



Formulas of Szegő Type for the Periodic Schrödinger Operator

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Abstract: We prove asymptotic formulas of Szegő 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 $\alpha \rightarrow \infty$ to the position of the spectral parameter μ relative to the spectrum of H .

1. Introduction

The classical Szegő 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

$$W(a; I) = \chi_I \mathcal{F}^* a \mathcal{F} \chi_I,$$

where $\mathcal{F} : L^2(\mathbb{R}) \mapsto L^2(\mathbb{R})$ is the unitary Fourier transform, and χ_I is the indicator of the interval I . Both a and χ_I are to be interpreted as multiplication operators on $L^2(\mathbb{R})$ in this context. There is a vast literature studying the behaviour of the trace

$$\mathrm{tr} h(W(a; \alpha I))$$

with a test function h , as the scaling parameter $\alpha > 0$ tends to infinity. The above trace is known to be finite if the functions a and h are smooth, $h(0) = 0$, and a decays sufficiently fast at infinity. We do not intend to give an extensive survey of known results, but only

mention that, under these assumptions, there exists a complete asymptotic expansion of this trace in powers of α^{-1} , see e.g. [3,33]. This expansion consists of two terms:

$$\text{tr } h(W(a; \alpha I)) = \frac{\alpha}{2\pi} |I| \int h(a(\xi)) d\xi + \mathcal{B} + \mathcal{O}(\alpha^{-\infty}), \quad \alpha \rightarrow \infty, \quad (1.1)$$

with an explicitly computable coefficient $\mathcal{B} = \mathcal{B}(a; h)$, independent of the interval I . Note that in the multidimensional case, in general, the asymptotics contain infinitely many terms, see [33].

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^∞ -function such that $h(0) = 0$. Then the results of [16,32] imply the asymptotic formula

$$\text{tr } h(W(\chi_J; \alpha I)) = \frac{\alpha}{2\pi} h(1) |I| |J| + \log(\alpha) \mathcal{W}(h) + o(\log(\alpha)), \quad \alpha \rightarrow \infty, \quad (1.2)$$

with a coefficient $\mathcal{W}(h)$ independent of the intervals I and J , see (1.9) 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 non-smooth functions h was done in [18,26,27]. The formula (1.1) is a continuous analogue of the second-order Szegő limit theorem, see [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

$$\text{tr } h(W(\chi_J; \alpha I)) = \log(\alpha) \mathcal{W}(h) + o(\log(\alpha)), \quad \alpha \rightarrow \infty, \quad \text{if } h(0) = h(1) = 0. \quad (1.3)$$

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. [9,10,18,19]. For instance, the formula (1.2), used with the function

$$\eta_1(t) = -t \log t - (1 - t) \log(1 - t), \quad t \in [0, 1], \quad (1.4)$$

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 [9,13]. The function (1.4) is just one representative of the family

$$\eta_\gamma(t) = \frac{1}{1 - \gamma} \log [t^\gamma + (1 - t)^\gamma], \quad t \in [0, 1], \quad (1.5)$$

with $\gamma > 0$, where η_1 is defined as the limit of η_γ as $\gamma \rightarrow 1, \gamma \neq 1$. Picking $h = \eta_\gamma$ one obtains from (1.2) the asymptotics of the γ -Rényi EE, see e.g. [18]. Due to the condition $\eta_\gamma(0) = \eta_\gamma(1) = 0$, formula (1.3) applies and the EE behaves as $\log(\alpha)$ as $\alpha \rightarrow \infty$.

Let us remark at this point that there is an extensive physics literature on the topic of EE. However, we do not enter a detailed discussion of it in the context of this paper. For the interested reader, we refer to general reviews [1,4,5,15,17] on the importance of EE in the study of black holes, condensed matter systems and quantum information theory.

Having in mind the application to EE, a natural generalization of discussed questions is to move from free fermions to fermions in an external field. In mathematical terms, that amounts to studying the trace of the operator

$$h(\chi_{\alpha I} a(H) \chi_{\alpha I}), \tag{1.6}$$

where H is some general self-adjoint one-particle Hamiltonian. Such an analysis for ergodic Hamiltonians H was conducted in [6, 12, 20], including multidimensional results. In this new setting, a number of new and rather unexpected effects emerge. To give just one example, as follows from [6], the EE for Fermions at zero temperature in a disordered one-dimensional medium remains bounded as $\alpha \rightarrow \infty$, in contrast to the free case, mentioned above.

Our objective in the present paper is to obtain formulas of Szegő type for the operator (1.6) with the function $a = \chi_{(-\infty, \mu)}$, $\mu \in \mathbb{R}$, and with H being the Schrödinger operator with a periodic potential in dimension one. More precisely, set

$$H := -\frac{d^2}{dx^2} + V(x), \text{ dom}(H) = H^2(\mathbb{R}), \tag{1.7}$$

where V is a real-valued periodic L^2_{loc} -function, so that the operator H is self-adjoint on $H^2(\mathbb{R})$. Without loss of generality we assume that the period equals 2π . The spectrum $\sigma(H)$ is known to be absolutely continuous, and it is the union of infinitely many spectral bands (closed intervals whose interiors are disjoint). We introduce the notation $P_{\mu} := \chi_{(-\infty, \mu)}(H)$ for the spectral projection of H associated with the interval $(-\infty, \mu)$. The parameter μ is naturally interpreted as the *Fermi energy*. Without loss of generality, in the operator (1.6), we choose a symmetric interval $I = (-1, 1)$, i.e. we obtain an asymptotic formula for the trace

$$\text{tr } h(B_{\alpha, \mu}), \quad B_{\alpha, \mu} = \chi_{(-\alpha, \alpha)} P_{\mu} \chi_{(-\alpha, \alpha)}, \tag{1.8}$$

as $\alpha \rightarrow \infty$. A mild condition is imposed on the test-function h .

Condition 1.1. *The function $h : [0, 1] \mapsto \mathbb{C}$ is piece-wise continuous, it is Hölder continuous at $t = 0$ and 1, and $h(0) = 0$.*

For a function h satisfying Condition 1.1, define the integral

$$\mathcal{W}(h) := \frac{1}{\pi^2} \int_0^1 \frac{[h(t) - th(1)]}{t(1-t)} dt. \tag{1.9}$$

The next theorem is the main result of the paper.

Theorem 1.2. *Let H be the operator defined in (1.7) and suppose that $V \in C^{\infty}(\mathbb{R})$. Assume that the function h satisfies Condition 1.1. Then for any $\mu \in (\sigma(H))^{\circ}$ we have the asymptotic formula*

$$\text{tr}[h(B_{\alpha, \mu})] = 2\alpha h(1)N(\mu, H) + \log(\alpha)\mathcal{W}(h) + o(\log(\alpha)), \text{ as } \alpha \rightarrow \infty. \tag{1.10}$$

If $\mu \notin (\sigma(H))^{\circ}$, then

$$\text{tr}[h(B_{\alpha, \mu})] = 2\alpha h(1)N(\mu, H) + \mathcal{O}(1), \text{ as } \alpha \rightarrow \infty. \tag{1.11}$$

Here, $(\sigma(H))^{\circ}$ is the set of interior points of the spectrum, and $N(\mu, H)$ denotes the integrated density of states for the operator H , defined in (2.5).

- Remark 1.3.* (1) The two terms in (1.10) are of different nature: the first one (linear in α) depends on both the potential V and the parameter μ , but the second one (log-term) is - remarkably - independent of V or μ , as long as μ remains an interior point of the spectrum $\sigma(H)$.
- (2) To emphasize the dependence of the asymptotics on the spectral parameter μ consider a function h such that $h(0) = h(1) = 0$. Then $\text{tr } h(B_{\alpha,\mu})$ remains bounded if μ is in a spectral gap. If however, μ is inside a spectral band, then the asymptotics are exactly as in the case $V \equiv 0$, described by the formula (1.3).
- (3) We point out that the function h in Theorem 1.2 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 relaxed to $V \in L^2_{\text{loc}}(\mathbb{R})$. This can be observed at the first step of Sect. 7, where we take the closure of the asymptotics, starting from polynomial test functions h . 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.

Let us describe the strategy of the proof of Theorem 1.2, focusing on the case where $\mu \in (\sigma(H))^\circ$. The proof of (1.11) is considerably easier, and we do not comment on it now.

To prove formula (1.10) we proceed in three steps. First we represent the function h as the sum

$$h(t) = th(1) + h_1(t) \tag{1.12}$$

so that the function h_1 satisfies Condition 1.1 and, in addition, $h_1(1) = 0$. The function $th(1)$ is responsible for the first term in (1.10) and the trace asymptotics for this function are found easily (see Sect. 2.2).

