FORMULAS OF SZEGÖ TYPE FOR THE PERIODIC SCHRÖDINGER OPERATOR

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ABSTRACT. We prove asymptotic formulas of Szegö type for the periodic Schrödinger operator
\[ H = -\frac{d^2}{dx^2} + V \] in dimension one. Admitting fairly general functions \( h \) with \( h(0) = 0 \), we study
the trace of the operator \( h(\chi(-\alpha,\alpha))\chi(-\infty,\mu)(H)\chi(-\alpha,\alpha) \) and link its subleading behaviour as
\( \alpha \to \infty \) to the position of the spectral parameter \( \mu \) relative to the spectrum of \( H \).

1. Introduction

The classical Szegö formula (see [30]) describes the determinant of the truncated Toeplitz
matrix as the truncation parameter tends to infinity, we refer to survey [14] for discussion and
further references. Our interest is closer to the continuous variant of this problem, i.e. to
truncated Wiener-Hopf operators. Let \( I \subset \mathbb{R} \) be a finite (open) interval, and let \( a = a(\xi), \xi \in \mathbb{R} \)
be a bounded, in general complex-valued function, which we call symbol. By the truncated
Wiener-Hopf operator we understand the operator of the form
\[ W(a; I) = \chi_I F^* a F \chi_I, \]
where \( F : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \) is the unitary Fourier transform, and \( \chi_I \) is the indicator of the interval
\( I \). There is a vast literature studying the behaviour of the trace
\[ \text{tr} h(W(a; \alpha I)) \]
with a test function \( h \), as the scaling parameter \( \alpha \) tends to infinity. Assuming for simplicity that
\( h \) is continuous, one can claim that the above trace is finite if \( h(0) = 0 \) and the function \( a \) decays
sufficiently fast at infinity. We do not intend to give an extensive survey of known results, but
only mention that, under the assumption that the functions \( a \) and \( h \) are smooth, one can find a
complete asymptotic expansion of this trace in powers of \( \alpha^{-1} \), see e.g. [3], [33]. Limited to two
terms only, this expansion has the form
\[ \text{tr} h(W(a; \alpha I)) = \frac{\alpha^2}{2\pi} |I| \int h(a(\xi)) d\xi + \mathcal{B} + O(\alpha^{-1}), \quad \alpha \to \infty, \quad (1.1) \]
with an explicitly computable coefficient \( \mathcal{B} = \mathcal{B}(a; h) \), independent of the interval \( I \). Note that
[33] contains even the multidimensional version of the result.

In this paper we do not need the precise value of \( \mathcal{B} \), since our main concern is the case of a
non-smooth symbol \( a \). Assume for the sake of discussion that \( a = \chi_J \) where \( J \subset \mathbb{R} \) is a bounded
interval, and that \( h \) is a \( C^\infty \)-function such that \( h(0) = 0 \). Then the results of [16], and [32] imply
the asymptotic formula
\[ \text{tr} h(W(\chi_J; \alpha I)) = \frac{\alpha}{2\pi} h(1)|I|\|J\| + \log(\alpha) W(h) + o(\log(\alpha)), \quad \alpha \to \infty, \quad (1.2) \]
with a coefficient \( W(h) \) independent of the intervals \( I \) and \( J \), see (3.1) for the definition. Thus,
one observes that the first term on the right-hand side is the same as in (1.1), but the second
one exhibits a behaviour different from (1.1). The multidimensional generalization of this result,
even with more general discontinuous symbols \( a \) was obtained in [23], [24]. Further extension to

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non-smooth functions \( h \) was done in \cite{18, 26, 27}. The formula (1.1) is a continuous analogue of the second-order Szegő limit theorem, see \cite{30}, so we loosely refer to (1.1) and (1.2) as Szegő formulas, or formulas of Szegő type. It is clear that under the condition \( h(0) = h(1) = 0 \) the leading term in (1.2) vanishes, and the formula takes the form

\[
\text{tr} h(W(\chi_J; \alpha I)) = \log(\alpha) W(h) + o(\log(\alpha)), \quad \alpha \to \infty, \text{ if } h(0) = h(1) = 0. \tag{1.3}
\]

The increased recent interest in the asymptotic results of the described type with possibly non-smooth functions \( h \) is partly due to their connection with the study of the bipartite entanglement entropy (EE), see e.g. \cite{9}, \cite{10}, \cite{18}, \cite{19}. For instance, the formula (1.2), used with the function

\[
\eta_1(t) = -t \log t - (1 - t) \log(1 - t), \quad t \in [0, 1],
\]

which is not differentiable at the endpoints of the interval \([0, 1]\), would describe the scaling asymptotics of the von Neumann EE for free fermions in the Fermi sea \( J \) at zero temperature, see \cite{13}, \cite{9}. The function (1.3) is just one representative of the family

\[
\eta_\gamma(t) = \frac{1}{1 - \gamma} \log \left[ t^\gamma + (1 - t)^\gamma \right], \quad t \in [0, 1],
\]

with \( \gamma > 0 \), where \( \eta_1 \) is defined as the limit of \( \eta_\gamma \) as \( \gamma \to 1 \), \( \gamma \neq 1 \). Picking \( h = \eta_\gamma \) one obtains from (1.2) the asymptotics of the \( \gamma \)-Rényi EE, see e.g. \cite{18}. Due to the condition \( \eta_1(0) = \eta_1(1) = 0 \), formula (1.3) applies and the EE behaves as \( \log(\alpha) \) as \( \alpha \to \infty \).

Let us remark at this point that there is an extensive physics literature on the topic of EE. Without loss of generality we assume that the period equals 2.

Another new element is the extended choice of the test function \( h \), see Condition 5.3. In our paper the function \( h = h(t), \ t \in [0, 1] \), is allowed to be piece-wise continuous,
although we require $h$ to be Hölder-continuous at the endpoints $t = 0, 1$. This is made possible by adjusting the Schatten-von Neumann class estimates for pseudo-differential operators with discontinuous symbols, obtained in [25]. Consequently, functions such as (1.5) are covered by our result.

A few comments on the structure of this paper are in order. We begin with recalling some fundamental properties of one-dimensional periodic Schrödinger operators (cf. Section 2) and afterwards state our results in Section 3. The very first step of the proof is to obtain an approximation of the kernel of the spectral projection $P_\mu$ in terms of Bloch eigenfunctions corresponding to the Fermi energy $\mu$, see Section 4. Section 5 contains some elementary trace class estimates, similar to the ones obtained in [16]. Here we also introduce an averaging procedure for a particular type of integral operators (see sub-Section 5.4) that allows us to average out the precise dependence on the Bloch eigenfunctions at Fermi energy $\mu$. This is sufficient to prove Theorem 3.2 for polynomial functions $h$, see Section 7 and sub-Section 8.1. As mentioned earlier, the extension to non-smooth functions calls for more advanced bounds in Schatten-von Neumann classes. These bounds are collected in Section 6. The extension to non-smooth $h$, i.e. the closure of the asymptotics from the polynomial $h$, is implemented in sub-Section 8.2.

To conclude the introduction let us fix some general notation. If $f, g$ are non-negative functions, we write $f \ll g$ if $f \leq Cg$ for some constant $C \geq 0$. This constant may depend on the potential $V$ but does not depend on the dilation parameter $\alpha$. To avoid confusion we sometimes make explicit comments on the nature of (implicit) constants in the bounds.

For a set $I \subset \mathbb{R}$ the notation $I^\circ$ is used for the set of all interior points of $I$ and its Lebesgue measure is denoted by $|I|$. In many situation (e.g. for the intervals $I, J, K$ in Section 5) it will not matter whether considered intervals are open, semi-open or closed. Whenever this is the case we shall use open intervals only.

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2. Preliminaries

We consider a periodic Schrödinger operator
\[ H = -\frac{d^2}{dx^2} + V(x), \quad \text{dom}(H) = H^2(\mathbb{R}), \]
in dimension 1. More precisely, let the potential $V$ be a real-valued $2\pi$-periodic $L^2_{\text{loc}}$-function, so that the operator $H$ is self-adjoint on $H^2(\mathbb{R})$. For $\mu \in \mathbb{R}$, we introduce the notation $P_\mu := \chi_{(-\infty, \mu]}(H)$ for the spectral projection of $H$. We shall use $\alpha > 0$ as a dilation parameter and write $\chi_I$ for the indicator function of the interval $I \subset \mathbb{R}$ as well as for the corresponding multiplication operator on $L^2(\mathbb{R})$. For an appropriate choice of the function $h$, we are interested in an asymptotic formula for the trace
\[ \text{tr} h(B_{a,\mu}), \quad B_{a,\mu} = \chi_{(-a,a)} P_\mu \chi_{(-a,a)}, \quad (2.1) \]
as $\alpha \to \infty$.

We heavily rely on the standard Floquet-Bloch theory for periodic operators, see e.g. [21], [31]. In particular, we make use of the Floquet-Bloch-Gelfand transform
\[ U : L^2(\mathbb{R}) \to L^2(\mathbb{T}, L^2(0, 2\pi)), \quad \mathbb{T} = \mathbb{R}/\mathbb{Z}. \]
For Schwartz class functions or $L^2(\mathbb{R})$-function with compact support, it is given by
\[ (U\psi)(x, k) := \sum_{\gamma \in 2\pi \mathbb{Z}} e^{-ik\gamma} \psi(x + \gamma), \quad k \in \mathbb{T}, \quad x \in [0, 2\pi]. \]
The operator $U$ is easily checked to be isometric, and hence it extends by continuity as a unitary operator to the entire $L^2(\mathbb{R})$. Under $U$ the periodic Schrödinger operator $H$ transforms into the
direct integral

\[ \int H(k) \, dk, \]

with self-adjoint fibres

\[ H(k) = -\frac{d^2}{dx^2} + V(x), \]

\[ \text{dom}(H(k)) = \{ f \in H^2(0, 2\pi) : f(2\pi) = e^{2\pi ik} f(0), f'(2\pi) = e^{2\pi ik} f'(0) \}, \]

that are well-defined for \( k \in \mathbb{T} \). It is well-known that each fibre operator \( H(k) \) has compact resolvent and, therefore, a discrete spectrum that consists of eigenvalues \( \lambda_j(k), \ j = 1, 2, \ldots \), labelled in ascending order counting multiplicity. Denote the corresponding normalized eigenfunctions by \( \phi_j(k) = \phi_j(\cdot, k) \in H^2(0, 2\pi), \ j = 1, 2, \ldots \).

It is clear that for all \( k \in \mathbb{R} \) the functions

\[ e_j(x, k) := e^{-ikx} \phi_j(x, k) \]

and their derivatives \( de_j/dx \) can be extended to all \( x \in \mathbb{R} \) as 2\( \pi \)-periodic functions, which induces a corresponding extension of \( \phi_j(\cdot, k) \). Using the eigenfunctions \( \phi_j(k) \) we can write out the kernel \( P_\mu(x, y) \) of the projection \( P_\mu \).

\[ P_\mu(x, y) = \sum_j \int_\mathbb{T} \chi(\mu_j, \nu_j)(\lambda_j(k)) \phi_j(x, k) \overline{\phi_j(y, k)} \, dk. \]

In the next proposition we summarize the properties of the functions \( \phi_j(k) \) and eigenvalues \( \lambda_j(k) \) that we use further on. The points \( k = 0 \) and \( k = \frac{1}{2} \) will play a special role, so it makes sense to introduce temporarily the notation

\[ \mathbb{T}_0 = \mathbb{T} \setminus \{0\} \cup \left\{ \frac{1}{2} \right\}. \]

**Proposition 2.1.** Let \( H(k), k \in \mathbb{T} \), be as defined above. Then

1. For every \( k \in \mathbb{T} \) the operators \( H(k) \) and \( H(-k) \) are antiunitarily equivalent under complex conjugation. In particular, \( \lambda_j(k) = \lambda_j(-k) \) for all \( j = 1, 2, \ldots \).
2. The eigenfunctions \( \phi_j(\cdot, k), j = 1, 2, \ldots \), can be chosen to be analytic in \( k \in \mathbb{T}_0 \), and such that \( \phi_j(-k) = \overline{\phi_j(k)} \), \( k \in \mathbb{T}_0 \).
3. The eigenvalues \( \lambda_j(k), j = 1, 2, \ldots \), are even continuous functions of \( k \in \mathbb{T} \). These eigenvalues are simple and analytic on \( \mathbb{T}_0 \).
4. For \( j \) odd (resp. even) each \( \lambda_j(\cdot) \) is strictly increasing (resp. decreasing) on \( (0, \frac{1}{2}) \).

