SZEGÖ LIMIT THEOREM FOR OPERATORS WITH DISCONTINUOUS SYMBOLS AND APPLICATIONS TO ENTANGLEMENT ENTROPY

DIMITRI GIOEV

Abstract. The main result in this paper is a one term Szegő type asymptotic formula with a sharp remainder estimate for a class of integral operators of the pseudodifferential type with symbols which are allowed to be non-smooth or discontinuous in both position and momentum. The simplest example of such symbol is the product of the characteristic functions of two compact sets, one in real space and the other in momentum space. The results of this paper are used in a study of the violation of the area entropy law for free fermions in [18]. This work also provides evidence towards a conjecture due to Harold Widom.

1. Introduction

The problem of estimating entanglement entropy (EE) is currently of considerable interest in the physics community, in particular in condensed matter physics and in the theory of quantum information. The interest in EE in condensed matter systems is due, in particular, to its scaling behavior and universal properties near quantum phase transitions, see for example [9, 25, 31, 32] and in particular [38]. EE is an accepted measure of entanglement: in the quantum information context, entanglement is necessary for performing quantum computations, see e.g. [5, 44, 29, 4, 30, 37]. An experimental demonstration of entanglement effects in a macroscopic system was reported in [14]. A connection between EE for spin chain models and Random Matrix Theory was found in [23, 24].

The evaluation of EE in physical systems of interest presents considerable mathematical difficulties [12, 22, 21, 13]. In several models EE turns out to be closely related to various versions of the strong Szegő limit theorem (SSLT) for dimension one [22] and also for the higher dimensional case [18], see Remark 2.4 below. More precisely, the asymptotic behavior of EE as the size of the subsystem of interest becomes large for the XX spin chain model with a transverse magnetic field was analyzed rigorously in [22] using a certain Fisher–Hartwig theorem for large Toeplitz determinants established in [1], see also [2, 11] (self-correlations for a translation invariant spin chain can be expressed in terms of Toeplitz determinants). For the more general XY model with a transverse magnetic field, the authors in [21] used the Riemann–Hilbert approach and the steepest descent method to find an explicit expression for EE (in the asymptotic regime where XY \( \rightarrow \) XX, the results in [22] are recovered from the corresponding expression in [21]).

2000 Mathematics Subject Classification. Primary: 81P15, 58J37, 47B35. Secondary: 35S05, 82B10.
Note that the above mentioned results are for the one dimensional case only (we refer the reader e.g. to the references in [21, 34] for further results concerning spin chains and also harmonic chain systems). Much less is known about the higher dimensional case. It was shown in [34] that for the harmonic lattice model the entanglement entropy of a cubic region of size $\lambda$ behaves like $\lambda^{d-1}$, $\lambda \to \infty$, where $d > 1$ is the dimension, i.e. the EE is of the order of the area of the boundary of the cube. In the physics community this type of behavior is referred to as the area law for the entropy. The area law was initially discovered in the context of the so-called geometric entropy, which is a component of the Bekenstein–Hawking black hole entropy, see [6, 35] and the references in [34].

It is known that there is a correspondence between 1D spin models and systems of non-interacting fermions on a 1D lattice by means of the Wigner–Jordan transformation. It is therefore natural to consider EE for fermionic systems in higher dimensions. It was noticed recently [18, 43], that the EE for a system of free fermions of arbitrary dimension on a lattice or in the continuum at zero temperature violates the area law and is, in particular, of larger order than the boundary area of the region in which the entropy is evaluated. In [18] the authors make a connection between the asymptotics of EE and a conjecture due to Widom [41, 42] (see (2.14) below), and then utilize this connection to posit a formula for EE of a continuous system, see (1.4) below. The conjecture of Widom appeared originally in the context of time–frequency limiting problems, i.e. problems that involve the extraction of information about a signal from a measurement in a finite time–finite frequency window.

In [18], some of the results are presented without proof. In this paper, we study Szegö type asymptotics for operators of pseudodifferential type with discontinuous symbols in the higher dimensional case: Various specializations of these asymptotics provide the proofs of most, but not all, of the results left open in [18], as explained below.

To fix ideas we recall first some basic facts concerning EE (see e.g. [3]). Let $H_A, H_B$ be two Hilbert spaces, which we assume for simplicity to be finite dimensional. Using the Schmidt decomposition [33], any state $\psi \in H_A \otimes H_B$ can be expressed in the form $\psi = \sum_i c_i \phi_{A,i} \otimes \phi_{B,i}$, where $0 < c_i \leq 1$, $\sum_i c_i^2 = 1$ and $\phi_{A,i}, \phi_{B,i}$ are orthonormal in $H_A, H_B$, respectively. Associate with $\psi$ the density matrix $\rho = \psi \psi^*$ acting on $H_A \otimes H_B$. The reduced density matrix $\rho_A$ acting on $H_A$ is defined as $\rho_A = \text{Tr}_{H_B} \rho = \sum_i c_i^2 \phi_{A,i} \phi_{A,i}^*$ and similarly $\rho_B = \text{Tr}_{H_A} \rho = \sum_i c_i^2 \phi_{B,i} \phi_{B,i}^*$. It is easy to check that the matrices $\rho_A$ and $\rho_B$ are well-defined independent of the choice of the orthonormal vectors $\phi_{A,i}, \phi_{B,j}$.

The entanglement entropy of a state $\psi \in H_A \otimes H_B$ measures how far the state $\psi$ is from a product state of the form $\phi_A \otimes \phi_B$, and is defined as the von Neumann entropy of either of the reduced density matrices

$$S \equiv - \text{Tr}(\rho_A \log_2 \rho_A) = - \text{Tr}(\rho_B \log_2 \rho_B) = - \sum_i c_i^2 \log_2 c_i^2$$

which is precisely the Shannon entropy of the (squared) Schmidt coefficients $c_i$.

In many problems, one is interested in finding EE for $\psi$ which is the ground state of some general many body system. In [26] the EE of a system of non-interacting (free) fermions in the ground state was studied. We note that the case of a general system with interactions is very difficult and at present time very little seems to be
known for dimensions higher than one (see however [14] and [24] where the area law is derived for the Kitaev model and for the harmonic lattice model, respectively).

Let $\Gamma \subset \mathbb{R}^d$ (resp., $\Gamma \subset \mathbb{T}^d$) denote a compact set in momentum space and fix a compact region $\Omega \subset \mathbb{R}^d$ (resp., $\Omega \subset \mathbb{Z}^d$) in position space for the continuous (resp., lattice) case. The ground state of the system is defined by the projection $P$ in $L^2(\mathbb{R}^d)$ (resp., $l^2(\mathbb{Z}^d)$) onto the modes in the Fermi sea $\Gamma$. We study the entropy of entanglement between fermions located in a compact region $\Omega$, scaled by some large $\lambda$, in position space, and its complement. Let $Q = \chi_{\lambda\Omega}$ be the projection onto $\lambda\Omega$ in $L^2(\mathbb{R}^d)$ (resp., $l^2(\mathbb{Z}^d)$).

For the system at hand, all the important quantities for the entanglement problem can be described in terms of the operator $PQP$ [26]; in particular the average number of fermions in $\lambda\Omega$ is given by $<N> = \text{Tr} PQP$, the particle number variance is

$$(\Delta N)^2 = \text{Tr}[PQP(1 - PQP)]$$

and the EE is given by

$$(1.2) \quad S = S_{\Omega, \Gamma}(\lambda) = \text{Tr} h(PQP)$$

where

$$(1.3) \quad h(t) = -t \log_2 t - (1 - t) \log_2(1 - t).$$

Note that $P = \mathcal{F} \chi_{\Gamma} \mathcal{F}^{-1}$ where $\mathcal{F}$ denotes either the Fourier transform or the Fourier series in the continuous, lattice case, respectively.

Assuming the applicability of the Widom conjecture (2.14) below to the function (1.3) the authors in [18] suggest the following explicit leading order asymptotics for the EE of a continuous system as $\lambda \to \infty$

$$(1.4) \quad S_{\Omega, \Gamma}(\lambda) = \frac{\lambda^{d-1} \log_2 \lambda}{(2\pi)^{d-1}} \frac{1}{12} \int_{\partial\Omega} \int_{\partial\Gamma} |n_x \cdot n_p| dS_x dS_\xi + o(\lambda^{d-1} \log_2 \lambda),$$

where $n_x, n_\xi$ are outward unit normals to the (smooth) boundaries $\partial\Omega, \partial\Gamma$ and $dS_x, dS_\xi$ are the area elements. Although the formula (1.4) was conjectured in [18] only for continuous models with smooth boundaries, it is probably also true for piecewise smooth boundaries in both the continuous and the lattice case. Indeed, (1.4) was recently checked numerically in the lattice case for $d = 2$ in [3] and for $d = 2, 3$ in [28], and an extremely close agreement concerning both the order and the (leading) coefficient was found.