The analysis of the asymptotic behaviour of $\text{tr } h_1(B_{\alpha,\mu})$, which yields the logarithmic correction in (1.10), is the second and main part of the proof. Here we follow the strategy of [16], where the asymptotics (1.2) were derived. As in [16], we focus first on polynomial functions h_1 , choosing $p_n(t) = [t(1-t)]^n$ and $q_n(t) = t[t(1-t)]^n$, $n = 1, 2, \dots$, as basis elements for polynomials that vanish at $t = 0$ and $t = 1$. However, the method of [16] is not directly applicable since the kernel of the operator $B_{\alpha,\mu}$ contains the Bloch eigenfunctions of H instead of the plain waves. One of the central points of our proof is to show that, at the cost of constant order errors, for the operators $p_n(B_{\alpha,\mu})$ one can replace the terms involving the Bloch functions by their mean values. This reduces the problem to the case $V \equiv 0$, and enables us to use the known formula (1.2) with $h = p_n$. Exploiting the periodicity of H , the study of polynomials q_n can be reduced to the polynomials p_n . This requires extra work since, in contrast to [16], the reflection symmetry and translation invariance of H which were essential for [16], are not available in our problem.

At the final stage of the proof, we extend the asymptotics to functions h_1 satisfying Condition 1.1. To this end, we approximate h_1 by polynomials, for which the sought formula has been proved at the previous step of the proof. The error term is shown to be of order $o(\log(\alpha))$ with the help of bounds for pseudo-differential operators in Schatten-von Neumann classes, that are due to the second author (see [25]). The required extension of the bounds from [25] to the periodic setting is relatively straightforward. This finishes the proof.

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. Sect. 2). An approximation of the kernel of the spectral projection P_μ in terms of Bloch eigenfunctions corresponding to the Fermi energy μ is given in Sect. 3. Section 4 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 Sect. 4.4) that allows us to average out the precise dependence on the Bloch eigenfunctions at Fermi energy μ . This is sufficient to prove Theorem 1.2 for polynomial functions h , see Sect. 6. As mentioned earlier, the extension to non-smooth functions calls for more advanced bounds in Schatten-von Neumann classes. These bounds are collected in Sect. 5. The extension to non-smooth h , i.e. the closure of the asymptotics from the polynomial h , is implemented in Sect. 7.

To conclude the introduction, let us fix some general notation. If f, g are non-negative functions, we write $f \lesssim g$ or $g \gtrsim f$ if $f \leq Cg$ for some constant $C > 0$. This constant may depend on the potential V but does not depend on the dilation parameter α . 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° 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 Sect. 4) it will not matter whether considered intervals are open, semi-open or closed. Whenever this is the case we shall use open intervals only.

2. Preliminaries

As introduced in (1.7) we consider a periodic Schrödinger operator

$$H = -\frac{d^2}{dx^2} + V(x), \text{ dom}(H) = H^2(\mathbb{R}),$$

in dimension 1. For now, let the potential V be a real-valued 2π -periodic L^2_{loc} -function, so that the operator H is self-adjoint on $H^2(\mathbb{R})$.

2.1. Floquet-Bloch theory. 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

$$U : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{T}, L^2(0, 2\pi)), \mathbb{T} = \mathbb{R}/\mathbb{Z}.$$

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

$$UHU^* = \int_{\mathbb{T}}^{\oplus} H(k)dk,$$

with self-adjoint fibres

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

$$\text{dom}(H(k)) = \{f \in H^2(0, 2\pi) : f(2\pi) = e^{2\pi ik} f(0), f'(2\pi) = e^{2\pi ik} f'(0)\}, \quad (2.1)$$

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 $\lambda_j(k)$, $j = 1, 2, \dots$, labelled in ascending order counting multiplicity. Denote the corresponding normalized eigenfunctions by $\phi_j(k) = \phi_j(\cdot, k) \in H^2(0, 2\pi)$, $j = 1, 2, \dots$

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

$$e_j(x, k) := e^{-ikx} \phi_j(x, k) \quad (2.2)$$

and their derivatives de_j/dx can be extended to all $x \in \mathbb{R}$ as 2π -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 spectral projection P_μ :

$$P_\mu(x, y) = \sum_j \int_{\mathbb{T}} \chi_{(-\infty, \mu)}(\lambda_j(k)) \phi_j(x, k) \overline{\phi_j(y, k)} dk. \quad (2.3)$$

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

$$\mathbb{T}_0 = \mathbb{T} \setminus \left(\{0\} \cup \left\{ \frac{1}{2} \right\} \right).$$

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 $j = 1, 2, \dots$*
- (2) *The eigenfunctions $\phi_j(\cdot, k)$, $j = 1, 2, \dots$, 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 $\lambda_j(k)$, $j = 1, 2, \dots$, 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

$$k_j = \begin{cases} 0, & j \text{ odd,} \\ \frac{1}{2}, & j \text{ even.} \end{cases} \quad (2.4)$$

Denote

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

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

$$\sigma(H) = \bigcup_{j=1}^{\infty} \sigma_j.$$

It follows from Proposition 2.1(4) that the bands σ_j are non-degenerate, i.e. $|\sigma_j| > 0$ for every $j = 1, 2, \dots$. Introduce the counting function of $H(k)$:

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

and the (integrated) density of states:

$$N(\mu; H) = \frac{1}{2\pi} \int_{\mathbb{T}} N(\mu, k) dk. \tag{2.5}$$

In view of Proposition 2.1(4) again, the function (2.5) is continuous. The definition (2.5) 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. [29, Theorem 4.2] or [21, Ch. XIII].

2.2. *The main term in the trace asymptotics.* Having established formula (2.3) for the kernel of the spectral projection, we are ready to prove Theorem 1.2 for the special case $h(t) = t$. Via the decomposition (1.12) this gives the main term in the trace asymptotics (1.10), (1.11), as explained in the introduction. Indeed, according to (2.3),

$$\|B_{\alpha, \mu}\|_{\mathfrak{S}_1} = \text{tr } B_{\alpha, \mu} = \sum_j \int_{-\alpha}^{\alpha} \int_{k \in \mathbb{T}: \lambda_j(k) < \mu} |\phi_j(x, k)|^2 dk dx.$$

Assume for simplicity that α is a multiple of 2π . Since the ϕ_j 's are normalized on $(0, 2\pi)$, by the definition (2.5), 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 α is not a multiple of 2π , then one easily checks, using the monotonicity of the trace in α , that

$$4\pi \left\lfloor \frac{\alpha}{2\pi} \right\rfloor N(\mu, H) \leq \text{tr } B_{\alpha, \mu} \leq 4\pi \left\lceil \frac{\alpha}{2\pi} \right\rceil N(\mu, H), \forall \alpha > 1. \tag{2.6}$$

Consequently, we conclude that

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

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.

2.3. *Touching spectral bands.* Note also that the spectral bands of the operator H 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 σ_{j-1} and σ_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 $v_{j-1} = \mu_j$, i.e. $\lambda_{j-1}(k_j) = \lambda_j(k_j)$, then in a neighbourhood of k_j , the eigenvalues λ_{j-1} and λ_j , and the eigenfunctions $\phi_{j-1}(x, \cdot)$ and $\phi_j(x, \cdot)$ are analytic continuations of each other. Moreover, $\lambda'_l(k_j \pm) \neq 0$, $\phi_l(k_j -) = \overline{\phi_l(k_j +)}$, and the limits $\phi_l(k_j -)$ and $\phi_l(k_j +)$ 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 ϕ_j are described in [7] and [8]. Also, the relation $\lambda'_l(k_j \pm) \neq 0$ from Proposition 2.2(2) can be found e.g. in [8, formula (3.1)].

Assume again that $v_{j-1} = \mu_j$, i.e. the bands σ_{j-1} and σ_j have one common point. Since $\phi_{j-1}(k)$ and $\phi_j(k)$ are orthogonal for all $k \in \mathbb{T}_0$, and $\phi_{j-1}(k_j \pm) = \phi_j(k_j \mp)$, 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 $\phi_j(k_j -) = \overline{\phi_j(k_j +)}$, this implies that

$$\int_0^{2\pi} \phi_j(x, k_j \pm)^2 dx = 0, \text{ if } v_{j-1} = \mu_j. \tag{2.7}$$

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

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

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

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

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

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

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

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

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

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

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

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

built out of the functions (2.2) 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 2π -periodic in $x \in \mathbb{R}$.

