$\int_0^1 \mathrm{d}u \left(\mathrm{Li}_2\Big(\frac{u-1}{u}\Big)\right)^2 = \frac{17}{180}\pi^4, \tag{8.22}$$

where $\mathrm{Li}_2(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2}$ denotes the dilogarithm. To prove (8.22), start from the first form in (8.7) and parameterize the simplex using the Jacobi map [Kön93, Sec. 9.3], then evaluate four of the five resulting integrals.

It is also possible to prove (8.22) without using (8.2). It follows for instance by using the more complicated integral identities of Freitas [Fre05, Table 3]; the expression for $\int_0^1 \mathrm{d}x\ \mathrm{Li}_2^2(x)$ there implies (8.22), which in turn implies (8.2) for the case $n = 6$.

As the last step in the current section, we determine the even part of the generating function of $(J_n)_{n\geq 2}$.

8.5 Proposition. For $n \in \mathbb{N}_{\geq 2}$, let J_n be given by (8.3). Then

$$\sum_{n=1}^{\infty} J_{2n} x^{2n} = \pi^{-2}\big(\arcsin(\pi x)\big)^2 \qquad (|x| \leq \tfrac{1}{\pi}). \tag{8.23}$$

Proof. The well-known power series of arcsin,

$$\arcsin(x) = \sum_{n=0}^{\infty} \binom{2n}{n} \frac{x^{2n+1}}{4^n(2n+1)} =: \sum_{n=0}^{\infty} a_n x^{2n+1} \qquad (|x| \leq 1), \tag{8.24}$$

implies

$$\big(\arcsin(x)\big)^2 = \sum_{n=0}^{\infty} b_n x^{2n+2} \qquad (|x| \leq 1), \tag{8.25}$$

with

$$b_n := \sum_{k=0}^{n} a_k a_{n-k} = 2^{2n+1} \frac{(n!)^2}{(2n+2)!} \qquad (n \in \mathbb{N}_0), \tag{8.26}$$

as can be shown by induction (or looked up in a table of series, e.g., [GR07, eq. 1.645 2]). By Theorem 8.1,

$$I_{2n+2} = (2\pi)^{2n} \frac{(n!)^2}{(2n+1)!} \qquad (n \in \mathbb{N}_0) \tag{8.27}$$

and thus $J_{2n+2} = \frac{2}{2n+2} I_{2n+2} = \pi^{2n} b_n$. This implies

$$\big(\arcsin(x)\big)^2 = \sum_{n=0}^{\infty} b_n x^{2n+2} = \pi^2 \sum_{n=0}^{\infty} J_{2n+2} \Big(\frac{x}{\pi}\Big)^{2n+2} \qquad (|x| \leq 1). \tag{8.28}$$

□

9 RELATIONS TO SCATTERING THEORY

In this section, the coefficient $\eta^{2n}(E)$ in Definition 7.2, which entered the asymptotics in Theorem 7.8, is given a scattering theoretic interpretation.

We fix some notation: Let H_{ac} and H'_{ac} be the absolutely continuous parts of H and H'. Let $\mathcal{H} := L_2(\mathbb{R}^d)$ and let $\mathcal{H}_{\mathrm{ac}} := 1(H_{\mathrm{ac}})\mathcal{H}$ be the absolutely continuous subspace of the operator H. Let (f_n) be an orthonormal basis of $\mathcal{H}$, such that

$$\mathcal{L} := \mathrm{lin}\{f_n;\ n \in \mathbb{N}\} \subseteq \mathcal{H} \tag{9.1}$$

is dense. We begin with a definition.

9.1 Definition. Let $\hat{\sigma} \subseteq \sigma(H)$ be a *core of the spectrum of* H in the sense of [Yaf92, Def. 1.3.8], i.e., a measurable set $\hat{\sigma} \subseteq \mathbb{R}$ that

(I) has full measure with respect to the projection-valued measure $A \mapsto 1_A(H)$ and

(II) has the property that for any other set $Z \subseteq \mathbb{R}$ of full measure with respect to $A \mapsto 1_A(H)$, the set $\hat{\sigma} \setminus Z$ has Lebesgue measure zero.

9.2 Remark. Note that $\sigma(T)$ itself need not be a core of the spectrum of a general self-adjoint operator T: There is an open dense set $G \subseteq [0,1]$ with $|G| < 1$, where $|G|$ denotes the Lebesgue measure of G. Taking $(Tf)(x) := 1_G(x)$ as a self-adjoint operator in $L_2(0,1)$, its spectrum is $\sigma(T) = \overline{G} = [0,1]$, but $\sigma(T) \setminus G$ does not have Lebesgue measure zero, even though G has full measure with respect to $A \mapsto 1_A(T)$.

Next we mention four statements from the literature that we will use in the sequel. The first one can be found in [Yaf92, §1.5].

9.3 Proposition. For a.e. $\lambda \in \hat{\sigma}$, there is a Hilbert space $\mathcal{H}_\lambda$ such that $\mathcal{H}_{\mathrm{ac}}$ is decomposed into a direct integral on which H acts as a multiplication by $\lambda \mapsto \lambda$; i.e., there is a unitary operator between

$$\mathcal{H}_{\mathrm{ac}} \text{ and } \int_{\hat{\sigma}}^{\oplus} \mathrm{d}\lambda\, \mathcal{H}_\lambda, \tag{9.2}$$

such that a vector $f \in \mathcal{H}_{\mathrm{ac}}$ corresponds to a vector-valued function $\lambda \mapsto f_\lambda \in \mathcal{H}_\lambda$ that is defined for a.e. $\lambda \in \hat{\sigma}$, and for $f \in D(H) \cap \mathcal{H}_{\mathrm{ac}}$, the vector Hf corresponds to $\lambda \mapsto (Hf)_\lambda = \lambda f_\lambda$. By extending the unitary mapping in (9.2) by zero to $\mathcal{H}$, every $f \in \mathcal{H}$ corresponds to a function $\lambda \mapsto f_\lambda \in \mathcal{H}_\lambda$.

If $f, g \in \mathcal{H}$, then for a.e. $\lambda \in \hat{\sigma}$, with a null set depending on f and g, one has

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle g, 1_{(-\infty,\lambda)}(H)f\rangle = \langle g_\lambda, f_\lambda\rangle_{\mathcal{H}_\lambda}. \tag{9.3}$$

9.4 Remark. In (9.2), one could also take a core of the absolutely continuous spectrum as the domain of integration. This is because for any such core $\hat{\sigma}_{\mathrm{ac}} \subseteq \sigma_{\mathrm{ac}}(H)$, the set $\hat{\sigma} \setminus \hat{\sigma}_{\mathrm{ac}}$ has Lebesgue measure zero, i.e., $\hat{\sigma}$ itself is a core of the absolutely continuous spectrum of H.

In the special case $V_0 = 0$, the direct integral in (9.2) can be made more explicit using the Fourier transformation; namely in that case

$$\mathcal{H} \leftrightarrow L_2\big((0,\infty); L_2(S_{d-1})\big) = L_2(0,\infty) \otimes L_2(S_{d-1}), \tag{9.4}$$

where S_{d-1} is the unit sphere in $\mathbb{R}^d$. See [Yaf10a, §1.2] for details; a similar computation is done in Appendix A.

The second statement is a part of [Yaf92, proof of Lemma 1.5.1].

9.5 Proposition. There is a null set $\mathcal{N}_0$ such that

$$\forall \lambda \in \hat{\sigma} \setminus \mathcal{N}_0 : \{f_\lambda;\ f \in \mathcal{L}\} \subseteq \mathcal{H}_\lambda \text{ is dense.} \tag{9.5}$$

The third statement we take from [BÈ67, Lemma 4.3, 4.4, and 4.5]; part (B) was already mentioned in Proposition 6.1.

9.6 Proposition. (A) For fixed $f \in \mathcal{H}$ there is a null set $\mathcal{N}_f$ such that the derivative

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\sqrt{V} 1_{(-\infty,\lambda)}(H) f \tag{9.6}$$

exists for all $\lambda \in \mathbb{R} \setminus \mathcal{N}_f$.

(B) There is a null set $\mathcal{N}_1$ such that the derivative

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\sqrt{V} 1_{(-\infty,\lambda)}(H)\sqrt{V} = A(\lambda) \tag{9.7}$$

exists in the sense of convergence in trace class for all $\lambda \in \mathbb{R} \setminus \mathcal{N}_1$.

