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Peter Müller[a] and Ruth Schulte

AFFILIATIONS

Mathematisches Institut, Ludwig-Maximilians-Universität München, Theresienstraße 39, 80333 München, Germany

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[a] **Author to whom correspondence should be addressed:** mueller@lmu.de

ABSTRACT

We consider a multi-dimensional continuum Schrödinger operator H, which is given by a perturbation of the negative Laplacian by a compactly supported bounded potential. We show that for a fairly large class of test functions, the second-order Szegő-type asymptotics for the spatially truncated Fermi projection of H is independent of the potential and, thus, identical to the known asymptotics of the Laplacian.

I. INTRODUCTION AND RESULT

A classical result of Szegő describes the asymptotic growth of the determinant of a truncated Toeplitz matrix as the truncation parameter tends to infinity.[24,25] Jump discontinuities in the spectral function (or symbol) of the Toeplitz matrix are of crucial importance for the growth of the subleading term in such an asymptotic expansion.[1,7]

Recent years have witnessed considerable interest in Szegő-type asymptotics for spectral projections of Schrödinger operators.[2,3,6,12,14–17,19–21,27] The first mathematical proof of such an asymptotics was established by Leschke, Sobolev, and Spitzer[12] and relies on extensive work of Sobolev,[22,23] making rigorous a long-standing conjecture of Widom.[26] The authors of Ref. 12 consider the simplest and most prominent Schrödinger operator, the self-adjoint (negative) Laplacian $H_0 := -\Delta$. It acts on a dense domain in the Hilbert space $L^2(\mathbb{R}^d)$ of complex-valued square-integrable functions over d-dimensional Euclidean space $\mathbb{R}^d$. More precisely, given a (Fermi) energy $E > 0$, they consider the spectral projection $1_{<E}(H_0)$ of H_0 associated with the interval $]-\infty, E[$. Besides physical motivation, this spectral projection provides a prototypical example for a symbol with a single discontinuity. The spectral projection $1_{<E}(H_0)$ gives rise to a Wiener–Hopf operator by truncation with the multiplication operator 1_{Λ_L} from the left and from the right. The truncation corresponds to multiplication with the indicator function of the spatial subset $\Lambda_L := L \cdot \Lambda \subset \mathbb{R}^d$, $L > 0$, which is the scaled version of some "nice" bounded subset $\Lambda \subset \mathbb{R}^d$. We state the details for Λ in Assumption 1.1(i). The final ingredient is a "test function" $h : [0,1] \to \mathbb{C}$, which is piecewise continuous and vanishes at zero, $h(0) = 0$. Furthermore, it is required that h grows at most algebraically near the endpoints of the interval, that is, there exists a "Hölder exponent" $\alpha > 0$ such that

$$h(\lambda) = O(\lambda^\alpha) \quad \text{and} \quad h(1) - h(1-\lambda) = O(\lambda^\alpha) \qquad \text{as} \quad \lambda \searrow 0. \tag{1.1}$$

Here, we employed the Bachmann–Landau notation for asymptotic equalities: We will use the big-O and little-o symbols throughout this paper. Under these hypotheses, the second-order asymptotic formula for the trace

$$\operatorname{tr}\{h(1_{\Lambda_L} 1_{<E}(H_0) 1_{\Lambda_L})\} = N_0(E) h(1) |\Lambda| L^d + \Sigma_0(E) I(h)\ |\partial\Lambda| L^{d-1} \ln L + o(L^{d-1} \ln L) \tag{1.2}$$

as $L \to \infty$ is proved in Ref. 12. Here, $|\Lambda|$ denotes the (Lebesgue) volume of Λ, and $|\partial\Lambda|$ denotes the surface area of the boundary $\partial\Lambda$ of Λ. The leading-order coefficient in (1.2) is determined by the integrated density of states,

$$N_0(E) := \frac{1}{\Gamma[(d+1)/2]}\left(\frac{E}{4\pi}\right)^{d/2}, \tag{1.3}$$

of H_0. Here, Γ denotes Euler's gamma function. The coefficient of the subleading term factorizes into a product of

$$I(h) := \frac{1}{4\pi^2}\int_0^1 \mathrm{d}\lambda\ \frac{h(\lambda)-\lambda h(1)}{\lambda(1-\lambda)} \tag{1.4}$$

and

$$\Sigma_0(E) := \frac{2}{\Gamma[(d+1)/2]}\left(\frac{E}{4\pi}\right)^{(d-1)/2}. \tag{1.5}$$

We follow the usual terminology and refer to (1.2) as a (second-order) Szegő-type asymptotics. The occurrence of the logarithmic factor $\ln L$ multiplying the surface area L^{d-1} in the subleading term of (1.2) is attributed to the discontinuity of the symbol $1_{<E}$ together with the *dynamical* delocalization of the Schrödinger time evolution generated by the Laplacian.[15] In the context of entanglement entropies for non-interacting Fermi gases [see (1.8)], the occurrence of this additional $\ln L$-factor is also coined an *enhanced area law*.[12]

A natural question concerns the fate of the asymptotics (1.2) when $H_0 = -\Delta$ is replaced by general self-adjoint Schrödinger operators $H := -\Delta + V$ with a (suitable) electric potential V. Unfortunately, there exists no general approach, which allows us to derive a two-term asymptotics like (1.2) for H. Mathematical proofs are restricted to special examples or classes of examples. The exact determination of the coefficient in the subleading term beyond bounds poses a particularly challenging task.

First, we describe two situations in which—in contrast to (1.2)—the subleading term does not exhibit a logarithmic enhancement. Such a behavior is generally referred to as an *area law* and caused an enormous attraction in the physics literature over several decades until now (see, e.g., Refs. 5 and 10 and references therein). An area law is typically expected if H has a mobility gap in its spectrum and if the Fermi energy falls inside the mobility gap. It was proved for discrete random Schrödinger operators, a Fermi energy lying in the region of complete localization, and for test functions obeying some smoothness assumption, including the ones for entanglement entropies in (1.7).[6,17,18] An area law also shows up in the Szegő asymptotics for rather general test functions when H equals the Landau Hamiltonian in two dimensions with a perpendicular constant magnetic field and if the Fermi energy E coincides with one of the Landau levels[14] (see also Ref. 2). Very recently, Ref. 19 established the stability of this area law under suitable magnetic and electric perturbations and for the test functions (1.7) corresponding to entanglement entropies.