Of course, it may happen that *all* bands starting with σ_j touch. In this case the above construction still works and yields analytic functions Φ , Λ , 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 Λ and Φ 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 (2.8). 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 (2.3) leads to the following formula for the kernel $P_\mu[S](x, y)$ of the projection $P_\mu[S] := P_\mu P[S]$:

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

2.4. Mean values of Bloch eigenfunctions. Given the properties of the Bloch eigenfunction $\Phi(\cdot, k)$, for every $k \in n\mathbb{T}$, it belongs to the algebra $CAP(\mathbb{R})$ 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^∞ -norm. For any $f \in CAP(\mathbb{R})$ the *almost-periodic mean*

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

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 $\Phi(k)$, see (2.10).

Lemma 2.3. *Let $\Phi = \Phi(\cdot, k)$ be the eigenfunction associated with the band S , see (2.8). Then*

$$\mathcal{M}(|\Phi|^2) = \frac{1}{2\pi}, \quad \forall k \in n\mathbb{T}, \tag{2.13}$$

and

$$\mathcal{M}(\Phi^2) = 0, \quad \forall k \neq k_j, k \neq k_j + n/2. \tag{2.14}$$

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

To prove (2.14), suppose first that $2k \not\equiv 1 \pmod{\mathbb{Z}}$, so that $k \neq k_j \pm l/2$, $l = 0, 1, \dots, n$. We use the representation (2.11), so

$$\mathcal{M}(\Phi^2) = \mathcal{M}(e^{2ikx} E^2).$$

The function $w = E(\cdot, k)^2$ is continuous and 2π -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:

$$\int_{-T}^T e^{2ikx+isx} dx = \frac{e^{i(2k+s)x}}{i(2k+s)} \Big|_{-T}^T,$$

which is bounded uniformly in T for all $s = -N, -N+1, \dots, N$. Thus $\mathcal{M}(e^{2ikx} p) = 0$, and hence

$$|\mathcal{M}(\Phi^2)| = |\mathcal{M}(e^{2ikx} \tilde{p})| \leq \varepsilon.$$

As $\varepsilon > 0$ is arbitrary, this entails that $\mathcal{M}(\Phi^2) = 0$, as required.

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

3. 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 3.1. *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*

$$P_\mu[S](x, y) = \Pi_\mu(x, y) + R_\mu[S](x, y), \tag{3.1}$$

where

$$\Pi_\mu(x, y) = \frac{\Phi(x, \delta)\overline{\Phi(y, \delta)} - \overline{\Phi(x, \delta)}\Phi(y, \delta)}{i(x - y)}, \tag{3.2}$$

and

$$R_\mu[S](x, y) = \mathcal{O}((1 + |x - y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}. \tag{3.3}$$

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

$$|P_\mu[S](x, y)| + |\Pi_\mu(x, y)| = \mathcal{O}((1 + |x - y|)^{-1}), \quad \forall x, y \in \mathbb{R}. \tag{3.4}$$

If $\mu \notin S^\circ$, then $P_\mu[S](x, y)$ is a continuous function of $x, y \in \mathbb{R}$, and it satisfies the bound

$$P_\mu[S](x, y) = \mathcal{O}((1 + |x - y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}. \tag{3.5}$$

Proof. Let us deduce the bound (3.5) first. Observe that if $\mu \notin S^\circ$, then either $P_\mu[S] = 0$ (if μ is below S°), or $P_\mu[S] = P_{\mu_0}[S]$ 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 (3.5) is trivial. In the second case the function $\Phi(\delta)$ is real-valued, so that $\Pi_{\mu_0}(x, y) = 0$, and hence the bound (3.5) follows from (3.1) and (3.3).

It remains to prove the continuity and the bounds (3.3) and (3.4) for $\mu \in S$. Note that the kernel $P_\mu[S]$ (cf. (2.12)) is bounded uniformly in x, y , as $\Phi(x, k)$ is uniformly bounded due to (2.11). It is also continuous in x, y . Furthermore, since $E(x, k)$ are continuous and periodic in x , the kernel (3.2) is continuous and bounded by $|x - y|^{-1}$ for all $x, y : |x - y| \geq 1$. Due to the continuity of the derivative Φ_x , the kernel (3.2) is continuous and uniformly bounded for $|x - y| < 1$. As a consequence, $\Pi_\mu(x, y)$ satisfies (3.4), and the remainder $R_\mu[S](x, y)$ is continuous and uniformly bounded. Thus it remains to prove the bounds (3.3) and (3.4) for $P_\mu(x, y)$ with $|x - y| \geq 1$.

Using (2.11), we rewrite

$$P_\mu[S](x, y) = \int_{2k_j - \delta}^{\delta} e^{ik(x-y)} E(x, k) \overline{E(y, k)} dk, \tag{3.6}$$

and integrate by parts to arrive at

$$\begin{aligned} P_\mu[S](x, y) &= \frac{e^{i\delta(x-y)}}{i(x-y)} E(x, \delta) \overline{E(y, \delta)} \\ &\quad - \frac{e^{i(2k_j - \delta)(x-y)}}{i(x-y)} E(x, 2k_j - \delta) \overline{E(y, 2k_j - \delta)} + R_\mu[S](x, y) \end{aligned}$$

with

$$R_\mu[S](x, y) = - \int_{2k_j - \delta}^{\delta} \frac{e^{ik(x-y)}}{i(x-y)} \partial_k (E(x, k) E(y, k)) dk.$$

Due to (2.11) and the symmetry property (2.10) one obtains the representation (3.1). Another integration by parts for $R_\mu[S]$ gives

$$\begin{aligned} R_\mu[S](x, y) &= \frac{e^{ik(x-y)} \partial_k (E(x, k) E(y, k))}{(x-y)^2} \Bigg|_{2k_j - \delta}^{\delta} \\ &\quad - \int_{2k_j - \delta}^{\delta} \frac{e^{ik(x-y)}}{(x-y)^2} \partial_k^2 (E(x, k) E(y, k)) dk. \end{aligned} \tag{3.7}$$

Hence, estimate (3.3) follows from the fact that the functions E , $\partial_k E$, and $\partial_k^2 E$ are uniformly bounded. \square

Now Lemma 3.1 may be used for each “genuine” spectral band separately to get the corresponding expansion of the kernel $P_\mu(x, y)$.

Lemma 3.2. *Let $\mu \in S$, where S is the band defined in (2.8), and let $\delta = \delta(\mu)$ be as in Lemma 3.1. Then for all $x, y \in \mathbb{R}$ we have*

$$P_\mu(x, y) = \Pi_\mu(x, y) + R_\mu(x, y), \tag{3.8}$$

where Π_μ is as defined in (3.2), and

$$R_\mu(x, y) = \mathcal{O}((1 + |x - y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}. \tag{3.9}$$

Moreover, $R_\mu(x, y)$, $\Pi_\mu(x, y)$ and $P_\mu(x, y)$ are continuous functions of $x, y \in \mathbb{R}$, and

$$|P_\mu(x, y)| + |\Pi_\mu(x, y)| = \mathcal{O}((1 + |x - y|)^{-1}), \quad \forall x, y \in \mathbb{R}. \tag{3.10}$$

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

$$P_\mu(x, y) = \mathcal{O}((1 + |x - y|^2)^{-1}), \quad \forall x, y \in \mathbb{R}. \tag{3.11}$$

Proof. The continuity of the projection kernel $P_\mu(x, y)$ follows immediately from Lemma 3.1. If $\mu \notin (\sigma(H))^\circ$, then (3.11) follows directly from (3.5).

Assume now that $\mu \in S$. Let S_1, S_2, \dots, S_N , be “genuine” spectral bands lying below the band S . Using Lemma 3.1, we can write

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

where

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

By Lemma 3.1, the kernel $R_\mu[S]$ and each term $P_\mu[S_l]$, $l = 1, 2, \dots, N$ satisfy (3.9), whence (3.8). The bound (3.10) for the kernel $P_\mu[S](x, y)$ follows from (3.4). \square

4. Elementary Trace Norm Estimates

Throughout the proof of Theorem 1.2 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

$$\chi_I P_\mu \chi_J P_\mu \chi_K, \tag{4.1}$$

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

4.1. *Schatten-von Neumann classes.* Throughout this paper, we make use of the standard notation for the Schatten-von Neumann classes of operators $\mathfrak{S}_q, q > 0$, in a Hilbert space, see e.g. [2,22]. The class \mathfrak{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 $A \in \mathfrak{S}_q$ 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 \mathfrak{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 $A \in \mathfrak{S}_p$ and $B \in \mathfrak{S}_q$. While in this section we limit ourselves to estimates in the trace class \mathfrak{S}_1 , Sect. 5 treats operators in the classes \mathfrak{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 4.1. *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 $A : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$ which is defined via the form

$$\langle u, Av \rangle_{L^2} := \int_M \langle u, f(z) \rangle_{L^2} \langle g(z), v \rangle_{L^2} dz, \quad u, v \in L^2(\mathbb{R}),$$

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

$$\begin{aligned} \sum_n |\langle d_n, Ae_n \rangle| &\leq \sum_n \int_M |\langle d_n, f(z) \rangle \langle g(z), e_n \rangle| dz \\ &= \int_M \sum_n |\langle d_n, f(z) \rangle \langle g(z), e_n \rangle| dz. \end{aligned}$$

The Cauchy-Schwartz inequality and Parseval’s identity yield

$$\begin{aligned} \sum_n |\langle d_n, f(z) \rangle \langle g(z), e_n \rangle| &\leq \left(\sum_n |\langle d_n, f(z) \rangle|^2 \right)^{\frac{1}{2}} \left(\sum_n |\langle g(z), e_n \rangle|^2 \right)^{\frac{1}{2}} \\ &= \|f(z)\| \|g(z)\|. \end{aligned}$$

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. \square

Equipped with these basic trace norm estimates, we can start now our investigation of the operator (4.1).