The following two results proven in [18] provide corroborating evidence towards (1.4). For the cubic domains $\Gamma = [-\frac{1}{2}, \frac{1}{2}]^d$ and $\Omega = [0, 1]^d$ (resp., $\Omega = \{0, 1\}^d$) in the continuous (resp., lattice) case, the following holds as $\lambda \to \infty$

$$(1.5) \quad \frac{1}{2} \left( \frac{\lambda}{2\pi} \right)^{d-1} S_1(\lambda) \leq S_{\Omega, \Gamma}(\lambda) \leq d \left( \frac{\lambda}{2\pi} \right)^{d-1} S_1(\lambda)$$

where $S_1(\lambda)$ is the entanglement entropy for the one dimensional system with $\Gamma_1 = [-\frac{1}{2}, \frac{1}{2}]$ and $\Omega_1 = [0, 1]$ (resp., $\{0, 1\}$). We note that (1.5) together with a result in [22] for the lattice case

$$(1.6) \quad S_1(\lambda) = \frac{1}{3} \log_2 \lambda + o(\log_2 \lambda), \quad \lambda \to \infty,$$
implies

\begin{equation}
\frac{1}{6} \left( \frac{\lambda}{2\pi} \right)^{d-1} \log_2 \lambda \leq S_{\Omega,\Gamma}(\lambda) \leq \frac{d}{3} \left( \frac{\lambda}{2\pi} \right)^{d-1} \log_2 \lambda
\end{equation}

thereby demonstrating the violation of the entropy area law for cubic domains in the lattice case in a way which is consistent with (1.4).

In [18] the authors also prove that for arbitrary (measurable) compact \( \Omega, \Gamma \) in both the continuous and lattice cases

\begin{equation}
4(\Delta N)^2 \leq S_{\Omega,\Gamma}(\lambda) \leq C \cdot (\log_2 \lambda) \cdot (\Delta N)^2
\end{equation}

where the constant \( C \) depends only on the dimension \( d \). (The estimate (1.8) for the lattice case with \( d = 1 \) was proved in [12]. The proof of (1.8) in [18] for all \( d \geq 1 \) in the lattice case is analogous, but the continuous case requires a new idea as provided in [18].)

The fact that Theorem 2.1 below is sharp implies, together with (1.1), that in the continuous case if \( \Omega, \Gamma \) have \( C^1 \) boundaries then for some \( c_1, c_2 > 0 \)

\begin{equation}
c_1 \lambda^{d-1} \log_2 \lambda \leq (\Delta N)^2 \leq c_2 \lambda^{d-1} \log_2 \lambda, \quad \lambda \to \infty,
\end{equation}

and also that for any \( \beta \in (0,1) \) there exists (a Cantor-like) set \( \Gamma \) such that for \( \Omega = [0,1]^d \) for some \( c_1, c_2 > 0 \)

\begin{equation}
c_1 \lambda^{d-\beta} \leq (\Delta N)^2 \leq c_2 \lambda^{d-\beta}, \quad \lambda \to \infty.
\end{equation}

The inequalities (1.8), (1.9) yield the following: In the continuous case, if \( \Omega, \Gamma \) have \( C^1 \) boundaries then for some \( c_1, c_2 > 0 \) that depend on \( \Omega, \Gamma \)

\begin{equation}
c_1 \lambda^{d-1} \log_2 \lambda \leq S_{\Omega,\Gamma}(\lambda) \leq c_2 \lambda^{d-1}(\log_2 \lambda)^2, \quad \lambda \to \infty.
\end{equation}

Note that (1.11) proves the violation of the area law in the continuous case for arbitrary domains with \( C^1 \) boundary and also gives the expected order for the lower estimate (and also the expected upper estimate, up to a power of \( \log_2 \lambda \)) consistent with (1.4).

**Remark 1.1.** It was proved independently in [43] that for cubic domains in the lattice case the estimate (1.11) holds. Note that in this case we have the stronger estimate (1.12).

Concerning irregular boundaries, (1.8) together with (1.10) shows that in the continuous case in any dimension \( d \) and for any \( \beta \in (0,1) \), there exists a set \( \Gamma \) so that for \( \Omega = [0,1]^d \) for some \( c_1, c_2 > 0 \)

\begin{equation}
c_1 \lambda^{d-\beta} \leq S_{\Omega,\Gamma}(\lambda) \leq c_2 \lambda^{d-\beta} \log_2 \lambda, \quad \lambda \to \infty.
\end{equation}

Finally, we note that in the one dimensional lattice case the following result is proved in [12]: For any \( \beta_1 \in (0,1) \) there exists a set \( \Gamma_1 \subset \mathbb{T} \) such that for \( \Omega_1 = [0,1] \) for some \( c_1, c_2 > 0 \)

\begin{equation}
c_1 \lambda^{1-\beta_1} \leq S_{\Omega_1,\Gamma_1}(\lambda) \leq c_2 \lambda^{1-\beta_1} \log_2 \lambda, \quad \lambda \to \infty.
\end{equation}

Combining this result with a straightforward generalization of (1.5) to the case \( \Gamma = \Gamma_1^d, \Omega = \Omega_1^d \), we see that (1.12) holds also for the lattice case (where \( \beta = 1-\beta_1 \)).

\footnote{The fractal set \( \Gamma \) in [12] is very similar to the fractal set appearing in Lemma 2.4 below, which was constructed in earlier work of the author, see math.FA/0212215, math.CA/0212254.}
The outline of the paper is as follows: In Section 2, we describe the main results, the proofs of these results together with various technical lemmas are given in Section 3.

2. Main results

We now state the main results of the paper. As noted above, some of these results were used in [13] to estimate EE for certain physical systems.

The problem of evaluating the Szegő type asymptotics for operators of pseudodifferential type with symbols discontinuous in both position and momentum in the higher dimensional case was introduced in [42] (see Remark 2.3 below), we refer also to [40, 27] where certain related results can be found. See e.g., [39] for a more detailed account of the results in this area.

Let $d \in \mathbb{N}$, let $\text{mes}$ denote the Lebesgue measure in $\mathbb{R}^d$, set $H = L^2(\mathbb{R}^d)$ and let $\| \cdot \|_k$ be the standard norm in $L^k(\mathbb{R}^d)$, $k = 1, 2, \infty$. Denote by $\| \cdot \|_{\mathcal{S}_2}$, $\| \cdot \|_{\mathcal{E}_1}$, the operator norm, the Hilbert–Schmidt and the trace-class norm in $H$, respectively. Let $\mathcal{S}(\mathbb{R}^d)$ stand for the Schwartz space and denote by $\int$ the integration over $\mathbb{R}^d$. Let $\mathcal{F}$ and $\hat{}$ denote the Fourier transform: $\mathcal{F}_{x \to u}[g(x)] \equiv \hat{g}(u) = \int e^{-iu \cdot x} g(x) \, dx$, $g \in H$. For a function $g \in L^2(\mathbb{R}^d)$ denote its $L^2$ modulus of continuity by $\omega_2[g](h) = \|g(\cdot + h) - g(\cdot)\|_2$, $h \in \mathbb{R}^d$. For a set $\Omega \subset \mathbb{R}^d$ denote by $\chi_\Omega$ its characteristic function. We characterize the regularity of the set $\Omega$ in terms of $\omega_2[\chi_\Omega]$: assume that $\chi_\Omega \in L^2(\mathbb{R}^d)$ (i.e. $\text{mes}(\Omega) < \infty$) and that there exist $0 < \beta_\Omega \leq 1$ and $c_\Omega > 0$ such that for small enough $|h|$

\begin{equation}
(\omega_2[\chi_\Omega](h))^2 \leq c_\Omega |h|^{2\beta_\Omega}
\end{equation}

where $|h| = \left( \sum_{j=1}^d |h_j|^2 \right)^{1/2}$. Let $\Omega_h = \{ x - h \mid x \in \Omega \}$, $h \in \mathbb{R}^d$. The left-hand side of (2.1) equals

\begin{equation}
\|\chi_\Omega(\cdot + h) - \chi_\Omega(\cdot)\|_2^2 = \text{mes}(\Omega \setminus \Omega_h) + \text{mes}(\Omega \setminus \Omega_{-h}),
\end{equation}

which gives the geometrical meaning of (2.1). Introduce a projection $P : H \to H$ by $(Pg)(x) = \chi_\Omega(x)g(x)$, $x \in \mathbb{R}^d$, $g \in H$. Following [42] we consider a family of integral operators $A_\lambda : H \to H$, $\lambda \geq 2$, of pseudodifferential type with a non-smooth or discontinuous symbol. Let $A_\lambda$, $\lambda \geq 2$, have the kernel

\begin{equation}
K_{A_\lambda}(x,y) = \left( \frac{\lambda}{2\pi} \right)^d \int e^{i\lambda \xi \cdot (x-y)} \sigma(x,y,\xi) \, d\xi
\end{equation}

where $\sigma$ (is measurable and) satisfies the following mild condition: Define

\begin{equation}
\phi(u) = \sup_{x,y} |\mathcal{F}_{\xi \to u}[\sigma(x,y,\xi)]|, \quad \psi(u) = \phi(u)\phi(-u)
\end{equation}

and assume $\psi \in L^1(\mathbb{R}^d)$ and for certain $0 < \beta \leq 1$ and $c > 0$

\begin{equation}
\int_{|u| \geq \rho} \psi(u) \, du \leq c\rho^{-\beta}, \quad \rho \geq 1.
\end{equation}

See Remark 2.5 below for an example of such $\sigma$. Setting $\lambda = h^{-1}$, $h > 0$, in (2.4) we can obtain semiclassical type asymptotics. We study the asymptotics of the trace of

\begin{equation}
Pf(PA_\lambda P) - Pf(A_\lambda)P,
\end{equation}

as $\lambda \to \infty$, for suitable functions $f$. For the particular choice $\sigma(x,y,\xi) = \chi_\Gamma(\xi)$, $\Gamma \subset \mathbb{R}^d$, such a study is motivated by the following question: what can be said
about a function if its restriction to \( \Omega \) and the restriction of its Fourier transform to \( \Gamma \) are known, see [12]. An order sharp estimate for the trace of (2.6) is found in Theorem 2.2 below in two settings; we assume either that \( f \) is analytic, or \( A_\lambda \) is self-adjoint and \( f \) has a bounded second derivative. Theorem 2.2 is a generalization of the classical Szeg"{o} limit theorem [36], see e.g., [39, 27] for a review of related results. Let \( \log \) denote the natural logarithm. The following result is basic for the proof of Theorem 2.2.