Now, we return to situations where the subleading term exhibits a logarithmic enhancement as in (1.2). One-dimensional Schrödinger operators $H = -\Delta + V$ with an arbitrarily often differentiable periodic potential V were studied in Ref. 21. If the Fermi energy lies in the interior of a Bloch band, Pfirsch and Sobolev[21] established an enhanced area law for the same class of test functions as considered in (1.2). Surprisingly, the coefficient of the subleading term of the Szegő asymptotics remains the same as for $H_0 = -\Delta$ in (1.2). However, as the integrated density of states of the periodic Schrödinger operator H differs from that of H_0, in general, this affects the leading-order term of the asymptotics. In contrast to the area law in the two-dimensional Landau model,[14] a logarithmic enhancement occurs when this model is considered in three space dimensions due to the free motion in the direction parallel to the magnetic field.[20] Another situation was studied by the present authors in Ref. 16. There, H_0 is perturbed by a compactly supported and bounded potential. The enhanced area law for H_0 is then proven to persist for the test function $h = h_1$ from (1.7), which corresponds to the von Neumann entropy. Yet, the bounds in Ref. 16 are not good enough as to allow for a conclusion concerning the coefficient.

The purpose of this paper is to show that the second-order Szegő asymptotics (1.2) remains valid with the same coefficients if H_0 is replaced by $H = -\Delta + V$ with a compactly supported and bounded potential $V \in L^\infty(\mathbb{R}^d)$. This improves the result in Ref. 16 in two ways: (i) the statement is strengthened as to cover also universality of the coefficients and (ii) it is extended from the von Neumann entropy to a fairly large class of test functions. The general approach we follow here is different from that in Ref. 16. It combines the traditional way[11] for proving (1.2) (see also, e.g., Refs. 12 and 21) with improved estimates from Ref. 16.

Our assumptions on the spatial domain coincide with those in Ref. 16.

Assumption 1.1. We consider a bounded Borel set $\Lambda \subset \mathbb{R}^d$ such that

(i) it is a Lipschitz domain with, if $d \geqslant 2$, a piecewise C^1-boundary and
(ii) the origin $0 \in \mathbb{R}^d$ is an interior point of Λ.

Remark 1.2. Assumption 1.1(i) is taken from Ref. 12 and guarantees the validity of (1.2) (see also Condition 3.1 in Ref. 13 for the notion of a Lipschitz domain). Assumption 1.1(ii) can always be achieved by a translation of the potential V in Theorem 1.6.

We specify the set of test functions to which our main result applies.

Definition 1.3. For $d \in \mathbb{N}\backslash\{1\}$, we set

$$\mathbb{H}_d := \{h : [0,1] \to \mathbb{C}\ \text{ piecewise continuous, } h(0) = 0 \text{ and } \exists\ \alpha > d^{-1} \text{ such that } h(\lambda) = O(\lambda^\alpha) \text{ and } h(1) - h(1-\lambda) = O(\lambda^\alpha) \text{ as } \lambda \searrow 0\}.$$

In $d = 1$ space dimension, we require test functions to have an additional mirror symmetry at $\lambda = 1/2$ and to vanish faster at zero (and one) than linear times a logarithm,

$$\mathbb{H}_1 := \{h : [0,1] \to \mathbb{C} \text{ piecewise continuous}, h(0) = 0, h = h(1-\cdot) \text{ and } h(\lambda) = o(\lambda \ln \lambda) \text{ as } \lambda \searrow 0\}.$$

The main result of this paper is about the first two terms in the asymptotics (1.6). These terms coincide with the ones in (1.2) and, thus, do not depend on the potential V.

Theorem 1.4. *Let $d \in \mathbb{N}$, and let $\Lambda \subset \mathbb{R}^d$ be as in Assumption 1.1. Let $V \in L^\infty(\mathbb{R}^d)$ be a compactly supported potential, and let $h \in \mathbb{H}_d$ be a test function. Then, for every Fermi energy $E > 0$, we obtain*

$$\operatorname{tr}\{h(1_{\Lambda_L} 1_{<E}(H) 1_{\Lambda_L})\} = N_0(E)h(1)|\Lambda|L^d + \Sigma_0(E)I(h)|\partial\Lambda|L^{d-1} \ln L + o(L^{d-1} \ln L) \tag{1.6}$$

as $L \to \infty$.

Remark 1.5. (i) The restriction to symmetric test functions in $\mathbb{H}_1$ is technical. It relates to the incommodious fact that the trace of a sequence of operators may converge, whereas convergence in trace norm need not hold. We refer to Remark 2.5(ii) for more details.

(ii) The class of test functions for which (1.2) holds requires less regularity for h near the endpoints of the interval [0,1] as compared to $\mathbb{H}_d$. We expect that Theorem 1.4 extends to this more general class, i.e., to test functions h with arbitrarily small "Hölder exponents" α. Possibly, such an extension requires additional smoothness of the potential V.

(iii) It is only for the sake of simplicity that we confined ourselves to compactly supported and bounded potentials. The theorem should remain valid for potentials with sufficient integrability properties.