4.2. Replacing the spectral projection by its approximation. Let us recall the following general notation. If f, g are real-valued functions we shall write $|f| \lesssim |g|$ if and only if $|f| \leq C|g|$ for some constant $C > 0$ which might depend on the potential V but does not depend on the dilation parameter α . Let Π_μ be as defined in Lemma 3.1.

Lemma 4.2. *Let $I, J, K \subset \mathbb{R}$ be intervals such that $I \cap J = \emptyset$ and $K \cap J = \emptyset$. Then we have*

$$\|\chi_I P_\mu \chi_J P_\mu \chi_K - \chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K\|_1 \lesssim 1, \tag{4.2}$$

where the integral kernel of Π_μ is defined in (3.2).

Proof. With the notation of Lemma 3.2 we may write

$$\chi_I P_\mu \chi_J P_\mu \chi_K = \chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K + \chi_I \Pi_\mu \chi_J R_\mu \chi_K + \chi_I R_\mu \chi_J P_\mu \chi_K.$$

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 4.1 with

$$f(x, z) = \chi_I(x) R_\mu(x, z), \quad g(y, z) = \chi_K(y) \overline{P_\mu(z, y)} = \chi_K(y) P_\mu(y, z),$$

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 (3.9) and (3.10) yield

$$\begin{aligned} \|\chi_I R_\mu \chi_J P_\mu \chi_K\|_1 &\lesssim \int_J \left[\int_I (1 + |x - z|)^{-4} dx \right]^{\frac{1}{2}} \left[\int_K (1 + |z - y|)^{-2} dy \right]^{\frac{1}{2}} dz \\ &\lesssim \int_J (1 + \text{dist}(z, I))^{-\frac{3}{2}} (1 + \text{dist}(z, K))^{-\frac{1}{2}} dz \\ &\lesssim \int_J [(1 + \text{dist}(z, I))^{-2} + (1 + \text{dist}(z, K))^{-2}] dz \lesssim 1. \end{aligned}$$

The operator $\chi_I \Pi_\mu \chi_J R_\mu \chi_K$ satisfies the same bound. Hence, the claim follows. \square

4.3. Uniform trace norm bounds. Under particular assumptions on the intervals I, J and K the operator (4.1) is of trace class with uniformly bounded trace norm. We list some of these conditions in the following proposition.

Proposition 4.3. *Let $I, J, K \subset \mathbb{R}$ be intervals such that one of the following conditions holds:*

- (i) $|J| \lesssim 1$,
- (ii) *Either*
 - (a) $|J| \lesssim \max\{\text{dist}(I, J), \text{dist}(J, K)\}$, or
 - (b) $|K| \lesssim \text{dist}(J, K)$, $|I| \lesssim \text{dist}(I, J)$, or
 - (c) $|K| \lesssim \text{dist}(J, K)$, $|J| \lesssim \text{dist}(I, J)$.
- (iii) J is finite, and I and K lie on opposite sides of J , i.e.

$$x \leq y \leq z \text{ or } z \leq y \leq x, \text{ for all } (x, y, z) \in I \times J \times K. \tag{4.3}$$

- (iv) $|I| \lesssim 1$ 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 α) in trace norm, i.e.

$$\|\chi_I P_\mu \chi_J P_\mu \chi_K\|_1 \lesssim 1. \tag{4.4}$$

Remark 4.4. At this point we emphasize again that the intervals I, J , and K may depend on α . In particular, assumption (iii) includes intervals J of size α . In the free case, i.e. for $V \equiv 0$, Proposition 4.3 with assumptions similar to ((i)) and (iii) has been obtained in [16, Lemma].

Proof of Proposition 4.3. According to Lemma 4.2 and bound (3.10),

$$\|\chi_I P_\mu \chi_J P_\mu \chi_K\|_1 \lesssim \int_J \left[\int_I (1 + |z - x|)^{-2} dx \right]^{\frac{1}{2}} \left[\int_K (1 + |z - y|)^{-2} dy \right]^{\frac{1}{2}} dz. \tag{4.5}$$

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

Assume condition (i). i.e. $|J| \lesssim 1$. Both integrals inside (4.5) are uniformly bounded, even if I and K are unbounded. Thus the trace norm does not exceed $|J| \lesssim 1$, as required.

Assume now condition (ii). Using the Cauchy-Schwarz inequality, we estimate the right-hand side of (4.5) by

$$\left[\int_J \int_I (1 + |z - x|)^{-2} dx dz \right]^{\frac{1}{2}} \left[\int_J \int_K (1 + |z - y|)^{-2} dy dz \right]^{\frac{1}{2}}.$$

The first integral is bounded by

$$|J|(1 + \text{dist}(I, J))^{-1} \quad \text{or} \quad |I|(1 + \text{dist}(I, J))^{-1}.$$

The second integral is bounded by

$$|K|(1 + \text{dist}(J, K))^{-1} \quad \text{or} \quad |J|(1 + \text{dist}(J, K))^{-1}.$$

Thus, under any of the conditions (ii), the right-hand side of (4.5) is uniformly bounded, as required.

Assume that the first of the conditions (4.3) holds. Let

$$I = (s_1, t_1), J = (s_2, t_2), K = (s_3, t_3) \tag{4.6}$$

with

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

Using (4.5), we get the bound

$$\begin{aligned} \|\chi_I P_\mu \chi_J P_\mu \chi_K\|_1 &\lesssim \int_{s_2}^{t_2} \left[\int_{s_1}^{t_1} |z - x|^{-2} dx \right]^{\frac{1}{2}} \left[\int_{s_3}^{t_3} |z - y|^{-2} dy \right]^{\frac{1}{2}} dz \\ &\lesssim \int_{s_2}^{t_2} (z - t_1)^{-\frac{1}{2}} (s_3 - z)^{-\frac{1}{2}} dz \\ &\leq \int_{s_2}^{t_2} (z - s_2)^{-\frac{1}{2}} (t_2 - z)^{-\frac{1}{2}} dz = \int_0^s z^{-\frac{1}{2}} (s - z)^{-\frac{1}{2}} dz, \end{aligned}$$

with $s = t_2 - s_2$. By rescaling, the last integral equals

$$\int_0^1 z^{-\frac{1}{2}} (1 - z)^{-\frac{1}{2}} dz \lesssim 1,$$

which leads to (4.4) again.

Finally, assume that (iv) holds. The right-hand side of (4.5) is bounded by

$$\begin{aligned} &|I|^{\frac{1}{2}} \int_J (1 + \text{dist}(z, I))^{-1} (1 + \text{dist}(z, K))^{-\frac{1}{2}} dz \\ &\lesssim \int_J (1 + \text{dist}(z, I))^{-\frac{3}{2}} dz + \int_J (1 + \text{dist}(z, K))^{-\frac{3}{2}} dz \lesssim 1. \end{aligned}$$

The proof is complete.