**Theorem 2.1.** Let \( \beta, \sigma, A_\lambda, \Omega \) be as above. Then there exist two constants \( c(\Omega, \sigma) \) and \( C(\Omega, \sigma) \) such that one has, for \( \lambda \geq 2 \),

\[
\| P A_\lambda \|_2^2 \leq c(\Omega, \sigma) \cdot \lambda^d,
\]

and

\[
\| P A_\lambda (I - P) \|_2^2 \leq C(\Omega, \sigma) \cdot \begin{cases} \lambda^{d - \min(\beta, \beta_\Omega)}, & \beta \neq \beta_\Omega \\ \lambda^{d - \beta} \log \lambda, & \beta = \beta_\Omega. \end{cases}
\]

and the same estimate holds for \( \|(I - P) A_\lambda P \|_2^2 \). The estimate (2.8) is sharp on the described class of \( \sigma \), that is for a certain \( \sigma \) (which can be chosen so that the corresponding \( A_\lambda \) is self-adjoint), the reverse inequality to (2.8) holds for some (different) constant \( C(\Omega, \sigma) \).

For an analytic on some disc \( f(z) = \sum_{m=0}^\infty c_m z^m \) set

\[
f_*(z) = \sum_{m=2}^\infty m(m - 1)|c_m|z^{m-2}
\]

and

\[
S(\sigma) = \sup_{\lambda \geq 2} \| A_\lambda \|.
\]

The condition \( S(\sigma) < \infty \) holds for a wide class of \( \sigma \), see Remark 2.5 below.

**Theorem 2.2.** Let the assumptions of Theorem 2.1 hold. Assume further that either

(i) \( S(\sigma) < \infty \) and \( f \) is analytic on a neighborhood of \( \{ z : |z| \leq S(\sigma) \} \), or

(ii) \( A_\lambda \) is self-adjoint for all \( \lambda \geq 2 \), and \( f \) is such that \( f'' \in L^\infty(\mathbb{R}) \).

Then the operator (2.6) is trace-class. Moreover, there exists a constant \( C(\Omega, \sigma) \) such that one has, for \( \lambda \geq 2 \),

\[
\left| \text{Tr} \left[ Pf(P A_\lambda P) - Pf(A_\lambda) P \right] \right| \leq C(\Omega, \sigma) \cdot \tilde{C}(f) \cdot \begin{cases} \lambda^{d - \min(\beta, \beta_\Omega)}, & \beta \neq \beta_\Omega \\ \lambda^{d - \beta} \log \lambda, & \beta = \beta_\Omega, \end{cases}
\]

where

\[
\tilde{C}(f) = \frac{1}{2} \cdot \begin{cases} f_*(S(\sigma)), & \text{in case (i)} \\ \| f'' \|_\infty, & \text{in case (ii)}. \end{cases}
\]

In both cases, the estimate (2.11) is sharp, that is for certain \( f \) and \( \sigma \), the reverse inequality to (2.11) holds for some (different) constant \( C(\Omega, \sigma) \).

In the case of analytic \( f \) we prove slightly more, namely that the sharp estimate (2.11) holds with the trace-class norm of (2.6) in the left-hand side. See subsections 3.1 and 3.2 for the proofs of Theorem 2.1 and Theorem 2.2 respectively. It is possible to compute the leading term in the asymptotics of \( \text{Tr} Pf(P A_\lambda P) P \) in certain special cases.
Corollary 2.3. (i) Let \( \Omega \) and \( \Gamma \) be two bounded domains with \( C^\infty \) boundaries. Assume that the symbol \( \sigma \) does not depend on \( y \), and that \( \sigma(x, \xi) = \tau(x, \xi) \chi_\Gamma(\xi) \), where \( \tau \in \mathcal{S}(\mathbb{R}^d) \). Let \( f \) be analytic on a neighborhood of the disc \( \{ z : |z| < \frac{1}{\|\tau\|_\infty} \} \) and satisfy \( f(0) = 0 \). Then the operator \( f(PA_\lambda P) \) is trace-class, and furthermore, for any small enough \( \epsilon > 0 \) there exist two constants \( C(\Omega, \Gamma, \tau, \epsilon) \) and \( \Lambda(\epsilon) \geq 2 \) so that, for \( \lambda \geq \Lambda(\epsilon) \),

\[
\left| \operatorname{Tr} f(PA_\lambda P) - \left( \frac{\lambda}{2\pi} \right)^d \int_\Gamma \int_\Omega f(\tau(x, \xi)) \, dx \, d\xi \right| \leq C(\Omega, \Gamma, \tau, \epsilon) \cdot f_*(\|\tau\|_\infty) \cdot \lambda^{d-1} \log \lambda.
\]

(ii) Let \((2.11)\) hold and assume that the symbol \( \sigma \) is real-valued, depends only on \( \xi \) and \((2.3)\) holds. Let \( f'' \in L^\infty([-\|\sigma\|_\infty, \|\sigma\|_\infty]) \) and assume \( f(\sigma(\xi)) \in L^1(\mathbb{R}^d) \). Then \( f(PA_\lambda P) \) is trace-class and there exists a constant \( C(\Omega, \sigma) \) such that, for \( \lambda \geq 2 \),

\[
\left| \operatorname{Tr}(Pf(PA_\lambda P)P) - \left( \frac{\lambda}{2\pi} \right)^d \operatorname{mes}(\Omega) \int f(\sigma(\xi)) \, d\xi \right| \leq C(\Omega, \sigma) \cdot \|f''\|_\infty \cdot \left\{ \begin{array}{ll} \lambda^{d-\min(\beta, \beta_0)}, & \beta \neq \beta_0 \vspace{1mm} \\ \lambda^{d-\beta} \log \lambda, & \beta = \beta_0. \end{array} \right.
\]

The proof of part (i) follows from the functional calculus results developed in [12], see subsection 3.3. Part (ii) is proved as follows. Under the above assumptions \( A_\lambda \) is self-adjoint, \( \lambda \geq 2 \), and also the operator \( f(A_\lambda) \) is well-defined and has the kernel

\[
K_{f(A_\lambda)}(x, y) = \left( \frac{\lambda}{2\pi} \right)^d \int e^{i\lambda \xi \cdot (x-y)} f(\sigma(\xi)) \, d\xi.
\]

The operator \( Pf(A_\lambda)P \), \( \lambda \geq 2 \), is trace-class since it is a composition of two Hilbert–Schmidt operators \( PF^{-1}|f|^{1/2}F, \quad F^{-1}|f|^{1/2}(\text{sgn} f)FP \). Note also that \( K_{f(A_\lambda)}(x, y) \) is continuous, since \( f(\sigma(\xi)) \in L^1(\mathbb{R}^d) \). Now we simply write the trace of \( Pf(A_\lambda)P \) as the integral of its kernel over the diagonal.

Remark 2.1. Let \( \chi_\Omega, \chi_\Gamma \) satisfy \((2.10)\) below with \( 0 < \beta_0, \beta \leq 1 \), respectively, and set \( \sigma(x, y, \xi) = \chi_\Gamma(\xi) \) (this example is considered in the proof of Theorem 2.4). The order sharp remainder estimate in \((2.13)\) for \( \beta_0 \neq \beta \) shows that the set with less regular boundary contributes to the order of the remainder. In the case \( \beta_0 = \beta \) the logarithmic factor persists even for \( \Omega, \Gamma \) with \( C^\infty \) boundaries (in which case \( \beta_0 = \beta = 1 \)) due to the fact that the symbol \( \chi_\Omega(x) \chi_\Gamma(\xi) \chi_\Omega(y) \) has discontinuities in both the position variables \( x, y \) and the momentum variable \( \xi \). (This should be compared with the power type asymptotics in e.g. [27] when a discontinuity in momentum only is present.)

Remark 2.2. The leading term \( \operatorname{Tr} Pf(A_\lambda)P \) in the asymptotics of \( \operatorname{Tr} Pf(PA_\lambda P)P \) in \((2.12)\) and \((2.13)\) is of Weyl type. It is written as an integral over the diagonal \((x, x, \xi)\) of the corresponding to \( \lambda \) phase volume.

Remark 2.3. In \((2.11)\) the following second order generalization of \((2.24)\) was conjectured: Under the assumptions of Corollary 2.3(i) the following holds, as
\[ \lambda \to \infty \]

\[
\text{Tr } f(P A_\lambda P) = \left( \frac{\lambda}{2\pi} \right)^d \int_{\Omega} \int_{\Gamma} f(\tau(x, \xi)) \, dx d\xi \\
+ \left( \frac{\lambda}{2\pi} \right)^{d-1} \log \lambda \frac{4\pi^2}{d} \int_{\partial \Omega} \int_{\partial \Gamma} |n_x \cdot n_p| U(0, \tau(x, \xi); f) \, dS_x dS_\xi \\
+ o(\lambda^{d-1} \log \lambda)
\]

where \( n_x, n_\xi \) are the outward unit normals to \( \partial \Omega, \partial \Gamma \), respectively, and

\[
U(a, b; f) = \int_0^1 \frac{f((1 - t)a + tb) - [(1 - tf) + tf(b)]}{t(1 - t)} \, dt.
\]

This conjecture is still open and it was one of the motivations for the present work.