(C) There is a null set $\mathcal{N}_1$ such that the limits

$$\lim_{\varepsilon \downarrow 0} \sqrt{V}(\lambda \pm i\varepsilon - H^{(\prime)})^{-1}\sqrt{V} \tag{9.8}$$

exist in operator norm for $\lambda \in \mathbb{R} \setminus \mathcal{N}_1$, and

$$\lim_{\varepsilon \downarrow 0} \sqrt{V}(\lambda - i\varepsilon - H)^{-1}\sqrt{V} - \lim_{\varepsilon \downarrow 0} \sqrt{V}(\lambda + i\varepsilon - H)^{-1}\sqrt{V} = 2\pi i A(\lambda), \tag{9.9}$$

$$\lim_{\varepsilon \downarrow 0} \sqrt{V}(\lambda - i\varepsilon - H')^{-1}\sqrt{V} - \lim_{\varepsilon \downarrow 0} \sqrt{V}(\lambda + i\varepsilon - H')^{-1}\sqrt{V} = 2\pi i B(\lambda). \tag{9.10}$$

Here, $\lim_{z \to \lambda \pm i0} f(z)$ denotes the limit $\lim_{\varepsilon \downarrow 0} f(\lambda \pm i\varepsilon)$. We also define the operator norm limit

$$\Phi_{\lambda \pm i0} := \lim_{\varepsilon \downarrow 0}\Big(I + \sqrt{V}(\lambda \pm i\varepsilon - H')^{-1}\sqrt{V}\Big). \tag{9.11}$$

The fourth and final statement we quote from the literature is from [BÈ67, §7 and formula (7.14)]

9.7 Proposition. Let S be the *scattering operator* of the pair H and H', which exists since the wave operators exist, and is a unitary operator on $\mathcal{H}_{\mathrm{ac}}$. Then the corresponding operator on $\mathcal{H}_\lambda$, the *scattering matrix* S_λ, exists for a.e. $\lambda \in \hat{\sigma}$. Moreover, for $f, g \in \mathcal{H}_{\mathrm{ac}}$ there is a null set $\mathcal{N}_{f,g}$ depending on f and g such that

$$\begin{aligned}\langle g_\lambda, (S_\lambda - I_\lambda) f_\lambda \rangle_{\mathcal{H}_\lambda} &= \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle g, 1_{(-\infty,\lambda)}(H)(S - I) f \rangle \\ &= -2\pi i \Big\langle \frac{\mathrm{d}}{\mathrm{d}\lambda} \sqrt{V} 1_{(-\infty,\lambda)}(H) g, \Phi_{\lambda + i0} \frac{\mathrm{d}}{\mathrm{d}\lambda} \sqrt{V} 1_{(-\infty,\lambda)}(H) f \Big\rangle \end{aligned} \tag{9.12}$$

holds for $\lambda \in \hat{\sigma} \setminus \mathcal{N}_{f,g}$. Here, I_λ stands for the identity on $\mathcal{H}_\lambda$.

Using Propositions 9.3 to 9.7, we are now able to prove the following lemma, which is at the core of our arguments relating $\eta^{2n}(E)$ to objects from scattering theory. The general idea of the proof is taken from [BW83, Lemma 6, p. 388], adopted to our more concrete setting.

9.8 Lemma. Define

$$\mathcal{L}_V := \mathcal{L} + \operatorname{lin}\{\sqrt{V} f_n;\ n \in \mathbb{N}\} = \operatorname{lin}\{f_n, \sqrt{V} f_n;\ n \in \mathbb{N}\}. \tag{9.13}$$

Then there is a null set $\mathcal{N}_2$ such that for $\lambda \in \hat{\sigma} \setminus \mathcal{N}_2$ the set

$$D(G_\lambda) := \{f_\lambda;\ f \in \mathcal{L}_V\} \subseteq \mathcal{H}_\lambda \tag{9.14}$$

is dense and there is an operator $G_\lambda : D(G_\lambda) \to \mathcal{H}$ such that

$$G_\lambda f_\lambda = \frac{\mathrm{d}}{\mathrm{d}\lambda} \sqrt{V} 1_{(-\infty,\lambda)}(H) f \qquad (f \in \mathcal{L}_V). \tag{9.15}$$

Moreover,

$$\langle g, G_\lambda f_\lambda \rangle = \langle (\sqrt{V} g)_\lambda, f_\lambda \rangle_{\mathcal{H}_\lambda} \qquad (f, g \in \mathcal{L}_V). \tag{9.16}$$

Proof. By Proposition 9.5, $\{f_\lambda;\ f \in \mathcal{L}\} \subseteq D(G_\lambda)$ is dense in $\mathcal{H}_\lambda$ for $\lambda \in \hat{\sigma} \setminus \mathcal{N}_0$. By Proposition 9.6, $\frac{\mathrm{d}}{\mathrm{d}\lambda} \sqrt{V} 1_{(-\infty,\lambda)}(H) f$ exists for $f \in \mathcal{H}$ outside of a null set depending on f. By countability and linearity, one can find a common null set $\mathcal{N} \supseteq \mathcal{N}_0$ such that $\frac{\mathrm{d}}{\mathrm{d}\lambda} \sqrt{V} 1_{(-\infty,\lambda)}(H) f$ exists for all $f \in \mathcal{L}_V$ and $\lambda \in \hat{\sigma} \setminus \mathcal{N}$. For $\lambda \in \hat{\sigma} \setminus \mathcal{N}$ and $f, g \in \mathcal{L}_V$, we can compute

$$\Big\langle g, \frac{\mathrm{d}}{\mathrm{d}\lambda} \sqrt{V} 1_{(-\infty,\lambda)}(H) f \Big\rangle = \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle g, \sqrt{V} 1_{(-\infty,\lambda)}(H) f \rangle = \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \sqrt{V} g, 1_{(-\infty,\lambda)}(H) f \rangle. \tag{9.17}$$

Looking at (9.3), we find a bigger null set $\mathcal{N}_2 \supseteq \mathcal{N}$ such that the right-hand side of (9.17) is equal to

$$\left\langle g, \frac{\mathrm{d}}{\mathrm{d}\lambda}\sqrt{V}1_{(-\infty,\lambda)}(H)f \right\rangle = \langle (\sqrt{V}g)_\lambda, f_\lambda \rangle_{\mathcal{H}_\lambda} \tag{9.18}$$

for every $f, g \in \mathcal{L}_V$ and $\lambda \in \hat{\sigma} \setminus \mathcal{N}_2$. Let $\lambda \in \hat{\sigma} \setminus \mathcal{N}_2$. For fixed $g \in \mathcal{L}_V$, the expression on the right-hand side of (9.18) only depends on f_λ, and therefore the expression on the left-hand side only depends on f_λ. This renders

$$\mathcal{L}_V \times D(G_\lambda) \ni (g, f_\lambda) \mapsto \left\langle g, \frac{\mathrm{d}}{\mathrm{d}\lambda}\sqrt{V}1_{(-\infty,\lambda)}(H)f \right\rangle \tag{9.19}$$

well-defined. Since $\mathcal{L}_V \subseteq \mathcal{H}$ is dense, this defines $G_\lambda : D(G_\lambda) \to \mathcal{H}$. □

We state an immediate consequence of (9.16).

9.9 Corollary. For $\lambda \in \hat{\sigma} \setminus \mathcal{N}_2$, the adjoint $G_\lambda^* : D(G_\lambda^*) \to \mathcal{H}_\lambda$ satisfies $\mathcal{L}_V \subseteq D(G_\lambda^*) \subseteq \mathcal{H}$ and

$$G_\lambda^* g = (\sqrt{V}g)_\lambda \qquad (g \in \mathcal{L}_V). \tag{9.20}$$

9.10 Corollary. Let $\lambda \in \hat{\sigma} \setminus \mathcal{N}_2$. Then $D(G_\lambda^*) = \mathcal{H}$ and $G_\lambda^{**}G_\lambda^* = A(\lambda)$.

Proof. The adjoint G_λ^* is densely defined. The biadjoint G_λ^{**} is an extension of G_λ, the operator $G_\lambda^{**}G_\lambda^*$ is positive self-adjoint and

$$D(G_\lambda^{**}G_\lambda^*) = \left\{ f \in D(G_\lambda^*);\ G_\lambda^* f \in D(G_\lambda^{**}) \right\} \tag{9.21}$$

is a core of G_λ^*, see [Wei80, Thm. 5.39]. Let $f \in \mathcal{L}$. Then $G_\lambda^* f = (\sqrt{V}f)_\lambda \in D(G_\lambda) \subseteq D(G_\lambda^{**})$. Thus $f \in D(G_\lambda^{**}G_\lambda^*)$, and

$$G_\lambda^{**}G_\lambda^* f = G_\lambda^{**}(\sqrt{V}f)_\lambda = G_\lambda(\sqrt{V}f)_\lambda = \frac{\mathrm{d}}{\mathrm{d}\lambda}\sqrt{V}1_{(-\infty,\lambda)}(H)\sqrt{V}f = A(\lambda)f. \tag{9.22}$$

The bounded linear operator $A(\lambda)$ acts on $\mathcal{L}$ as the closed densely defined operator $G_\lambda^{**}G_\lambda^*$ does. This implies $G_\lambda^{**}G_\lambda^* = A(\lambda)$. In particular, $D(G_\lambda^*) = \mathcal{H}$. □

9.11 Theorem. As in Proposition 9.7, let S_λ be the scattering matrix and $\Phi_{\lambda+i0}$ be given by (9.11) for $\lambda \in \hat{\sigma} \setminus \mathcal{N}$ with some null set $\mathcal{N}$. Then there is a larger null set $\mathcal{N}_3 \supseteq \mathcal{N}$ such that for $\lambda \in \hat{\sigma} \setminus \mathcal{N}_3$ the *transition matrix*

$$T_\lambda := S_\lambda - I_\lambda \tag{9.23}$$

satisfies

$$T_\lambda = -2\pi i G_\lambda^* \Phi_{\lambda+i0} G_\lambda^{**} \tag{9.24}$$

and is unitarily equivalent to

$$\tilde{T}_\lambda := -2\pi i\sqrt{A(\lambda)}\Phi_{\lambda+i0}\sqrt{A(\lambda)}, \tag{9.25}$$

which is an operator on $\mathcal{H}$. This operator can be viewed as the pullback of T_λ into $\mathcal{H}$, cf. [BW83, Remark after Lemma 12, p. 394].