4.4. *Replacing almost periodic functions by their mean value.* Looking at the formula (3.2) we see that the kernel of $\chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K$ contains kernels of the form

$$S_{I,J,K}(x, y; f) = \chi_I(x) \chi_K(y) \int_J \frac{f(z)}{(z-x)(z-y)} dz, \tag{4.7}$$

where f is a product of functions such as $\Phi(\cdot, \delta)$ and $\overline{\Phi(\cdot, \delta)}$. 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 4.5. *Let $\Theta \subset \mathbb{R}$ be a countable set, and let $(a_\theta)_\theta \subset \mathbb{C}$ be such that*

$$\sum_{\substack{\theta \in \Theta \\ \theta \neq 0}} |a_\theta| (1 + |\theta|^{-1}) < \infty. \tag{4.8}$$

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 $\text{dist}(I, J), \text{dist}(J, K) \gtrsim 1$ and consider the operator $S_{I,J,K}(f)$ in $L^2(\mathbb{R})$ with the integral kernel (4.7). Then we have

$$\|S_{I,J,K}(f) - S_{I,J,K}(\mathcal{M}(f))\|_1 \lesssim 1. \tag{4.9}$$

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 (4.8) implies that F is uniformly bounded:

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

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

$$\begin{aligned} S_{I,J,K}(x, y; f) &= \chi_I(x) \chi_K(y) \frac{F(z)}{(z-x)(z-y)} \Big|_{z=s}^t \\ &\quad + \chi_I(x) \chi_K(y) \int_J \left[\frac{F(z)}{(z-x)^2(z-y)} + \frac{F(z)}{(z-x)(z-y)^2} \right] dz. \end{aligned} \tag{4.10}$$

The first term in (4.10) constitutes the kernel of a rank two operator, whose norm, and hence trace norm as well, is easily estimated by a constant times $\text{dist}(I, J)^{-1/2} \text{dist}(J, K)^{-1/2}$. The second term on the right-hand side of (4.10) is treated with the help of Lemma 4.1, as in the proof of Lemma 4.2. Thus (4.9) follows. \square

5. 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 4.1. 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 4.1 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 (Ψ DO). For a complex-valued function $p = p(x, y, \xi)$, $x, y, \xi \in \mathbb{R}$, that we call *amplitude*, we define the Ψ DO $\text{Op}(p)$ that acts on Schwartz class functions u as follows:

$$\text{Op}(p)u(x) = \frac{1}{2\pi} \iint e^{i\xi(x-y)} p(x, y, \xi) u(y) dy d\xi. \tag{5.1}$$

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

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

$$A_{\alpha,\mu} = B_{\alpha,\mu}(\mathbb{1} - B_{\alpha,\mu}) \tag{5.2}$$

(see Corollary 5.3).

Lemma 5.1. *Let $I, \Omega \subset \mathbb{R}$ be bounded intervals, and let the function p be C^∞ in all three variables, 2π -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

$$\|\chi_{\alpha I} \text{Op}(p)(\mathbb{1} - \chi_{\alpha I})\|_q \lesssim 1, \tag{5.3}$$

and

$$\|\chi_{\alpha I} \text{Op}(p[\Omega])(\mathbb{1} - \chi_{\alpha I})\|_q \lesssim (\log(\alpha))^{\frac{1}{q}}. \tag{5.4}$$

The implicit constants in (5.3) and (5.4) depend on the amplitude p , number R and also on the intervals I and Ω .

Our proof relies on similar results from [25]. We state these results in the form adjusted for our purposes.

Proposition 5.2. *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*

$$N_q(p) := \max_{0 \leq m \leq \lfloor 2q^{-1} \rfloor + 1} \sup_{\xi} |p^{(m)}(\xi)| < \infty. \tag{5.5}$$

Then

$$\|\chi_{\alpha I} \text{Op}(p)(\mathbb{1} - \chi_{\alpha I})\|_q \lesssim N_q(p), \tag{5.6}$$

and

$$\|\chi_{\alpha I} \text{Op}(p[\Omega])(\mathbb{1} - \chi_{\alpha I})\|_q \lesssim (\log(\alpha))^{\frac{1}{q}} N_q(p). \tag{5.7}$$

The implicit constants in (5.6) and (5.7) depend on the intervals I , Ω and number R , but are independent of the amplitude p .

Thus, our task is to extend Proposition 5.2 to amplitudes, that are periodic in x and y .

A few remarks are in order. Proposition 5.2 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 5.1. We prove only the bound (5.4). The bound (5.3) can be derived in a similar way.

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

$$p(x, y, \xi) = \sum_{nl} e^{inx+ily} a_{nl}(\xi),$$

where $a_{nl}(\cdot)$ are C_0^∞ in ξ 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

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

for arbitrary $t, s = 0, 1, \dots$, so that

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

with a constant independent of n, l , but depending on s, t, q (see (5.5) for the definition of N_q). Consequently, the operator $\text{Op}(p[\Omega])$ can be represented as follows:

$$\text{Op}(p[\Omega]) = \sum_{nl} e^{inx} A_{nl} e^{ily}, \quad A_{nl} = \text{Op}(a_{nl} \chi_\Omega).$$

Using (5.7), we immediately obtain the bound

$$\|\chi_{\alpha I} A_{nl} (\mathbb{1} - \chi_{\alpha I})\|_q^q \lesssim (1 + |n|)^{-sq} (1 + |l|)^{-tq} \log(\alpha).$$

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

$$\begin{aligned} \|\chi_{\alpha I} \text{Op}(p[\Omega])(\mathbb{1} - \chi_{\alpha I})\|_q^q &\leq \sum_{nl} \|\chi_{\alpha I} A_{nl} (\mathbb{1} - \chi_{\alpha I})\|_q^q \\ &\lesssim \log(\alpha) \sum_{nl} (1 + |n|)^{-sq} (1 + |l|)^{-tq}. \end{aligned}$$

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

Corollary 5.3. *Assume that $V \in C^\infty(\mathbb{R})$. Let $A_{\alpha,\mu}$ be as defined in (5.2).*

(1) *Let $I \subset \mathbb{R}$ be an interval. If $\mu \in (\sigma(H))^\circ$, then for any $q \in (0, 1]$,*

$$\|\chi_{\alpha I} P_\mu(\mathbb{1} - \chi_{\alpha I})\|_q^q \lesssim \log(\alpha). \tag{5.8}$$

If $\mu \notin (\sigma(H))^\circ$, then for any $q \in (0, 1]$,

$$\|\chi_{\alpha I} P_\mu(\mathbb{1} - \chi_{\alpha I})\|_q^q \lesssim 1. \tag{5.9}$$

(2) *For any $q \in (0, 1]$,*

$$\|A_{\alpha,\mu}\|_q^q \lesssim \begin{cases} 1, & \mu \notin (\sigma(H))^\circ, \\ \log(\alpha), & \mu \in (\sigma(H))^\circ. \end{cases} \tag{5.10}$$

Moreover, assume that h satisfies Condition 1.1. Then $h(B_{\alpha,\mu})$ is of trace class and

$$\|h(B_{\alpha,\mu})\|_1 \lesssim \begin{cases} \alpha|h(1)| + 1, & \mu \notin (\sigma(H))^\circ, \\ \alpha|h(1)| + \log(\alpha), & \mu \in (\sigma(H))^\circ. \end{cases} \tag{5.11}$$

(3) *If $\mu \notin (\sigma(H))^\circ$, then (1.11) holds.*

The implicit constants in the inequalities (5.8), (5.9), (5.10) and (5.11) are independent of α .

Proof. It suffices to prove (5.8) and (5.9) 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 (3.6), the operator $P_\mu[S]$ has the form $\text{Op}(p[\Omega])$ with

$$p(x, y, \xi) = E(x, \xi)\overline{E(y, \xi)} \quad \text{and} \quad \Omega = (2k_j - \delta, \delta),$$

where k_j is as defined in (2.4), 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 2π -periodic in x , and due to the C^∞ -smoothness of V , it is also C^∞ -smooth in x . Now (5.8) follows from (5.4).

Suppose that $\mu \notin S^\circ$. According to (2.12), either $P_\mu[S] = 0$, in which case (5.9) is trivial, or

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

Using a straightforward partition of unity on the circle $n\mathbb{T}$ one can represent $P_\mu[S]$ as a finite sum of operators of the form $\text{Op}(p)$ with

$$p(x, y, \xi) = E(x, \xi)\overline{E(y, \xi)}\zeta(\xi), \quad \zeta \in C_0^\infty(\mathbb{R}).$$

Therefore, (5.9) is a consequence of (5.3).

From $\|P_\mu\chi_{(-\alpha,\alpha)}\| \leq 1$ we get that

$$\|A_{\alpha,\mu}\|_q = \|\chi_{(-\alpha,\alpha)}P_\mu(\mathbb{1} - \chi_{(-\alpha,\alpha)})P_\mu\chi_{(-\alpha,\alpha)}\|_q \leq \|\chi_{(-\alpha,\alpha)}P_\mu(\mathbb{1} - \chi_{(-\alpha,\alpha)})\|_q,$$

and (5.10) follows from (5.9).