Let

\[ k_j = \begin{cases} 0, & j \text{ odd}, \\ \frac{1}{2}, & j \text{ even}. \end{cases} \]

Denote

\[ \mu_j = \lambda_j(k_j), \nu_j = \lambda_j\left(k_j + \frac{1}{2}\right), \quad \sigma_j = [\mu_j, \nu_j], \ j = 1, 2, \ldots. \]

The spectrum \( \sigma(H) \) of \( H \) is represented as the union of spectral bands \( \sigma_j \):

\[ \sigma(H) = \bigcup_{j=1}^{\infty} \sigma_j. \]
It follows from Proposition 2.1(4) that the bands \( \sigma_j \) are non-degenerate, i.e. \(|\sigma_j| > 0\) for every \( j = 1, 2, \ldots \). Introduce the counting function of \( H(k) \):

\[
N(\mu, k) = \# \{ j : \lambda_j(k) < \mu \}, \quad \mu \in \mathbb{R}, \ k \in \mathbb{T},
\]

and the (integrated) density of states:

\[
N(\mu; H) = \frac{1}{2\pi} \int_{\mathbb{T}} N(\mu, k) \, dk. \tag{2.6}
\]

In view of Proposition 2.1(4) again, the function (2.6) is continuous. The definition (2.6) agrees with the standard definition of the density of states which is given via the Hamiltonian with Dirichlet boundary condition on a large cube, see e.g. [20, Theorem 4.2] or [21, Ch. XIII].

Note also that the spectral bands cannot overlap, but they may touch. This situation is our main concern in the next proposition.

**Proposition 2.2.** Let \( \lambda_j = \lambda_j(k), \ \phi_j = \phi_j(k) \) be as described in Proposition 2.1. Then

1. If for some \( j \) the bands \( \sigma_{j-1} \) and \( \sigma_j \) are separated from each other, i.e. \( \nu_{j-1} < \mu_j \), then the eigenvalues \( \lambda_{j-1}(\cdot) \), \( \lambda_j(\cdot) \) and eigenfunctions \( \phi_{j-1}(x, \cdot), \phi_j(x, \cdot) \) are analytic in \( k \) in a neighbourhood of \( k_j \), for each \( x \in \mathbb{R} \). Furthermore, the functions \( \phi_{j-1}(\cdot, k_j) \) and \( \phi_j(\cdot, k_j) \) are real-valued.
2. If for some \( j \) we have \( \nu_{j-1} = \mu_j \), i.e. \( \lambda_{j-1}(k_j) = \lambda_j(k_j) \), then in a neighbourhood of \( k_j \), the eigenvalues \( \lambda_{j-1} \) and \( \lambda_j \), and the eigenfunctions \( \phi_{j-1}(x, \cdot) \) and \( \phi_j(x, \cdot) \) are analytic continuations of each other. Moreover, \( \lambda'_j(k_j) \neq 0 \), \( \phi_i(k_j) = \phi_i(k_j+) \) and the limits \( \phi_i(k_j-) \) and \( \phi_i(k_j+) \) are mutually \( L^2 \)-orthogonal for \( l = j - 1, j \).

Although Propositions 2.1 and 2.2 are well-known, we need to make some comments. The analyticity on \( \mathbb{T}_0 \) in Proposition 2.1 is a straightforward consequence of the analytic perturbation theory, see [11] or [21]. The analyticity of \( \phi_j(k) \) and \( \lambda_j(k) \) in the vicinity of points \( k_j \) in Proposition 2.2 is a more subtle fact, and it follows from abstract theorems [11, Ch. II, Theorems 1.9, 1.10] and [21, Theorems XII.12, XII.13]. In the context of the periodic operators the analytic properties of eigenfunctions \( \phi_j \) are described in [2] and [8]. Also, the relation \( \lambda'_j(k_j) \neq 0 \) from Proposition 2.2 can be found e.g. in [8, formula (3.1)].

Assume again that \( \nu_{j-1} = \mu_j \), i.e. the bands \( \sigma_{j-1} \) and \( \sigma_j \) have one common point. Since \( \phi_{j-1}(k) \) and \( \phi_j(k) \) are orthogonal for all \( k \in \mathbb{T}_0 \), and \( \phi_{j-1}(k_j) = \phi_j(k_j+) \), the functions \( \phi_j(k_j-) \) and \( \phi_j(k_j+) \) are mutually orthogonal, as claimed in Proposition 2.2(2). In view of the identity \( \phi_j(k_j-) = \phi_j(k_j+) \), this implies that

\[
\int_{0}^{2\pi} \phi_j(x, k_j \pm)^2 \, dx = 0, \quad \text{if} \quad \nu_{j-1} = \mu_j. \tag{2.7}
\]

It is natural to group the bands that have common points (i.e. touch) together. Suppose that the bands \( \sigma_j, \sigma_{j+1}, \ldots, \sigma_{j+n-1} \) are of this type and that \( \sigma_j \cap \sigma_j = \emptyset, \ \sigma_{j+n-1} \cap \sigma_{j+n} = \emptyset \). Thus the interval

\[
S = \bigcup_{l=0}^{n-1} \sigma_{j+l} = [\mu_j, \nu_{j+n-1}], \tag{2.8}
\]

is a “genuine” spectral band. Sometimes we informally use this term, “genuine”, to distinguish the bands \( \{ \sigma_j \} \) and \( S \). Using this construction, we can somewhat simplify the description of the
spectral structure of $H$ inside $S$. Indeed, define on $[k_j - n/2, k_j + n/2]$ the real-valued function

$$
\Lambda(k) = \lambda_{j+l}(k), \ k \in \left[ k_j + \frac{l}{2}, k_j + \frac{l+1}{2} \right], \ l = 0, 1, \ldots, n - 1,
$$

$$
\Lambda(k) = \Lambda(2k_j - k), \ k \in \left[ k_j - \frac{n}{2}, k_j \right].
$$

According to Propositions 2.1 and 2.2, the above function is analytic on the circle $n \mathbb{T} = \mathbb{R}/n \mathbb{Z}$, monotone increasing in $k \in [k_j, k_j + n/2]$, and symmetric in $k = k_j$. Note also that

$$
\Lambda(k_j) = \mu_j > \nu_j - 1, \ \Lambda(k_j + n/2) = \nu_j + n/2 < \mu_{j+1}. \quad (2.9)
$$

In the same way, one defines the eigenfunction $\Phi(x, k)$ that incorporates all of the $\phi_{j+l}$, $l = 0, 1, \ldots, n - 1$:

$$
\Phi(k) = \phi_{j+l}(k), \ k \in \left[ k_j + \frac{l}{2}, k_j + \frac{l+1}{2} \right], \ l = 0, 1, \ldots, n - 1,
$$

$$
\Phi(k) = \Phi(2k_j - k), \ k \in \left[ k_j - \frac{n}{2}, k_j \right]. \quad (2.10)
$$

Similarly to $\Lambda(\cdot)$, the function $\Phi(x, \cdot)$ is analytic on the circle $n \mathbb{T}$. The functions $\Phi(\cdot, k_j)$ and $\Phi(\cdot, k_j + n/2)$, associated with the ends of the band $S$, are real-valued. It is also useful to define the function

$$
E(x, k) = e^{-ixk}\Phi(x, k), \quad (2.11)
$$

built out of the functions (2.3) in the same way as $\Phi(k)$ is built out of $\phi_j(k)$’s. The functions $E(x, k)$ are analytic in $k \in \mathbb{R}$, and $2\pi$-periodic in $x \in \mathbb{R}$.

Of course, it may happen that all bands starting with $\sigma_j$, touch. In this case the above construction still works and yields analytic functions $\Phi$, $\Lambda$, and $E$ on $\mathbb{R}$. To keep the notation simple we shall allow in the following $n = \infty$ and use the convention $\infty \mathbb{T} = \mathbb{R}$.

Using the functions $\Lambda$ and $\Phi$ we can write the spectral representation of the operator $H$ as follows. Let $P[S]$ be the spectral projection of $H$ corresponding to a band $S$ defined as in (2.3). Then

$$
UHP[S]U^* = \int_{n \mathbb{T}} \Lambda(k)P[\Phi(k)] \, dk,
$$

where $P[\psi]$ is the orthogonal projection in $L^2(0, 2\pi)$ on the span of the function $\psi \in L^2(0, 2\pi)$. As a consequence, the formula (2.4) leads to the following formula for the kernel $P_\mu[S](x, y)$ of the projection $P_\mu[S] := P_\mu P[S]$:

$$
P_\mu[S](x, y) = \int_{k \in n \mathbb{T} : \Lambda(k) < \mu} \Phi(x, k)\overline{\Phi(y, k)} \, dk. \quad (2.12)
$$

Given the properties of the eigenfunction $\Phi(\cdot, k_j), j = 1, 2, \ldots$, for every $k \in n \mathbb{T}$, it belongs to the algebra $\text{CAP}(\mathbb{R})$ of continuous almost-periodic functions on $\mathbb{R}$, which is defined as the closure of the span of exponentials $e^{i\xi x}, \ \xi \in \mathbb{R}$, in the $L^\infty$-norm. For any $f \in \text{CAP}(\mathbb{R})$ the almost-periodic mean

$$
\mathcal{M}(f) := \lim_{T \to \infty} (2T)^{-1} \int_{-T}^{T} dt \, f(t)
$$

is well-defined. For an introduction to almost periodic functions and their properties we refer to [29] or [28].

For the future use we need to evaluate some means for the eigenfunctions $\Phi(k)$. 

...
Lemma 2.3. Let $\Phi = \Phi(\cdot, k)$ be the eigenfunction associated with the band $S$, see (2.8). Then
\[ M(|\Phi|^2) = \frac{1}{2\pi}, \quad \forall k \in n\mathbb{T}, \quad (2.13) \]
and
\[ M(\Phi^2) = 0, \quad \forall k \neq k_j, k \neq k_j + n/2. \quad (2.14) \]

Proof. The function $\Phi$ is normalised in $L^2(0, 2\pi)$, whence $M(|\Phi|^2) = (2\pi)^{-1}$, as claimed in (2.13).

To prove (2.14), suppose first that $2k \neq 1 \mod \mathbb{Z}$, so that $k \neq k_j \pm 1/2$, $l = 0, 1, \ldots, n$. We use the representation (2.11), so
\[ M(\Phi^2) = M(e^{2ikx} E^2). \]
The function $w = E(\cdot, k)^2$ is continuous and $2\pi$-periodic. Picking an $\varepsilon > 0$ we can approximate $w$ by trigonometric polynomials
\[ p(x) = \sum_{s=-N}^{N} p_s e^{isx}, \]
so that $w = p + \tilde{p}$, where $\tilde{p}$ is a continuous periodic function such that $|\tilde{p}| < \varepsilon$. Let us find the mean for each component of the polynomial $p$ separately:
\[ \int_{-T}^{T} e^{2ikx + isx} dx = \frac{e^{i(2k+s)x}}{i(2k+s)} \bigg|_{-T}^{T}, \]
which is bounded uniformly in $T$ for all $s = -N, -N+1, \ldots, N$. Thus $M(e^{2ikx} p) = 0$, and hence
\[ |M(\Phi^2)| = |M(e^{2ikx} \tilde{p})| \leq \varepsilon. \]
As $\varepsilon > 0$ is arbitrary, this entails that $M(\Phi^2) = 0$, as required.