Proof. From Proposition 9.7, we deduce that there is a null set $\mathcal{N} \supseteq \mathcal{N}_2$ such that

$$\langle g_\lambda, (S_\lambda - I_\lambda) f_\lambda\rangle_{\mathcal{H}_\lambda} = -2\pi i\langle G_\lambda g_\lambda, \Phi_{\lambda+i0}\, G_\lambda f_\lambda\rangle = -2\pi i\langle g_\lambda, G_\lambda^* \Phi_{\lambda+i0}\, G_\lambda^{**} f_\lambda\rangle_{\mathcal{H}_\lambda} \tag{9.26}$$

for all $f, g \in \mathcal{L}_V$ and $\lambda \in \hat{\sigma} \setminus \mathcal{N}$. Since $\{g_\lambda;\, g \in \mathcal{L}\} \subseteq \mathcal{H}_\lambda$ is dense for such λ, we conclude

$$(S_\lambda - I_\lambda) f_\lambda = -2\pi i G_\lambda^* \Phi_{\lambda+i0}\, G_\lambda^{**} f_\lambda, \tag{9.27}$$

which implies (9.24). To see (9.25), we take the polar decomposition $G_\lambda^* = U_\lambda |G_\lambda^*| = U_\lambda\sqrt{A(\lambda)}$. Then $U_\lambda : \operatorname{ran}(\sqrt{A(\lambda)}) \to \operatorname{ran}(G_\lambda^*)$ is an isometry and

$$T_\lambda = -2\pi i U_\lambda \sqrt{A(\lambda)}\Phi_{\lambda+i0}\sqrt{A(\lambda)}U_\lambda^*. \tag{9.28}$$

□

Using Theorem 9.11, we can prove the following identity relating the operators $A(\lambda)$ and $B(\lambda)$ from Proposition 6.1 to the transition matrix.

9.12 Corollary. Let $\lambda \in \hat{\sigma} \setminus \mathcal{N}_3$. Then

$$\tilde{T}_\lambda^* \tilde{T}_\lambda = (2\pi)^2\sqrt{A(\lambda)}B(\lambda)\sqrt{A(\lambda)}. \tag{9.29}$$

In particular,

$$\|T_\lambda\|_{2n}^{2n} = (2\pi)^{2n}\operatorname{tr}\big(A(\lambda)B(\lambda)\big)^n = (2\pi)^{2n}\eta^{2n}(\lambda) \tag{9.30}$$

for $n \in \mathbb{N}$, where $\|T_\lambda\|_{2n} := \sqrt[2n]{\operatorname{tr}|T_\lambda|^{2n}}$ is a Schatten norm of T_λ. By setting $T_\lambda := 0$ whenever $A(\lambda) = 0$ or $B(\lambda) = 0$, (9.30) is true for all $\lambda \in \mathbb{R} \setminus \mathcal{N}_3$.

Proof. The definition (9.25) of $\tilde{T}_\lambda$ implies

$$\tilde{T}_\lambda^* \tilde{T}_\lambda = (2\pi)^2\sqrt{A(\lambda)}\Phi_{\lambda+i0}^* A(\lambda)\Phi_{\lambda+i0}\sqrt{A(\lambda)}, \tag{9.31}$$

where $\Phi^*_{\lambda+i0} = \Phi_{\lambda-i0}$, as can be seen from (9.11). For $z \in \mathbb{C} \setminus \mathbb{R}$, we abbreviate the resolvents with $R^{(\prime)}(z) := (z - H^{(\prime)})^{-1}$. Then (9.9) implies

$$\begin{aligned}\Phi^*_{\lambda+i0}A(\lambda)\Phi_{\lambda+i0} &= \frac{1}{2\pi i}\lim_{\varepsilon\downarrow 0}\Big(\big(I + \sqrt{V}R'(\lambda - i\varepsilon)\sqrt{V}\big) \\ &\qquad \times \sqrt{V}\big(R(\lambda - i\varepsilon) - R(\lambda + i\varepsilon)\big)\sqrt{V}\big(I + \sqrt{V}R'(\lambda + i\varepsilon)\sqrt{V}\big)\Big) \\ &= \frac{1}{2\pi i}\lim_{\varepsilon\downarrow 0}\sqrt{V}\big(I + R'(\lambda - i\varepsilon)V\big)\big(R(\lambda - i\varepsilon) - R(\lambda + i\varepsilon)\big)\big(I + VR'(\lambda + i\varepsilon)\big)\sqrt{V}.\end{aligned} \tag{9.32}$$

For fixed $\varepsilon > 0$, define $R^{(\prime)}_{\pm} := R^{(\prime)}(\lambda \pm i\varepsilon)$. Then the middle part of (9.32) is

$$\begin{aligned}&(I + R'_- V)(R_- - R_+)(I + VR'_+) \\ &\quad = R_- - R_+ + R_- VR'_+ - R_+ VR'_+ + R'_- VR_- - R'_- VR_+ + R'_- VR_- VR'_+ - R'_- VR_+ VR'_+ \\ &\quad = R'_- - R'_+,\end{aligned} \tag{9.33}$$

where we used the second resolvent identity $R'_\pm - R_\pm = R'_\pm VR_\pm = R_\pm VR'_\pm$ several times. Together with (9.10), this implies

$$\Phi^*_{\lambda+i0}A(\lambda)\Phi_{\lambda+i0} = \frac{1}{2\pi i}\lim_{\varepsilon\downarrow 0}\sqrt{V}\big(R'(\lambda - i\varepsilon) - R'(\lambda + i\varepsilon)\big)\sqrt{V} = B(\lambda). \tag{9.34}$$

From this and (9.31), (9.29) follows. The unitary equivalence in Theorem 9.11 then implies (9.30). □

10 THE CATASTROPHE

The bound we set out to prove was proven in § 7. In §§ 8 and 9, we examined the right-hand side of that bound. What remains to do is to gather the individual statements into a final one and discuss this result. This we do in the this final section.

10.1 Theorem (Orthogonality Catastrophe)**.** Assume conditions (v_0) and (v) from page 1. Let $(L_m)_{m\in\mathbb{N}}$ be a sequence in $(0,\infty)$ with $L_m \to \infty$. Then there exists a subsequence $(L_{m_k})_{k\in\mathbb{N}}$, a null set $\mathcal{N} \subseteq \mathbb{R}$, and a function $\gamma : \mathbb{R} \setminus \mathcal{N} \to [0,\infty)$ such that for $E \in \mathbb{R}\setminus\mathcal{N}$ the ground-state overlap (1.5) obeys

$$|\mathcal{S}_{L_{m_k}}(E)|^2 \le \exp\big(-\gamma(E)\ln L_{m_k} + o(\ln L_{m_k})\big) = L_{m_k}^{-\gamma(E)+o(1)} \tag{10.1}$$

as $k\to\infty$. The decay exponent γ is given by

$$\gamma(E) := \frac{1}{\pi^2}\big\|\arcsin|T_E/2|\big\|_{\mathrm{HS}}^2, \tag{10.2}$$

where $T_E = S_E - I_E$ is the transition matrix for the energy E defined in § 9.

Proof. Let $0 < a < 1$. Let $M \in \mathbb{N}$. Let $\mathcal{N}$ be the union of the null sets from Lemma 2.1 and Theorem 9.11. Let $E \in \mathbb{R}\setminus\mathcal{N}$. We start from Lemma 1.2 and Lemma 2.1, which imply

$$\begin{aligned} -\ln|\mathcal{S}_{L_{m_k}}(E)| &\ge \frac{1}{2}\sum_{n=1}^{M}\frac{1}{n}\operatorname{tr}\Big(\mathrm{P}_{L_{m_k}}^{N_{L_{m_k}}(E)}\big(I-\Pi_{L_{m_k}}^{N_{L_{m_k}}(E)}\big)\Big)^n \\ &= \frac{1}{2}\sum_{n=1}^{M}\frac{1}{n}\operatorname{tr}\Big(1_{(-\infty,E]}(H_{L_{m_k}})1_{(E,\infty)}(H'_{L_{m_k}})\Big)^n + o(\ln L_{m_k}) \end{aligned} \tag{10.3}$$

as $k \to \infty$, for a subsequence $(L_{m_k})_{k\in\mathbb{N}}$, and with an M-dependent error term $o(\ln L_{m_k})$. Looking at Remark 6.8 and Theorem 7.8, this is

$$\ge \frac{a}{2}\sum_{n=1}^{M}\frac{I_{2n}}{n}\operatorname{tr}\big(A(E)B(E)\big)^n\ln L_{m_k} + o(\ln L_{m_k})$$

as $k\to\infty$, with an M and a-dependent error term $o(\ln L_{m_k})$. Using Corollary 9.12, this is

$$\begin{aligned} &= \frac{a}{2}\sum_{n=1}^{M}\frac{I_{2n}}{n}(2\pi)^{-2n}\operatorname{tr}(|T_E|^{2n})\ln L_{m_k} + o(\ln L_{m_k}) \\ &= \frac{a}{2}\operatorname{tr}\sum_{n=1}^{M}J_{2n}|T_E/(2\pi)|^{2n}\ln L_{m_k} + o(\ln L_{m_k}). \end{aligned} \tag{10.4}$$

Proposition 8.5 yields $\sum_{n=1}^{M} J_{2n}|T_E/(2\pi)|^{2n} \to \pi^{-2}(\arcsin|T_E/2|)^2$ in operator norm as $M \to \infty$, and therefore

$$\operatorname{tr}\sum_{n=1}^{M} J_{2n}|T_E/(2\pi)|^{2n} \to \pi^{-2}\big\|\arcsin|T_E/2|\big\|_{\mathrm{HS}}^2 \qquad (M \to \infty) \tag{10.5}$$

monotonically. We find $M \in \mathbb{N}$ such that

$$\operatorname{tr}\sum_{n=1}^{M} J_{2n}|T_E/(2\pi)|^{2n} \geq a\pi^{-2}\big\|\arcsin|T_E/2|\big\|_{\mathrm{HS}}^2. \tag{10.6}$$