**Remark 2.4.** In a broader context, the Widom conjecture \[2.14\] is a generalization of the strong (two-term) Szegö limit theorem (SSLT) for the continuous setting. (As noted earlier, a generalization of the SSLT plays a central role in the computation of the EE for the XX spin chain model in \[22\].) The SSLT was initially used by Onsager in his celebrated computation of the spontaneous magnetization for the 2D Ising model (see e.g. \[7\] and the references therein). It is interesting to note that in Onsager’s computation (and also in \[22\]) the leading asymptotic term vanishes, and one needs to compute the sub-leading term. This is exactly the situation in \[13\]: the leading term should vanish since for the entropy function \( h \) in \[13\], \( h(1) = 0 \) (and also \( h(0) = 0 \) holds).

**Remark 2.5.** Let \( \Gamma \subset \mathbb{R}^d \) be such that for some \( 0 < \beta \leq 1 \) the function \( \chi_\Gamma \) satisfies \[2.4\] with \( \gamma = \beta \) (see also Lemmas \[2.4, 2.5\] below). Set \( \sigma(x, y, \xi) = \tau(x, y, \xi) \chi_\Gamma(\xi) \), where \( \tau \) is satisfies for some \( c = c(\tau) < \infty \)

\[
\sup_{x, y} \left| \mathcal{F}_{\xi \to u} \tau(x, y, \xi) \right| \leq c (1 + |u|)^{d-1}, \quad u \in \mathbb{R}^d.
\]

A standard application of the Cauchy inequality implies that there is \( C = C(\tau, d) < \infty \) so that \( \psi(u) \leq C \int |\hat{\chi}_\Gamma(u - v)|^2 (1 + |v|)^{-d-1} \, dv \in L^1(\mathbb{R}^d) \), and \[2.5\] holds (see, for instance, \[13\] Section 3.4.2). For \( \sigma(x, y, \xi) = \chi_\Gamma(\xi) \) we can take \( \psi(u) = |\hat{\chi}_\Gamma(u)|^2 \). Now for \[2.10\]. If \( \sigma(x, y, \xi) \) is a classical zeroth order (parameter dependent) symbol in the sense of pseudodifferential operators, then \( S(\sigma) < \infty \) is a standard result, see e.g. \[10, 12\]. However we are interested here in \( \sigma \) with limited regularity for which no such general results are available. We restrict ourselves to the following standard example in which irregularities in \( x \) and, most importantly, in \( \xi \) are allowed. Assume \( \sigma = \sigma(x, \xi) \) (we only need \( S(\sigma) < \infty \) when \( A_\lambda \) is not assumed to be self-adjoint) is of the form \( \tau(x, \xi) \chi(\xi) \). Then \( A_\lambda = \tilde{A}_\lambda \mathcal{F}^{-1} \chi \mathcal{F} \) where \( \tilde{A}_\lambda \) has integral kernel \( \left( \frac{4\pi}{2\pi} \right)^d e^{i\lambda(x - y) - \xi \tau(x, \xi)} \, d\xi \). Assume that \( \chi \in L^\infty(\mathbb{R}^d) \), then \( \|\mathcal{F}^{-1} \chi \mathcal{F}\| \leq \|\chi\|_\infty \) (the factor \( \chi \) is allowed to be quite irregular). Now \( \sup_{\lambda > 2} \|\tilde{A}_\lambda\| < \infty \) follows from the standard estimate for the bilinear form under the sole assumption that \( \tilde{\phi}(u) = \sup_x |\mathcal{F}_{\xi \to u} \tau(x, \xi)| \in L^1(\mathbb{R}^d) \). Indeed, by the Cauchy inequality for any
(2π)^d |(A_λ f, g)| \leq |λ|^d \int \int \tilde{φ}(λ(x-y)) |f(y)||g(x)| \, dx \, dy \\
\leq \left( |λ|^d \int \int \tilde{φ}(λ(x-y)) |f(y)|^2 \, dx \, dy \right)^{1/2} \left( |λ|^d \int \int \tilde{φ}(λ(x-y)) |g(x)|^2 \, dx \, dy \right)^{1/2} \\
\leq \|\tilde{φ}\|_1 \|f\|_2 \|g\|_2

which implies \( S(σ) \leq (2π)^{-d} \|\tilde{φ}\|_1 \). Note that if \( σ(x, ξ) = τ(x, ξ)χ_Γ(ξ) \) where Γ is as before, and \( \sup_x |F_{ξ→u}τ(x, ξ)| \leq c (1 + |u|)^{-d-1} \) as in (2.15), then both (2.5) and \( S(σ) < \infty \) hold.

In the proof of Theorem 2.1 we use the following auxiliary results. They are concerned with a two-sided version of the estimate (2.1): assume that \( g \in L^2(\mathbb{R}^d) \) is such that there exist \( 0 < γ < 2 \) and \( c_1, c_2 > 0 \) so that for small enough \( |h| \)

\[(2.16)\]
\[c_1|h|^γ \leq (ω_2|g|(h))^2 \leq c_2|h|^γ.\]

**Lemma 2.4.** For any \( d ∈ \mathbb{N} \) and \( 0 < β_1 \leq 1 \) there exists a compact set \( Ω ⊂ \mathbb{R}^d \) such that \( χ_Ω \) satisfies (2.16) with \( γ = β_1 \).

**Lemma 2.5.** Assume that a function \( f \in L^2(\mathbb{R}^d) \) satisfies (2.16) for some \( 0 < γ < 2 \) and \( c_1, c_2 > 0 \). Then

(i) there exist \( b_1, b_2 > 0 \) such that

\[(2.17)\]
\[b_1 ρ^{-γ} \leq \int_{|ξ| ≥ ρ} |\hat{f}(ξ)|^2 \, dξ \leq b_2 ρ^{-γ}, \quad ρ ≥ 1;\]

(ii) the upper estimate in (2.16) implies the upper estimate in (2.17).

Lemma 2.4 is proved in subsection 3.1. Lemma 2.5 for \( γ = 1 \) was proved in [10, Lemma 2.10, 4.2], the proof for \( γ ∈ (0, 2) \) is analogous and is left to the reader, see also [17] and [15, Lemma 3.4.1]. (If one introduces an average of \( ω_2|g|(h) \) over \( \|h\|_d \leq ε \), then the upper estimates in this modification of (2.16), and in (2.17) become equivalent, and so do the lower ones, see [10, 17].)

3. Proofs

3.1. **Proof of Theorem 2.1** We denote \( λ \)-independent constants (that may depend on \( Ω, σ \)) by \( c_k, k \in \mathbb{N} \). Let us consider \( \|PA_λ(I - P)\|_{ℓ^2} \) only, the case of \( \|(I - P)A_λ P\|_{ℓ^2} \) is completely analogous.

1. Let us prove first the upper estimate (2.8). Using (2.4) we obtain

\[(3.1)\]
\[\|PA_λ(I - P)\|_{ℓ^2}^2 = (\frac{λ}{2π})^{2d} \int \int \int \int e^{iλξ(x-y)} e^{-iλη(x-y)} σ(x, y, ξ) \bar{σ}(x, y, η) \chi_Ω(x) (1 - χ_Ω(y)) \, dξ \, dy \, dη \, dx \]
\[\times \chi_Ω(ξ) (1 - χ_Ω(η)) \, dx \, dy \]
\[= (\frac{λ}{2π})^{2d} \int \int \int \int \psi(λ(x-y)) σ(x, y, ξ) \bar{σ}(x, y, η) \chi_Ω(x) (1 - χ_Ω(y)) \, dx \, dy \]
\[≤ (\frac{λ}{2π})^{2d} \int \int \int \psi(λ(x-y)) \chi_Ω(x) [1 - χ_Ω(y)] \, dx \, dy.\]
Changing variables $x - y = 2x'$, $x + y = 2y'$ and dropping the primes we rewrite the right-hand side of (3.1) in the form

$$\left(\frac{\lambda}{2\pi}\right)^{2d} \int \psi(2\lambda x) \, dx \int \chi_\Omega(x + y) \left[1 - \chi_\Omega(-x + y)\right] \, dy.$$

(3.2)

Since $\chi_\Omega$ takes on values 0 or 1 only, we have

$$\int \chi_\Omega(x + y) \left[1 - \chi_\Omega(-x + y)\right] \, dy = \|\chi_\Omega\|^2 - \int \chi_\Omega(x + y) \chi_\Omega(-x + y) \, dy$$

$$= \frac{1}{2} \left|\int \chi_\Omega(x + y) - \chi_\Omega(-x + y)\right|^2 \, dy = \frac{1}{2} \left(\omega_2[\chi_\Omega](2x)\right)^2.$$

(3.3)

Therefore (3.1) and (3.2) imply

$$\text{PA}_\lambda(I - P)^3 \leq \lambda^{2d} c_1 \int \psi(2\lambda x) \left(\omega_2[\chi_\Omega](2x)\right)^2 \, dx$$

(3.4)

Using (2.1) and making a change of variables $u = 2\lambda x$ we estimate the first integral in (3.3) as follows

$$\lambda^{2d} c_1 \int_{|x| \leq 1/\lambda} \psi(2\lambda x) \left(\omega_2[\chi_\Omega](2x)\right)^2 \, dx \leq \lambda^{2d} c_2 \int_{|x| \leq 1/\lambda} \psi(2\lambda x) |x|^\beta_0 \, dx$$