The points $k = k_j \pm l/2$, $l = 1, 2, \ldots, (n-1)$ are exactly those, where the bands $\sigma_{j+l-1}$ and $\sigma_{j+l}$ touch. Thus the equality $M(\Phi^2) = 0$ for these values of $k$ follows from (2.7). This leads to (2.14) again. \qed

3. Results

Our main result concerns the trace defined in (2.1) with a test-function which satisfies the following condition.

Condition 3.1. The function $h : [0, 1] \to \mathbb{C}$ is piece-wise continuous, it is Hölder continuous at $t = 0$ and $1$, and $h(0) = 0$.

For a function $h$ satisfying Condition 3.1, define the integral
\[ \mathcal{W}(h) := \frac{1}{\pi^2} \int_{0}^{1} \frac{[h(t) - th(1)]}{t(1-t)} dt. \quad (3.1) \]
The next theorem contains a Szegő type formula for the operator $B_{\alpha, \mu}$ (see (2.1)), and it constitutes the main result of the paper.

Theorem 3.2. Suppose that $V \in C^{\infty}(\mathbb{R})$. Assume that the function $h$ satisfies Condition 3.1. Then for any $\mu \in (\sigma(H))^0$ we have the asymptotic formula
\[ \text{tr}[h(B_{\alpha, \mu})] = 2\alpha h(1) N(\mu, H) + \log(\alpha) \mathcal{W}(h) + o(\log(\alpha)), \quad \text{as} \quad \alpha \to \infty. \quad (3.2) \]
If $\mu \notin (\sigma(H))^0$, then
\[ \text{tr}[h(B_{\alpha, \mu})] = 2\alpha h(1) N(\mu, H) + \mathcal{O}(1), \quad \text{as} \quad \alpha \to \infty. \quad (3.3) \]
Here, $N(\mu, H)$ denotes the integrated density of states for the operator $H$, defined in (2.6).
**Remark 3.3.**

1. The two terms in (3.2) are of different nature: the first one (linear in $\alpha$) depends on both the potential $V$ and the parameter $\mu$, but the second one (log-term) is independent of $V$ or $\mu$, as long as $\mu$ remains an interior point of the spectrum $\sigma(H)$.

2. The ways in which one finds the main term and the log-term in (3.2) are completely different. To explain this, represent the function $h$ as the sum

$$h(t) = th(1) + h_1(t),$$

so that the function $h_1$ satisfies Condition 3.1 and, in addition, $h_1(1) = 0$. The function $th(1)$ is responsible for the first term in (3.2). Indeed, according to (2.4),

$$\|B_{\alpha,\mu}\|_{\mathcal{S}} = \text{tr} B_{\alpha,\mu} = \sum_{j} \int_{-\alpha}^{\alpha} \int_{k \in \mathbb{T} : \lambda_j(k) < \mu} |\phi_j(x,k)|^2 dk dx.$$

Assume for simplicity that $\alpha$ is a multiple of $2\pi$. Since the $\phi_j$’s are normalized on $(0, 2\pi)$, by the definition (2.6), we have

$$\text{tr} B_{\alpha,\mu} = \frac{\alpha}{\pi} \sum_{j} \int_{k \in \mathbb{T} : \lambda_j(k) < \mu} dk = 2\alpha N(\mu, H).$$

If $\alpha$ is not a multiple of $2\pi$, then one easily checks, using the monotonicity of the trace in $\alpha$, that

$$4\pi \left[ \frac{\alpha}{2\pi} \right] N(\mu, H) \leq \text{tr} B_{\alpha,\mu} \leq 4\pi \left[ \frac{\alpha}{2\pi} \right] N(\mu, H), \forall \alpha > 1. \quad (3.5)$$

Consequently, we conclude that

$$\text{tr} B_{\alpha,\mu} = 2\alpha N(\mu, H) + O(1), \alpha \to \infty.$$

The study of $\text{tr} h_1(B_{\alpha,\mu})$ is much more difficult, and the rest of the paper is focused on this task.

3. We point out that the function $h$ in Theorem 3.2 is not required to be smooth, not even at the endpoints $t = 0, 1$. If we do assume that $h$ is differentiable at the endpoints, then the conditions on the potential $V$ can be reduced to $V \in L^2_{loc}(\mathbb{R})$, as in Section 2. This can be observed at the first step of the proof of Theorem 3.2, see Subsection 3.2.

The increased smoothness of $V$, i.e. the condition $V \in C^\infty(\mathbb{R})$ is required to handle the functions $h$ that are Hölder-continuous at $t = 0, 1$. To be precise, a finite smoothness of $V$, depending on the Hölder exponent, would have been sufficient, but we do not go into these details to avoid excessive technicalities.

4. An Expansion of the Integral Kernel of the Spectral Projection

Let us temporarily assume that $\mu \in S$ where $S$ is a “genuine” band of $\sigma(H)$ defined in (2.8). Inspecting the formula (2.12), we observe that the set $\{k : \Lambda(k) < \mu\}$ is the interval $(2k_j - \delta, \delta)$ where $\delta = \delta(\mu) \in [k_j, k_j + n/2]$ is the uniquely defined value such that $\Lambda(\delta) = \mu$. The following lemma provides a convenient expansion of $P_\mu[S]$ in powers of $|x - y|^{-1}$.

**Lemma 4.1.** Let $\mu \in S$, where $S$ is the band defined in (2.8), and let $\delta = \delta(\mu)$ be as defined above. Then for all $x, y \in \mathbb{R}$ we have

$$P_\mu[S](x, y) = \Pi_\mu(x, y) + R_\mu[S](x, y), \quad (4.1)$$

where

$$\Pi_\mu(x, y) = \frac{\Phi(x, \delta)\Phi(y, \delta) - \Phi(x, \delta)\Phi(y, \delta)}{i(x - y)}, \quad (4.2)$$

and

$$R_\mu[S](x, y) = O\left((1 + |x - y|^2)^{-1}\right), \forall x, y \in \mathbb{R}. \quad (4.3)$$
Moreover, $R_{\mu}[S](x,y)$, $P_{\mu}[S](x,y)$ and $\Pi_{\mu}(x,y)$ are continuous functions of $x, y \in \mathbb{R}$, and
\[
|P_{\mu}[S](x,y)| + |\Pi_{\mu}(x,y)| = O((1 + |x-y|)^{-1}), \quad \forall x, y \in \mathbb{R}.
\] (4.4)

If $\mu \notin S^0$, then $P_{\mu}[S](x,y)$ is a continuous function of $x, y \in \mathbb{R}$, and it satisfies the bound
\[
P_{\mu}[S](x,y) = O((1 + |x-y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}.
\] (4.5)

**Proof.** Let us deduce the bound (4.5) first. Observe that if $\mu \notin S^0$, then either $P_{\mu}[S] = 0$ (if $\mu$ is below $S^0$), or $P_{\mu}[S] = P_{\mu}\circ [S]$ where $\mu_0 = \nu_{j+n-1}$, i.e. $\delta(\mu_0) = k_j + n/2$ (if $S$ is bounded). In the first case the bound (4.5) follows from the fact that the function $\Phi(\cdot)$ is real-valued, and in the second case it is trivial, so that $\Pi_{\mu}(x,y) = 0$, and hence the bound (4.5) follows from (1.1) and (1.3).

It remains to prove the continuity and the bounds (4.3) and (4.4) for $\Pi_{\mu}(x,y)$ with $|x-y|^r \geq 1$. Due to (2.11) and the symmetry property (2.10) one obtains the representation (4.1). Another integration by parts for $R_{\mu}[S]$ gives
\[
R_{\mu}[S](x,y) = \frac{\partial}{\partial k}(E(x,k)\Phi(y,k))\bigg|_{x \to y} - \int_{2k_j-\delta}^{\delta} \frac{\partial}{\partial k}(E(x,k)\Phi(y,k))dk.
\] (4.7)

Hence, estimate (4.3) follows from the fact that the functions $E$, $\partial_k E$, and $\partial_k^2 E$ are uniformly bounded.

Now Lemma 4.1 may be used for each “genuine” spectral band separately to get the corresponding expansion of the kernel $P_{\mu}(x,y)$.

**Lemma 4.2.** Let $\mu \in S$, where $S$ is the band defined in (2.3), and let $\delta = \delta(\mu)$ be as in Lemma 4.1. Then for all $x, y \in \mathbb{R}$ we have
\[
P_{\mu}(x,y) = \Pi_{\mu}(x,y) + R_{\mu}(x,y),
\] (4.8)

where $\Pi_{\mu}$ is as defined in (4.2), and
\[
R_{\mu}(x,y) = O((1 + |x-y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}.
\] (4.9)

Moreover, $R_{\mu}(x,y)$, $\Pi_{\mu}(x,y)$ and $P_{\mu}(x,y)$ are continuous functions of $x, y \in \mathbb{R}$, and
\[
|P_{\mu}(x,y)| + |\Pi_{\mu}(x,y)| = O((1 + |x-y|)^{-1}), \quad \forall x, y \in \mathbb{R}.
\] (4.10)
If $\mu \notin (\sigma(H))^\circ$, then $P_\mu(x,y)$ is a continuous function of $x, y \in \mathbb{R}$, and it satisfies the bound

$$P_\mu(x,y) = O((1 + |x - y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}. \quad (4.11)$$

**Proof.** The continuity of the projection kernel $P_\mu(x,y)$ follows immediately from Lemma 4.1. If $\mu \notin (\sigma(H))^\circ$, then $(4.11)$ follows directly from $(4.5)$. Assume now that $\mu \in S$. Let $S_1, S_2, \ldots, S_N$ be “genuine” spectral bands lying below the band $S$. Using Lemma 4.1, we can write

$$P_\mu(x,y) = \sum_{l=1}^N P_\mu[S_l](x,y) + P_\mu[S](x,y) = \Pi_\mu(x,y) + R_\mu(x,y),$$

where

$$R_\mu(x,y) = \sum_{l=1}^N P_\mu[S_l](x,y) + R_\mu[S](x,y).$$

By Lemma 4.1, the kernel $R_\mu[S]$ and each term $P_\mu[S_l]$, $l = 1, 2, \ldots, N$ satisfy $(4.9)$, whence $(4.8)$. The bound $(4.10)$ for the kernel $P_\mu[S](x,y)$ follows from $(4.4)$. \qed

5. **Elementary Trace Norm Estimates**

Throughout the proof of Theorem 3.2 we need various trace class bounds for operators involved. It is interesting that for most of our needs we can get away with rather elementary bounds, as in [16]. This fact is due to the specific form of the operators studied. As we see in the next few pages, many of the technical issues that we come across, boil down to trace class bounds for the operators of the form

$$\chi_I P_\mu \chi_J P_\mu \chi_K,$$

where $I, J, K \subset \mathbb{R}$ are some intervals that may depend on the parameter $\alpha > 0$.

### 5.1. **Schatten-von Neumann Classes.**

Throughout this paper, we make use of the standard notation for the Schatten-von Neumann classes of operators $S_q$, $q > 0$ in a Hilbert space, see e.g. [2], [22]. The class $S_q$ consists of all compact operators $A$ whose singular values $(s_k(A))_{k \in \mathbb{N}}$ are $q$-summable, i.e.

$$\sum_{k \in \mathbb{N}} s_k(A)^q < \infty.$$ 

For $A \in S_q$ we denote by

$$\|A\|_q := \left(\sum_{k \in \mathbb{N}} s_k(A)^q\right)^{\frac{1}{q}},$$

the norm (for $q \geq 1$) or quasi-norm (for $q \in (0, 1)$) on $S_q$. Note the “Hölder’s inequality”

$$\|AB\|_1 \leq \|A\|_p \|B\|_q, \quad \frac{1}{p} + \frac{1}{q} = 1,$$

which holds for any $A \in S_p$ and $B \in S_q$. While in this section we limit ourselves to estimates in the trace class $S_1$, Section 6 treats operators in the classes $S_q$ for $q \in (0, 1]$.