We conclude this section with an application of Theorem 1.4 to entanglement entropies for the ground state of a system of non-interacting fermions with single-particle Hamiltonian H. We introduce the one-parameter family of test functions $h_\alpha : [0,1] \to [0,1]$, given by

$$\lambda \mapsto h_\alpha(\lambda) := \begin{cases} (1-\alpha)^{-1} \log_2[\lambda^\alpha + (1-\lambda)^\alpha] & \text{if } \alpha \in]0,\infty[\setminus\{1\}, \\ -\lambda \log_2 \lambda - (1-\lambda)\log_2(1-\lambda) & \text{if } \alpha = 1 \end{cases} \tag{1.7}$$

and refer to them as Rényi entropy functions. The particular case h_1 is also called the von Neumann entropy function, for which we use the convention $0 \log_2 0 := 0$ for the binary logarithm. Following Ref. 8, the quantity

$$S_\alpha(H, E, \Omega) := \operatorname{tr}\{h_\alpha(1_\Omega 1_{<E}(H) 1_\Omega)\}, \tag{1.8}$$

$\alpha > 0$, defines the Rényi-entanglement entropy with respect to a spatial bipartition for the ground state of a quasi-free Fermi gas characterized by the single-particle Hamiltonian H and Fermi energy E. Here, $\Omega \subset \mathbb{R}^d$ is any bounded Borel set. It is obvious from the definition of the space of test functions that

$$h_\alpha \in \mathbb{H}_d \quad \text{if and only if} \quad d > \alpha^{-1}. \tag{1.9}$$

Therefore, Theorem 1.4 has the following immediate:

Corollary 1.6. Let $d \in \mathbb{N}$, and let $\Lambda \subset \mathbb{R}^d$ be as in Assumption 1.1. Let $V \in L^\infty(\mathbb{R}^d)$ be a compactly supported potential. We fix a Fermi energy $E > 0$ and a Rényi index $\alpha > d^{-1}$. Then, the Rényi entanglement entropy exhibits an enhanced area law,

$$\lim_{L\to\infty} \frac{S_\alpha(H, E, \Lambda_L)}{L^{d-1} \ln L} = \Sigma_0(E)I(h_\alpha)|\partial\Lambda|, \tag{1.10}$$

the limit being independent of V.

Remark 1.7. Again, it would be desirable to remove the restriction $\alpha > d^{-1}$ in the corollary.

II. PROOF OF THEOREM 1.4

Theorem 1.4 follows from (1.2), which was proven in Ref. 12, and the next theorem.

Theorem 2.1. *Let $d \in \mathbb{N}$, and let $\Lambda \subset \mathbb{R}^d$ be as in Assumption 1.1. Let $V \in L^\infty(\mathbb{R}^d)$ be a compactly supported potential, and let $h \in \mathbb{H}_d$ be a test function. Then, for every Fermi energy $E > 0$, we have*

$$\operatorname{tr}\{h(1_{\Lambda_L} 1_{<E}(H) 1_{\Lambda_L}) - h(1_{\Lambda_L} 1_{<E}(H_0) 1_{\Lambda_L})\} = o(L^{d-1} \ln L) \qquad \text{as } L \to \infty. \tag{2.1}$$

The following notion will be useful in the proof of Theorem 2.1.

Definition 2.2. For every $d \in \mathbb{N}$, we set

$$\mathbb{H}_{d,0} := \{h \in \mathbb{H}_d : h(1) = 0\}. \tag{2.2}$$

We note that $\mathbb{H}_{1,0} = \mathbb{H}_1$ due to the additional symmetry constraint in $d = 1$.

Proof of Theorem 2.1. We fix $E > 0$, and let $L > 1$. For a given $h \in \mathbb{H}_d$, we have $\tilde{h} := h - h(1)\ \mathrm{id} \in \mathbb{H}_{d,0}$. Throughout this paper, we use the notation $H_{(0)}$ as a placeholder for either H or H_0 and similarly for other quantities, such as

$$P_{L(,0)} := 1_{\Lambda_L} 1_{<E}(H_{(0)}) 1_{\Lambda_L}. \tag{2.3}$$

By definition of $\tilde{h}$, we observe

$$h(P_L) - h(P_{L,0}) = \tilde{h}(P_L) - \tilde{h}(P_{L,0}) + h(1)(P_L - P_{L,0}). \tag{2.4}$$

We recall that if $d = 1$, then $h(1) = 0$ by symmetry. Thus, Lemma 2.11 implies that the proof of the theorem is reduced to showing the claim for test functions from $\mathbb{H}_{d,0}$ only. This will be accomplished in four steps for test functions of increasing generality.

Step (i). $h \in \mathbb{H}_{d,0}$ is a polynomial.

We define even and odd polynomials s_n and a_n, $n \in \mathbb{N}$, on [0,1] by

$$s_n(\lambda) := [\lambda(1-\lambda)]^n \quad \text{and} \quad a_n(\lambda) := \lambda s_n(\lambda), \quad \lambda \in [0,1], \tag{2.5}$$

and note that the family $\{s_n, a_n : n \in \mathbb{N}\}$ constitutes a basis of the space of polynomials in $\mathbb{H}_{d,0}$ for $d \geqslant 2$ because the linear spans

$$\operatorname{span}\{s_n, a_n : n \in \mathbb{N}\} = \operatorname{span}\{s_1\, \mathrm{id}^k : k \in \mathbb{N}_0\} \tag{2.6}$$

coincide. For $d = 1$, only the symmetric polynomials are to be considered for the basis due to the symmetry constraint. Therefore, the claim of step (i) amounts to proving

$$\operatorname{tr}\{s_n(P_L) - s_n(P_{L,0})\} = o(L^{d-1} \ln L) \tag{2.7}$$

and, if $d \geqslant 2$, also

$$\operatorname{tr}\{a_n(P_L) - a_n(P_{L,0})\} = o(L^{d-1} \ln L) \tag{2.8}$$

as $L \to \infty$ for every $n \in \mathbb{N}$.