To prove (5.11) we use the representation (1.12): $h(t) = th(1) + h_1(t)$, so that $h_1(0) = h_1(1) = 0$ and $|h_1(t)| \lesssim t^q(1 - t)^q$, where $q \in (0, 1]$ is the Hölder parameter of the function h . The first term on the right-hand side of (5.11) follows from the bound (2.6). For the second term write:

$$\|h_1(B_{\alpha,\mu})\|_1 \lesssim \|A_{\alpha,\mu}^q\|_1 = \|A_{\alpha,\mu}\|_q^q,$$

and hence the required bounds follow from (5.10). Together with Remark 1.3, this also implies Part (3) of the corollary. \square

6. Proof of Theorem 1.2: Polynomial Test Functions

By virtue of Corollary 5.3(3), the formula (1.11) is already proved. Thus it remains to prove Theorem 1.2 for $\mu \in (\sigma(H))^\circ$. From now on we assume that μ 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 $\Phi = \Phi(\cdot, \delta)$.

6.1. *Polynomial classes.* We begin the proof of (1.10) with studying polynomial test functions. The following classes of polynomials on the interval $[0, 1]$ will be relevant:

$$\begin{aligned} \mathfrak{P} &:= \{p : [0, 1] \mapsto \mathbb{C}, \text{ polynomial}\}, \\ \mathfrak{P}_0 &:= \{p \in \mathfrak{P} : p(0) = p(1) = 0\}, \\ \mathfrak{P}_s &:= \{p \in \mathfrak{P} : p(t) = p(1 - t) \text{ for all } t\}, \\ \mathfrak{P}_{s,0} &:= \mathfrak{P}_s \cap \mathfrak{P}_0. \end{aligned} \tag{6.1}$$

As explained in Remark 1.3, it suffices to prove (1.10) for the functions h_1 satisfying Condition 1.1, such that $h_1(0) = h_1(1) = 0$. Thus we need to study polynomials $p \in \mathfrak{P}_0$. In fact, it is enough to consider a basis of \mathfrak{P}_0 . As in [16] we choose the basis

$$\{(p_n, q_n) : p_n(t) = (t(1 - t))^n, q_n(t) = t(t(1 - t))^n, n = 1, 2, \dots\},$$

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

$$p_n(B_{\alpha,\mu}) = A_{\alpha,\mu}^n, \quad A_{\alpha,\mu} = B_{\alpha,\mu}(\mathbb{1} - B_{\alpha,\mu}).$$

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 4.5.

6.2. *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

$$\begin{cases} A_{\alpha,\mu}^- : &= \chi_{(-\alpha,\alpha)} P_\mu \chi_{(-\infty,-\alpha)} P_\mu \chi_{(-\alpha,\alpha)}, \\ A_{\alpha,\mu}^+ : &= \chi_{(-\alpha,\alpha)} P_\mu \chi_{(\alpha,\infty)} P_\mu \chi_{(-\alpha,\alpha)}. \end{cases} \tag{6.2}$$

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

Definition 6.1. Let A and B be bounded operators on $L^2(\mathbb{R})$. We write $A \sim B$ if $\|A - B\|_1 \lesssim 1$, uniformly in $\alpha \gtrsim 1$. We write $A \approx B$ if A and B are trace class and $|\operatorname{tr} A - \operatorname{tr} B| \lesssim 1$ uniformly in $\alpha \gtrsim 1$.

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 for operators A and B with uniformly bounded operator norm (in α), $A \sim B$ implies $A^n \sim B^n$ for any $n = 1, 2, \dots$

To begin with, by virtue of Proposition 4.3(i),

$$A_{\alpha,\mu}^+ \sim \chi_{(-\alpha,\alpha)} P_\mu \chi_{(\alpha+1,\infty)} P_\mu \chi_{(-\alpha,\alpha)}. \tag{6.3}$$

and

$$A_{\alpha,\mu}^- \sim \chi_{(-\alpha,\alpha)} P_\mu \chi_{(-\infty,-\alpha-1)} P_\mu \chi_{(-\alpha,\alpha)}. \tag{6.4}$$

6.2.1. Operators D_α^\pm The next step is to replace $A_{\alpha,\mu}^\pm$ with operators that do not contain any information on the function $\Phi(x, k)$. These are the operators $D_\alpha^\pm : L^2(\mathbb{R}) \mapsto L^2(\mathbb{R})$, 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_α^+ and D_α^- are unitarily equivalent via the change $x \mapsto -x$. The crucial fact is that the asymptotic formulas for the traces of powers $(D_\alpha^\pm)^n$ can be easily deduced from the results of [16]:

Lemma 6.2. *Let $p_n(t) = t^n(1-t)^n, n = 1, 2, \dots$ Then*

$$\operatorname{tr}(D_\alpha^\pm)^n = \frac{1}{4} \log \alpha \mathcal{W}(p_n) + o(\log(\alpha)), \quad \alpha \rightarrow \infty, \tag{6.5}$$

where $\mathcal{W}(\cdot)$ is as defined in (1.9).

Proof. Since D_α^+ and D_α^- are unitarily equivalent, we show (6.5) for $D_\alpha := D_\alpha^+$ only. By translation and reflection, the operator D_α 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 (6.5) immediately follows from [16, formula (19), p. 477]. \square

A useful way to write D_α^\pm is

$$D_\alpha^\pm = (Z_\alpha^\pm)^* Z_\alpha^\pm,$$

where Z_α^\pm have kernels

$$Z_\alpha^+(x, y) = \frac{\chi_{(\alpha+1, \infty)}(x)\chi_{(-\alpha, \alpha)}(y)}{2\pi(x - y)}, \quad \text{and} \quad Z_\alpha^-(x, y) = \frac{\chi_{(-\infty, -\alpha-1)}(x)\chi_{(-\alpha, \alpha)}(y)}{2\pi(x - y)} \tag{6.6}$$

respectively. Now we need to establish a few facts for operators D_α^\pm and Z_α^\pm . Recall that we abbreviate $\Phi = \Phi(x, \delta)$, $\delta = \delta(\mu)$, remembering that μ is strictly inside the band S .

Lemma 6.3. *Denote by Y_α^\pm any of the two operators Z_α^\pm or $(Z_\alpha^\pm)^*$. With the notation as above,*

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

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_α instead of Z_α^+ .

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

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

see the definition (4.7). Thus by Lemma 4.5,

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

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

Corollary 6.4. *Let*

$$K_{\alpha, n}^\pm = 2\pi [\Phi (D_\alpha^\pm)^n \bar{\Phi} + \bar{\Phi} (D_\alpha^\pm)^n \Phi], \quad n = 1, 2, \dots \tag{6.7}$$

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

$$(K_{\alpha, 1}^\pm)^n \sim K_{\alpha, n}^\pm, \tag{6.8}$$

and

$$(K_{\alpha, 1}^\pm)^n \approx 2(D_\alpha^\pm)^n, \quad \alpha \rightarrow \infty. \tag{6.9}$$

Proof. For brevity we omit the superscript “±” and write $K_{\alpha, 1}$, D_α instead of $K_{\alpha, 1}^\pm$, D_α^\pm etc. The powers of $K_{\alpha, 1}$ contain terms of the form $D_\alpha f D_\alpha$ with $f = |\Phi|^2$, Φ^2 or $\bar{\Phi}^2$. The operator $D_\alpha f D_\alpha$, is written as

$$Z_\alpha^* Z_\alpha f Z_\alpha^* Z_\alpha.$$

Thus by Lemma 6.3,

$$K_{\alpha, 1}^n \sim (2\pi)^n [(\Phi D_\alpha \bar{\Phi})^n + (\bar{\Phi} D_\alpha \Phi)^n] \sim 2\pi [\Phi D_\alpha^n \bar{\Phi} + \bar{\Phi} D_\alpha^n \Phi],$$

as claimed.

In order to prove (6.9), use the cyclicity of the trace. If $n = 1$, then, again by Lemma 6.3,

$$\Phi D_\alpha \bar{\Phi} \approx Z_\alpha |\Phi|^2 Z_\alpha^* \sim \frac{1}{2\pi} Z_\alpha Z_\alpha^* \approx \frac{1}{2\pi} D_\alpha.$$

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

$$\Phi D_\alpha^n \bar{\Phi} \approx Z_\alpha D_\alpha^{n-2} Z_\alpha^* Z_\alpha |\Phi|^2 Z_\alpha^* \sim \frac{1}{2\pi} Z_\alpha D_\alpha^{n-2} Z_\alpha^* Z_\alpha Z_\alpha^* \approx \frac{1}{2\pi} D_\alpha^n$$

The same is done with the component containing Φ and $\bar{\Phi}$ in the other order. This implies (6.9). Thus the proof is complete. \square

6.2.2. *Approximating operators $A_{\alpha,\mu}^\pm$* Assume that μ is as before and $K_{\alpha,n}^\pm$ are as defined in (6.7).