Therefore, continuing from (10.4),

$$\begin{aligned} -\ln|\mathcal{S}_{L_{m_k}}(E)| &\geq \frac{a^2}{2\pi^2}\big\|\arcsin|T_E/2|\big\|_{\mathrm{HS}}^2 \ln L_{m_k} + \mathrm{o}(\ln L_{m_k}) \\ &= \frac{a^2}{2}\gamma(E)\ln L_{m_k} + \mathrm{o}(\ln L_{m_k}) \end{aligned} \tag{10.7}$$

as $k \to \infty$, which implies

$$-\frac{\ln|\mathcal{S}_{L_{m_k}}(E)|}{\ln L_{m_k}} \geq \frac{a^2}{2}\gamma(E) + \mathrm{o}(1) \tag{10.8}$$

as $k \to \infty$, and therefore

$$\limsup_{k\to\infty} \frac{\ln|\mathcal{S}_{L_{m_k}}(E)|}{\ln L_{m_k}} \leq -\frac{1}{2}\gamma(E). \tag{10.9}$$

Let $\varepsilon > 0$. By the definition of the limit superior there is $k_0 \in \mathbb{N}$ such that

$$\frac{\ln|\mathcal{S}_{L_{m_k}}(E)|}{\ln L_{m_k}} \leq -\frac{1}{2}\gamma(E) + \varepsilon \tag{10.10}$$

for $k \geq k_0$, which implies (10.1). □

10.2 Remark. In [GKM14], a similar statement to Theorem 10.1 was proven, but with the smaller exponent

$$\eta^2(E) = \operatorname{tr}\big(A(E)B(E)\big) = \frac{1}{\pi^2}\big\|T_E/2\big\|_{\mathrm{HS}}^2. \tag{10.11}$$

In the special case he considers, this exponent is exactly the one that Anderson initially gave as a bound in [And67a], except for a factor $\frac{1}{2}$ which seems to be an oversight on Anderson's part. Anderson considers the case $d = 3$ with a spherically symmetric perturbation, and in that case $\eta^2(E)$ can be written as

$$\eta^2(E) = \frac{1}{\pi^2}\sum_{\ell=0}^{\infty}(2\ell+1)\big(\sin\delta_\ell(E)\big)^2, \tag{10.12}$$

with the scattering phases $(\delta_\ell(E))_{\ell\in\mathbb{N}_0}$. Later that same year, Anderson suggested a larger exponent for the exact asymptotics, mentioning that »[i]t is interesting that the main difference from the previous result is to replace $\sin^2\delta$ by δ^2« [And67b, p. 164].

Comparing the smaller exponent $\eta^2(E)$ in (10.11) to the larger exponent $\gamma(E)$ in (10.2), the only difference is the arcsin function in the definition of $\gamma(E)$ where $\eta^2(E)$ has the identity function. This is somewhat analogous to the difference between [And67a] and [And67b]. It should be noted that the particle number N in [And67b] refers to the number of s-orbital states below the Fermi energy, see [Ham71], and therefore $N \sim L$ in that publication – in contrast to [And67a], where $N \sim L^3$. This accounts for the absence of the dimension factor $\frac{1}{3}$ in [And67b].

Since (10.1) is also just a bound instead of an exact asymptotic, the exact decay of the overlap $\mathcal{S}_L(E)$ might be faster still. We conjecture that this is not the case, i.e., that

$$|\mathcal{S}_L(E)|^2 = L^{-\gamma(E)+o(1)} \qquad (L\to\infty) \tag{10.13}$$

for a.e. $E\in\mathbb{R}$. For $d = 1$, some headway towards (10.13) has been made by [KOS13] using explicit computations. For $V_0 = 0$ and a slightly different class of perturbations V, the statement there can be rendered as

$$\operatorname{tr}\Big(\mathrm{P}_L^{N_L(E)}\big(I - \Pi_L^{N_L(E)}\big)\Big) = \eta^2(E)\ln L + o(1) \qquad (L\to\infty); \tag{10.14}$$

thus the exact asymptotics of the first term of (1.14) has been treated in that case. Since Theorem 7.8 for $n = 1$ yields

$$\operatorname{tr}\Big(\mathrm{P}_L^{N_L(E)}\big(I - \Pi_L^{N_L(E)}\big)\Big) \geq \eta^2(E)\ln L + o(\ln L) \tag{10.15}$$

as $L\to\infty$ with $L\in\{L_{m_k};\, k\in\mathbb{N}\}$, we know that for $d = 1$ this bound on the $n = 1$ term is asymptotically exact in the setting considered in [KOS13]. (For $d = 1$, it might be possible to prove the equivalent of (10.14) for any $n\in\mathbb{N}$ using the methods of this thesis: in the $d = 1$ case the subsequences in L are not necessary as per Remark 2.2, and the error introduced by smoothing could be controlled as per Remark 4.2.) It is therefore reasonable to expect the equivalent of the bound (10.15) to be asymptotically exact for any $n\in\mathbb{N}$, and for V_0 and V satisfying (v_0) and (v). However, this alone would still not imply (10.13), since the bounds on the individual errors we proved in this thesis are not summable in $n\in\mathbb{N}$. The methods we employed seem unlikely to yield summable bounds even when further refined.

Another approach would be to establish upper bounds on the terms of (1.14). But there the errors would need to be summable if we want to deduce something about the overlap, since truncating the series like we did in Theorem 10.1 always yields a lower bound on $-\ln|\mathcal{S}_L|$. In the case considered there, [KOS13] give a nonoptimal lower bound on the overlap of the form $|\mathcal{S}_L(E)| \geq CL^{-\varepsilon}$. The catastrophe therefore is not qualitatively worse than L to some negative power.

Yet another problem, and probably a much harder one, is to include interactions in the model. Judging from the physics literature, the catastrophe should then still occur, and probably with the same behavior in first order. There seem to be no mathematical results in that direction.

APPENDIX

In the main matter of the text, we proved an upper bound on the overlap $|S_L|$ under the assumptions given in Theorem 10.1. In Section A of this appendix, we will give a result regarding the strict positivity of the decay exponent $\gamma(E)$; this is of interest since Theorem 10.1 is a trivial statement whenever $\gamma(E) = 0$. In Section B, we state and prove some additional propositions mentioned but not needed in the main matter of the text. Finally, and as a convenience for the reader, we give a proof in Section C of the geometric resolvent inequality as we used it in § 5.

A POSITIVITY OF THE EXPONENT

In this additional section, we give conditions for the decay exponent $\gamma(E)$ in (10.2) to be strictly positive. Intuitively, one might hope that

$$\gamma(E) > 0 \Leftrightarrow E \in \sigma_{\mathrm{ac}}(H), \tag{A.1}$$

at least for a.e. $E \in \mathbb{R}$. It is not clear if this in fact holds for the general type of Schrödinger operators $H = -\Delta + V_0$ we consider. However, (A.1) is true for almost all $E > 0$ in the case $V_0 = 0$, which we treat below. At the end of the section, we comment upon the case $V_0 \neq 0$.

In the whole section, we assume that V is one fixed representative of a function satisfying (V), with the property that $0 \leq V(x) < \infty$ for all $x \in \mathbb{R}^d$ and $V \neq 0$ in the a.e.-sense.

A.1 Theorem. Let $V_0 = 0$. Let $E > 0$. Then the operator $A(E)$ from (6.2) has the integral kernel

$$A(E; x, y) = \frac{E^{d/2-1}}{2(2\pi)^d} \sqrt{V(x)} \sqrt{V(y)} \int_{S_{d-1}} \mathrm{d}S(\xi)\, e^{i\sqrt{E}\xi\cdot(x-y)} \qquad (x, y \in \mathbb{R}^d). \tag{A.2}$$

(The surface integral can be evaluated, see Theorem B.4. However, we will not need its value.)

Proof. For $f \in L_1(\mathbb{R}^d)$, denote the Fourier transform by

$$\mathcal{F}(f)(\xi) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{d}x \, e^{-i\xi\cdot x} f(x). \tag{A.3}$$

Let $\varepsilon > 0$. Let $f \in L_2(\mathbb{R}^d)$ and $x \in \mathbb{R}^d$. Then

$$\begin{aligned}
\Big(\sqrt{V}1_{(E-\varepsilon,E+\varepsilon)}(-\Delta)\sqrt{V}f\Big)(x) &= \frac{\sqrt{V(x)}}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{d}\xi \, 1_{(E-\varepsilon,E+\varepsilon)}(|\xi|^2) e^{i\xi\cdot x} \mathcal{F}(\sqrt{V}f)(\xi) \\
&= \frac{\sqrt{V(x)}}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{d}\xi \int_{\mathbb{R}^d} \mathrm{d}y \, 1_{(E-\varepsilon,E+\varepsilon)}(|\xi|^2) e^{i\xi\cdot(x-y)} \sqrt{V(y)} f(y) \\
&= \frac{\sqrt{V(x)}}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{d}y \, \sqrt{V(y)} f(y) \int_0^\infty \mathrm{d}r \, r^{d-1} \int_{S_{d-1}} \mathrm{d}S(\xi) \, 1_{(E-\varepsilon,E+\varepsilon)}(r^2) e^{ir\xi\cdot(x-y)} \\
&= \frac{\sqrt{V(x)}}{2(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{d}y \, \sqrt{V(y)} f(y) \int_{E-\varepsilon}^{E+\varepsilon} \mathrm{d}r \, r^{d/2-1} \int_{S_{d-1}} \mathrm{d}S(\xi) \, e^{i\sqrt{r}\xi\cdot(x-y)},
\end{aligned} \tag{A.4}$$

and therefore

$$\begin{aligned}
\Big(\frac{1}{2\varepsilon}\sqrt{V}1_{(E-\varepsilon,E+\varepsilon)}(-\Delta)\sqrt{V}f\Big)(x) &\xrightarrow{\varepsilon\to 0} \\
&\frac{\sqrt{V(x)}}{2(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{d}y \, \sqrt{V(y)} f(y) E^{d/2-1} \int_{S_{d-1}} \mathrm{d}S(\xi) \, e^{i\sqrt{E}\xi\cdot(x-y)},
\end{aligned} \tag{A.5}$$

since the integrand in (A.4) is continuous in r. This implies (A.2). □

A.2 Corollary. Let $d \geq 2$. Let $V_0 = 0$. Then for any $E > 0$ the operator $A(E)$ from (6.2) has infinite rank.