We turn to (2.7) first and observe that $s_1(P_{L(,0)}) = |Q_{L(,0)}|^2$ with

$$Q_{L(,0)} := 1_{\Lambda_L^c} 1_{<E}(H_{(0)}) 1_{\Lambda_L}, \tag{2.9}$$

where $|A|^2 := A^* A$ for any bounded operator A and the superscript ^{c} indicates the complement of a set. The telescope-sum identity

$$a^n = b^n + \sum_{j=1}^{n} a^{n-j}(a-b) b^{j-1} \tag{2.10}$$

for $a, b \in \mathbb{R}$ and $n \in \mathbb{N}$ does not use the commutativity of a and b and, thus, implies

$$s_n(P_L) = \left(|Q_L|^2\right)^n = s_n(P_{L,0}) + \sum_{j=1}^{n} |Q_L|^{2(n-j)}\left(|Q_L|^2 - |Q_{L,0}|^2\right)|Q_{L,0}|^{2(j-1)}. \tag{2.11}$$

Hence, we obtain

$$|\mathrm{tr}\{s_n(P_L) - s_n(P_{L,0})\}| \leqslant n\left\| |Q_L|^2 - |Q_{L,0}|^2 \right\|_1, \tag{2.12}$$

where $\|\cdot\|_p$, $p > 0$, denotes the von Neumann–Schatten (quasi-) norm. We infer from the identity

$$|Q_L|^2 - |Q_{L,0}|^2 = (Q_L^* - Q_{L,0}^*)(Q_L - Q_{L,0}) + (Q_L^* - Q_{L,0}^*)Q_{L,0} + Q_{L,0}^*(Q_L - Q_{L,0}) \tag{2.13}$$

and (2.12) that

$$|\mathrm{tr}\{s_n(P_L) - s_n(P_{L,0})\}| \leqslant n\left(\|Q_L - Q_{L,0}\|_2^2 + 2\|Q_L - Q_{L,0}\|_2\|Q_{L,0}\|_2\right) =: n\phi(L). \tag{2.14}$$

The boundedness of Hilbert–Schmidt norms,

$$\sup_{L>1}\|Q_L - Q_{L,0}\|_2 < \infty, \tag{2.15}$$

(see Lemma 2.3 in Ref. 16) and the asymptotics (1.2) applied to the test function s_1,

$$\|Q_{L,0}\|_2 = [\mathrm{tr}\, s_1(P_{L,0})]^{1/2} = O\left(L^{(d-1)/2}(\ln L)^{1/2}\right) \qquad \text{as } L \to \infty, \tag{2.16}$$

yield

$$\phi(L) = O\left(L^{(d-1)/2}(\ln L)^{1/2}\right) \qquad \text{as } L \to \infty. \tag{2.17}$$

Therefore, (2.7) follows from (2.14) and (2.17).

Now, we turn to the proof of (2.8) and equate, using (2.11),

$$a_n(P_L) = a_n(P_{L,0}) + (P_L - P_{L,0})s_n(P_{L,0}) + P_L\sum_{j=1}^{n} |Q_L|^{2(n-j)}\left(|Q_L|^2 - |Q_{L,0}|^2\right)|Q_{L,0}|^{2(j-1)}. \tag{2.18}$$

This leads to the estimate

$$\begin{aligned}|\mathrm{tr}\{a_n(P_L) - a_n(P_{L,0})\}| &\leqslant |\mathrm{tr}\{(P_L - P_{L,0})s_n(P_{L,0})\}| + n\phi(L)\\ &\leqslant \|P_L - P_{L,0}\|_2\ \|s_n(P_{L,0})\|_2 + n\phi(L).\end{aligned} \tag{2.19}$$

The first factor of the first term in the second line of (2.19) is of the order $O(\sqrt{\ln L})$ as $L \to \infty$ according to Lemma 2.3. The second factor of the first term behaves like

$$\|s_n(P_{L,0})\|_2 = (\mathrm{tr}\{s_{2n}(P_{L,0})\})^{1/2} = O(L^{(d-1)/2}(\ln L)^{1/2}) \qquad \text{as } L \to \infty, \tag{2.20}$$

according to (1.2) applied to the test function s_{2n}. Together with (2.17), we conclude from (2.19) that

$$|\mathrm{tr}\{a_n(P_L) - a_n(P_{L,0})\}| = O(L^{(d-1)/2}\ \ln L) \qquad \text{as } L \to \infty, \tag{2.21}$$

which proves (2.8) for $d \geqslant 2$.

Steps (ii)–(iv) establish the "closure" of the asymptotics.

Step (ii). $h \in \mathbb{H}_{d,0}$ is of the form $h = s_1 f$ with $f \in C([0,1])$.

Let $\varepsilon > 0$. The Stone–Weierstraß theorem guarantees the existence of a polynomial ζ over [0,1] such that

$$\sup_{\lambda\in[0,1]} |f(\lambda) - \zeta(\lambda)| \leqslant \varepsilon. \tag{2.22}$$

We estimate with the triangle inequality,

$$
\begin{aligned}
|\mathrm{tr}\{(s_1 f)(P_L) - (s_1 f)(P_{L,0})\}| &\leqslant \|(s_1(f-\zeta))(P_L)\|_1 + \|(s_1(\zeta - f))(P_{L,0})\|_1 \\
&\quad + |\mathrm{tr}\{(s_1\zeta)(P_L) - (s_1\zeta)(P_{L,0})\}| \\
&\leqslant \varepsilon(\|s_1(P_L)\|_1 + \|s_1(P_{L,0})\|_1) + o(L^{d-1}\ln L)
\end{aligned}
\tag{2.23}
$$

as $L \to \infty$, where the last estimate uses Hölder's inequality, (2.22), and the result of step (i) for the polynomial $s_1\zeta \in \mathbb{H}_{d,0}$. We observe $\|s_1(P_{L(,0)})\|_1 = \mathrm{tr}\, s_1(P_{L(,0)})$ and conclude with (1.2) plus another application of step (i) to the difference $\mathrm{tr}\, s_1(P_L) - \mathrm{tr}\, s_1(P_{L,0})$ that

$$
\lim_{L\to\infty} \frac{|\mathrm{tr}\{(s_1 f)(P_L) - (s_1 f)(P_{L,0})\}|}{L^{d-1}\ln L} \leqslant 2\varepsilon\Sigma_0(E) I(s_1)|\partial\Lambda|. \tag{2.24}
$$

As $\varepsilon > 0$ is arbitrary, the claim follows.

Step (iii). $h \in \mathbb{H}_{d,0}$ is continuous.