The next elementary trace class estimate (see [16, formula (12)]) plays a central role in our paper. We provide a proof for the reader’s convenience.

**Lemma 5.1.** Let $M \subset \mathbb{R}$ be a Borel-measurable set. Consider (weakly) measurable mappings $f, g : M \mapsto L^2(\mathbb{R})$, such that

$$\int_M \|f(z)\|_{L^2} \|g(z)\|_{L^2} \, dz < \infty.$$
Then the operator $A : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ which is defined via the form
$$\langle u, Av \rangle_{L^2} := \int_M \langle u, f(z) \rangle_{L^2} \langle g(z), v \rangle_{L^2} \, dz,$$

is of trace class with
$$\|A\|_1 \leq \int_M \|f(z)\|_{L^2} \|g(z)\|_{L^2} \, dz.$$

Proof. Let $(d_n)_n$ and $(e_n)_n$ be orthonormal bases (ONB’s) of $L^2(\mathbb{R})$ and denote by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ the scalar product and the norm respectively, on $L^2(\mathbb{R})$. Then we have
$$\sum_n |\langle d_n, Ae_n \rangle| \leq \sum_n \int_M |\langle d_n, f(z) \rangle \langle g(z), e_n \rangle| \, dz
= \int_M \sum_n |\langle d_n, f(z) \rangle \langle g(z), e_n \rangle| \, dz.$$ 

The Cauchy-Schwartz inequality and Parseval’s identity yield
$$\sum_n |\langle d_n, f(z) \rangle \langle g(z), e_n \rangle| \leq \left( \sum_n |\langle d_n, f(z) \rangle|^2 \right)^{\frac{1}{2}} \left( \sum_n |\langle g(z), e_n \rangle|^2 \right)^{\frac{1}{2}}
= \|f(z)\| \|g(z)\|.$$ 

This implies that
$$\sum_n |\langle d_n, Ae_n \rangle| \leq \int_M \|f(z)\| \|g(z)\| \, dz.$$ 

The supremum of the left-hand side over all ONB’s coincides with the trace norm, whence the claimed estimate. □

Equipped with these basic trace norm estimates, we can start now our investigation of the operator $A$.

5.2. Replacing the Spectral Projection by its Approximation. Let us recall the following general notation. If $f, g$ are real-valued functions we shall write $f \ll g$ if and only if $|f| \leq C|g|$ for some constant $C \geq 0$ which might depend on the potential $V$ but does not depend on the dilation parameter $\alpha$. Let $\Pi_\mu$ be as defined in Lemma 4.1.

Lemma 5.2. Let $I, J, K \subset \mathbb{R}$ be intervals such that $I \cap J = \emptyset$ and $K \cap J = \emptyset$. Then we have
$$\|\chi_I P_\mu \chi_J P_\mu \chi_K - \chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K\|_1 \ll 1,$$ 

where the integral kernel of $\Pi_\mu$ is defined in (4.2).

Proof. With the notation of Lemma 4.1 we may write
$$\chi_I P_\mu \chi_J P_\mu \chi_K = \chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K + \chi_I \Pi_\mu \chi_J R_\mu \chi_K + \chi_I R_\mu \chi_J \Pi_\mu \chi_K.$$ 

Let us then estimate the trace norm of the operator $\chi_I R_\mu \chi_J P_\mu \chi_K$, which has the integral kernel
$$\chi_I(x) \chi_K(y) \int_J R_\mu(x, z) P_\mu(z, y) \, dz.$$ 

We apply Lemma 5.1 with
$$f(x, z) = \chi_I(x) R_\mu(x, z), \quad g(y, z) = \chi_K(y) P_\mu(z, y) = \chi_K(y) P_\mu(y, z),$$
leading to
$$\|\chi_I R_\mu \chi_J P_\mu \chi_K\|_1 \leq \int_J \|R_\mu(\cdot, z)\|_{L^2(I)} \|P_\mu(\cdot, z)\|_{L^2(K)} \, dz.$$
Thus estimates (4.9) and (4.10) yield
\[
\left\| \chi_I R_{\mu} \chi_J P_\mu \chi_K \right\|_1 \ll \int_J \left( \int_I (1 + |x - z|)^{-4} \, dx \right)^{\frac{1}{2}} \left[ \int_K (1 + |z - y|)^{-2} \, dy \right]^{\frac{1}{2}} \, dz \\
\ll \int_J \left( 1 + \text{dist}(z, I) \right)^{-\frac{3}{2}} \left( 1 + \text{dist}(z, K) \right)^{-\frac{1}{2}} \, dz \\
\ll \int_J \left[ (1 + \text{dist}(z, I))^{-2} + (1 + \text{dist}(z, K))^{-2} \right] \, dz \ll 1.
\]

The operator \( \chi_I \Pi R\mu \chi_J R\mu \chi_K \) satisfies the same bound. Hence, the claim follows. \( \Box \)

5.3. Uniform Trace Norm Bounds. Under particular assumptions on the intervals \( I, J \) and \( K \) the operator (5.1) is of trace class with uniformly bounded trace norm. We list some of these conditions in the following proposition.

**Proposition 5.3.** Let \( I, J, K \subset \mathbb{R} \) be intervals such that one of the following conditions holds:

(i) \( |J| \ll 1 \),

(ii) Either
   (a) \( |J| \ll \max\{\text{dist}(I, J), \text{dist}(J, K)\} \), or
   (b) \( |K| \ll \text{dist}(J, K), |I| \ll \text{dist}(I, J) \), or
   (c) \( |K| \ll \text{dist}(J, K), |J| \ll \text{dist}(I, J) \).

(iii) \( J \) is finite, and \( I \) and \( K \) lie on opposite sides of \( J \), i.e.
\[
x \leq y \leq z \text{ or } z \leq y \leq x, \quad \text{for all } (x, y, z) \in I \times J \times K.
\]

(iv) \( |I| \ll 1 \) and \( I \cap J = \emptyset, K \cap J = \emptyset \).

Then the operator \( \chi_I P_\mu \chi_J P_\mu \chi_K \) is uniformly bounded (independently of \( \alpha \)) in trace norm, i.e.
\[
\| \chi_I P_\mu \chi_J P_\mu \chi_K \|_1 \ll 1. \tag{5.4}
\]

In the free case, i.e. for \( V \equiv 0 \), Proposition 5.3 with assumptions similar to (i) and (iii) has been obtained in [16, Lemma].

**Proof of Proposition 5.3.** According to Lemma 5.2 and bound (4.10),
\[
\| \chi_I P_\mu \chi_J P_\mu \chi_K \|_{S^1} \ll \int_J \left( \int_I (1 + |x - z|)^{-4} \, dx \right)^{\frac{1}{2}} \left[ \int_K (1 + |z - y|)^{-2} \, dy \right]^{\frac{1}{2}} \, dz. \tag{5.5}
\]

Let us estimate this integral under the conditions of the lemma.

Assume condition (i) i.e. \( |J| \ll 1 \). Both integrals inside (5.5) are uniformly bounded, even if \( I \) and \( K \) are unbounded. Thus the trace norm does not exceed \( |J| \ll 1 \), as required.

Assume now condition (iii). Using the Cauchy-Schwarz inequality, we estimate the right-hand side of (5.5) by
\[
\left[ \int_J \int_I (1 + |x - z|)^{-2} \, dxdz \right]^{\frac{1}{2}} \left[ \int_J \int_K (1 + |z - y|)^{-2} \, dydz \right]^{\frac{1}{2}}.
\]

The first integral is bounded by
\[
|J| \left( 1 + \text{dist}(I, J) \right)^{-1} \text{ or } |I| \left( 1 + \text{dist}(I, J) \right)^{-1}.
\]

The second integral is bounded by
\[
|K| \left( 1 + \text{dist}(J, K) \right)^{-1} \text{ or } |J| \left( 1 + \text{dist}(J, K) \right)^{-1}.
\]

Thus, under any of the conditions (iii) the right-hand side of (5.5) is uniformly bounded, as required.
Assume that the first of the conditions (5.3) holds. Let

\[ I = (s_1, t_1), J = (s_2, t_2), K = (s_3, t_3) \]  

(5.6)

with

\[-\infty \leq s_1 < t_1 \leq s_2 < t_2 \leq s_3 < t_3 \leq \infty.\]

Using (5.5), we get the bound

\[
\|\chi_I P_\mu \chi_J P_\mu \chi_K\|_1 \ll t_2 \int_{s_2}^{t_2} \left[ \int_{s_1}^{t_1} (z-x)^{-2} \, dx \right]^{1/2} \left[ \int_{s_3}^{t_3} (z-y)^{-2} \, dy \right]^{1/2} \, dz 
\]

\[
\ll \int_{s_2}^{t_2} (z-t_1)^{-1/2} (s_3-z)^{-1/2} \, dz 
\]

\[
\leq \int_{s_2}^{t_2} (z-s_2)^{-1/2} (t_2-z)^{-1/2} \, dz = \int_{0}^{s} z^{-1/2} (s-z)^{-1/2} \, dz,
\]

with \( s = t_2 - s_2 \). By rescaling, the last integral equals

\[
\int_{0}^{1} z^{-1/2} (1-z)^{-1/2} \, dz \ll 1,
\]

which leads to (5.4) again.

Finally, assume that (iv) holds. The right-hand side of (5.5) is bounded by

\[
|I|^{1/2} \int_{J} (1 + \text{dist}(z, I))^{-1} (1 + \text{dist}(z, K))^{-1/2} \, dz 
\]

\[
\ll \int_{J} (1 + \text{dist}(z, I))^{-1/2} \, dz + \int_{J} (1 + \text{dist}(z, K))^{-1/2} \, dz \ll 1.
\]

The proof is complete. \( \square \)

5.4. Replacing Almost Periodic Functions by their Mean Value. Looking at the formula (4.2) we see that the kernel of \( \chi_I P_\mu \chi_J P_\mu \chi_K \) contains kernels of the form

\[
S_{I,J,K}(x,y; f) = \chi_I(x) \chi_K(y) \int_{J} \frac{f(z)}{(z-x)(z-y)} \, dz,
\]

(5.7)

where \( f \) is a product of functions such as \( \Phi(\cdot, \delta) \) and \( \Phi(\cdot, \delta) \). The following lemma gives conditions for the intervals \( I, J, K \) under which we may replace \( f \) in \( S_{I,J,K}(x,y; f) \) by its almost periodic mean value while the resulting error is uniformly bounded in trace norm.

Lemma 5.4. Let \( \Theta \subset \mathbb{R} \) be a countable set, and let \( (a_\theta)_{\theta} \subset \mathbb{C} \) be such that

\[
\sum_{\theta \in \Theta} |a_\theta| (1 + |\theta|^{-1}) < \infty.
\]

(5.8)

Let the function \( f \in \text{CAP}(\mathbb{R}) \) be defined by

\[
f(x) = \sum_{\theta \in \Theta} a_\theta e^{i\theta x}.
\]

Assume that the intervals \( I, J, K \subset \mathbb{R} \) satisfy \( \text{dist}(I, J), \text{dist}(J, K) \gg 1 \) and consider the operator \( S_{I,J,K}(f) \) in \( L^2(\mathbb{R}) \) with the integral kernel (5.7). Then we have

\[
\|S_{I,J,K}(f) - S_{I,J,K}(M(f))\|_1 \ll 1.
\]

(5.9)
Proof. Without loss of generality we may assume that $\mathcal{M}(f) = 0$, i.e. $0 \notin \Theta$. (otherwise consider $f - \mathcal{M}(f)$). Consider the primitive $F(x) := \int_0^x f(t)dt$ of $f$. Then the assumption (5.8) implies that $F$ is uniformly bounded:

$$|F(x)| = \left| \sum_{\theta \in \Theta} a_{\theta} \int_0^x e^{i\theta t}dt \right| \leq \sum_{\theta \in \Theta} \left| \frac{a_{\theta}}{i\theta}(e^{i\theta x} - 1) \right| \ll 1, \ \forall x \in \mathbb{R}.$$ 

Let $J = (s, t)$, so integrating by parts gives

$$S_{I,J,K}(x, y; f) = \chi_I(x)\chi_K(y) \frac{F(z)}{(z-x)(z-y)} \bigg|_{z=s}^{t} + \chi_I(x)\chi_K(y) \int_s^t \left[ \frac{F(z)}{(z-x)^2(z-y)} + \frac{F(z)}{(z-x)(z-y)^2} \right] dz.$$ 

(5.10)

The first term in (5.10) constitutes the kernel of a rank two operator, whose norm, and hence trace norm as well, is easily estimated by a constant times $\text{dist}(I,J)$, $\text{dist}(J,K)$.