Proof. We first show that the set of functions

$$\big\{\mathbb{R}^d \ni x \mapsto \sqrt{V(x)} e^{i\xi\cdot x}; \; \xi \in \mathbb{R}^d\big\} \tag{A.6}$$

is linearly independent in the sense of equality almost everywhere. For this, notice that $\{\mathbb{C} \ni z \mapsto e^{isz}; \, s \in \mathbb{R}\}$ is linearly independent, since for $z = -ix$, these functions have different asymptotic behavior for $x \to \infty$. Given a finite nonempty set $M \subseteq \mathbb{R}$ and $c_s \neq 0$ for $s \in M$, the analytic function $\mathbb{C} \ni z \mapsto \sum_{s\in M} c_s e^{isz}$ is therefore not identically zero, and thus $\mathbb{R} \ni x \mapsto \sum_{s\in M} c_s e^{isx}$ is zero only on a discrete subset of $\mathbb{R}$.

Given another finite nonempty set $M \subseteq \mathbb{R}^d$ and $c_\xi \neq 0$ for $\xi \in M$, define $F\colon \mathbb{R}^d \to \mathbb{C}$ via $F(x) := \sum_{\xi \in M} c_\xi e^{i\xi\cdot x}$. We show that $F^{-1}(\{0\}) \subseteq \mathbb{R}^d$ is a null set. Since F is continuous, it is measurable, and its measure is

$$\int_{\mathbb{R}^d} \mathrm{d}x\, 1_{F^{-1}(\{0\})}(x) = \int_{S_{d-1}} \mathrm{d}S(\eta) \int_0^\infty \mathrm{d}r\, r^{d-1} 1_{\{0\}}\big(F(r\eta)\big) = 0, \tag{A.7}$$

where the r-integral is zero, since for $\eta \in S_{d-1}$ fixed the function $r \mapsto F(r\eta) = \sum_{\xi \in M} c_\xi e^{ir\xi\cdot\eta}$ is zero only on a discrete subset of $\mathbb{R}$, as shown above. To show that the set (A.6) is linearly independent, it suffices to show that

$$\Big\{x \in \mathbb{R}^d;\ \sqrt{V(x)}F(x) \neq 0\Big\} = \Big\{x \in \mathbb{R}^d;\ V(x) \neq 0\Big\} \cap \Big\{x \in \mathbb{R}^d;\ F(x) \neq 0\Big\} \tag{A.8}$$

has positive measure. This is the case, since the first set in the intersection has positive measure and the second set is the complement of the null set $F^{-1}(\{0\})$.

Now, let $f \in \ker A(E)$. Then

$$0 = \langle f, A(E)f\rangle = \frac{E^{d/2-1}}{2(2\pi)^d} \int_{S_{d-1}} \mathrm{d}S(\xi) \Big| \int_{\mathbb{R}^d} \mathrm{d}x \sqrt{V(x)} e^{i\sqrt{E}\xi\cdot x} f(x)\Big|^2, \tag{A.9}$$

and therefore

$$\int_{\mathbb{R}^d} \mathrm{d}x \sqrt{V(x)} e^{i\sqrt{E}\xi\cdot x} f(x) = 0 \tag{A.10}$$

for a.e. $\xi \in S_{d-1}$. Since the left-hand side of (A.10) is continuous in ξ, the orthogonality in (A.10) holds in fact for all $\xi \in S_{d-1}$. Since $f \in \ker A(E)$ was arbitrary, we conclude that

$$\Big\{\mathbb{R}^d \ni x \mapsto \sqrt{V(x)} e^{i\sqrt{E}\xi\cdot x};\ \xi \in S_{d-1}\Big\} \subseteq (\ker A(E))^\perp. \tag{A.11}$$

Since S_{d-1} is an infinite set for $d \geq 2$, the set of functions on the left-hand side is infinite and linearly independent, and thus $\dim(\ker A(E))^\perp = \infty$. Since the coimage $(\ker A(E))^\perp$ of the linear map $A(E)$ is isomorphic to $\operatorname{ran} A(E)$ (the restriction $A(E)\big|_{(\ker A(E))^\perp}\colon (\ker A(E))^\perp \to \operatorname{ran} A(E)$ being bijective), this shows $\dim \operatorname{ran} A(E) = \infty$. □

A.3 Remark. (A) The second part of the argument in Corollary A.2 can be made in a more abstract way. A preliminary form would be the following: Given an inner product space $\mathcal{H}$, let $\mathcal{M} \subseteq \mathcal{H}$ be a linearly independent countable set with the property that the series

$$Kf := \sum_{\varphi \in \mathcal{M}} \langle \varphi, f\rangle \varphi \tag{A.12}$$

converges for all $f \in \mathcal{H}$ and defines a linear operator $K\colon \mathcal{H} \to \mathcal{H}$. Then $\dim \operatorname{ran} K = \#\mathcal{M}$.

Still more abstract formulations could be devised using Bochner-integrable functions on a measure space. The argument in Corollary A.2 can be seen as the application of such an abstract result. We remark upon this since this can be a useful way to determine the rank of an integral operator.

(B) For background potentials V_0 with suitable decay, a generalization of Corollary A.2 that uses generalized eigenfunctions due to Ikebe-Povzner (see [Sim82, §C5] and references therein) in place of $e^{i\sqrt{E}\xi\cdot x}$ might hold.

The infinite rank of $A(E)$ implies the positivity of $\gamma(E)$.[2]

A.4 Theorem. Let $d \geq 2$, let $E > 0$ and let S_E be the scattering matrix corresponding to the pair $H = -\Delta$ and $H' = -\Delta + V$. Then the transition matrix $T_E = S_E - I_E$ has infinite rank for a.e. $E > 0$. In particular, it is nonzero, and therefore the decay exponent $\gamma(E) = \pi^{-2}\left\|\arcsin|T_E/2|\right\|_{\mathrm{HS}}^2$ from (10.2) is strictly positive in the case $V_0 = 0$ for a.e. $E > 0$.

Proof. By Theorem 9.11, it suffices to show that $\tilde{T}_E = -2\pi i\sqrt{A(E)}\Phi_{E+i0}\sqrt{A(E)}$ has infinite rank, with $\Phi_{E\pm i0} = \lim_{\varepsilon\downarrow 0}\big(I + \sqrt{V}(E \pm i\varepsilon - H')^{-1}\sqrt{V}\big)$. We show that its imaginary part $\operatorname{Im}\tilde{T}_E = \frac{1}{2i}(\tilde{T}_E - \tilde{T}_E^*)$ has infinite rank. For brevity, set $R := \lim_{z\to E+i0}\sqrt{V}(z - H')^{-1}\sqrt{V}$. Recall that by the limiting absorption principle, this limit exists in operator norm for a.e. $E > 0$. In particular, R is compact. Then

$$\begin{aligned}\operatorname{Im}\tilde{T}_E &= \frac{1}{2i}\Big(-2\pi i\sqrt{A(E)}\Phi_{E+i0}\sqrt{A(E)} - 2\pi i\sqrt{A(E)}\Phi_{E-i0}\sqrt{A(E)}\Big)\\ &= -2\pi\sqrt{A(E)}(I + \operatorname{Re}R)\sqrt{A(E)}.\end{aligned} \tag{A.13}$$

Since $\operatorname{Re}R$ is compact, we can write it as $\operatorname{Re}R = R_1 + R_2$, where $\|R_1\| < 1/2$ and R_2 has finite rank. Thus

$$-\frac{1}{2\pi}\operatorname{Im}\tilde{T}_E = \sqrt{A(E)}(I + R_1)\sqrt{A(E)} + \tilde{A}, \tag{A.14}$$

where $\tilde{A}$ is a finite rank operator. Now, since $I + R_1 \geq I - \frac{1}{2}I = \frac{1}{2}I$, we get

$$\sqrt{A(E)}(I + R_1)\sqrt{A(E)} \geq \tfrac{1}{2}A(E). \tag{A.15}$$

By Corollary A.2, this operator has infinite rank. $\square$

2 The argument in Theorem A.4 was communicated to me by Dr. Alexander Pushnitski, for which I am very thankful.

A.5 Remarks. (A) Theorem A.4 shows positivity of $\gamma(E)$ in the case $V_0 = 0$ and $d \geq 2$. The argument of Theorem A.4 does not work for $d = 1$, since in that case $A(E)$ has finite rank – its rank being not more than points on the sphere $S_0 = \{-1, 1\}$ in $\mathbb{R}$. However, we expect that using a direct computation it is nonetheless possible to treat the $d = 1$ case as well.