Boundedness of h and the growth conditions at 0 and 1 provide the existence of a constant $C > 0$ and of a function $g : [0, 1/4] \to [0, \infty[$ with $g(0) = 0$ and $\lim_{x\searrow 0} g(x) = 0$ such that

$$
|h| \leqslant \begin{cases} C s_1^{\alpha} & \text{if } d \geqslant 2 \ \text{ with } \alpha > 1/d, \\ -s_1 \log_2(s_1)\, g(s_1) & \text{if } d = 1. \end{cases} \tag{2.25}
$$

For $\varepsilon \in\,]0, 1/2[$ arbitrary but fixed, we consider a non-negative switch function $\tilde{\psi}_\varepsilon \in C^\infty([0,1])$ with $0 \leqslant \tilde{\psi}_\varepsilon \leqslant 1$ and with restrictions,

$$
\tilde{\psi}_\varepsilon|_{[0,\varepsilon/2]} = 1 \qquad \text{and} \qquad \tilde{\psi}_\varepsilon|_{[\varepsilon,1]} = 0. \tag{2.26}
$$

We set $\psi_\varepsilon := \tilde{\psi}_\varepsilon \circ s_1$. Since $(1-\psi_\varepsilon)h$ is of the form of the previous step (ii), we conclude that

$$
\begin{aligned}
\frac{|\mathrm{tr}\{h(P_L) - h(P_{L,0})\}|}{L^{d-1}\ln L} &\leqslant \frac{|\mathrm{tr}\{(\psi_\varepsilon h)(P_L) - (\psi_\varepsilon h)(P_{L,0})\}|}{L^{d-1}\ln L} + o(1) \\
&\leqslant \frac{\|(\psi_\varepsilon h)(P_L)\|_1}{L^{d-1}\ln L} + \Sigma_0(E) I(|\psi_\varepsilon h|)|\partial\Lambda| + o(1)
\end{aligned}
\tag{2.27}
$$

as $L \to \infty$, where we used the Szegő asymptotics (1.2) for the unperturbed operator $P_{L,0}$.

First, we consider the case $d \geqslant 2$. Let $\delta \in\,]0, \alpha - 1/d[$ so that $\alpha' := \alpha - \delta > 1/d$. We observe that

$$
|\psi_\varepsilon h| \leqslant C s_1^{\alpha}\psi_\varepsilon \leqslant C\varepsilon^{\delta} s_1^{\alpha'}, \tag{2.28}
$$

whence

$$
\|(\psi_\varepsilon h)(P_L)\|_1 \leqslant C\varepsilon^{\delta}\|Q_L\|_{2\alpha'}^{2\alpha'} \leqslant C_{\alpha'}\varepsilon^{\delta}\Big(\|Q_{L,0}\|_{2\alpha'}^{2\alpha'} + \|Q_L - Q_{L,0}\|_{2\alpha'}^{2\alpha'}\Big). \tag{2.29}
$$

Here, $C_{\alpha'} \geqslant C$ is a constant needed to cover the case $2\alpha' > 1$. The difference term satisfies $\|Q_L - Q_{L,0}\|_{2\alpha'}^{2\alpha'} = o(L^{d-1})$ as $L \to \infty$ by Corollary 2.7 if $\alpha' \in\,]1/d, 1[$. For the remaining case $\alpha' > 1$, we refer to the general von Neumann–Schatten-norm estimate $\|\cdot\|_{2\alpha'} \leqslant \|\cdot\|_2$ and (2.15). Thus, we infer from (2.27) that

$$
\begin{aligned}
\lim_{L\to\infty} \frac{|\mathrm{tr}\{h(P_L) - h(P_{L,0})\}|}{L^{d-1}\ln L} &\leqslant \Sigma_0(E) I(|\psi_\varepsilon h|)|\partial\Lambda| + C_{\alpha'}\varepsilon^{\delta} \lim_{L\to\infty} \frac{\mathrm{tr}\{s_1^{\alpha'}(P_{L,0})\}}{L^{d-1}\ln L} \\
&= \Sigma_0(E)|\partial\Lambda|\,\Big[I(|\psi_\varepsilon h|) + C_{\alpha'}\varepsilon^{\delta} I(s_1^{\alpha'})\Big],
\end{aligned}
\tag{2.30}
$$

where we (ab-)used the notation (2.5) for the symmetric polynomials to include also positive real exponents and appealed to the unperturbed asymptotics (1.2) in the last step. The bound (2.28) implies $I(|\psi_\varepsilon h|) \leqslant C\varepsilon^{\delta} I(s_1^{\alpha'}) < \infty$ so that the claim follows from (2.30) and the fact that $\varepsilon > 0$ can be chosen arbitrarily small.

It remains to treat the case $d = 1$. In this case, (2.28) and (2.29) are to be replaced by

$$
|\psi_\varepsilon h| \leqslant -s_1 \log_2(s_1) g(s_1)\psi_\varepsilon \leqslant -s_1\log_2(s_1)\psi_\varepsilon G(\varepsilon), \tag{2.31}
$$

where $G(\varepsilon) := \sup_{x\in[0,\varepsilon]} g(x)$, and

$$\|(\psi_\varepsilon h)(P_L)\|_1 \leqslant G(\varepsilon)\ \big\||Q_L|^2\log_2(|Q_L|^2)\big\|_1 = G(\varepsilon)\mathrm{tr}\{f(|Q_L|)\}, \tag{2.32}$$

where $f : [0,\infty[\ \to [0,1]$, $x \mapsto 1_{[0,1]}(x)(-x^2)\log_2(x^2)$. The "Proof of the upper bound in Theorem 1.3" in Ref. 16 demonstrates

$$\mathrm{tr}\{f(|Q_L|)\} = O(\ln L) \qquad \text{as } L \to \infty \tag{2.33}$$

[see Eq. (2.49) in Ref. 16]. Thus, we conclude with (2.27) and (2.31)–(2.33) that there exists a constant $c > 0$ such that

$$\begin{aligned}\varlimsup_{L\to\infty} \frac{|\mathrm{tr}\{h(P_L) - h(P_{L,0})\}|}{\ln L} &\leqslant cG(\varepsilon) + \Sigma_0(E)I(|\psi_\varepsilon h|)|\partial\Lambda| \\ &\leqslant G(\varepsilon)\big[c + \Sigma_0(E)I(s_1|\log_2 s_1|)|\partial\Lambda|\big].\end{aligned} \tag{2.34}$$

The claim follows because of $I(s_1|\log_2 s_1|) < \infty$ and $\lim_{\varepsilon\downarrow 0} G(\varepsilon) = 0$, which is consequence of the right-continuity of g.