The second term on the right-hand side of (5.10) is treated with the help of Lemma 5.1, as in the proof of Lemma 5.2. Thus (5.9) follows.

□

6. SCHATTEN-VON NEUMANN CLASS ESTIMATES FOR PSEUDO-DIFFERENTIAL OPERATORS WITH PERIODIC AMPLITUDES

So far our main tool for getting trace-class estimates has been Lemma 5.1. At the final stages of the proof, however, when we pass to non-smooth functions $h$, we also need some estimates in more general Schatten-von Neumann classes $\mathfrak{S}_q$ with $q \in (0,1]$. Lemma 5.1 is not applicable any longer, and we have to appeal to other results available in the literature.

We use the formalism of pseudo-differential operators (ΨDO). For a complex-valued function $p = p(x, y, \xi)$, $x, y, \xi \in \mathbb{R}$, that we call amplitude, we define the ΨDO $\text{Op}(p)$ that acts on Schwartz class functions $u$ as follows:

$$\text{Op}(p)u(x) = \frac{1}{2\pi} \int \int e^{i\xi(x-y)} p(x, y, \xi) u(y)dyd\xi.$$ 

(6.1)

This integral is well-defined, e.g. for any amplitude $p$ which is uniformly bounded and compactly supported in the variable $\xi$.

The main result of this section is the following proposition that implies Schatten-(quasi)norm estimates for the operator

$$A_{\alpha,\mu} = B_{\alpha,\mu}(1 - B_{\alpha,\mu})$$ 

(6.2)

(see Corollary 6.3).

Lemma 6.1. Let $I$, $\Omega \subset \mathbb{R}$ be bounded intervals, and let the function $p$ be $C^\infty$ in all three variables, $2\pi$-periodic in $x$ and $y$, and such that $p(x, y, \xi) = 0$ for all $x, y \in \mathbb{R}$, and $|\xi| \geq R$ with some $R > 0$. Denote

$$p[\Omega](x, y, \xi) = p(x, y, \xi) \chi_\Omega(\xi).$$

Then, for any $q \in (0,1]$ we have

$$\|\chi_{\alpha I} \text{Op}(p)(1 - \chi_{\alpha I})\|_q \ll 1,$$ 

(6.3)

and

$$\|\chi_{\alpha I} \text{Op}(p[\Omega])(1 - \chi_{\alpha I})\|_q \ll (\log \alpha)^{\frac{1}{q}},$$ 

(6.4)

The implicit constants in (6.3) and (6.4) depend on the amplitude $p$, number $R$ and also on the intervals $I$ and $\Omega$.

Our proof relies on similar results from [23]. We state these results in the form adjusted for our purposes.
FORMULAS OF SZEG˝O TYPE FOR THE PERIODIC SCHR¨ODINGER OPERATOR

Proposition 6.2. Let \( I, \Omega \subset \mathbb{R} \) be bounded intervals, and let the function \( p = p(\xi) \) be \( C_0^\infty(\mathbb{R}) \) with \( p(\xi) = 0 \) for \( |\xi| \geq R \) with some \( R > 0 \). For \( q \in (0, 1] \) denote

\[
N_q(p) := \max_{0 \leq m \leq \lfloor 2q^{-1} \rfloor + 1} \sup_\xi |p^{(m)}(\xi)| < \infty.
\]

Then

\[
\|\chi_{\alpha l} \operatorname{Op}(p)(1 - \chi_{\alpha l})\|_q \ll N_q(p),
\]

and

\[
\|\chi_{\alpha l} \operatorname{Op}(p(\omega))(1 - \chi_{\alpha l})\|_q \ll (\log \alpha)^{\frac{q}{2}} N_q(p).
\]

The implicit constants in (6.6) and (6.7) depend on the intervals \( I, \Omega \) and number \( R \), but are independent of the amplitude \( p \).

Thus, our task is to extend Proposition 6.2 to amplitudes, that are periodic in \( x \) and \( y \).

A few remarks are in order. Proposition 6.2 is a direct consequence of [25, Corollary 4.4, Theorem 4.6]. At this point it is important to emphasize that the main focus of [25] was the quasi-classical asymptotics, whereas our objective in the current paper is the scaling asymptotics. In the context of pseudo-differential operators, these two types of asymptotics are equivalent if the amplitude \( p \) is \( x, y \)-independent.

Proof of Lemma 6.1. We prove only the bound (6.4). The bound (6.3) can be derived in a similar way.

Performing translations, dilations and renormalization of \( \alpha \), one may assume that \( I = \Omega = (0, 1) \). Since \( p \) is \( 2\pi \)-periodic in \( x \) and \( y \), we can represent it as

\[
p(x, y, \xi) = \sum_{n,l} e^{inx + iyl} a_{nl}(\xi),
\]

where \( a_{nl}(\cdot) \) are \( C_0^\infty \) in \( \xi \) with supports in \((-R, R)\), and decay in \( n \) and \( l \) faster than any reciprocal polynomial, uniformly in \( \xi \in (-R, R) \). Precisely, a straightforward integration by parts shows that

\[
|a_{nl}^{(m)}(\xi)| \ll (1 + |n|)^{-s}(1 + |l|)^{-t} \int_0^{2\pi} \int_0^{2\pi} \left| \partial_x^s \partial_y^t \partial_{\xi}^m p(x, y, \xi) \right| dx dy, \quad n, l \in \mathbb{Z},
\]

for arbitrary \( t, s = 0, 1, \ldots \), so that

\[
N_q(a_{nl}) \ll (1 + |n|)^{-s}(1 + |l|)^{-t}, \quad n, l \in \mathbb{Z},
\]

with a constant independent of \( n, l \), but depending on \( s, t, q \) (see (6.5) for the definition of \( N_q \)). Consequently, the operator \( \operatorname{Op}(p(\omega)) \) can be represented as follows:

\[
\operatorname{Op}(p(\omega)) = \sum_{n,l} e^{inx} A_{nl} e^{ily}, \quad A_{nl} = \operatorname{Op}(a_{nl} \chi_{\Omega}).
\]

Using (6.7), we immediately obtain the bound

\[
\|\chi_{\alpha l} A_{nl}(1 - \chi_{\alpha l})\|_q^q \ll (1 + |n|)^{-sq}(1 + |l|)^{-tq} \log \alpha.
\]

Employing the \( q \)-triangle inequality for the ideals \( \mathcal{S}_q \) (see [2, p. 262]), we arrive at the bound

\[
\|\chi_{\alpha l} \operatorname{Op}(p(\omega))(1 - \chi_{\alpha l})\|_q^q \leq \sum_{nl} \|\chi_{\alpha l} A_{nl}(1 - \chi_{\alpha l})\|_q^q \ll \log \alpha \sum_{nl} (1 + |n|)^{-sq}(1 + |l|)^{-tq}.
\]

The sum on the right-hand side is finite if \( sq, tq > 1 \). This completes the proof.

\[\square\]

Corollary 6.3. Assume that \( V \in C_0^\infty(\mathbb{R}) \). Let \( A_{\alpha,\mu} \) be as defined in (6.2).
(1) Let \( I \subset \mathbb{R} \) be an interval. If \( \mu \in (\sigma(H))^{\circ} \), then for any \( q \in (0, 1) \),
\[
\| \chi_{\alpha}P_{\mu}(1 - \chi_{\alpha}) \|_q^q \ll \log(\alpha). \tag{6.8}
\]
If \( \mu \notin (\sigma(H))^{\circ} \), then for any \( q \in (0, 1) \),
\[
\| \chi_{\alpha}P_{\mu}(1 - \chi_{\alpha}) \|_q^q \ll 1. \tag{6.9}
\]

(2) For any \( q \in (0, 1) \),
\[
\| A_{\alpha,\mu} \|_q^q \ll \begin{cases} 
1, & \mu \notin (\sigma(H))^{\circ}, \\
\log(\alpha), & \mu \in (\sigma(H))^{\circ}.
\end{cases} \tag{6.10}
\]
Moreover, assume that \( h \) satisfies Condition [3.7]. Then \( h(B_{\alpha,\mu}) \) is of trace class and
\[
\| h(B_{\alpha,\mu}) \|_1 \ll \begin{cases} 
\alpha|h(1)| + 1, & \mu \notin (\sigma(H))^{\circ}, \\
\alpha|h(1)| + \log(\alpha), & \mu \in (\sigma(H))^{\circ}.
\end{cases} \tag{6.11}
\]

(3) If \( \mu \notin (\sigma(H))^{\circ} \), then [3.3] holds.

The implicit constants in the inequalities (6.8), (6.9), (6.10) and (6.11) are independent of \( \alpha \).

Proof. It suffices to prove (6.8) and (6.9) for the projections \( P_{\mu}[S] \) under the conditions \( \mu \in S^{\circ} \)
and \( \mu \notin S^{\circ} \) respectively, for any “genuine” band \( S \) of the type (2.8).

Suppose that \( \mu \in S^{\circ} \). By virtue of (4.6), the operator \( P_{\mu}[S] \) has the form \( \text{Op}(\rho[\Omega]) \) with
\[
p(x, y, \xi) = E(x, \xi)E(y, \xi) \quad \text{and} \quad \Omega = (2k_j - \delta, \delta),
\]
where \( k_j \) is as defined in (2.5), and \( \delta \in (k_j, k_j + n/2) \) is the unique solution of the equation
\( \Lambda(\delta) = \mu \). The function \( E(x, \xi) \) is \( 2\pi \)-periodic in \( x \), and due to the \( C^\infty \)-smoothness of \( V \), it is also \( C^\infty \)-smooth in \( x \). Now (6.8) follows from (6.3).

Suppose that \( \mu \notin S^{\circ} \). According to (2.12), either \( P_{\mu}[S] = 0 \), in which case (6.9) is trivial, or
\[
P_{\mu}[S](x, y) = \int_{nT} \Phi(x, k)\Phi(y, k)dk.
\]
Using a straightforward partition of unity on the circle \( nT \) one can represent \( P_{\mu}[S] \) as a finite sum of operators of the form \( \text{Op}(p) \) with
\[
p(x, y, \xi) = E(x, \xi)E(y, \xi)\zeta(\xi), \quad \zeta \in C^\infty_0(\mathbb{R}).
\]
Therefore, (6.10) is a consequence of (6.3).

From \( \| P_{\mu}\chi_{(-\alpha,\alpha)} \|_q \leq 1 \) we get that
\[
\| A_{\alpha,\mu} \|_q = \| \chi_{(-\alpha,\alpha)}P_{\mu}(1 - \chi_{(-\alpha,\alpha)})P_{\mu}\chi_{(-\alpha,\alpha)} \|_q \leq \| \chi_{(-\alpha,\alpha)}P_{\mu}(1 - \chi_{(-\alpha,\alpha)}) \|_q,
\]
and (6.10) follows from (6.3).