(3.5)

$$\leq \lambda^{d-\beta_0} c_3 \int_{|u| \leq 2} \psi(u)|u|^\beta_0 \, du \leq \lambda^{d-\beta_0} c_4 \|\psi\|_1, \quad \lambda \geq 2.$$

Next, noting that $\left(\omega_2[\chi_\Omega](2x)\right)^2 \leq 2\|\chi_\Omega\|^2 = 2\beta_0(\Omega)$, setting $u = 2\lambda x$ and using (2.4) we estimate the third integral in (3.3) in the following way

$$\lambda^{2d} c_1 \int_{|x| \geq 1} \psi(2\lambda x) \left(\omega_2[\chi_\Omega](2x)\right)^2 \, dx \leq 2 \beta_0(\Omega) \lambda^{2d} \int_{|x| \geq 1} \psi(2\lambda x) \, dx$$

(3.6)

Consider now the second integral in (3.3). Set $\Psi(r) = \int_{\Omega_{d-1}} \psi(r \theta) \, dS_\theta$, $r \geq 1$, and note that by (2.5)

$$\int_r^\infty \Psi(s) \, s^{d-1} \, ds \leq c r^{-\beta}, \quad r \geq 1.$$

Then the second integral in (3.3) is estimated as follows

$$\lambda^{2d} c_1 \int_{1/\lambda \leq |x| \leq 1} \psi(2\lambda x) \left(\omega_2[\chi_\Omega](2x)\right)^2 \, dx \leq \lambda^{d-\beta_0} c_7 \int_{2 \leq |u| \leq 2\lambda} \psi(u)|u|^\beta_0 \, du$$

(3.7)

$$= \lambda^{d-\beta_0} c_7 \int_2^{2\lambda} \Psi(r) r^{\beta_0 + d - 1} \, dr.$$

Writing $\Psi(r) = -\frac{1}{\beta_0} \frac{d}{dr} \int_r^\infty \Psi(s) \, s^{d-1} \, ds$ and integrating by parts we obtain

$$\lambda^{d-\beta_0} c_7 \int_2^{2\lambda} \Psi(r) r^{\beta_0 + d - 1} \, dr = \lambda^{d-\beta_0} c_7 \left[2^{2\beta_0} \int_2^\infty \Psi(s) \, s^{d-1} \, ds \right.$$

$$- 2^{\beta_0} \beta_0 \int_2^\infty \Psi(s) \, s^{d-1} \, ds + \beta_0 \int_2^{2\lambda} \left(\int_r^\infty \Psi(s) \, s^{d-1} \, ds\right) r^{\beta_0 - 1} \, dr \right].$$
Discarding the negative term above and using \( \Omega \) we obtain
\[
\lambda^{d-\beta_\Omega} c_7 \int_2^{2^\lambda} \Psi(r) r^{\beta_\Omega + d - 1} dr \leq \lambda^{d-\beta_\Omega} c_8 \cdot \left( 1 + \begin{cases} 1, & \beta_\Omega < \beta \\ \log \lambda, & \beta_\Omega = \beta \\ \lambda^{\beta_\Omega - \beta}, & \beta_\Omega > \beta \end{cases} \right)
\]
\[
\leq c_9 \cdot \left\{ \begin{array}{ll}
\lambda^{d-\min(\beta, \beta_\Omega)}, & \beta \neq \beta_\Omega \\
\lambda^{d-\beta} \log \lambda, & \beta = \beta_\Omega.
\end{array} \right.
\]
Substituting the latter estimate in (3.7) and collecting the estimates (3.4), (3.5) we complete the proof of (2.8).

2. Let us now prove the sharpness of the estimate (2.8). We choose arbitrary \( 0 < \beta_\Omega, \beta \leq 1 \). By Lemma 2.4 there exist two sets \( \Omega, \Gamma \) such that \( \chi_{\Omega}, \chi_{\Gamma} \in L^2(\mathbb{R}^d) \) satisfy the two-sided estimate (2.10) with the power \( \beta_\Omega \) and \( \beta \), respectively. Set \( \sigma(x,y,\xi) = \chi_{\Gamma}(\xi) \) (then the corresponding \( A_\lambda \) is self-adjoint) and let \( \psi(u) = |\chi_{\Gamma}(u)|^2 \). Apply Lemma 2.4(i) to \( \chi_{\Gamma} \). Then for some \( b_1, b_2 > 0 \), \( b_1 \rho^{-\beta} \leq \int_{|u| \geq \rho} \psi(u) du \leq b_2 \rho^{-\beta} \) for \( \rho \geq 1 \). Let \( \kappa \) be such that \( b_2 \kappa^{-\beta} < \frac{b_1}{2} \) and \( \kappa > 1 \). Then
\[
\frac{b_1}{2} \rho^{-\beta} \leq \int_{\rho \leq |u| \leq \kappa \rho} \psi(u) du, \quad \rho \geq 1.
\]

In place of (3.1) we now have an equality and therefore
\[
\| P A_\lambda (I - P) \|_{\mathfrak{E}_2}^2 = \lambda^{2d} c_{10} \int \psi(2\lambda x) \left( \omega_2[\chi_{\Omega}](2x) \right)^2 dx
\]
\[
\geq \lambda^{2d} c_{10} \int_{1/\lambda \leq |x| \leq 1} \psi(2\lambda x) \left( \omega_2[\chi_{\Omega}](2x) \right)^2 dx
\]
\[
\geq \lambda^{2d} c_{11} \int_{1/\lambda \leq |x| \leq 1} \psi(2\lambda x) |x|^{\beta_\Omega} dx
\]
\[
\geq \lambda^{d-\beta_\Omega} c_{12} \int_{2 \leq |x| \leq 2\lambda} \psi(u)|u|^{\beta_\Omega} du
\]
where we have used the lower estimate in (2.10) for \( \chi_{\Omega} \). Let \( \lambda \geq \kappa \), set \( L = \lfloor \log_\kappa \lambda \rfloor \) where \( \lfloor . \rfloor \) denotes the integer part of a number. Now we split the domain of integration as a union of concentric domains in the standard way (see e.g. [8])
\[
\lambda^{d-\beta_\Omega} c_{12} \int_{2 \leq |x| \leq 2\lambda} \psi(u)|u|^{\beta_\Omega} du \geq \lambda^{d-\beta_\Omega} c_{12} \sum_{l=0}^L \int_{2\kappa^l \leq |u| \leq \kappa(2\kappa^l)} \psi(u)|u|^{\beta_\Omega} du
\]
\[
\geq \lambda^{d-\beta_\Omega} c_{12} \sum_{l=0}^L (2\kappa^l)^{\beta_\Omega} \cdot \frac{b_1}{2} (2\kappa^l)^{-\beta}
\]
\[
= \lambda^{d-\beta_\Omega} c_{13} \sum_{l=0}^L (\kappa^{\beta_\Omega - \beta})^l
\]
where we have used (3.8). Considering the three cases when \( \beta_\Omega \) is smaller than, equal to, and greater than \( \beta \) separately, and using the fact that \( \kappa^{-1} \lambda < \kappa^L \leq \lambda \) together with (3.9) we conclude that for the operator \( A_\lambda \)
\[
\| PA_\lambda (I - P) \|_{\mathfrak{E}_2} \geq c_{14} \cdot \begin{cases} \lambda^{d-\min(\beta, \beta_\Omega)}, & \beta \neq \beta_\Omega \\
\lambda^{d-\beta} \log \lambda, & \beta = \beta_\Omega
\end{cases}
\]
for \( \lambda \geq \kappa \). The sharpness of the estimate (2.8) is proved.

3. Finally we prove (2.7). Analogously to (3.1), (3.2) we obtain

\[
\|PA_\lambda\|^2_{\mathcal{S}_2} \leq \left( \frac{\lambda}{2\pi} \right)^{2d} \int \psi(2\lambda x) dx \int \chi_\Omega(x+y) \chi_\Omega(-x+y) dy
\leq (2\pi)^{-2d} 2^{-d} \|\psi\|_1 \text{mes}(\Omega) \cdot \lambda^d,
\]

for all \( \lambda \geq 2 \). This finishes the proof of Theorem 2.1.