Step (iv). $h \in \mathbb{H}_{d,0}$.

We follow the argument in Ref. 21 and assume—without restriction—that h is real-valued. Otherwise, we decompose h into its real part $\mathrm{Re}h$ and imaginary part $\mathrm{Im}\,h$.

Since h is piecewise continuous and continuous at 0 and at 1, there exists $\delta > 0$ such that h is continuous in $[0,2\delta] \cup [1-2\delta,1]$. Let $\varepsilon > 0$. We choose continuous functions $h_1, h_2 \in \mathbb{H}_{d,0} \cap C([0,1])$ such that

(1) h, h_1, and h_2 coincide on $[0,\delta] \cup [1-\delta,1]$,
(2) $h_1 \leqslant h \leqslant h_2$, and
(3) $\int_0^1 \mathrm{d}\lambda\ |h_2(\lambda) - h_1(\lambda)| < \varepsilon$.

The monotonicity (2) and an application of step (iii) to h_1, respectively, h_2, imply

$$\frac{\mathrm{tr}\{h_1(P_{L,0}) - h(P_{L,0})\}}{L^{d-1}\ \ln L} + o(1) \leqslant \frac{\mathrm{tr}\{h(P_L) - h(P_{L,0})\}}{L^{d-1}\ \ln L} \leqslant \frac{\mathrm{tr}\{h_2(P_{L,0}) - h(P_{L,0})\}}{L^{d-1}\ \ln L} + o(1) \tag{2.35}$$

as $L \to \infty$. The unperturbed asymptotics (1.2) for $h_1 - h$, respectively, $h_2 - h$, thus gives

$$\Sigma_0(E)I(h_1 - h)|\partial\Lambda| \leqslant \varliminf_{L\to\infty} \frac{\mathrm{tr}\{h(P_L) - h(P_{L,0})\}}{L^{d-1}\ \ln L} \leqslant \Sigma_0(E)I(h_2 - h)|\partial\Lambda|. \tag{2.36}$$

By (1) and (3), we estimate $I(|h_2 - h_1|) \leqslant \eta\varepsilon$ with $\eta := 1/[4\pi^2\delta(1-\delta)]$. Combining this with the monotonicity (2), we infer

$$-\eta\varepsilon \leqslant I(h_1 - h) \qquad \text{and} \qquad I(h_2 - h) \leqslant \eta\varepsilon. \tag{2.37}$$

Since $\varepsilon > 0$ is arbitrary, the claim follows from (2.36). □

Lemma 2.3. Assume the hypotheses of Theorem 2.1. Then, we have

$$\|P_L - P_{L,0}\|_2 = O(\sqrt{\ln L}) \qquad \text{as } L \to \infty. \tag{2.38}$$

Proof. Let $\Gamma_x := x + [0,1]^d \subset \mathbb{R}^d$ denote the closed unit cube translated by $x \in \mathbb{R}^d$. By Eq. (2.25) in Ref. 16, there exist $c_2 \equiv c_2(E,V) > 0$ and $\ell \equiv \ell(E,V) > 0$ such that

$$\|1_{\Gamma_n}(1_{<E}(H) - 1_{<E}(H_0))1_{\Gamma_m}\|_2 \leqslant \frac{c_2}{(|n||m|)^{(d-1)/2}(|n| + |m|)} \tag{2.39}$$

for all $n, m \in \mathbb{Z}^d \setminus [-\ell,\ell]^d$. In order to deal also with centers in the excluded cube $[-\ell,\ell]^d$, we use the estimate

$$\|A\|_2^2 \leqslant 3\|1_\Omega A\|_2^2 + \|1_{\Omega^c}A1_{\Omega^c}\|_2^2 \tag{2.40}$$

for any self-adjoint Hilbert–Schmidt operator A and any measurable subset $\Omega \subset \mathbb{R}^d$, together with the norm bound

$$\sup_{x\in\mathbb{R}^d} \| 1_{\Gamma_x} 1_{<E}(H_{(0)}) \|_p \leqslant \gamma, \tag{2.41}$$

which holds for any $p > 0$ (see Lemma B.1 in Ref. 4). Here, $\gamma \equiv \gamma(E, p, V) > 0$ is a constant. As to the applicability of Lemma B.1 in Ref. 4, we remark that the result of that lemma is formulated with two spatial indicator functions: one to the left and one to the right of the spectral projection. Yet, only one of them is needed in the proof. The other one drops out in Eq. (155) of Ref. 4.

Combining (2.39)–(2.41), we infer the existence of constants $C \equiv C(\ell, E, V) > 0$, $C' \equiv C'(\ell, E, V) > 0$, and $a \equiv a(\Lambda) > 0$, which are independent of L, such that

$$\begin{aligned} \|P_L - P_{L,0}\|_2^2 &\leqslant C + \sum_{\substack{n,m\in\mathbb{Z}^d\setminus[-\ell,\ell]^d:\\ \Gamma_n\cap\Lambda_L\neq\emptyset,\ \Gamma_m\cap\Lambda_L\neq\emptyset}} \frac{c_2^2}{(|n||m|)^{d-1}(|n|+|m|)^2} \\ &\leqslant C' \int_\ell^{aL} \mathrm{d}x \int_\ell^{aL} \mathrm{d}y \, \frac{1}{(x+y)^2} = O(\ln L) \end{aligned} \tag{2.42}$$

as $L \to \infty$. □

Lemma 2.4. Assume the hypotheses of Theorem 2.1. Then, we have

$$|\mathrm{tr}\{P_L - P_{L,0}\}| = O(\ln L) \qquad \text{as } L \to \infty. \tag{2.43}$$