If the background potential V_0 is present, the situation is more complicated and we know of no argument that yields (A.1). In fact, for the most general case of two self-adjoint operators differing by a perturbation, (A.1) is not necessarily true for all energies: Let T be a self-adjoint operator with spectral measure ρ (in the sense of [Sim82, §C5]; see also the discussion in [Yaf92, §1.3] of elements of maximal spectral type). Then the density of the absolutely continuous part of ρ need not be strictly positive almost everywhere on $\sigma_{\mathrm{ac}}(T)$. This fact gives rise to the concept of the core of the spectrum, see Definition 9.1, and see Remark 9.2 for an example of such a T. The absolutely continuous part of ρ corresponds to the trace of the operator function $E \mapsto A(E)$ from Proposition 6.1. For general self-adjoint operators, one can therefore not expect a statement analogous to (A.1) to hold for a.e. $E \in \mathbb{R}$. The situation for Schrödinger operators might be different; in many cases, γ could possibly even be a continuous function. We don't know of any results in that direction.

(B) Looking at the definition of $\gamma(E)$ in (10.2) and the definition $T_E = S_E - I_E$ of the transition matrix, the question of strict positivity of $\gamma(E)$ is equivalent to asking whether $S_E = I_E$, i.e., whether S_E has any eigenvalue different from one. A series of papers by Pushnitski (see [Pus08], [Pus10], and references therein) gives another equivalent statement: The operator $D(E) := 1_{(-\infty,E)}(H) - 1_{(-\infty,E)}(H')$ is compact if and only if $S_E = I_E$. This result, however, seems more useful for extracting information about the spectrum of $D(E)$ from information about S_E than the other way around.

Since the scattering matrix S_E has some relation to the spectral shift function ξ of H and H', one could also ask for conditions when ξ is nonzero. Since V is not trace class, ξ is not integrable on all of $\mathbb{R}$, so the support of ξ is unbounded. However, we know of no concrete condition for some $E \in \mathbb{R}$ to be in spt ξ.

(C) The question of strict positivity of γ has some relation to the *unique continuation property* (UCP) of H as defined in [Sim82, §C9; see also the *open question* on page 510]: Every distributional solution u of $Hu = 0$ in an open connected set Ω with the property that u vanishes near some $x_0 \in \Omega$ is identically zero. This is the case for instance if V_0^2 is locally $-\Delta$-form bounded, in particular if V_0^2 is in $K_{\mathrm{loc}}(\mathbb{R}^d)$ (see [Sim82, Theorem C.9.3] and the references therein). It can be shown that if H satisfies the UCP, the operator $A(E)$ is nonzero on a dense subset of $\sigma_{\mathrm{ac}}(H)$. This does not imply strict positivity of $\gamma(E)$ though, since the operator Φ_{E+i0} in Theorem 9.11

(or equivalently $B(E)$ in Corollary 9.12) might map into the null space of $A(E)$. It is, however, possible to proof that $\{E \in \sigma_{\mathrm{ac}}(H);\ \gamma(E) > 0\}$ is not a null set if the perturbation V is sufficiently small.

B MISCELLANEOUS PROPOSITIONS

In this additional section, some additional statements mentioned in the main matter of the text are proven. In the whole section, let H and H' be as defined in § 1.

We begin with two statements regarding trace class properties of combinations of functions of the infinite-volume operators.

B.1 Lemma. Let $f \in C_c^\infty(\mathbb{R})$. Then $f(H') - f(H)$ is trace class.

Proof. Let T and T' be self-adjoint operators on a Hilbert space $\mathcal{H}$ with the property that $T' - T$ is trace class. Then $h(T') - h(T)$ is trace class for every $h \in C_c^\infty(\mathbb{R})$ by an argument involving the spectral shift function of T' and T [Yaf92, Thm. 8.3.3], see also [HM10, Sec. 5]. Moreover, $e^{-tH'} - e^{-tH}$ is trace class for every $t > 0$ [Hun+06, Remark after Thm. 1]. Set $T := e^{-H}$ and $T' := e^{-H'}$ as well as

$$h(x) := \begin{cases} f\big(-\ln(x)\big) & \text{if } x > 0, \\ 0 & \text{if } x \leq 0. \end{cases} \tag{B.1}$$

Then $T' - T$ is trace class, $h \in C_c^\infty(\mathbb{R})$, and $h(T^{(\prime)}) = f(H^{(\prime)})$. This implies that $h(T') - h(T) = f(H') - f(H)$ is trace class, proving the assertion. □

B.2 Corollary. Let $f \in C_c^\infty(\mathbb{R})$ and $g, g_1, g_2 \in L_\infty(\mathbb{R})$ with $\operatorname{spt} f \cap \operatorname{spt} g = \varnothing$ and $\operatorname{spt} g_1 \subseteq [c_1, E - \varepsilon]$, $\operatorname{spt} g_2 \subseteq [E + \varepsilon, c_2]$ for some $c_1 < E < c_2$ and $\varepsilon > 0$. Then the operators $f(H)g(H')$, $g(H)f(H')$, and $g_1(H)g_2(H')$ are trace class.

Proof. The first assertion follows from $f(H)g(H') = -\big(f(H') - f(H)\big)g(H')$ and Lemma B.1. The second assertion follows in the same way. For the third assertion, one finds $f_1, f_2 \in C_c^\infty(\mathbb{R})$ satisfying $\operatorname{spt} f_1 \subseteq [c_1, E)$ and $\operatorname{spt} f_2 \subseteq (E, c_1]$, as well as $g_1 \leq f_1$ and $g_2 \leq f_2$. Then $f_1(H)f_2(H')$ is trace class by Lemma B.1, and Lemma 2.3 implies the third assertion. □

Lemma B.1 allows us to prove that the integrated densities of state of H and H' are the same if they exist at all, which was mentioned in Remark 1.1.

B.3 Lemma. For $\varepsilon > 0$ and $f \in C_c^\infty(\mathbb{R})$,

$$\lim_{L\to\infty} \frac{1}{L^\varepsilon} \operatorname{tr}\big(1_{\Omega_L} f(H) - 1_{\Omega_L} f(H')\big) = 0. \tag{B.2}$$

Moreover, there is a set $\mathcal{N} \subseteq \mathbb{R}$ of measure zero, such that if $E \in \mathbb{R} \setminus \mathcal{N}$ and if either the integrated density of states of H or of H', given by

$$\rho^{(\prime)}(E) := \lim_{L\to\infty} \frac{1}{L^d |\Omega_1|} \operatorname{tr}\big(1_{\Omega_L} 1_{(-\infty,E)}(H^{(\prime)})\big), \tag{B.3}$$

exists, then the other exists and

$$\rho(E) = \rho'(E) = \lim_{L\to\infty} \frac{N_L(E)}{L^d\,|\Omega_1|}. \tag{B.4}$$

Proof. The statement in (B.2) is an immediate consequence of Lemma B.1. If it exists, the integrated density of states is the distribution function of the density of states measure, which is represented by the functional

$$F^{(\prime)}(f) := \lim_{L\to\infty} \frac{1}{L^d|\Omega_1|} \operatorname{tr}\big(1_{\Omega_L} f(H^{(\prime)})\big) \qquad (f \in C_c^\infty(\mathbb{R})). \tag{B.5}$$

If $E \in \mathbb{R}$ is a continuity point of this distribution function, the limit in (B.3) exists and is equal to the distribution function at E, see [Sim82, Prop. C.7.2]. Since distribution functions are monotone, the set of discontinuity points is countable. From (B.2) we infer that if $F(f)$ exists, so does $F'(f)$, and vice versa, and $F(f) = F'(f)$ in that case. This proves the first equation in (B.4). The second one follows from [Sim82, Thm. C.7.4]. □

We also compute the integral from Theorem A.1.

B.4 Theorem. Let $a \in \mathbb{R}^d$. Then

$$\int_{S_{d-1}} \mathrm{d}S(\xi)\, e^{i\xi\cdot a} = (2\pi)^{d/2} \frac{J_{d/2-1}(|a|)}{|a|^{d/2-1}}, \tag{B.6}$$

where the Bessel function J_ν of order $\nu = d/2 - 1$ is given by

$$J_\nu(x) = (\tfrac{1}{2}x)^\nu \sum_{k=0}^{\infty} (-1)^k \frac{(\frac{1}{2}x)^{2k}}{k!\,\Gamma(\nu+k+1)} \qquad (x > 0), \tag{B.7}$$

and the right-hand side of (B.6) is understood as its analytic continuation for $a = 0$.