Lemma 6.5. *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*

$$(A_{\alpha,\mu}^\pm)^n \sim (K_{\alpha,1}^\pm)^n, \tag{6.10}$$

and

$$A_{\alpha,\mu}^n \sim (A_{\alpha,\mu}^+)^n + (A_{\alpha,\mu}^-)^n \sim (K_{\alpha,1}^+)^n + (K_{\alpha,1}^-)^n. \tag{6.11}$$

for every $n = 1, 2, \dots$

Proof. To prove (6.10) it suffices to consider the case $n = 1$. As before, we do it for $A_{\alpha,\mu}^+$ only, omitting the superscript “+”. From (6.3) and Lemma 4.2 it follows that

$$A_{\alpha,\mu}^+ \sim \chi_{(-\alpha,\alpha)} \Pi_\mu \chi_{(\alpha+1,\infty)} \Pi_\mu \chi_{(-\alpha,\alpha)}.$$

By (3.2) and (6.6),

$$\begin{aligned} \chi_{(\alpha+1,\infty)} \Pi_\mu \chi_{(-\alpha,\alpha)} &= -2\pi i (\Phi Z_\alpha \bar{\Phi} - \bar{\Phi} Z_\alpha \Phi), \\ \chi_{(-\alpha,\alpha)} \Pi_\mu \chi_{(\alpha+1,\infty)} &= 2\pi i (\Phi Z_\alpha^* \bar{\Phi} - \bar{\Phi} Z_\alpha^* \Phi), \end{aligned}$$

so that

$$\begin{aligned} A_{\alpha,\mu}^+ &\sim 4\pi^2 (\Phi Z_\alpha^* |\Phi|^2 Z_\alpha \bar{\Phi} + \bar{\Phi} Z_\alpha^* |\Phi|^2 Z_\alpha \Phi) \\ &\quad - 4\pi^2 (\Phi Z_\alpha^* \bar{\Phi}^2 Z_\alpha \Phi + \bar{\Phi} Z_\alpha^* \Phi^2 Z_\alpha \bar{\Phi}). \end{aligned}$$

Consequently, by Lemma 6.3,

$$A_{\alpha,\mu}^+ \sim 2\pi (\Phi Z_\alpha^* Z_\alpha \bar{\Phi} + \bar{\Phi} Z_\alpha^* Z_\alpha \Phi) = K_{\alpha,1},$$

as required.

Proof of (6.11). By the definition (6.2),

$$A_{\alpha,\mu}^- A_{\alpha,\mu}^+ = \chi_{(-\alpha,\alpha)} P_\mu \left(\chi_{(-\infty,-\alpha)} P_\mu \chi_{(-\alpha,\alpha)} P_\mu \chi_{(\alpha,\infty)} \right) P_\mu \chi_{(-\alpha,\alpha)}.$$

By Proposition 4.3((iii)), the trace norm of the operator in the middle is uniformly bounded, and hence $A_{\alpha,\mu}^- A_{\alpha,\mu}^+ \sim 0$. In the same way one checks that $A_{\alpha,\mu}^+ A_{\alpha,\mu}^- \sim 0$. Thus

$$A_{\alpha,\mu}^n \sim (A_{\alpha,\mu}^+)^n + (A_{\alpha,\mu}^-)^n,$$

and (6.11) is now a consequence of (6.10). \square

6.3. *Proof of Theorem 1.2 for symmetric polynomials.* By (6.11), (6.9) and (6.5),

$$\begin{aligned} \operatorname{tr} A_{\alpha,\mu}^n &= \operatorname{tr}(K_{\alpha}^+)^n + \operatorname{tr}(K_{\alpha}^-)^n + \mathcal{O}(1) \\ &= 2 \operatorname{tr}(D_{\alpha}^+)^n + 2 \operatorname{tr}(D_{\alpha}^-)^n + \mathcal{O}(1) \\ &= \log(\alpha) \mathcal{W}(p_n) + o(\log(\alpha)), \quad n = 1, 2, \dots \end{aligned} \tag{6.12}$$

Hence, Theorem 1.2 for polynomials $p \in \mathfrak{P}_{s,0}$ follows from the identity $p_n(B_{\alpha,\mu}) = A_{\alpha,\mu}^n$. \square

6.4. *Arbitrary polynomials.* As above, we assume that $\mu \in S^\circ$, where S is a band of the type (2.8). So far we have proved Theorem 1.2 for polynomials $p \in \mathfrak{P}_{s,0}$ (cf. (6.1) for notation). To extend this result to arbitrary $p \in \mathfrak{P}_0$ it remains to treat basis elements of the form $q_n(t) = t[t(1-t)]^n$, $n = 1, 2, \dots$. Following [16] for the free case, this is done by a symmetry argument that reduces $\operatorname{tr} [B_{\alpha,\mu} A_{\alpha,\mu}^n]$ to $\operatorname{tr} A_{\alpha,\mu}^n$.

Lemma 6.6. *For every $n = 1, 2, \dots$, we have*

$$B_{\alpha,\mu}(A_{\alpha,\mu})^n \approx \frac{1}{2} \operatorname{tr}(A_{\alpha,\mu})^n, \tag{6.13}$$

as $\alpha \rightarrow \infty$.

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 periodicity of the operators. The operators $A_{\alpha,\mu}^+$ and $A_{\alpha,\mu}^-$ (see (6.2)) are considered separately. Applying Proposition 4.3 (ii)b, we get

$$A_{\alpha,\mu}^+ \sim \chi_{(-\alpha,\alpha)} P_{\mu} \chi_{(\alpha,3\alpha)} P_{\mu} \chi_{(-\alpha,\alpha)}. \tag{6.14}$$

Let U_{α}^{\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 (6.14) implies that

$$(U_{\alpha}^+)^* A_{\alpha,\mu}^+ U_{\alpha}^+ \sim \chi_{(-2\alpha,0)} P_{\mu} \chi_{(0,2\alpha)} P_{\mu} \chi_{(-2\alpha,0)}. \tag{6.15}$$

Indeed, (6.14) yields:

$$(U_{\alpha}^+)^* A_{\alpha,\mu}^+ U_{\alpha}^+ \sim \chi_{(-\alpha-\alpha_0,\alpha-\alpha_0)} P_{\mu} \chi_{(\alpha-\alpha_0,3\alpha-\alpha_0)} P_{\mu} \chi_{(-\alpha-\alpha_0,\alpha-\alpha_0)},$$

since $(U_{\alpha}^+)^* P_{\mu} U_{\alpha}^+ = P_{\mu}$. Now, to get (6.15), one needs to use repeatedly Proposition 4.3(i), (iv). We denote

$$\chi_{\alpha}^+ = \chi_{(0,2\alpha)}, \quad \chi_{\alpha}^- = \chi_{(-2\alpha,0)}$$

and

$$T_{\alpha,\mu}^{\pm} := \chi_{\alpha}^{\mp} P_{\mu} \chi_{\alpha}^{\pm} P_{\mu} \chi_{\alpha}^{\mp}.$$

Thus one can write

$$(U_{\alpha}^{\pm})^* A_{\alpha,\mu}^{\pm} U_{\alpha}^{\pm} \sim T_{\alpha,\mu}^{\pm}. \tag{6.16}$$

This relation with the “+” sign coincides with (6.15), and for the “−” sign it is proved in the same way. The proof of Lemma 6.6 begins with the following observation.

Lemma 6.7. *For any $n = 1, 2, \dots$, we have*

$$P_\mu(T_{\alpha,\mu}^\pm)^n \approx (\mathbb{1} - P_\mu)(T_{\alpha,\mu}^\mp)^n, \text{ as } \alpha \rightarrow \infty. \tag{6.17}$$

Proof. For brevity we write $\chi^\pm = \chi_\alpha^\pm$, $T^\pm = T_{\alpha,\mu}^\pm$, $P = P_\mu$, and $Q = \mathbb{1} - P$. We have

$$\begin{aligned} P(T^+)^n &= P\chi^-P\chi^+P\chi^-(T^+)^{n-1} = -P\chi^-Q\chi^+P\chi^-(T^+)^{n-1} \\ &= P(\mathbb{1} - \chi^-)Q\chi^+P\chi^-(T^+)^{n-1} \\ &= P\chi^+Q\chi^+P\chi^-(T^+)^{n-1} + R_1 + R_2, \end{aligned} \tag{6.18}$$

with

$$\begin{aligned} R_1 &= P\chi_{(2\alpha,\infty)}Q\chi^+P\chi^-(T^+)^{n-1}, \\ R_2 &= P\chi_{(-\infty,-2\alpha)}Q\chi^+P\chi^-(T^+)^{n-1}. \end{aligned}$$

We notice that $Q = \mathbb{1} - P$ can be replaced by $-P$ in R_1 . By Proposition 4.3(iii),

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

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

$$\chi^+P\chi^-(T^+)^{n-1} = (T^-)^{n-1}\chi^+P\chi^-, \tag{6.19}$$

and hence, by cyclicity of the trace,

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

Applying Proposition 4.3(iii) to the factor $\chi^+P\chi^-P\chi_{(-\infty,-2\alpha)}$ we infer that $R_2 \approx 0$.