Proof. The argument is similar to the one for the previous lemma. First, we claim that the estimate (2.39) also holds if the Hilbert–Schmidt norm is replaced by the trace norm; only the constant c_2 changes: there exists $c_1 \equiv c_1(E, V) > 0$ such that

$$\| 1_{\Gamma_n} (1_{<E}(H) - 1_{<E}(H_0)) 1_{\Gamma_m} \|_1 \leqslant \frac{c_1}{(|n||m|)^{(d-1)/2}(|n|+|m|)} \tag{2.44}$$

for all $n, m \in \mathbb{Z}^d\setminus[-\ell, \ell]^d$, with the same $\ell > 0$ as in (2.39). We prove (2.44) later. Assuming its validity for the time being, we proceed with the proof of the lemma and estimate

$$\begin{aligned} |\mathrm{tr}\{P_L - P_{L,0}\}| &= \left| \sum_{n\in\mathbb{Z}^d:\ \Gamma_n\cap\Lambda_L\neq\emptyset} \mathrm{tr}\{1_{\Gamma_n} 1_{\Lambda_L} (1_{<E}(H) - 1_{<E}(H_0)) 1_{\Gamma_n}\} \right| \\ &\leqslant \sum_{n\in\mathbb{Z}^d:\ \Gamma_n\cap\Lambda_L\neq\emptyset} \| 1_{\Gamma_n} 1_{\Lambda_L} (1_{<E}(H) - 1_{<E}(H_0)) 1_{\Gamma_n} \|_1 \\ &\leqslant C + \sum_{\substack{n\in\mathbb{Z}^d\setminus[-\ell,\ell]^d:\\ \Gamma_n\cap\Lambda_L\neq\emptyset}} \frac{c_1}{2|n|^d} = O(\ln L) \qquad \text{as } L \to \infty. \end{aligned} \tag{2.45}$$

Here, $C \equiv C(E, V) > 0$ is a constant, and we used (2.41) and (2.44) later for the second inequality.

It remains to show (2.44). To this end, we recall the pointwise estimate from Eq. (2.7) in Ref. 16 for the integral kernel $G_0(x, y;\ z)$ of the unperturbed resolvent $\frac{1}{H_0 - z}$, $z \in \mathbb{C}\setminus\mathbb{R}$, and apply it to

$$\begin{aligned} \left\| |V|^{1/2} \frac{1}{H_0 - z} 1_{\Gamma_n} \right\|_2 &= \left(\int_{\mathbb{R}^d} \mathrm{d}x \int_{\Gamma_n} \mathrm{d}y \, |V(x)| |G_0(x, y; z)|^2 \right)^{1/2} \\ &\leqslant C \left(\int_{\mathbb{R}^d} \mathrm{d}x \, |V(x)| \right)^{1/2} |z|^{(d-3)/4} \, \frac{\mathrm{e}^{-|\mathrm{Im}\sqrt{z}||n|/2}}{|n|^{(d-1)/2}}, \end{aligned} \tag{2.46}$$

where $n \in \mathbb{Z}^d\setminus[-\ell_0, \ell_0]^d$ for some suitable $\ell_0 \equiv \ell_0(z, V) > 0$, which is given in Lemma 2.1 of Ref. 16, and $C > 0$, which depends only on the dimension. The bound (2.46) is analogous to the statement of Lemma 2.1 in Ref. 16, except that (2.46) involves the 2-norm instead of the 4-norm. A double application of the resolvent identity yields

$$\begin{aligned} \left\| 1_{\Gamma_n} \left(\frac{1}{H_0 - z} - \frac{1}{H - z} \right) 1_{\Gamma_m} \right\|_1 &\leqslant \left\| 1_{\Gamma_n} \frac{1}{H_0 - z} |V|^{1/2} \right\|_2 \left\| |V|^{1/2} \frac{1}{H_0 - z} 1_{\Gamma_m} \right\|_2 \\ &\quad \times \left(1 + \left\| |V|^{1/2} \frac{1}{H - z} |V|^{1/2} \right\| \right). \end{aligned} \tag{2.47}$$

We observe that (2.47) and (2.46) are fully analogous to Eq. (2.15) and Lemma 2.1 in Ref. 16. Thus, (2.44) follows from (2.47) in the very same way as Eq. (2.25) in Ref. 16 follows from Eq. (2.15) in Ref. 16. □

Remark 2.5. (i) We expect that the trace in the claim of Lemma 2.4 remains bounded as $L \to \infty$. In fact, in their study of the spectral shift function, Kohmoto, Koma, and Nakamura proved the existence of the limit

$$\lim_{L\to\infty} \operatorname{tr}\{\vartheta_L(1_{<E}(H) - 1_{<E}(H_0))\vartheta_L\} \tag{2.48}$$

in Theorem 5 of Ref. 9, where $\vartheta_L := \vartheta(L^{-1}\cdot)$ is a smooth cut-off function determined by some $\vartheta \in C_c^\infty(\mathbb{R}^d)$, which obeys $\vartheta = 1$ in a neighborhood of the origin. Unfortunately, we cannot use this result in our study of the Szegő asymptotics with "sharp" indicator functions because the volume of the region where ϑ_L decays from 1 to 0 is of the order $O(L^d)$.

(ii) Likewise, we believe that the trace on the rhs of the first line of (2.19) remains bounded as $L \to \infty$. On the other hand, the trace norm $\|(P_L - P_{L,0})s_n(P_{L,0})\|_1$ may grow logarithmically in L in some one-dimensional situations, which is correctly captured by the product of Hilbert–Schmidt norms in the second line of (2.19). Thus, it is the second inequality in (2.19), which is responsible for the additional symmetry constraint in $\mathbb{H}_1$, respectively, $\mathbb{H}_{1,0}$, as compared to higher dimensions.

