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# Szegő-type Trace Asymptotics for Operators with Translational Symmetry

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## Declaration

I, Bernhard Pfirsch, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the work. Parts of this thesis have been published as [53, 54] (copyright for [53]: © 2019 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim) with the paper [54] being a result of joint work with Alexander V. Sobolev. Naturally, the thesis coincides both in content and writing partially with [53, 54].

Bernhard Pfirsch

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# Abstract

The classical Szegő limit theorem describes the asymptotic behaviour of Toeplitz determinants as the size of the Toeplitz matrix grows. The continuous analogue are trace asymptotics for Wiener–Hopf operators on intervals of growing length. We study two problems related to these scaling asymptotics.

The first problem concerns the higher-dimensional version of the trace asymptotics. Namely, consider a translation-invariant bounded linear operator in dimension two whose integral kernel exhibits super-polynomial off-diagonal decay. Then we study the spectral asymptotics of its spatial restriction to the interior of a scaled polygon, as the scaling parameter tends to infinity. To this end, we provide complete trace asymptotics for analytic functions of the truncated operator. These consist of three terms, which reflect the geometry of the polygon. If the polygon is substituted by a domain with smooth boundary, then the corresponding asymptotics are well-known. However, we show that the constant order term in the expansion for the polygon cannot be recovered from a formal approximation by smooth domains. This fact is reminiscent of the heat trace anomaly for the Dirichlet Laplacian.

A prominent application of trace asymptotics for Wiener–Hopf operators lies in quantum information theory: they can be used to compute the bipartite entanglement entropy for the ground state of a free Fermi gas in the absence of an external field. At zero temperature, this requires studying Wiener–Hopf operators with a discontinuous symbol, which causes notable difficulties. In the second part of the thesis, based on joint work with Alexander V. Sobolev, we prove a two-term asymptotic trace formula for the periodic Schrödinger operator in dimension one. This formula can be applied to compute the aforementioned entanglement entropy when the fermions are exposed to a periodic electric field. Moreover, the subleading order of the asymptotics identifies the spectrum of the periodic Schrödinger operator.

# Impact Statement

Among the mathematical research areas, this thesis is settled at the intersection of analysis, spectral theory, and mathematical physics. The thesis deals with advances of different nature in the context of Szegő-type trace asysmptotics, which have been an active field of research for more than a century. Firstly, trace asymptotics for truncated Wiener–Hopf operators are considered, where progress is made in the direction of truncation sets with non-smooth geometry. Secondly, this thesis implements an extension of known trace asymptotics for Wiener–Hopf operators to operators with less symmetries. The latter is of interdisciplinary interest: it can be used to study quantum entanglement in theoretical physics. The author hopes to stimulate further research in both mentioned directions. The results contained in the thesis have been communicated to the mathematical research community via the publications [53, 54].

# Acknowledgements

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To begin with, I would like to thank Alex for suggesting the mathematical problems considered in this thesis and for the smooth and respectful collaboration in our joint work. Thank you, Alex, for sharing with me not only your broad mathematical knowledge but also your positive attitude and love towards research. I have profited immensely from our countless and intensive discussions that at times kept you from your well-deserved evening with your family. Particularly, I would like to thank you for your patience and always honest opinion on my mathematical ideas. Moreover, I am at least equally grateful for your generous and selfless personal advice during my whole PhD.