Proof. For $d = 1$, the left-hand side of (B.6) is $2\cos a$, and so is the right-hand side since $J_{-1/2}(x) = (\frac{2}{\pi x})^{1/2} \cos x$. So let $d \geq 2$. For $a = 0$, the analytic continuation of (B.6) is

$$\frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})} = \sigma_{d-1}, \tag{B.8}$$

which is the surface volume σ_{d-1} of S_{d-1}. For any other $a \in \mathbb{R}^d$, there is an orthogonal matrix U such that $a = |a|Ue_1$, where e_1 is the first unit normal vector. Since the surface measure on S_{d-1} is orthogonally invariant,

$$\int_{S_{d-1}} \mathrm{d}S(\xi)\, e^{i\xi\cdot a} = \int_{S_{d-1}} \mathrm{d}S(\xi)\, e^{i|a|U^*\xi\cdot e_1} = \int_{S_{d-1}} \mathrm{d}S(\xi)\, e^{i|a|\xi\cdot e_1}. \tag{B.9}$$

Parameterizing the sphere, we arrive at

$$\int_{S_{d-1}} \mathrm{d}S(\xi)\, e^{i|a|\xi\cdot e_1} = \sum_{k=0}^{\infty} \frac{i^k|a|^k}{k!} \int_{S_{d-1}} \mathrm{d}S(\xi)\,(\xi\cdot e_1)^k$$
$$= \sum_{k=0}^{\infty} \frac{i^k|a|^k}{k!} \int_{-\pi}^{\pi} \mathrm{d}\varphi_1 \int_{(-\pi/2,\pi/2)^{d-2}} \mathrm{d}(\varphi_2,\dots,\varphi_{d-1}) \cos^k\varphi_1 \cdots \cos^{d-2+k}\varphi_{d-1}. \quad \text{(B.10)}$$

For odd k, the integration with respect to φ_1 yields zero. For even k, the integration yields

$$\int_{-\pi}^{\pi} \mathrm{d}\varphi_1 \int_{(-\pi/2,\pi/2)^{d-2}} \mathrm{d}(\varphi_2,\dots,\varphi_{d-1}) \cos^k\varphi_1 \cdots \cos^{d-2+k}\varphi_{d-1} = 2c_k \cdots c_{d-2+k} \quad \text{(B.11)}$$

with

$$c_k := \int_{-\pi/2}^{\pi/2} \mathrm{d}\varphi \cos^k\varphi \qquad (k \in \mathbb{N}_0). \quad \text{(B.12)}$$

An elementary computation shows that

$$c_k \cdots c_{d-2+k} = \frac{\omega_{d-2+k}}{\omega_{k-1}} = \pi^{d/2} \frac{k!}{4^{k/2}(\frac{k}{2})!\,\Gamma(\frac{k}{2}+\frac{1}{2})}, \quad \text{(B.13)}$$

where

$$\omega_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \quad \text{(B.14)}$$

is the volume of the unit ball. Inserting this back into (B.10) proves the assertion. □

C THE GEOMETRIC RESOLVENT INEQUALITY

In this section, we state and prove the geometric resolvent inequality. The formulation and the proof are an adaptation from [Sto01], generalized to allow for Kato decomposable potentials and complex points in the resolvent set.

Let $M > 0$ and let $a : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ be measurable with $M^{-1} \le a(x) \le M$ for all $x \in \mathbb{R}^d$ in the sense of positive semidefiniteness.

Let $V_+ \in K_{\mathrm{loc}}(\mathbb{R}^d)$ and $V_- \in K(\mathbb{R}^d)$ be positive. By [Sim82, p. 459], V_- is relatively $-\Delta$-form bounded with relative bound zero, i.e., for $\varepsilon > 0$ there is $C(\varepsilon) > 0$ such that $\langle \varphi, V_-\varphi\rangle \le \varepsilon \|\nabla\varphi\|^2 + C(\varepsilon)\|\varphi\|^2$. Consequently, we can define a self-adjoint operator H in $L_2(\mathbb{R}^d)$ that is formally given by

$$H = -\nabla \cdot a\nabla + V \tag{C.1}$$

via its form, where $V := V_+ - V_-$. Choosing Dirichlet or Neumann boundary conditions, we can also define a corresponding self-adjoint operator H_Ω in $L_2(\Omega)$ for some open set $\Omega \subseteq \mathbb{R}^d$.

Before we can prove the geometric resolvent inequality, we need a technical lemma.

C.1 Lemma ([Sto01, Lemma 2.5.3])**.** Let $\tilde\Omega \subset \Omega \subseteq \mathbb{R}^d$ with $\operatorname{dist}(\partial\Omega, \partial\tilde\Omega) =: \delta > 0$. Let $R > 0$ and $z \in \mathbb{C}$ with $|z| \le R$. Let $g \in L_2(\Omega)$. Let $u \in W_2^1(\Omega)$ be a weak solution of $(H + z)u = g$ in Ω, i.e.,

$$\langle a\nabla u, \nabla\varphi\rangle + \langle Vu, \varphi\rangle + \langle zu, \varphi\rangle = \langle g, \varphi\rangle \qquad (\varphi \in C_c^\infty(\Omega)). \tag{C.2}$$

Then there exists a constant C only depending on δ, M, V_-, and R, such that

$$\|\nabla u\|_{L^2(\tilde\Omega)} \le C(\|u\|_{L^2(\Omega)} + \|g\|_{L^2(\Omega)}). \tag{C.3}$$

Proof. By density, the condition (C.2) is satisfied for all $\varphi \in W_{2,0}^1(\Omega)$. There is $\psi \in C_c^\infty(\Omega)$ with $0 \le \psi \le 1$, $\psi = 1$ on $\tilde\Omega$ and $\|\nabla\psi\|_\infty \le C/\delta$, where C depends only upon the dimension d. For $w := u\psi^2 \in W_{2,0}^1(\Omega)$, it follows that

$$\langle a\nabla u, \nabla w\rangle + \langle Vu, w\rangle + \langle zu, w\rangle = \langle g, w\rangle, \tag{C.4}$$

and since $\nabla w = \psi^2\nabla u + 2u\psi\nabla\psi$,

$$\begin{aligned}\langle a\nabla u, \nabla w\rangle &= \langle a\nabla u, \psi^2\nabla u\rangle + \langle a\nabla u, 2u\psi\nabla\psi\rangle \\ &= \langle a\psi\nabla u, \psi\nabla u\rangle + 2\langle a\psi\nabla u, u\nabla\psi\rangle.\end{aligned} \tag{C.5}$$

Now,

$$
\begin{aligned}
\langle \psi\nabla u, \psi\nabla u\rangle &\le M\langle a\psi\nabla u, \psi\nabla u\rangle = M\big(\langle a\nabla u, \nabla w\rangle - 2\langle a\psi\nabla u, u\nabla\psi\rangle\big)\\
&= M\big(\langle g, w\rangle - \langle Vu, w\rangle - \langle zu, w\rangle - 2\langle a\psi\nabla u, u\nabla\psi\rangle\big)\\
&\le M\big(|\langle g, w\rangle| + \langle V_-\psi u, \psi u\rangle + R\|\psi u\|^2 + 2|\langle a\psi\nabla u, u\nabla\psi\rangle|\big)\\
&\le M\big(\|g\|\|u\| + \langle V_-\psi u, \psi u\rangle + R\|\psi u\|^2 + 2\|a\|_\infty\|\psi\nabla u\|\|u\|\|\nabla\psi\|_\infty\big). \quad \text{(C.6)}
\end{aligned}
$$

Using the $-\Delta$-form boundedness of V_- with relative bound zero, we set $\varepsilon = \frac{1}{4M}$ to conclude

$$
\begin{aligned}
M\langle V_-\psi u, \psi u\rangle &\le \frac{1}{4}\|\nabla(\psi u)\|^2 + C(M)\|\psi u\|^2\\
&\le \frac{1}{2}\|\psi\nabla u\|^2 + \frac{1}{2}\|u\nabla\psi\|^2 + C(M)\|\psi u\|^2\\
&\le \frac{1}{2}\|\psi\nabla u\|^2 + \frac{C^2}{2\delta^2}\|u\|^2 + C(M)\|u\|^2 \qquad \text{(C.7)}
\end{aligned}
$$

and therefore

$$
\frac{1}{2}\|\psi\nabla u\|^2 \le M\|g\|\|u\| + \Big(\frac{C^2}{2\delta^2} + C(M) + R\Big)\|u\|^2 + 2MC/\delta\,\|a\|_\infty\|\psi\nabla u\|\|u\|. \quad \text{(C.8)}
$$

This is a quadratic inequality for $\|\psi\nabla u\|$, which implies that there exists $C(\delta, M, R)$ with

$$
\|\psi\nabla u\| \le C(\delta, M, R)\big(\|u\| + \|g\|\big). \quad \text{(C.9)}
$$

Taking the supremum over ψ proves the lemma. □

We are now ready to prove the geometric resolvent inequality. To shorten formulas, let us write $R_\Lambda(z) := (z - H_\Lambda)^{-1}$, for $\Lambda \subseteq \mathbb{R}^d$ open and $z \in \rho(H_\Lambda)$.

C.2 Theorem (Geometric resolvent inequality, [Sto01, Lemma 2.5.2])**.** Let $\Lambda \subseteq \Lambda'$ be open sets, $A \subseteq \Lambda$ and $B \subseteq \Lambda'$. Let $\varphi \in C_c^1(\Lambda)$ and Ω an open neighborhood of $\operatorname{spt}\nabla\varphi$ with $\delta := \operatorname{dist}(\partial\Omega, \operatorname{spt}\nabla\varphi) > 0$ and $\Omega \cap A = \varnothing$. Let $K \subseteq \mathbb{C}$ be compact. Then there exists $C = C(\delta, M, \|\nabla\varphi\|_\infty, V, K)$ such that for all $z \in \rho(H_\Lambda) \cap \rho(H_{\Lambda'}) \cap K$ the operator norm estimate

$$
\|1_A(\varphi R_{\Lambda'}(z) - R_\Lambda(z)\varphi)1_B\| \le C\|1_A R_\Lambda(z)1_\Omega\|\|1_\Omega R_{\Lambda'}(z)1_B\| \quad \text{(C.10)}
$$

holds, where the functions are understood as their associated multiplication operators.