The difference $Q_L - Q_{L,0}$ was previously estimated in Lemma 2.5 of Ref. 16 in suitable von Neumann–Schatten norms $\|\cdot\|_s$. The next lemma improves that result by accessing smaller values of s and obtaining a weaker growth in L as compared to Lemma 2.5 of Ref. 16.

Lemma 2.6. Let $\Lambda \subset \mathbb{R}^d$, $d \in \mathbb{N}$, be as in Assumption 1.1(ii). Let $V \in L^\infty(\mathbb{R}^d)$ have compact support, and fix $E > 0$ and $s \in\ ]0,1]$. Then, for every $p_0 \in\ ]0, \min\{1, 2s\}]$, there exists a constant $C \equiv C(\Lambda, V, E, p_0) > 0$ such that for all $L \geqslant 1$, we have

$$\|Q_L - Q_{L,0}\|_{2s}^{2s} \leqslant CL^{2d(1-s)/(2-p_0)}. \tag{2.49}$$

Proof. We fix $E > 0$, $s \in\ ]0,1]$, and $p_0 \in\ ]0, \min\{1, 2s\}]$. Given any $L > 1$, the spatial domain $\Lambda_L \subseteq \bigcup_{n\in\Xi_L}\Gamma_n$ can be covered by finitely many unit cubes indexed by the set $\Xi_L \equiv \Xi_L(\Lambda) \subset \mathbb{Z}^d$. The number of required cubes can be bounded by $|\Xi_L| \leqslant \varkappa L^d$ where the constant $\varkappa \equiv \varkappa(\Lambda) > 0$ does not depend on L. We therefore conclude from (2.41) that

$$\|Q_L - Q_{L,0}\|_{p_0}^{p_0} \leqslant 2\gamma\varkappa L^d. \tag{2.50}$$

We will apply the interpolation inequality

$$\|\cdot\|_{p_\theta} \leqslant \|\cdot\|_{p_0}^{1-\theta}\|\cdot\|_{p_1}^{\theta} \qquad \text{with} \quad \frac{1}{p_\theta} = \frac{\theta}{p_1} + \frac{1-\theta}{p_0} \tag{2.51}$$

to von Neumann–Schatten (quasi-) norms. It is valid for every $0 < p_0 \leqslant p_1 < \infty$ and every $\theta \in [0,1]$. We choose $p_\theta := 2s$, $p_1 := 2$ and determine

$$\theta = 1 - \frac{p_0}{s}\,\frac{1-s}{2-p_0}. \tag{2.52}$$

Together with the boundedness of Hilbert–Schmidt norms (2.15), we infer the claim from (2.51) and (2.50). □

Corollary 2.7. Let $d \in \mathbb{N}\backslash\{1\}$ and $\Lambda \subset \mathbb{R}^d$ be as in Assumption 1.1(ii). Let $V \in L^\infty(\mathbb{R}^d)$ have compact support, and fix $E > 0$ and $s \in\ ]d^{-1}, 1]$. Then, we have

$$\|Q_L - Q_{L,0}\|_{2s}^{2s} = o(L^{d-1}) \qquad \text{as } L \to \infty. \tag{2.53}$$

Proof. For $s \in\ ]0,1]$ and $p_0 \in\ ]0,2[$, we observe

$$2d(1-s)/(2-p_0) < d-1 \quad \Longleftrightarrow \quad s > d^{-1} + p_0(d-1)/(2d). \tag{2.54}$$

Now, the claim follows from Lemma 2.6 because p_0 can be chosen arbitrarily close to zero. □

Remark 2.8. We summarize the results of this section in the following structural reformulation of Theorem 2.1, which is independent of the concrete forms of the unperturbed operator H_0 and of the perturbed operator H:

Let H_0 and H be two self-adjoint operators that are bounded below. Consider a Fermi energy $E \in \mathbb{R}$, a bounded subset $\Lambda \subset \mathbb{R}^d$, coefficients $N_0(E,\Lambda) > 0$ and $\Sigma_0(E,\Lambda) > 0$, and a linear functional $h \mapsto I(h)$, defined on test functions h as specified above (1.2) and depending on h only through $h - \mathrm{id}\, h(1)$ and such that

- $I(h) \geqslant 0 \quad whenever\ h \geqslant 0\ and\ h(1) = 0,$
- $\lim_{n\to\infty} I(h_n) = 0 \quad whenever\ \lim_{n\to\infty}\int_0^1 \mathrm{d}\lambda\ |h_n(\lambda)| = 0\ \ and\ h_n|_{\mathcal{N}} = 0$
  for all $n \in \mathbb{N}$ *with an* n*-independent neighbourhood* $\mathcal{N}$ *of both endpoints* 0 *and* 1.

Suppose that given any test function h as specified above (1.2), the asymptotics

$$\operatorname{tr}\{h(1_{\Lambda_L}1_{<E}(H_0)1_{\Lambda_L})\} = N_0(E,\Lambda)h(1)L^d + \Sigma_0(E,\Lambda)I(h)\ L^{d-1}\ln L + o(L^{d-1}\ln L) \tag{2.55}$$

holds as $L\to\infty$. *Assume further that the a-priori-norm bound (2.41) holds for both* H_0 *and* H. *Finally, suppose the validity of (2.15) and of the conclusions of Lemmas 2.3 and 2.4. Then, for every test function* $h \in \mathbb{H}_d$, *we have*

$$\operatorname{tr}\{h(1_{\Lambda_L}1_{<E}(H)1_{\Lambda_L}) - h(1_{\Lambda_L}1_{<E}(H_0)1_{\Lambda_L})\} = o(L^{d-1}\ln L) \tag{2.56}$$

as $L\to\infty$.

DEDICATION

This paper is dedicated to Abel Klein in honor of his numerous fundamental contributions to mathematical physics. As a mentor and friend of P. M., Abel has been a constant source of inspiration to him.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Peter Müller: Conceptualization (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (lead). **Ruth Schulte**: Conceptualization (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (supporting).

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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