To prove (6.11) we use the representation (5.4): \( h(t) = th(1) + h_1(t) \), so that \( h(0) = h_1(0) = 0 \)
and \( |h_1(t)| \ll t^{q}(1-t)^{q} \), where \( q \in (0, 1) \) is the Hölder parameter of the function \( h \). The first term on the right-hand side of (6.11) follows from the bound (5.5). For the second term write:
\[
\| h_1(B_{\alpha,\mu}) \|_1 \ll \| A_{\alpha,\mu} \|_q \ll \| A_{\alpha,\mu} \|_q,
\]
and hence the required bounds follow from (6.10). Together with Remark [3.3] this also implies Part (3) of the corollary. \( \square \)

7. Proof of Theorem 3.2: symmetric polynomial functions

By virtue of Corollary [3.3], the formula (5.3) is already proved. Thus it remains to prove Theorem 3.2 for \( \mu \in (\sigma(H))^{\circ} \). From now on we assume that \( \mu \) is an interior point of a band \( S \) of the type (2.8). As before, define \( \delta \in (k_j, k_j + n/2) \) as the unique solution of the equation \( \Lambda(\delta) = \mu \). For simplicity we abbreviate \( \Phi = \Phi(\cdot, \delta) \).
7.1. Polynomial Classes. We begin the proof of (5.2) with studying polynomial functions. The following classes of polynomials on the interval \([0, 1]\) will be relevant:

\[
\mathcal{P} := \{p : [0, 1] \rightarrow \mathbb{C}, \text{ polynomial}\},
\]
\[
\mathcal{P}_0 := \{p \in \mathcal{P} : p(0) = p(1) = 0\},
\]
\[
\mathcal{P}_s := \{p \in \mathcal{P} : p(t) = p(1 - t) \text{ for all } t\},
\]
\[
\mathcal{P}_{s,0} := \mathcal{P}_s \cap \mathcal{P}_0.
\]

As explained in Remark 3.3, it suffices to prove (3.2) for the functions \(h\) such that \(h_1(0) = h_1(1) = 0\). Thus we need to study polynomials \(p \in \mathcal{P}_0\). In fact, it is enough to consider a basis of \(\mathcal{P}_0\). As in [16], we choose the basis

\[
\{(p_n, q_n) : p_n(t) = (t(1 - t))^n, q_n(t) = t(t(1 - t))^n, n = 1, 2, \ldots\},
\]

and start by considering the symmetric elements \(p_n(t)\), which form a basis of \(\mathcal{P}_{s,0}\). So, we study the operators

\[
p_n(B_{\alpha,\mu}) = A^n_{\alpha,\mu}, \quad A_{\alpha,\mu} = B_{\alpha,\mu}(1 - B_{\alpha,\mu}).
\]

In so doing, we follow the strategy of [16], where a similar problem was analysed in the unperturbed case \(V = 0\). In fact, our objective is to reduce the calculations to the unperturbed case, by using Lemmas 2.3 and 5.4.

7.2. Trace Class Calculus for the Operator \(A_{\alpha,\mu}\). Rewrite the operator \(A_{\alpha,\mu}\) in the form

\[
A_{\alpha,\mu} = A^-_{\alpha,\mu} + A^+_{\alpha,\mu}
\]

with

\[
\begin{align*}
A^-_{\alpha,\mu} & = \chi(-\alpha,\alpha)P_{\mu}\chi(-\infty,\alpha)P_{\mu}\chi(-\alpha,\alpha), \\
A^+_{\alpha,\mu} & = \chi(-\alpha,\alpha)P_{\mu}\chi(\alpha,\infty)P_{\mu}\chi(-\alpha,\alpha).
\end{align*}
\]

Now we perform various transformations with each of these operators that constitute “small” perturbations in \(\mathcal{G}_1\). Thus, it is natural to adopt the following notational convention:

Definition 7.1. Let \(A\) and \(B\) be bounded operators on \(L^2(\mathbb{R})\). We write \(A \sim B\) if \(\|A - B\|_{\mathcal{G}_1} \ll 1\), uniformly in \(\alpha \gg 1\). We write \(A \approx B\) if \(A\) and \(B\) are trace class and \(|\text{tr } A - \text{tr } B| \ll 1\) uniformly in \(\alpha \gg 1\).

Clearly, for trace class operators \(A, B\) the relation \(A \sim B\) implies \(A \approx B\), but not the other way round. Note also, that \(A \sim B\) implies \(A^n \sim B^n\) for any \(n = 1, 2, \ldots\).

To begin with, by virtue of Proposition 5.3(ii),

\[
A^+_{\alpha,\mu} \sim \chi(-\alpha,\alpha)P_{\mu}\chi(\alpha,\infty)P_{\mu}\chi(-\alpha,\alpha),
\]

and

\[
A^-_{\alpha,\mu} \sim \chi(-\alpha,\alpha)P_{\mu}\chi(-\infty,-\alpha-1)P_{\mu}\chi(-\alpha,\alpha).
\]

7.2.1. Operators \(D^\pm_{\alpha}\). The next step is to replace \(A^\pm_{\alpha,\mu}\) with operators that do not contain any information on the function \(\Phi(x, k)\). These are the operators \(D^\pm_{\alpha} : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})\), defined via their integral kernels

\[
D^+_{\alpha}(x, y) := \frac{1}{4\pi^2}\chi(-\alpha,\alpha)(x)\chi(-\alpha,\alpha)(y) \int_{\alpha+1}^\infty \frac{1}{(z-x)(z-y)} \, dz,
\]
\[
D^-_{\alpha}(x, y) := \frac{1}{4\pi^2}\chi(-\alpha,\alpha)(x)\chi(-\alpha,\alpha)(y) \int_{-\infty}^{-\alpha-1} \frac{1}{(z-x)(z-y)} \, dz.
\]
Note that $D^{\pm}_\alpha$ and $D^{-}_\alpha$ are unitarily equivalent via the change $x \mapsto -x$. The crucial fact is that the asymptotic formulas for the traces of powers $(D^{\pm}_\alpha)^n$ can be easily deduced from the results of [16]:

**Lemma 7.2.** Let $p_n(t) = t^n(1 - t)^n$, $n = 1, 2, \ldots$. Then

$$\text{tr}(D^{\pm}_\alpha)^n = \frac{1}{4} \log \alpha \ W(p_n) + o(\log \alpha), \ \alpha \to \infty, \quad (7.5)$$

where $W(\cdot)$ is as defined in (3.1).

**Proof.** Since $D^{\pm}_\alpha$ and $D^{-}_\alpha$ are unitarily equivalent, we show (7.3) for $D_\alpha := D^{+}_\alpha$ only. By translation and reflection, the operator $D_\alpha$ is unitarily equivalent to the operator with kernel

$$\frac{1}{4\pi^2} \chi(1,2\alpha+1)(x)\chi(1,2\alpha+1)(y) \int_0^\infty \frac{1}{(z+x)(z+y)} dz,$$

This is the kernel of the operator which is denoted by $K_c$ in [16, p. 476]. Thus the formula (7.5) immediately follows from [16, formula (19), p. 477].

A useful way to write $D^{\pm}_\alpha$ is

$$D^{\pm}_\alpha = (Z^{\pm}_\alpha)^* Z^{\pm}_\alpha,$$

where $Z^{\pm}_\alpha$ have kernels

$$Z^{+}_\alpha(x, y) = \frac{\chi(x,1,\infty)(x)\chi(-\alpha,\alpha)(y)}{2\pi(x-y)}, \quad \text{and} \quad Z^{-}_\alpha(x, y) = \frac{\chi(\alpha,1,\infty)(x)\chi(-\alpha,\alpha)(y)}{2\pi(x-y)}, \quad (7.6)$$

respectively. Now we need to establish a few facts for operators $D^{\pm}_\alpha$ and $Z^{\pm}_\alpha$. Recall that we abbreviate $\Phi = \Phi(x, \delta)$, $\delta = \delta(\mu)$, remembering that $\mu$ is strictly inside the band $S$.

**Lemma 7.3.** Denote by $Y^{\pm}_\alpha$ any of the two operators $Z^{\pm}_\alpha$ or $(Z^{\pm}_\alpha)^*$. With the notation as above,

$$Y^{\pm}_\alpha |\Phi|^2(Y^{\pm}_\alpha)^* \sim \frac{1}{2\pi} Y^{\pm}_\alpha (Y^{\pm}_\alpha)^*, \quad Y^{\pm}_\alpha \Phi^2(Y^{\pm}_\alpha)^* \sim 0.$$

**Proof.** We prove the lemma for the “$+$” sign and for the case $Y^{+}_\alpha = Z^{+}_\alpha$ only. The remaining cases are treated in the same way. For brevity we omit the superscript “$+$” and write $Z_\alpha$ instead of $Z^{+}_\alpha$.

The operator $Z_\alpha f Z_\alpha^*$ coincides with the operator $(4\pi^2)^{-1} S_{I,J,K}(f)$ with

$$I = K = (\alpha + 1, \infty), J = (-\alpha, 0),$$

see the definition (5.7). Thus by Lemma 3.4

$$Z_\alpha f Z_\alpha^* \sim M(f) Z_\alpha Z_\alpha^*.$$

In view of (2.13) and (2.14), $M(|\Phi|^2) = (2\pi)^{-1}$ and $M(\Phi^2) = 0$, whence the claimed result. \hfill $\square$

**Corollary 7.4.** Let

$$K^{\pm}_\alpha = 2\pi [\Phi(D^{\pm}_\alpha)^n \Phi + \Phi(D^{\pm}_\alpha)^n \Phi], \quad n = 1, 2, \ldots, \quad (7.7)$$

Then for all $n = 1, 2, \ldots$, we have

$$(K^{\pm}_\alpha)^n \sim K^{\pm}_{\alpha,n}, \quad (7.8)$$

and

$$(K^{\pm}_{\alpha,1})^n \approx 2(D^{\pm}_\alpha)^n, \quad \alpha \to \infty. \quad (7.9)$$
Proof. For brevity we omit the superscript “±” and write $K_{a,1}, D_a$ instead of $K^±_{a,1}, D^±_a$ etc. The powers of $K_{a,1}$ contain terms of the form $D_a f D_a$ with $f = |\Phi|^2$, $\Phi^2$ or $\overline{\Phi}^2$. The operator $D_a f D_a$, is written as

$$Z^*_a Z_a f Z^*_a Z_a.$$ 

Thus by Lemma 7.3

$$K^n_{a,1} \sim (2\pi)^n [(\Phi D_a \overline{\Phi})^n + (\overline{\Phi} D_a \Phi)^n] \sim 2\pi [\Phi D^n_{a} \overline{\Phi} + \overline{\Phi} D^n_{a} \Phi],$$

as claimed.

In order to prove (7.9), use the cyclicity of the trace. If $n = 1$, then, again by Lemma 7.3

$$\Phi D_a \overline{\Phi} \approx Z_a |\Phi|^2 Z^*_a \sim \frac{1}{2\pi} Z_a Z^*_a \approx \frac{1}{2\pi} D_a.$$ 

If $n \geq 2$, then, in the same way,

$$\Phi D^n_{a} \overline{\Phi} \approx Z_a D^{n-2}_a Z^*_a |\Phi|^2 Z^*_a \sim \frac{1}{2\pi} Z_a D^{n-2}_a Z^*_a Z^*_a Z^*_a \sim \frac{1}{2\pi} D^n_a$$

The same is done with the component containing $\Phi$ and $\overline{\Phi}$ in the other order. This implies (7.3). Thus the proof is complete. \hfill $\Box$

7.2. Approximating Operators $A^\pm_{a,\mu}$. Assume that $\mu$ is as before and $K^\pm_{a,n}$ are as defined in (7.7).

Lemma 7.5. Let $S$ be a band of the spectrum of $H$, and let $\mu \in S^\circ$. Let $\delta \in (k_j, k_j + n/2)$ be the unique solution of the equation $\Lambda(\delta) = \mu$. Then we have

$$(A^\pm_{a,\mu})^n \sim (K^\pm_{a,1})^n,$$ (7.10)

and

$$(A^+_{a,\mu})^n \sim (A^-_{a,\mu})^n + (K^-_{a,1})^n.$$ (7.11)

for every $n = 1, 2, \ldots$.