3.2. Proof of Theorem 2.2. It is important that in both cases the fact \( PA_\lambda \in \mathcal{S}_2 \) implies that the operator (2.6) is trace-class, and also that in this case the absolute value of the trace of (2.6) can be estimated as follows: there exists a constant \( C(\Omega, \sigma) \) such that one has, for \( \lambda \geq 2 \),

(3.11)

\[
\text{Tr} \left[ Pf(PA_\lambda P) - Pf(A_\lambda P) \right] \leq C(\Omega, \sigma) \cdot \tilde{C}(f) \cdot \|PA_\lambda(I-P)\|_{\mathcal{S}_2} \cdot \|(I-P)A_\lambda P\|_{\mathcal{S}_2}.
\]

In the case of self-adjoint \( A_\lambda \), (3.11) was proved in [27, Theorem 1.2] (note that \( \cup_{0 \leq k \leq 1} \cup_{\lambda \geq 2} \text{spec} \ A_\lambda \subset \mathbb{R} \)). In the case of analytic \( f \), the idea of the proof goes back to [10]. More precisely, denote \( Q = I - P \) and note that for any \( m \in \mathbb{N}, m \geq 2 \) we can write

\[
PA_\lambda^m P = PA_\lambda(P + Q)A_\lambda^{m-1} P = PA_\lambda(P + Q)A_\lambda^{m-2} P + (PA_\lambda)QA_\lambda^{m-1} P
= P(A_\lambda P)^{m-1}(P + Q)A_\lambda P + (PA_\lambda)QA_\lambda^{m-1} P
\]

(3.12)

\[
= P(A_\lambda P)^{m-2}A_\lambda^{m-2} P + (PA_\lambda)^2QA_\lambda^{m-2} P + (PA_\lambda)QA_\lambda^{m-1} P = \cdots =
\]

\[
= P(A_\lambda P)^m + \sum_{j=1}^{m-1} (PA_\lambda)^{m-j} QA_\lambda^j P.
\]

Also for \( j \geq 2 \)

\[
A_\lambda^j P = A_\lambda^{j-1}(P + Q)A_\lambda P = A_\lambda^{j-1}PA_\lambda P + A_\lambda^{j-1}QA_\lambda P
= A_\lambda^{j-2}(P + Q)A_\lambda PA_\lambda P + A_\lambda^{j-1}QA_\lambda P
\]

(3.13)

\[
= A_\lambda^{j-2}(PA_\lambda)^2 P + A_\lambda^{j-2}Q(A_\lambda P)^2 + A_\lambda^{j-1}QA_\lambda P = \cdots =
\]

\[
= A_j(PA_\lambda)^{j-1} P + \sum_{k=1}^{j-1} A_k^j Q(A_\lambda P)^{j-k} P.
\]

Substituting (3.13) in (3.12) we obtain

(3.14)

\[
P(A_\lambda)^m P - (PA_\lambda)^m = \sum_{j=1}^{m-1} (PA_\lambda)^{m-j} QA_\lambda^j P
\]

\[
= \sum_{j=1}^{m-1} (PA_\lambda)^{m-j} QA_\lambda(PA_\lambda)^{j-1} P + \sum_{j=2}^{m-1} (PA_\lambda)^{m-j} Q \sum_{k=1}^{j-1} A_k^j Q(A_\lambda P)^{j-k} P.
\]

There are \( \frac{m(m-1)}{2} \) terms on the right-hand side in (3.14) each containing both \( PA_\lambda Q \) and \( QA_\lambda P \). Hence

(3.15)

\[
\|(PA_\lambda P)^m - P(A_\lambda)^m P\|_{\mathcal{S}_1} \leq \frac{m(m-1)}{2} \|A_\lambda\|^{m-2} \|PA_\lambda Q\|_{\mathcal{S}_2} \|QA_\lambda P\|_{\mathcal{S}_2}.
\]
Recall (3.11) and note that (3.11) (even with \( \| Pf(PA_\lambda P)P - Pf(A_\lambda P) \|_{\mathcal{S}_1} \) in the left-hand side) holds for any \( f(z) \) analytic on a neighborhood of \( \{ z : |z| \leq S(\sigma) \} \).

Note finally that for \( f(z) = z^2 \) and a self-adjoint \( A_\lambda \)

\[
\text{Tr} [ Pf(PA_\lambda P)P - Pf(A_\lambda P) ] = \| PA_\lambda (I - P) \|_{\mathcal{S}_2}^2
\]

This together with the sharpness in Theorem 2.1 implies sharpness in Theorem 2.2

3.3. Proof of Corollary 2.3. We need to prove the case (i). By Theorem 2.2 we only have to analyze \( \text{Tr}(Pf(A_\lambda P), f \) analytic. We use the functional calculus developed in [12]. Denote by \( \text{op} \tau \) the depending on the parameter \( \lambda \geq 2 \) operator with integral kernel \((2\pi)^{-d} \int e^{i\xi \cdot (x-y)} \tau(x, \xi/\lambda) \, d\xi \) and let \( Q_{\lambda \Gamma} = \text{op} \lambda \Gamma \cdot (\xi) \). Then \( A_\lambda = (\text{op} \tau) Q_{\lambda \Gamma} \). By [12, Lemma D(iii)] for any \( \epsilon > 0 \) there is a constant \( \Lambda(\epsilon) \geq 2 \) such that for all \( \lambda \geq \Lambda(\epsilon) \)

\[
\| A_\lambda \| \leq (1 + \epsilon) \| \tau \|_{\mathcal{S}_1}.
\]

Next, by [12, Lemma 2], for any \( \epsilon > 0 \) there exist \( C(\epsilon) \) and \( \Lambda(\epsilon) \geq 2 \) such that for all \( m \in \mathbb{N} \) and \( \lambda \geq \Lambda(\epsilon) \)

(3.16) \[
\| P(A_\lambda)^m P - P(\text{op} \tau^m) Q_{\lambda \Gamma} P \|_{\mathcal{S}_1} \leq C(\epsilon) (1 + \epsilon)^m \| \tau \|_{\mathcal{S}_1}^m \cdot \lambda^{d-1}.
\]

Clearly \( \text{Tr}(P(\text{op} \tau^m) Q_{\lambda \Gamma} P) = \left( \frac{\lambda}{2\pi} \right)^d \int \int_{\Omega} (\tau(x, \xi))^m \, dx \, d\xi \). By the argument [12, p. 184], as \( \lambda \to \infty \)

\[
\text{Tr}(P(f(\text{op} \tau)) Q_{\lambda \Gamma} P) = \left( \frac{\lambda}{2\pi} \right)^d \int \int_{\Omega} f(\tau(x, \xi)) \, dx \, d\xi + O(\lambda^{d-1}).
\]

Now for any \( f(z) = \sum_{m=1}^{\infty} c_m z^m \) analytic on a neighborhood of \( \{ z : |z| \leq \| \tau \|_{\mathcal{S}_1} \} \) we have \( c_m = O((1 + \delta)^{-m} \| \tau \|_{\mathcal{S}_1}^m) \) for some \( \delta > 0 \). Taking \( \epsilon < \delta \) in (3.16) finishes the proof of Corollary 2.3

3.4. Proof of Lemma 2.4. We start with \( d = 1 \). Here we write \( \beta = \beta_0 \) for brevity and denote the Lebesgue measure in \( \mathbb{R} \) by \( m_{\mathbb{R}} \). The case \( \beta = 1 \) is trivial, any finite interval with non-empty interior would do. Let us therefore assume \( 0 < \beta < 1 \). We construct a set \( \Omega \) with the required properties as a (finite union of sets each of which is a) countable union of closed intervals obtained by a process similar to the construction of a Cantor set. The difference is that we do not remove but rather add intervals. Let \( 0 < \alpha < \infty, I_\alpha = [0, \alpha] \) and \( 0 < q < 1 \). We explain how \( q \) is related to the given \( \beta \) later. We construct the set \( \Omega_\alpha \) as follows. We start with an empty set and at the \( i \)th step we add the middle \( q^i \)th part of \( I_\alpha \) to \( \Omega_\alpha \). Each of the remaining intervals has length \( \alpha Q \), where we denote \( Q = \frac{1}{q} \). Note that \( 0 < Q < \frac{1}{2} \). Then we take the middle \( q^i \)th part of each of the two remaining intervals and do not add it to the set \( \Omega_\alpha \). Each of the four remaining intervals has length \( \alpha Q^2 \). Now we take the \( q^i \)th middle part of each of the four intervals and add it to \( \Omega_\alpha \). This completes the 1st step of the construction of \( \Omega_\alpha \). We continue in this manner. The set \( \Omega_\alpha \) we obtain has the following properties:

1. For each \( k \in \mathbb{N} \), it contains \( 2^{2k} \) intervals of length \( \alpha Q^{2k} \);
2. Half of these \( 2^{2k} \) intervals will have an interval of length \( \alpha Q^{2k-1} \), at a distance of \( \alpha Q^{2k+1} \) to the right, which does not contain points from \( \Omega_\alpha \).