Apply (6.19) to the first operator on the right-hand side of (6.18) and use again the cyclicity:

$$\begin{aligned} P\chi^+Q\chi^+P\chi^-(T^+)^{n-1} &= P\chi^+Q(T^-)^{n-1}\chi^+P\chi^- \\ &\approx Q(T^-)^{n-1}\chi^+P\chi^-P\chi^+ = Q(T^-)^n. \end{aligned}$$

Together with (6.18) this yields (6.17) for the “+” sign. The relation (6.17) for the “-” sign is obtained in the same way. \square

Proof of Lemma 6.6. We shall use the simplified notation as in the proof of Lemma 6.7 and also write $A = A_{\alpha,\mu}$, $A^\pm = A_{\alpha,\mu}^\pm$, and $B = B_{\alpha,\mu}$. First observe that $BA^n \approx PA^n$. Thus by (6.11) and (6.16),

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

By Lemma 6.7,

$$2P(T^\pm)^n \approx P(T^\pm)^n + (\mathbb{1} - P)(T^\mp)^n,$$

so that

$$\begin{aligned} 2P(T^+)^n + 2P(T^-)^n &\approx P(T^+)^n + (\mathbb{1} - P)(T^-)^n + P(T^-)^n + (\mathbb{1} - P)(T^+)^n \\ &= (T^+)^n + (T^-)^n. \end{aligned}$$

Using (6.16) and (6.11) again, we get

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

which leads to (6.13), and hence completes the proof.

As a consequence of Lemma 6.6, Theorem 1.2 can be proved for arbitrary $p \in \mathfrak{P}_0$.

Proof of Theorem 1.2 for arbitrary polynomials. It remains to prove the theorem for polynomials of the form $q_n(t) = tp_n(t)$, $n = 1, 2, \dots$. From Lemma 6.6 and (6.12) we deduce that

$$\text{tr} [B_{\alpha,\mu}(A_{\alpha,\mu})^n] = \frac{1}{2} \log(\alpha) \mathcal{W}(p_n) + o(\log(\alpha)), \quad \alpha \rightarrow \infty. \tag{6.20}$$

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

$$\pi^2 \mathcal{W}(q_n) = \int_0^1 \frac{tp_n(t)}{t(1-t)} dt = \int_0^1 \frac{p_n(t)}{1-t} dt = \int_0^1 \frac{p_n(t)}{t} dt.$$

Therefore

$$2\pi^2 \mathcal{W}(q_n) = \int_0^1 p_n(t) \left(\frac{1}{1-t} + \frac{1}{t} \right) dt = \int_0^1 \frac{p_n(t)}{t(1-t)} dt = \pi^2 \mathcal{W}(p_n).$$

Together with (6.20) this leads to Theorem 1.2 for arbitrary polynomials $p \in \mathfrak{P}_0$.

7. Proof of Theorem 1.2: Closure of the Asymptotics

Throughout this final section we assume that h satisfies Condition 1.1. Also, without loss of generality we may assume that h is real-valued (otherwise treat real and imaginary part separately). 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 $t = 1$. 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

$$h(t) \leq t(1-t)(p(t) + \epsilon) = \tilde{p}(t) + \epsilon t(1-t), \tag{7.1}$$

and

$$h(t) \geq t(1-t)(p(t) - \epsilon) = \tilde{p}(t) - \epsilon t(1-t). \tag{7.2}$$

The monotonicity of the trace in combination with (7.1) gives

$$\text{tr} [h(B_{\alpha,\mu})] \leq \text{tr} [\tilde{p}(B_{\alpha,\mu})] + \epsilon \text{tr} [B_{\alpha,\mu}(1 - B_{\alpha,\mu})].$$

From Theorem 1.2 for polynomials from \mathfrak{P}_0 , we get

$$\limsup_{\alpha \rightarrow \infty} \frac{\text{tr} [h(B_{\alpha,\mu})]}{\log(\alpha)} \leq \mathcal{W}(\tilde{p}) + \epsilon \mathcal{W}(t(1-t)) = \mathcal{W}(\tilde{p}) + \frac{\epsilon}{\pi^2},$$

where we have used that $\mathcal{W}(t(1-t)) = \pi^{-2}$, see (1.9). Moreover, we notice that

$$|\mathcal{W}(h) - \mathcal{W}(\tilde{p})| = |\mathcal{W}(h - \tilde{p})| \leq \frac{\epsilon}{\pi^2},$$

and hence,

$$\limsup_{\alpha \rightarrow \infty} \frac{\text{tr} [h(B_{\alpha,\mu})]}{\log(\alpha)} \leq \mathcal{W}(h) + \frac{2\epsilon}{\pi^2}.$$

In the same way (7.2) implies

$$\liminf_{\alpha \rightarrow \infty} \frac{\text{tr} [h(B_{\alpha,\mu})]}{\log(\alpha)} \geq \mathcal{W}(h) - \frac{2\epsilon}{\pi^2},$$

and as $\epsilon > 0$ was chosen arbitrarily we deduce (1.10) 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

$$|h(t)| \lesssim t^q(1-t)^q, \quad t \in [0, 1].$$

Fix again $\epsilon > 0$ and choose a smooth function ζ_ϵ 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

$$|(\zeta_\epsilon h)(t)| \lesssim [t(1-t)]^q \zeta_\epsilon(t) \lesssim \epsilon^r [t(1-t)]^r, \quad r = \frac{q}{2},$$

we have

$$\|(\zeta_\epsilon h)(B_{\alpha,\mu})\|_1 \lesssim \epsilon^r \|B_{\alpha,\mu}(\mathbb{1} - B_{\alpha,\mu})\|_r^r.$$

By Corollary 5.3, the right-hand side does not exceed $\log(\alpha)$, $\alpha \geq 2$. Consequently,

$$\frac{|\text{tr} [(\zeta_\epsilon h)(B_{\alpha,\mu})]|}{\log(\alpha)} \lesssim \epsilon^r, \quad \alpha \geq 2. \tag{7.3}$$

On the other hand, $h_\epsilon = (1 - \zeta_\epsilon)h$ vanishes in a vicinity of 0 and 1 and, therefore, by Step 1, we have

$$\text{tr} [h_\epsilon(B_{\alpha,\mu})] = \log(\alpha)\mathcal{W}(h_\epsilon) + o(\log(\alpha)), \quad \alpha \rightarrow \infty. \tag{7.4}$$

It is clear that

$$\mathcal{W}(h) - \mathcal{W}(h_\epsilon) \lesssim \left(\int_0^\epsilon + \int_{1-\epsilon}^1 \right) t^{q-1}(1-t)^{q-1} dt \lesssim \epsilon^q. \tag{7.5}$$

Combining (7.3), (7.4), and (7.5) gives

$$\limsup_{\alpha \rightarrow \infty} \left| \frac{\text{tr}[h(B_{\alpha,\mu})]}{\log(\alpha)} - \mathcal{W}(h) \right| \lesssim \epsilon^r.$$

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

Step 3 Suppose that h satisfies Condition 1.1. Fix an $\epsilon > 0$. Let h_1, h_2 be two continuous functions, such that

- (1) $h_1(t) = h_2(t) = h(t)$ in a neighbourhood of the endpoints $t = 0, 1$,
- (2) $h_1(t) \leq h(t) \leq h_2(t)$ a.e. $t \in (0, 1)$, and
- (3) $\|h_1 - h_2\|_{L^1} < \epsilon$.

By (1.9), this implies that

$$|\mathcal{W}(h_1) - \mathcal{W}(h)| \lesssim \epsilon, \quad |\mathcal{W}(h_2) - \mathcal{W}(h)| \lesssim \epsilon.$$

Also, in view of monotonicity, we have

$$\operatorname{tr} h_1(B_{\alpha,\mu}) \leq \operatorname{tr} h(B_{\alpha,\mu}) \leq \operatorname{tr} h_2(B_{\alpha,\mu}).$$

Thus, by Step 2,

$$\limsup_{\alpha \rightarrow \infty} \left| \frac{\operatorname{tr} h(B_{\alpha,\mu})}{\log(\alpha)} - \mathcal{W}(h) \right| \lesssim \epsilon.$$

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

This completes the proof of Theorem 1.2.

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