Proof. To prove (7.10) it suffices to consider the case $n = 1$. As before, we do it for $A^+_{a,\mu}$ only, omitting the superscript “+”. From (7.3) and Lemma 5.3 it follows that

$$A^+_{a,\mu} \sim \chi(-a, a) P\mu \chi(a+1, \infty) P\mu \chi(-a, a).$$

By (4.2) and (7.3),

$$\chi(a+1, \infty) P\mu \chi(-a, a) = -2\pi i (\Phi Z^*_a \overline{\Phi} - \overline{\Phi} Z^*_a \Phi),$$

so that

$$A^+_{a,\mu} \sim 4\pi^2 (\Phi Z^*_a |\Phi|^2 Z^*_a \overline{\Phi} + \overline{\Phi} Z^*_a |\Phi|^2 Z^*_a \Phi) - 4\pi^2 (\Phi Z^*_a \overline{\Phi} Z^*_a Z^*_a \Phi)$$

Consequently, by Lemma 7.3

$$A^+_{a,\mu} \sim 2\pi (\Phi Z^*_a Z^*_a \overline{\Phi} + \overline{\Phi} Z^*_a Z^*_a \Phi) = K_{a,1},$$

as required.

Proof of (7.11). By the definition (7.2),

$$A^-_{a,\mu} A^+_{a,\mu} = \chi(-a, a) P\mu \left(\chi(-\infty, -a) P\mu \chi(-a, a) P\mu \chi(a, \infty)\right) P\mu \chi(-a, a).$$

By Proposition 5.3(iii)), the trace norm of the operator in the middle is uniformly bounded, and hence $A^-_{a,\mu} A^+_{a,\mu} \sim 0$. In the same way one checks that $A^+_{a,\mu} A^-_{a,\mu} \sim 0$. Thus

$$A^+_{a,\mu} \sim (A^+_{a,\mu})^n + (A^-_{a,\mu})^n,$$

and (7.11) is now a consequence of (7.10). \hfill $\Box$
7.3. Proof of Theorem 3.2 for Symmetric Polynomials. By (7.11), (7.9) and (7.5),
\[
\text{tr} A_{\alpha,\mu}^n = \text{tr}(K_+^n) + \text{tr}(K_-^n) + O(1)
\]
\[= 2\text{tr}(D_+^n) + 2\text{tr}(D_-^n) + O(1)
\]
\[= \log(\alpha) W(p_n) + o(\log(\alpha)), \quad n = 1, 2, \ldots. \tag{7.12}
\]
Hence, Theorem 3.2 for polynomials \(p \in \mathcal{P}_{s,0}\) follows from the identity \(p_n(B_{\alpha,\mu}) = A_{\alpha,\mu}^n\). \(\square\)

8. Proof of Theorem 3.2 Conclusion

As above, we assume that \(\mu \in S^o\), where \(S\) is a band of the type (2.8).

8.1. Arbitrary Polynomials. So far we have proved Theorem 3.2 for polynomials \(p \in \mathcal{P}_{s,0}\) (cf. (7.1) for notation). To extend this result to arbitrary \(p \in \mathcal{P}_s\) it remains to treat basis elements of the form \(q_n(t) = t[t(1-t)]^n, \quad n = 1, 2, \ldots. \) Following [16] for the free case, this is done by a symmetry argument that reduces \(\text{tr} [B_{\alpha,\mu} A_{\alpha,\mu}^n]\) to \(\text{tr} A_{\alpha,\mu}^n\).

Lemma 8.1. For every \(n = 1, 2, \ldots, \) we have
\[
B_{\alpha,\mu}(A_{\alpha,\mu})^n \approx \frac{1}{2} \text{tr} (A_{\alpha,\mu})^n, \tag{8.1}
\]
as \(\alpha \to \infty\).

Compared to [16], the proof requires some extra work. The main difference is that instead of the reflection symmetry used in [16], we use the translation symmetry of the operators. The operators \(A_{\alpha,\mu}^+\) and \(A_{\alpha,\mu}^-(\text{see (7.2)})\) are considered separately. Applying Proposition 5.3 (i)(b), we get
\[
A_{\alpha,\mu}^\pm \sim \chi(-\alpha, \mu)p_\chi(\alpha, 3\alpha) P_\mu \chi(-\alpha, \mu). \tag{8.2}
\]
Let \(U_\alpha^\pm\) be the unitary shift operators defined by
\[
U_\alpha^\pm f(x) = f(x \mp \alpha_0), \quad \alpha_0 = 2\pi \left\lfloor \frac{\alpha}{2\pi} \right\rfloor.
\]
The equivalence (8.2) implies that
\[
(U_\alpha^+) A_{\alpha,\mu} A_{\alpha,\mu}^+ \sim \chi(-2\alpha, 0)P_\mu \chi(2\alpha, 0). \tag{8.3}
\]
Indeed, (8.2) yields:
\[
(U_\alpha^+) A_{\alpha,\mu} A_{\alpha,\mu}^+ \sim \chi(-\alpha_0, \alpha - \alpha_0) P_\mu \chi(-\alpha_0, 3\alpha - \alpha_0) P_\mu \chi(-\alpha_0, \alpha - \alpha_0),
\]
since \((U_\alpha^+)^* P_\mu U_\alpha^+ = P_\mu\). Now, to get (8.3), one needs to use repeatedly Proposition 5.3 (i)(b) (iv). We denote
\[
\chi_\alpha^+ = \chi(2\alpha, 0), \quad \chi_\alpha^- = \chi(-2\alpha, 0)
\]
and
\[
T_{\alpha,\mu} := \chi_\alpha^+ P_\mu \chi_\alpha^- P_\mu \chi_\alpha^+.
\]
Thus one can write
\[
(U_\alpha^+) A_{\alpha,\mu} A_{\alpha,\mu}^+ \sim T_{\alpha,\mu}^\pm. \tag{8.4}
\]
This relation with the “+” sign coincides with (8.3), and for the “-” sign it is proved in the same way. The proof of Lemma 8.1 begins with the following observation.

Lemma 8.2. For any \(n = 1, 2, \ldots, \) we have
\[
P_\mu(T_{\alpha,\mu}^\pm)^n \approx (1 - P_\mu)(T_{\alpha,\mu}^\pm)^n, \quad \text{as} \quad \alpha \to \infty. \tag{8.5}
\]
Proof. For brevity we write $\chi^\pm = \chi^\pm_\alpha$, $T^\pm = T^\pm_{\alpha, \mu}$, $P = P_\mu$, and $Q = 1 - P$. We have

$$P(T^+)^n = P(1 - P)^n Q \chi^+ P \chi^- (T^+)^n -1,$$

$$= P \chi^+ Q \chi^- (T^+)^n -1 + R_1 + R_2,$$

(8.6)

with

$$R_1 = P \chi_{(2\alpha, \infty)} Q \chi^+ P \chi^- (T^+)^n -1,$$

$$R_2 = P \chi_{(-\infty, -2\alpha)} Q \chi^+ P \chi^- (T^+)^n -1.$$

We notice that $Q = 1 - P$ can be replaced by $-P$ in $R_1$. By Proposition 5.3(iii),

$$\chi_{(2\alpha, \infty)} P \chi^+ P \chi^- \sim 0,$$

so that $R_1 \sim 0$. To handle $R_2$, observe that

$$\chi^+ P \chi^- (T^+)^n -1 = (T^-) n -1 \chi^+ P \chi^-,$$

(8.7)

and hence, by cyclicity of the trace,

$$R_2 \sim Q \chi^+ (T^-)^n -1 \chi^+ P \chi^- P \chi_{(-\infty, -2\alpha)}.$$

Applying Proposition 5.3(iii) to the factor $\chi^+ P \chi^- P \chi_{(-\infty, -2\alpha)}$, we infer that $R_2 \approx 0$.

Apply (8.7) to the first operator on the right-hand side of (8.6) and use again the cyclicity:

$$P \chi^+ Q \chi^+ P \chi^- (T^+)^n -1 = P \chi^+ Q (T^-)^n -1 \chi^+ P \chi^-,$$

$$\approx Q (T^-)^n -1 \chi^+ P \chi^- = Q (T^-)^n.$$

Together with (8.6), this yields (8.5) for the “+” sign. The relation (8.5) for the “-” sign is obtained in the same way.

Proof of Lemma 8.1. We shall use the simplified notation as in the proof of Lemma 8.2 and also write $A = A_{\alpha, \mu}$, $A^\pm = A^\pm_{\alpha, \mu}$, and $B = B_{\alpha, \mu}$. First observe that $BA^n \approx PA^n$. Thus by (7.11) and (8.4),

$$BA^n \approx P(A^+)^n + P(A^-)n \approx P(T^+)^n + P(T^-)^n.$$

By Lemma 8.2

$$2P(T^\pm)^n \approx P(T^\pm)^n + (1 - P)(T^\pm)^n,$$

so that

$$2P(T^+)^n + 2P(T^-)^n \approx P(T^+)^n + (1 - P)(T^-)^n + P(T^-)^n + (1 - P)(T^+)^n$$

$$= (T^+)^n + (T^-)^n.$$

Using (8.4) and (7.11) again, we get

$$2BA^n \approx A^n,$$

which leads to (8.1), and hence completes the proof.

As a consequence of Lemma 8.1, Theorem 3.2 can be proved for arbitrary $p \in \mathbb{N}_0$.

Proof of Theorem 3.2 for arbitrary polynomials. It remains to prove the theorem for polynomials of the form $q_n(t) = tp_n(t)$, $n = 1, 2, \ldots$. From Lemma 8.1 and (7.12) we deduce that

$$\text{tr } [B_{\alpha, \mu} (A_{\alpha, \mu})^n] = \frac{1}{2} \log(\alpha) W(p_n) + o(\log(\alpha)), \ \alpha \to \infty.$$

(8.8)

To convert $W(p_n)$ into $W(q_n)$ we perform a very elementary calculation:

$$\pi^2 W(q_n) = \int_0^1 \frac{tp_n(t)}{t(1 - t)} dt = \int_0^1 \frac{p_n(t)}{1 - t} dt = \int_0^1 \frac{p_n(t)}{t} dt.$$
Therefore
\[ 2\pi^2 W(q_n) = \int_0^1 p_n(t) \left( \frac{1}{1-t} + 1 \right) dt = \int_0^1 \frac{p_n(t)}{t(1-t)} dt = \pi^2 W(p_n). \]
Together with (8.8) this leads to Theorem 3.2 for arbitrary polynomials \( p \in \mathfrak{P}_0 \).

8.2. Closure of the Asymptotics. Throughout this final section we assume that \( h \) satisfies Condition 3.1. The proof splits into three steps.