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# List of Symbols

## General Notation

| | |
|---|---|
| $d$ | dimension |
| $L$ | scaling parameter |
| $\partial\mathbb{D}$ | unit circle in the complex plane |
| $B_r(x)$ | closed ball of radius $r$ around $x \in \mathbb{R}^d$ (with respect to the Euclidean norm) |
| $Q_x$ | unit cube centered at $x \in \mathbb{R}^d$ |
| $G_+$ | lattice point neighbourhood for the set $G$, see (2.43) |
| $\mathsf{M} \triangle \Lambda$ | symmetric difference of the sets $\mathsf{M}$ and $\Lambda$ |
| $\Omega^\circ$ | interior of the set $\Omega$ |
| $\lvert\Omega\rvert$ | $d$-dimensional Lebesgue measure of the set $\Omega \subset \mathbb{R}^d$ |
| $\sharp\Omega$ | cardinality of the set $\Omega$ |
| $\varphi_k$ | $k$th Fourier coefficient of $\varphi \in \mathrm{L}^1(\mathbb{D})$ |
| $G[\varphi]$ | geometric mean of $\varphi$ |
| $\mathcal{F}$ | Fourier transform |
| $\check{f}$ | inverse Fourier transform of $f$ with modified constant, see (2.16) |
| $\mathcal{M}(\,\cdot\,)$ | mean value of an almost periodic function |
| $\langle x \rangle$ | $(1+\lvert x\rvert^2)^{1/2}$ |

## Function spaces and norms

| | |
|---|---|
| $\mathrm{L}^p_{(\mathrm{loc})}(Y)$ | measurable functions $Y \to \mathbb{C}$ such that the $p$th power of their modulus is (locally) integrable on $Y$ |
| $\mathrm{L}^p(Y,Z)$ | measurable functions $Y \to Z$ such that the $p$th power of their modulus is integrable on $Y$ |
| $\mathrm{L}^\infty(Y)$ | bounded, measurable functions $Y \to \mathbb{C}$ |
| $\mathrm{H}^N(\mathbb{R})$ | measurable functions $\mathbb{R} \to \mathbb{C}$ such that their weak derivatives up to order $N$ exist and are elements of $\mathrm{L}^2(\mathbb{R})$ |

| | |
|---|---|
| $\mathrm{W}^{N,1}(\mathbb{R}^d)$ | measurable functions $f : \mathbb{R}^d \to \mathbb{C}$ such that their weak derivatives up to order $N$ exist and are integrable |
| $\mathrm{W}^{\infty,1}(\mathbb{R}^d)$ | smooth functions $\mathbb{R}^d \to \mathbb{C}$ whose (partial) derivatives are Lebesgue-integrable |
| $\mathrm{CAP}(\mathbb{R})$ | uniformly almost-periodic functions $\mathbb{R} \to \mathbb{C}$ |
| $\mathrm{C}^k_{(0)}(Y)$ | $k$ times continuously differentiable functions $Y \to \mathbb{C}$ (with compact support) |
| $\mathcal{S}(\mathbb{R}^d)$ | smooth and rapidly decreasing functions $\mathbb{R}^d \to \mathbb{C}$ |
| $\lvert \cdot \rvert$ | Euclidean norm on $\mathbb{R}^d$ |
| $\lvert \cdot \rvert_N$ | norm on $\mathrm{W}^{N,1}(\mathbb{R}^d)$, see (2.29) |

## Operators

| | |
|---|---|
| $\mathscr{L} = \mathscr{L}(\varphi)$ | Laurent matrix with symbol $\varphi$ |
| $T_n(\varphi)$ | Toeplitz matrix with symbol $\varphi$ of size $n$ |
| $A = A(a)$ | Fourier multiplier with symbol $a$ |
| $A_\Omega = A_\Omega(a)$ | Truncated Wiener–Hopf operator with symbol $a$ and truncation set $\Omega$ |
| $W(a)$ | Wiener–Hopf operator with symbol $a$ |
| $M(f)$ | multiplication operator by the function $f$ |
| $\mathrm{Op}(p)$ | pseudo-differential operator with amplitude $p$, see (4.26) |
| $\mathbb{1}$ | identity operator |
| $-\Delta$ | non-negative Laplacian |
| $H$ | not necessarily bounded self-adjoint operator on $\mathrm{L}^2(\mathbb{R}^d)$; from page 29 on specified as periodic Schrödinger operator in dimension 1 |
| $\mathfrak{S}_p$ | compact operators whose singular values are $p$-summable |
| $\lVert \cdot \rVert_p$ | $p$th Schatten (quasi-)norm |