For any \( k \in \mathbb{N} \) introduce notation

\[
\begin{align*}
\alpha_k^{(\alpha)} &= \alpha(qQ^{2k} + Q^{2k+1}) = \alpha(q + Q)Q^{2k} \\
b_k^{(\alpha)} &= \alpha(Q^{2k} + qQ^{2k-1}) = \alpha(q^{-1} + Q)Q^{2k}
\end{align*}
\]
and consider the shift of the set $\Omega_\alpha$ to the right by
\[ h \in \left[ a_k^{(\alpha)}, b_k^{(\alpha)} \right], \quad k \in \mathbb{N}, \]
units. Recall that $Q \in (0, 1/2)$ and set $\beta = 1 - \frac{\log 2}{\log 1/Q} \in (0, 1)$. (Actually we start with a given $\beta \in (0, 1)$ and after that define $Q$ as above and $q = 1 - 2Q \in (0, 1)$.) By the properties 1 and 2 above for $h$ as in (3.18)
\[ \text{mes}_1((\Omega_\alpha - h) \setminus \Omega_\alpha) \geq \frac{1}{2} \cdot 2^{2k} \cdot \alpha q Q^{2k} = \frac{1}{2} \alpha q \cdot \left( Q^{2k} \right)^{1 - \frac{\log 2}{\log 1/Q}}. \]
We note that in (3.18), $c_1 Q^{2k} \leq h \leq c_2 Q^{2k}$, where $c_1 = \alpha(q + Q)$ and $c_2 = \alpha(qQ^{-1} + Q)$ do not depend on $k$. In particular $Q^{2k} \geq \frac{1}{\alpha(qQ^{-1} + q)} h$ for $h$ as in (3.18), and hence (3.19) implies
\[ \text{mes}_1((\Omega_\alpha - h) \setminus \Omega_\alpha) \geq \frac{\alpha q}{2(\alpha(qQ^{-1} + q))} \cdot h^{\beta} \]
for $h$ as in (3.18), and therefore for $h \in \bigcup_{k \in \mathbb{N}} [a_k^{(\alpha)}, b_k^{(\alpha)}]$. Using $q = 1 - 2Q$ we find that
\[ \frac{b_{k+1}^{(\alpha)}}{a_k^{(\alpha)}} = \frac{qQ + Q^2}{q + Q} = Q - Q^2 \in (0, 1/4), \quad q \in (0, 1), \]
and hence the set $\bigcup_{k \in \mathbb{N}} [a_k^{(\alpha)}, b_k^{(\alpha)}]$ has gaps. We need (3.20) to hold for all small $h$. In order to fulfill this condition, we consider a finite union of the scale $d$ sets $\Omega_\alpha$ for appropriate $\alpha$. More precisely, the first set in the union is the set $\Omega_1$ corresponding to $\alpha = 1$. Then (3.20) holds for $h \in \bigcup_{k \in \mathbb{N}} [a_k^{(1)}, b_k^{(1)}]$. Note that the ratio
\[ \gamma = \frac{b_k^{(\alpha)}}{a_k^{(\alpha)}} = \frac{q + Q^2}{qQ + Q^2} > 1 \]
is independent of $k$ and $\alpha$. Now for this $\gamma$ we construct the set $\Omega_\gamma$. For the set $\Omega_\gamma$, (3.20) holds (with a different constant) for $h \in \bigcup_{k \in \mathbb{N}} [\gamma a_k^{(1)}, \gamma b_k^{(1)}] = \bigcup_{k \in \mathbb{N}} [b_k^{(1)}, \gamma b_k^{(1)}]$ because $\gamma a_k^{(\alpha)} = b_k^{(\alpha)}$ for all $k \in \mathbb{N}$ and $\alpha > 0$, in particular for $\alpha = \gamma$. Now for the union $\Omega_1 \cup (\Omega_\gamma - 2)$, (3.20) holds (with a different constant) for
\[ h \in \left( \bigcup_{k \in \mathbb{N}} [a_k^{(1)}, b_k^{(1)}] \right) \cup \left( \bigcup_{k \in \mathbb{N}} [\gamma b_k^{(1)}, \gamma b_k^{(1)}] \right) = \bigcup_{k \in \mathbb{N}} [a_k^{(1)}, \gamma b_k^{(1)}]. \]
Now we construct the scaled sets $\Omega_{\gamma^2}, \ldots, \Omega_{\gamma^N}$, where the (finite) number $N \in \mathbb{N}$ is determined by the (independent of $k$ and $\alpha$) condition $\gamma^N a_k^{(\alpha)} \geq a_{k-1}^{(\alpha)}$ or $\gamma^N \geq \frac{q + Q}{qQ + Q^2}$ (recall that $\gamma > 1$ by (3.21)). Set finally
\[ \Omega = \Omega_1 \cup (\Omega_\gamma - 2) \cup (\Omega_{\gamma^2} - 3) \cup \cdots \cup \left( \Omega_{\gamma^N} - N \sum_{j=1}^{N-1} (1 + \gamma^{j-1}) \right). \]
Since $N$ is finite, (3.20) for the set $\Omega$ holds (with a different constant) for $h$ in
\[ \bigcup_{k=2}^{\infty} \left[ a_k^{(1)}, b_k^{(1)} \cup [b_k^{(1)}, \gamma b_k^{(1)}] \cup [\gamma b_k^{(1)}, \gamma^2 b_k^{(1)}] \cup \cdots \cup [\gamma^{N-1} b_k^{(1)}, \gamma^N b_k^{(1)}] \right] \]
and $\bigcup_{k=2}^{\infty} \left[ a_k^{(1)}, a_{k-1}^{(1)} \right] = (0, a_1^{(1)}].$
Therefore (3.24) holds for the set $\Omega$ with some constant for all $h \in (0, a_1^{(1)})$.

Now we explain why the estimate opposite to (3.24) holds for the same $\beta$. Again since $N$ is finite it suffices to consider one set $\Omega_\alpha$ with an arbitrary $\alpha > 0$. Choose first any $k = 2, 3, \cdots$ and $h \in [a_k^{(\alpha)}, a_{k-1}^{(\alpha)}]$. We estimate the contribution of the sets up to generation $k$ to $\text{mes}_1((\Omega_\alpha - h) \setminus \Omega_\alpha)$ by $a_k^{(\alpha)}$ times their total number. We estimate the contribution of the sets from generation $k + 1$ and onwards by their total length. As a result we obtain the following estimate

$$\text{mes}_1((\Omega_\alpha - h) \setminus \Omega_\alpha) \leq a_k^{(\alpha)} \sum_{l=0}^{k} 2^{2l} + \sum_{l=k+1}^{\infty} \alpha q 2^{2l} \cdot 2^{2l} \leq c \cdot Q^{2k} \cdot 2^{2k} = c \cdot (Q^{2k})^{1 - \frac{\log 2}{\log q}} \leq \tilde{c} \cdot h^\beta$$

for some $c, \tilde{c}$ independent of $k$ (recall (3.17)). Since the right-hand side in (3.22) does not depend on $k$, we conclude that (3.22) holds for $h \in \bigcup_{k=2}^{\infty} [a_k^{(\alpha)}, a_{k-1}^{(\alpha)}] = (0, a_1^{(\alpha)})$.

This completes the proof for $d = 1$.

In the case $d \geq 2$ for a given $\beta \in (0, 1)$, let $\Omega$ be the constructed above set and consider the direct product $\Omega^d$. Let $\text{mes}_d$ denote the Lebesgue measure in $\mathbb{R}^d$. Recall that $(\Omega^d)_h = \Omega^d - h, h \in \mathbb{R}^d$. Since for an arbitrary $h = (h_1, \cdots, h_d)$ we can write $\Omega^d$ as a disjoint union $\Omega^d = (\Omega^d \cap (\Omega^d)_h) \cup (\Omega^d \setminus (\Omega^d)_h)$ we have

$$\text{mes}_d(\Omega^d \cap (\Omega^d)_h) = \text{mes}_d(\Omega^d \setminus (\Omega^d)_h).$$

Noting that $\Omega^d \cap (\Omega^d)_h = (\Omega \cap \Omega_{h_1}) \times \cdots \times (\Omega \cap \Omega_{h_d})$ and using (3.23) for each of the factors we find

$$\text{mes}_d(\Omega^d \cap (\Omega^d)_h) = \prod_{j=1}^{d} \text{mes}_1(\Omega \cap \Omega_{h_j})$$

(3.24)

By the construction of the set $\Omega$, there are $c_1, c_2 > 0$ so that for $|h_j|$ small,

$$c_1 |h_j|^{\beta} \leq \text{mes}_1(\Omega \setminus \Omega_{h_j}) \leq c_2 |h_j|^{\beta}$$

which together with (3.24) implies

$$\prod_{j=1}^{d} (\text{mes}_1(\Omega) - c_2 |h_j|^{\beta}) \leq \text{mes}_d(\Omega^d \cap (\Omega^d)_h) \leq \prod_{j=1}^{d} (\text{mes}_1(\Omega) - c_1 |h_j|^{\beta}).$$

Recall that $|h| = \left(\sum_{j=1}^{d} |h_j|^2\right)^{1/2}, h \in \mathbb{R}^d$ (we hope that denoting the Euclidean length of a vector and the absolute value of a number does not lead to confusion below). Note that

$$\prod_{j=1}^{d} (\text{mes}_1(\Omega) - c_1 |h_j|^{\beta}) = (\text{mes}_1(\Omega))^{d} - c_1 \sum_{j=1}^{d} |h_j|^{\beta} + E(h_1, \cdots, h_d)$$

(3.26)

where the function $E$ has the property that it is a finite sum of terms each of which contains a factor $|h_{k_1}|^2 \cdot \cdots \cdot |h_{k_p}|^\beta$ for some $1 \leq k_1 < \cdots < k_p \leq d$ and $p \geq 2$. Note that each such factor is $\leq O(|h|^{2\beta})$ for small $|h|$. (Indeed, we can write $|h_1|^{\beta} |h_2|^{\beta} = |h_1|^{2\beta} \cdot (|h_1|/|h|)^{\beta} \cdot (|h_2|/|h|)^{\beta} \leq |h|^{2\beta}$ and for all other possible factors
again use the estimate $|h_j| \leq |h|$. Substituting (3.26) in (3.25) and returning to (3.23), we find

$$c_1 \sum_{j=1}^{d} |h_j|^\beta + O(|h|^{2\beta}) \leq \text{mes}_d(\Omega^d \setminus (\Omega^d)_h) \leq c_2 \sum_{j=1}^{d} |h_j|^\beta + O(|h|^{2\beta})$$

for small enough $|h|$ (we have used that $\text{mes}_d(\Omega^d) = (\text{mes}_1(\Omega))^d$). We note finally that for any fixed $\beta \in (0, 1)$ there exist $C_1, C_2 > 0$ so that for all $h$

$$C_1 |h|^\beta \leq \sum_{j=1}^{d} |h_j|^\beta \leq C_2 |h|^\beta.$$

(To see this, set $\tilde{h} = h/|h|$ and note that we just have to prove that for some $\tilde{C}_1, \tilde{C}_2 > 0$, $\tilde{C}_1 \leq \sum_{j=1}^{d} |\tilde{h}_j|^\beta \leq \tilde{C}_2$ if only $\sum_{j=1}^{d} |\tilde{h}_j|^2 = 1$. But this holds since the minimum and the maximum are attained at some points on the unit sphere.) Combining (3.27) and (3.28) completes the proof of Lemma 2.4.