Step 1. First we prove the theorem for continuous functions \( h \) such that \( h(0) = h(1) = 0 \) that are differentiable at \( t = 0 \) and \( t = 1 \). Without loss of generality we may assume that \( h \) is real-valued (otherwise treat real and imaginary part separately). The differentiability condition at \( t = 0 \) and \( t = 1 \) implies that \( h(t) = t(1-t)g(t) \) for a continuous real-valued function \( g \). Fix \( \epsilon > 0 \). Due to the Stone-Weierstrass theorem, there exist a real-valued polynomial \( p \in \mathfrak{P} \) with \( \|p - g\|_\infty < \epsilon \). Denoting \( \tilde{p}(t) := t(1-t)p(t) \) we estimate
\[ h(t) \leq t(1-t)(p(t) + \epsilon) = \tilde{p}(t) + \epsilon t(1-t), \quad (8.9) \]
and
\[ h(t) \geq t(1-t)(p(t) - \epsilon) = \tilde{p}(t) - \epsilon t(1-t). \quad (8.10) \]
The monotonicity of the trace in combination with (8.9) gives
\[ \text{tr} \left[ h(B_{\alpha,\mu}) \right] \leq \text{tr} \left[ \tilde{p}(B_{\alpha,\mu}) \right] + \epsilon \text{tr} \left[ B_{\alpha,\mu}(1 - B_{\alpha,\mu}) \right]. \]
From Theorem 3.2 for polynomials from \( \mathfrak{P}_0 \), we get
\[ \limsup_{\alpha \to \infty} \frac{\text{tr} \left[ h(B_{\alpha,\mu}) \right]}{\log(\alpha)} \leq W(\tilde{p}) + \epsilon W(t(1-t)) = W(\tilde{p}) + \frac{\epsilon}{\pi^2}, \]
where we have used that \( W(t(1-t)) = \pi^{-2} \), see (3.1). Moreover, we notice that
\[ |W(h) - W(\tilde{p})| = |W(h - \tilde{p})| \leq \frac{\epsilon}{\pi^2}, \]
and hence,
\[ \limsup_{\alpha \to \infty} \frac{\text{tr} \left[ h(B_{\alpha,\mu}) \right]}{\log(\alpha)} \leq W(h) + \frac{2\epsilon}{\pi^2}. \]
In the same way (8.11) implies
\[ \liminf_{\alpha \to \infty} \frac{\text{tr} \left[ h(B_{\alpha,\mu}) \right]}{\log(\alpha)} \geq W(h) - \frac{2\epsilon}{\pi^2}, \]
and as \( \epsilon > 0 \) was chosen arbitrarily we deduce (3.2) for our choice of \( h \).

Step 2. Now let \( h \) be a continuous function, which is Hölder-continuous at 0 and 1 with exponent \( q \in (0, 1] \), so that
\[ |h(t)| \ll t^q(1-t)^q, \quad t \in [0, 1]. \]
Fix again \( \epsilon > 0 \) and choose a smooth function \( \zeta_\epsilon \) such that \( 0 \leq \zeta_\epsilon \leq 1 \) and
\[ \zeta_\epsilon(t) = \begin{cases} 1, & t \in [0, \epsilon/2] \cup [1 - \epsilon/2, 1], \\ 0, & t \in [\epsilon, 1 - \epsilon]. \end{cases} \]
In view of the estimate
\[ |(\zeta_\epsilon h)(t)| \ll |t(1-t)|^q \zeta_\epsilon(t) \ll \epsilon^r|t(1-t)|^r, \quad r = \frac{q}{2}, \]
we have
\[ \|(\zeta_\epsilon h)(B_{\alpha,\mu})\|_1 \ll \epsilon^r \|B_{\alpha,\mu}(1 - B_{\alpha,\mu})\|_r. \]
By Corollary 6.3, the right-hand side does not exceed \( \log(\alpha) \), \( \alpha \geq 2 \). Consequently,
\[
\left| \frac{\text{tr} \left[ (\zeta h)(B_{\alpha,\mu}) \right]}{\log(\alpha)} \right| \ll \epsilon^r, \quad \alpha \geq 2.
\] (8.11)

On the other hand, \( h_\epsilon = (1 - \zeta)h \) vanishes in a vicinity of 0 and 1 and, therefore, by Step 1, we have
\[
\text{tr} \left[ h_\epsilon(B_{\alpha,\mu}) \right] = \log(\alpha)W(h_\epsilon) + o(\log(\alpha)), \quad \alpha \to \infty.
\] (8.12)

It is clear that
\[ W(h) - W(h_\epsilon) \ll \left( \int_0^\alpha + \int_{1-\epsilon}^1 \right) t^{q-1}(1-t)^{q-1} dt \ll \epsilon^q. \] (8.13)

Combining (8.11), (8.12), and (8.13) gives
\[
\limsup_{\alpha \to \infty} \frac{\text{tr}(h(B_{\alpha,\mu}))}{\log \alpha} - W(h) \ll \epsilon^r.
\]

Since \( \epsilon > 0 \) is arbitrary, this yields the claim.

Step 3. Suppose that \( h \) satisfies Condition 3.1. Let \( t_0 \in (0,1) \) be a point such that \( h \) is continuous on \([0,t_0]\) and \([1 - t_0,1]\). Fix an \( \epsilon > 0 \). Then one can find two continuous functions \( h_1, h_2 \) as at Step 2, such that
\[
h_1(t) = h_2(t) = h(t), \quad t \in [0,t_0] \cup [1 - t_0,1], \quad h_1(t) \leq h(t) \leq h_2(t), \quad t \in [0,1],
\]
and \( \| h_2 - h_1 \|_{1,1} < \epsilon \). This implies that
\[
|W(h_1) - W(h)|, |W(h_2) - W(h)| \ll \epsilon.
\]

Now, in view of monotonicity, we have
\[
\text{tr} h_1(B_{\alpha,\mu}) \leq \text{tr} h(B_{\alpha,\mu}) \leq \text{tr} h_2(B_{\alpha,\mu}).
\]

Thus, by Step 2,
\[
\limsup_{\alpha \to \infty} \frac{\text{tr}(h(B_{\alpha,\mu}))}{\log \alpha} - W(h) \ll \epsilon.
\]

Since \( \epsilon > 0 \) is arbitrary, the required result follows.

**References**

1. L. Amico, et al., *Entanglement in Many-Body Systems*. Rev. Mod. Phys. 80: 517–576, 2008.
2. M. S. Birman and M. Z. Solomjak, *Spectral Theory of Selfadjoint Operators in Hilbert Space*. Mathematics and its Applications (Soviet Series), D. Reidel, 1987. Translated from the 1980 Russian original by S. Khrushchëv and V. Peller.
3. A. Budylin and V. Buslaev, *On the Asymptotic Behaviour of the Spectral Characteristics of an Integral Operator with a Difference Kernel on Expanding Domains*. Differential equations, Spectral theory, Wave propagation (Russian) 13: 16–60, 1991.
4. P. Calabrese, J. Cardy, and B. Doyon, *Entanglement Entropy in Extended Quantum Systems*. Journal of Physics A: Mathematical and Theoretical 42(50): 500301, 2009.
5. S. Das and S. Shankaranarayanan, *Entanglement as a Source of Black Hole Entropy*. Journal of Physics: Conference Series 68(1): 012015, 2007.
6. A. Elgart, L. Pastur, and M. Shcherbina, *Large Block Properties of the Entanglement Entropy of Disordered Fermions*. ArXiv e-prints 2016. [1601.00294]
7. N. E. Firsova, *Resonances of the Perturbed Hill Operator with Exponentially Decreasing Extrinsic Potential*. Mat. Zametki 36(5): 711–724, 1984. English translation: Math. Notes 36(5-6): 854–861, 1984.
8. N. E. Firsova, *A Direct and Inverse Scattering Problem for a One-Dimensional Perturbed Hill Operator*. Mat. Sb. (N.S.) 130(172)(3): 349–385, 431, 1986. English translation: Math. USSR-Sb. 58(2): 351–388, 1987.
9. D. Gioev and I. Klich, *Entanglement Entropy of Fermions in Any Dimension and the Widom Conjecture*. Phys. Rev. Lett. **96**: 100503, 2006.

10. R. Helling, H. Leschke, and W. Spitzer, *A Special Case of a Conjecture by Widom with Implications to Fermionic Entanglement Entropy*. Int. Math. Res. Not. **2011**: 1451–1482, 2011.

11. T. Kato, *Perturbation Theory for Linear Operators*. Grundlehren der Mathematischen Wissenschaften, Band 132, second edn., Springer-Verlag, Berlin-New York, 1976.

12. W. Kirsch and L. A. Pastur, *Analogues of Szegő’s Theorem for Ergodic Operators*. Mat. Sb. **206**(1): 103–130, 2006.

13. I. Klich, *Lower Entropy Bounds and Particle Number Fluctuations in a Fermi Sea*. Journal of Physics A: Mathematical and General **39**(4): L85, 2006.

14. I. Krasovsky, *Aspects of Toeplitz Determinants*. Random Walks, Boundaries and Spectra, Progr. Probab., vol. 64, 305–324, Birkhäuser/Springer Basel AG, Basel, 2011.

15. N. Laflourenocie, *Quantum Entanglement in Condensed Matter Systems*. Physics Reports **646**: 1 – 59, 2016.

16. H. J. Landau and H. Widom, *Eigenvalue Distribution of Time and Frequency Limiting*. J. Math. Anal. Appl. **77**(2): 469–481, 1980.

17. J. I. Latorre and A. Riera, *A Short Review on Entanglement in Quantum Spin Systems*. Journal of Physics A: Mathematical and Theoretical **42**(50): 504002, 2009.

18. H. Leschke, A. V. Sobolev, and W. Spitzer, *Scaling of Rényi Entanglement Entropies of the Free Fermi-Gas Ground State: A Rigorous Proof*. Phys. Rev. Lett. **112**: 160403, 2014.

19. H. Leschke, A. V. Sobolev, and W. Spitzer, *Large-Scale Behaviour of Local and Entanglement Entropy of the Free Fermi Gas at Any Temperature*. Journal of Physics A: Mathematical and Theoretical **49**(30): 30LT04, 2016.

20. L. Pastur and V. Slavín, *Area Law Scaling for the Entropy of Disordered Quasifree Fermions*. Phys. Rev. Lett. **113**: 150404, 2014.

21. M. Reed and B. Simon, *Methods of Modern Mathematical Physics. IV. Analysis of Operators*. Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1978.

22. B. Simon, *Trace Ideals and Their Applications*, Mathematical Surveys and Monographs, vol. 120. Second edn., American Mathematical Society, Providence, RI, 2005.

23. A. V. Sobolev, *Quasi-Classical Asymptotics for Pseudodifferential Operators with Discontinuous Symbols: Widom’s Conjecture*. Functional Analysis and Its Applications **44**(4): 313–317, 2010.

24. A. V. Sobolev, *Pseudo-Differential Operators with Discontinuous Symbols: Widom’s Conjecture*. Mem. Amer. Math. Soc. **222**(1043): vi+104, 2013.

25. A. V. Sobolev, *On the Schatten-von Neumann Properties of Some Pseudo-Differential Operators*. J. Funct. Anal. **266**(9): 5886–5911, 2014.

26. A. V. Sobolev, *Functions of Self-Adjoint Operators in Ideals of Compact Operators*. Journal of LMS, 2016.

27. A. V. Sobolev, *Quasi-Classical Asymptotics for Functions of Wiener-Hopf Operators: Smooth vs Non-Smooth Symbols*. ArXiv e-prints 2016, [1609.02068](https://arxiv.org/abs/1609.02068).

28. M. A. Subin, *Almost Periodic Functions and Partial Differential Operators*. Uspehi Mat. Nauk **33**(2): 3–47, 247, 1978.

29. M. A. Subin, *Spectral Theory and the Index of Elliptic Operators with Almost-Periodic Coefficients*. Uspekhi Mat. Nauk **34**(2): 95–135, 1979. English translation: Russian Mathematical Surveys, **34**(2): 109–157, 1979.

30. G. Szegö, *On Certain Hermitian Forms Associated with the Fourier Series of a Positive Function*. Comm. Sém. Math. Univ. Lund, Tome Supplémentaire 228–238, 1952.

31. G. Teschl, *Ordinary Differential Equations and Dynamical Systems*, Graduate Studies in Mathematics, vol. 140. American Mathematical Society, Providence, RI, 2012.
32. H. Widom, *On a Class of Integral Operators with Discontinuous Symbol. Toeplitz Centennial (Tel Aviv, 1981)*, Operator Theory: Adv. Appl., vol. 4, 477–500, Birkhäuser, Basel-Boston, Mass., 1982.

33. H. Widom, *Asymptotic Expansions for Pseudodifferential Operators on Bounded Domains*, Lecture Notes in Mathematics, vol. 1152. Springer-Verlag, New York-Berlin, 1985.

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