Proof. We use the geometric resolvent equation (see [Sto01, Prop. 2.5.1], the proof there holds for Kato decomposable potentials and arbitrary open sets $\Lambda \subseteq \Lambda'$) to write

$$\begin{aligned}\|1_A(\varphi R_{\Lambda'}(z) - R_\Lambda(z)\varphi)1_B\| &= \|1_A\big(R_\Lambda(z)\big((\nabla\varphi)\cdot a\,\nabla + \nabla\cdot a\nabla\varphi\big)R_{\Lambda'}(z)\big)1_B\| \\ &\le \|1_A R_\Lambda(z)(\nabla\varphi)\cdot a\nabla R_{\Lambda'}(z)1_B\|\|1_A R_\Lambda(z)(\nabla\cdot)a\nabla\varphi R_{\Lambda'}(z)1_B\|. \end{aligned} \tag{C.11}$$

We estimate the second factor of (C.11). Choose $\tilde\Omega \subseteq \Omega$ with $\operatorname{spt}\nabla\varphi \subseteq \tilde\Omega$ and $\operatorname{dist}(\partial\Omega, \partial\tilde\Omega) = \frac{\delta}{2}$. Then the second factor is, since $\operatorname{spt}\varphi \subseteq \Lambda$,

$$\begin{aligned}&\|1_A R_\Lambda(z)(\nabla\cdot)1_{\tilde\Omega} a\nabla\varphi R_{\Lambda'}(z)1_B\| \\ &\qquad\le \|1_A R_\Lambda(z)(\nabla\cdot)1_{\tilde\Omega}\|\|a\|_\infty\|\nabla\varphi\|_\infty\|1_\Lambda R_{\Lambda'}(z)1_B\|. \end{aligned} \tag{C.12}$$

By adjoining, the first factor is $\|1_{\tilde\Omega}\nabla R_\Lambda(\overline{z})1_A\|$. We claim that

$$\|1_{\tilde\Omega}\nabla R_\Lambda(\overline{z})1_A\| \le C(K,\delta)\|1_\Omega R_\Lambda(\overline{z})1_A\|. \tag{C.13}$$

Let $f \in L_2(\Lambda)$ and set $u = R_\Lambda(\overline{z})1_A f$ and $g = 1_A f$. Then u is a weak solution of $(H-\overline{z})u = g$ in Λ and, in particular, in $\Omega \cap \Lambda$. Using Lemma C.1 and $\Omega \cap A = \varnothing$, we arrive at

$$\|1_{\tilde\Omega}\nabla u\| \le c(\delta, M, V, K)\|u\|_{L_2(\Omega)} = c(\delta, M, V, K)\|1_\Omega u\|.$$

This proves equation (C.13). The first factor of (C.11) can be treated similarly. □

In the main text, we did not use Theorem C.2 in its most general formulation stated here. We used it in the formulation of Lemma 5.3, which we state here as a corollary.

C.3 Corollary. Let $L > 1$ and let $A \subseteq \Omega_{L-1}$ be closed. Take $\varphi \in C_c^1(\Omega_L)$ with $\varphi(x) = 1$ for $x \in \Omega_{L-1}$. Then $U_L := \Omega_L \setminus \overline{\Omega_{L-1}}$ is an open neighborhood of $\operatorname{spt}\nabla\varphi$ and $\delta := \operatorname{dist}(\partial U_L, \operatorname{spt}\nabla\varphi) > 0$. Let $K \subseteq \mathbb{C}$ be compact. Then there exists $C_{\text{GR}} > 0$ depending on δ, $\|\nabla\varphi\|_\infty$, V, and K such that for all $z \in \rho(H_L^{(\prime)}) \cap \rho(H^{(\prime)}) \cap K$ the operator norm estimate

$$\begin{aligned}&\|1_A\big((z - H^{(\prime)})^{-1} - (z - H_L^{(\prime)})^{-1}\big)1_A\| \\ &\qquad\le C_{\text{GR}}\|1_A(z - H_L^{(\prime)})^{-1}1_{U_L}\|\|1_{U_L}(z - H^{(\prime)})^{-1}1_A\| \end{aligned} \tag{C.14}$$

holds, where the indicator functions are understood as their associated multiplication operators.

Proof. Let $a(x) = I$ be the identity matrix. As the potential, take either V_0 or $V_0 + V$. In Theorem C.2, choose $\Lambda = \Omega_L$ and $\Lambda' = \mathbb{R}^d$, as well as $A = B$ and $\Omega = U_L$. Then $1_A\varphi = \varphi 1_A$, and therefore (C.10) implies the assertion. □

NOTATION

$\langle \cdot, \cdot \rangle$	scalar product on some Hilbert space; antilinear in the first and linear in the second argument
$\sim$	asymptotic equality; $f(x) \sim \varphi(x)$ as $x \to c \iff f(x)/\varphi(x) \to 1$ as $x \to c$
$\ker T$	kernel (null space) of the linear operator T
$\operatorname{ran} T$	range (image) of the linear operator T
$\operatorname{lin} M$	linear span (hull) of the set of vectors M
L	length parameter
Ω_L	$\{Lx;\, x \in \Omega_1\} = L \cdot \Omega_1$, where $\Omega_1 \subseteq \mathbb{R}^d$ open and bounded with $0 \in \Omega_1$
$K(\mathbb{R}^d)$	Kato class
$K_{\text{loc}}(\mathbb{R}^d)$	locally Kato class
$\operatorname{spt} f$	support of a function f
$\#M$	number of elements in the set M; $\#M \in \mathbb{N}_0 \cup \{\infty\}$
V_0	background potential, see (v_0) on page 1
V	perturbation potential, see (v) on page 1
$H_L = -\Delta_L + V_0$	unperturbed finite-volume Schrödinger operator
$H'_L = H_L + V$	perturbed finite-volume Schrödinger operator
λ_j^L, μ_j^L	jth eigenvalue of H_L and H'_L, counting multiplicities

φ_j^L, ψ_j^L	normalized jth eigenfunction of H_L and H_L'
$H = -\Delta + V_0$	unperturbed infinite-volume Schrödinger operator
$H' = H + V$	perturbed infinite-volume Schrödinger operator
E	Fermi energy
$N_L(E)$	number of particles, see (1.4) on page 2
$\mathcal{S}_L(E)$	ground-state overlap, see (1.5) on page 2
P_L^N, Π_L^N	orthogonal projections on the first N eigenvalues of H_L and H_L', see (1.7) on page 2
$\mathrm{O}(g(x))$	Bachmann-Landau symbol; $f(x) = \mathrm{O}(g(x))$ as $x \to \infty \iff \exists C, x_0 \geq 0 \; \forall x \geq x_0 : \lvert f(x) \rvert \leq C \lvert g(x) \rvert$
$\mathrm{o}(g(x))$	Bachmann-Landau symbol; $f(x) = \mathrm{o}(g(x))$ as $x \to \infty$ for nonzero $g(x) \iff f(x)/g(x) \to 0$ as $x \to \infty$
1_A	indicator function of the set A
ξ_L	spectral shift function
$L_{1,\mathrm{loc}}(\mathbb{R})$	locally integrable functions
$\mathrm{Borel}(X)$	σ-algebra of all Borel sets of the topological space X
$\mathrm{d}S$	integration with respect to the surface measure on a manifold
$x \cdot y$	Euklidean scalar product of $x, y \in \mathbb{R}^n$
δ	Dirac distribution, used in an abbreviation for integration with respect to the surface measure, see Remark 3.3 on page 9
$\lvert \cdot \rvert_1$	1-norm on $\mathbb{R}^n$
Δ_n	n-dimensional standard simplex; $= \{x \in [0,1]^n; \lvert x \rvert_1 \leq 1\}$
Γ	Euler's Gamma function
B	Euler's Beta function
$C_c^\infty(\Omega)$	$\{f \in C^\infty(\Omega); \operatorname{spt} f \text{ kompakt}\}$
χ_L^+, χ_L^-	smooth cut-off functions, see Definition 4.1 on page 13
χ^+, χ^-	discontinuous cut-off functions, see Definition 6.5 on page 26
$\rho(T)$	resolvent set of a linear operator T

ν^1, μ^1	one-dimensional trace measures, see (6.1) on page 25
I_n	an integral related to the Hilbert matrix, see § 8
η^{2n}	coefficient in the asymptotics, see Definition 7.2 on page 32
$\mathbb{N}_{\geq n}$	set of natural numbers greater than or equal to n
Li_2	dilogarithm function; $\mathrm{Li}_2(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2}$
$\mathcal{H}_{\mathrm{ac}}$	absolutely continuous subspace of H
$\hat{\sigma}$	core of the spectrum of H, see Definition 9.1 on page 41
S_E, T_E	scattering matrix and transition matrix, see § 9
$\|\cdot\|_{\mathrm{HS}}$	Hilbert-Schmidt norm
S_{d-1}	unit sphere in $\mathbb{R}^d$
ω_d	volume of the unit ball in $\mathbb{R}^d$; $\omega_d = \pi^{d/2}/\Gamma(\frac{d}{2}+1)$
σ_{d-1}	volume of the $(d-1)$-dimensional unit sphere in $\mathbb{R}^d$; $\sigma_{d-1} = d\omega_d$

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EIDESSTATTLICHE VERSICHERUNG

(Siehe Promotionsordnung vom 12. 7. 2011, § 8, Abs. 2 Pkt. 5)

Hiermit erkläre ich an Eides statt, dass die Dissertation von mir selbständig ohne unerlaubte Beihilfe angefertigt ist.

Heinrich Küttler

Ort, Datum	Unterschrift Doktorand