**Acknowledgments.** The author would like to thank the following colleagues for useful discussions: A. Laptev for the suggestion to work on the Widom conjecture, Yu. Safarov for a simpler and more general proof of Theorem 2.1 than the original one in [15], S. Smirnov for the idea of the construction of the set in Lemma 2.4 and I. Klich, who represented the EE in a form amenable to the analysis related to the Widom conjecture (see [20]). The work in this paper was supported in part by the Royal Institute of Technology (KTH) in Stockholm, the Swedish Foundation for International Cooperation in Research and Higher Education (STINT) grant Dnr. PD2001–128, the NSF grant INT–0204308 U.S.–Sweden Collaborative Workshop on PDE’s and Spectral Theory, and the NSF grant DMS–0556049.

**References**

[1] E. L. Basor, *A localization theorem for Toeplitz determinants*, Indiana Univ. Math. J. 28 (1979), no. 6, 975–983.

[2] E. L. Basor and C. A. Tracy, *The Fisher–Hartwig conjecture and generalizations*, Phys. A 177 (1991), no. 1-3, 167–173.

[3] T. Barthel, M.-C. Chung and U. Schollwoeck, *Entanglement scaling in critical two-dimensional fermionic and bosonic systems*, preprint, 2006. quant-ph/0602077

[4] C. H. Bennett and D. P. DiVincenzo, *Quantum information and computation*, Nature 404 (2000), 247–255.

[5] C. H. Bennett, H. J. Bernstein, S. Popescu and B. Schumacher, *Concentrating partial entanglement by local operations*, Phys. Rev. A 53 (1996), no. 4, 2046–2052.

[6] L. Bombelli, R. K. Koul, J. Lee and R. D. Sorkin, *Quantum source of entropy for black holes*, Phys. Rev. D 34 (1986), no. 2, 373–383.

[7] A. Böttcher, *The Onsager formula, the Fisher-Hartwig conjecture, and their influence on research into Toeplitz operators*, Papers dedicated to the memory of Lars Onsager, J. Statist. Phys. 78 (1995), no. 1-2, 575–584.

[8] L. Brandolini, L. Colzani and G. Travaglini, *Average decay of Fourier transforms and integer points in polyhedra*, Ark. Mat. 35 (1997), no. 2, 253–275.

[9] P. Calabrese and J. Cardy, *Entanglement entropy and Quantum Field Theory*, J. Stat. Mech. Theory Exp. 2004, no. 6, 002, 27 pp. (electronic).

[10] D. B. H. Cline, *Regularly varying rates of decrease for moduli of continuity and Fourier transforms of functions on $\mathbb{R}^d$*, J. Math. Anal. Appl. 159 (1991), no. 2, 507–519.

[11] T. Ehrhardt, *A status report on the asymptotic behavior of Toeplitz determinants with Fisher-Hartwig singularities*, Recent advances in operator theory (Groningen, 1998), 217–241, Oper. Theory Adv. Appl., 124, Birkhäuser, Basel, 2001.
[12] M. Fannes, B. Haegeman and M. Mosonyi, Entropy growth of shift-invariant states on a quantum spin chain, J. Math. Phys. 44 (2003), no. 12, 6005–6019.

[13] A. Hamma, R. Ionicioiu and P. Zanardi, Bipartite entanglement and entropic boundary law in lattice spin systems, Phys. Rev. A 71 (2005), no. 2, 022315, 10 pp.

[14] S. Ghosh, T. F. Rosenbaum, G. Aeppli and S. N. Coppersmith, Entangled quantum state of magnetic dipoles, Nature 425 (2003), 48–51.

[15] D. Gioev, Generalizations of Szegő Limit Theorem: Higher Order Terms and Discontinuous Symbols. Ph.D. Thesis, Dept. of Mathematics, Royal Inst. of Technology (KTH), Stockholm, 2001. http://media.lib.kth.se:8080/dissengrefhit.asp?dissnr=3123

[16] D. Gioev, Lower order terms in Szegő type limit theorems on Zoll manifolds, Comm. Partial Differential Equations 28 (2003), no. 9-10, 1739–1785.

[17] D. Gioev, Moduli of continuity and average decay of Fourier transforms: two-sided estimates, submitted. math.CA/0212254

[18] D. Gioev and I. Klich, Entanglement entropy of fermions in any dimension and the Widom conjecture, Phys. Rev. Lett. 96 (2006), no. 10, 100503, 4 pp.

[19] A. Grigis and J. Sjöstrand, Microlocal analysis for differential operators. London Mathematical Society Lecture Note Series, 196. Cambridge University Press, Cambridge, 1994.

[20] V. Guillemin and K. Okikiolu, Spectral asymptotics of Toeplitz operators on Zoll manifolds, J. Funct. Anal. 146 (1997), no. 2, 496–516.

[21] A. R. Its, B.-Q. Jin and V. E. Korepin, Entanglement in the XY spin chain, J. Phys. A 38 (2005), no. 13, 2975–2990.

[22] B.-Q. Jin and V. E. Korepin, Quantum spin chain, Toeplitz determinants and the Fisher–Hartwig conjecture, J. Statist. Phys. 116 (2004), no. 1-4, 79–95.

[23] J. P. Keating and F. Mezzadri, Random matrix theory and entanglement in quantum spin chains, Comm. Math. Phys. 252 (2004), no. 1-3, 543–579.

[24] J. P. Keating and F. Mezzadri, Entanglement in quantum spin chains, symmetry classes of random matrices, and conformal field theory, Phys. Rev. Lett. 94 (2005), no. 5, 050501, 4 pp.

[25] V. E. Korepin, Universality of entropy scaling in one dimensional gapless models, Phys. Rev. Lett. 92 (2004), no. 9, 096402, 3 pp.

[26] I. Klich, Lower entropy bounds and particle number fluctuations in a Fermi sea, J. Phys. A 39 (2006), no. 4, L85–L91.

[27] A. Laptev and Yu. Safarov, Szegő type limit theorems, J. Funct. Anal. 138 (1996), no. 2, 544–559.

[28] W. Li, L. Ding, R. Yu, T. Roscilde and S. Haas, Scaling behavior of entanglement in two- and three-dimensional free Fermions, preprint, 2006. quant-ph/0602094

[29] N. Linden and S. Popescu, Good dynamics versus bad kinematics: Is entanglement needed for quantum computation? Phys. Rev. Lett. 87 (2001), no. 4, 047901, 4 pp.

[30] M. A. Nielsen and I. L. Chuang, Quantum computation and quantum information. Cambridge University Press, Cambridge, 2000.

[31] T. J. Osborne and M. A. Nielsen, Entanglement in a simple quantum phase transition, Phys. Rev. A 66 (2002), no. 3, 032110, 14 pp.

[32] A. Osterloh, L. Amico, G. Falci and R. Fazio, Scaling of entanglement close to a quantum phase transition, Nature 416 (2002), 608–610.

[33] A. Peres, Quantum theory: concepts and methods. Fundamental Theories of Physics, 57. Kluwer Academic Publishers Group, Dordrecht, 1993.

[34] M. B. Plenio, J. Eisert, J. Dreissig and M. Cramer, Entropy, entanglement, and area: Analytical results for harmonic lattice systems, Phys. Rev. Lett. 94 (2005), no. 6, 060503, 4 pp.

[35] M. Srednicki, Entropy and area, Phys. Rev. Lett. 71 (1993), no. 5, 666–669.

[36] G. Szegő, Ein Grenzwertsatz über die Toeplitzschen Determinanten einer reellen positiven Funktion, Math. Ann. 76 (1915), 490–503.

[37] G. Vidal, Efficient classical simulation of slightly entangled quantum computations, Phys. Rev. Lett. 91 (2003), no. 14, 147902, 4 pp.

[38] G. Vidal, J. I. Latorre, E. Rico and A. Kitaev, Entanglement in quantum critical phenomena, Phys. Rev. Lett. 90 (2003), no. 22, 227902, 4 pp.

[39] H. Widom, Asymptotic Expansions for Pseudodifferential Operators in Bounded Domains. Lecture Notes in Mathematics, 1152. Springer–Verlag, Berlin, 1985.
[40] H. Widom, *Eigenvalue distribution theorems for certain homogeneous spaces*, J. Funct. Anal. 32 (1979), no. 2, 139–147.

[41] H. Widom, *On a class of integral operators with discontinuous symbol*. Toeplitz centennial (Tel Aviv, 1981), pp. 477–500, Operator Theory: Adv. Appl., 4. Birkhäuser, Basel-Boston, Mass., 1982.

[42] H. Widom, *On a class of integral operators on a half-space with discontinuous symbol*, J. Funct. Anal. 88 (1990), no. 1, 166–193.

[43] M. M. Wolf, *Violation of the entropic area law for fermions*, Phys. Rev. Lett. 96 (2006), no. 1, 010404, 4 pp.

[44] W. K. Wootters, *Entanglement of formation of an arbitrary state of two qubits*, Phys. Rev. Lett. 80 (1998), no. 10, 2245–2248.

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF ROCHESTER, HYLAN BUILDING, ROCHESTER, NY 14627

E-mail address: gioev@math.rochester.edu