## Functions

| | |
|---|---|
| $h$ | test function |
| $h_0$ | $h_0(t) = h(t) - th(1)$ |
| $h_1$ | $h_1(z) = h(z) - zh'(0)$ |
| $\chi_\Omega$ | characteristic function for the set $\Omega$ and its corresponding multiplication operator |
| $\eta_1$ | von Neumann entanglement function |
| $\eta_\gamma$ | $\gamma$-Rényi entropy function |

| | |
|---|---|
| $F(E)$ | function of the angles adjacent to $E$, see (2.3) |
| $a_{E,t}$ | see (2.12) |
| $a_t$ | $a_t(\xi) = a(t, \xi)$ |

## Coefficients

| | |
|---|---|
| $\mathcal{W}(\,\cdot\,)$ | linear functional defined in (1.10) |
| $\mathcal{B}_j(\Omega, h, a)$ | coefficient for the term of order $L^j$ in the trace asymptotics for Wiener–Hopf operators with smooth symbol on domains with smooth boundary |
| $\mathrm{c}_j$ | coefficient for the term of order $L^j$ in the trace asymptotics for Wiener–Hopf operators on domains with piecewise smooth Lipschitz boundary |
| $\mathrm{a}_1(\nu_E)$ | see (2.5) |
| $\mathrm{a}_0(\nu_E)$ | see (2.6) |
| $\mathrm{b}_0(X)$ | see (2.9), (2.10) |

## Geometry of the polygon

| | |
|---|---|
| $\mathscr{P}$ | the (interior of the) polygon |
| $\mathcal{E}(\mathscr{P})$ | edges of the polygon $\mathscr{P}$ |
| $\Xi(\mathscr{P})$ | vertices of the polygon $\mathscr{P}$ |
| $\Xi_{\lessgtr}(\mathscr{P})$ | vertices at convex and concave corners, respectively |
| $\mathscr{H}_E$ | half-space extending into the direction $\nu_E$ with boundary passing through 0, parallel to the edge $E$ |
| $\nu_E$ | inward pointing unit normal for the edge $E$ |
| $\tau_E$ | unit tangent vector for the edge $E$ |
| $S_E$ | strip of unit width with base parallel to $E$ and one corner being equal to 0 |
| $\mathscr{C}(X)$ | (semi-)infinite sector modelling the corner of $\mathscr{P}$ at $X$ |
| $E^j(X)$ | edge adjacent to the vertex $X$ |
| $\mathscr{H}^{(j)}(X)$ | halfspace corresponding to the edge $E^{(j)}(X)$ |
| $\tau_X^{(j)}$, $j = 1, 2$ | tangent vectors corresponding to the vertex $X$, see (2.50) |
| $\nu_X^{(j)}$, $j = 1, 2$ | normal vectors corresponding to the vertex $X$, see (2.50) |
| $\Gamma^{(j)}(X)$ | see (2.60) |
| $\mathcal{V} = \mathcal{V}^\epsilon$ | one-sided $\epsilon$-neighbourhood of $\partial\mathscr{P}$ |
| $\mathcal{N}(X)$ | corner neighbourhood at $X$, see Figure 1, p. 41, and (2.53) |
| $\mathsf{N}(X)$ | shifted corner neighbourhood for $X$, see (2.52) and Figure 2, p. 52 |

$\mathsf{T}^{(j)}(X)$ tube parallel to the edge $E^{(j)}(X)$, see (2.51) and Figure 2, p. 52

## Periodic Schrödinger operator

| | |
|---|---|
| $H$ | periodic Schrödinger operator in dimension 1 |
| $V$ | $2\pi$-periodic potential |
| $\sigma(H)$ | spectrum of $H$ |
| $P_\mu$ | spectral projection $\chi_{(-\infty,\mu)}(H)$ |
| $N(\mu, H)$ | integrated density of states for the operator $H$ at energy $\mu$ |
| $U$ | Floquet-Bloch-Gelfand transform |
| $H(k)$ | fibre operator of $H$ with quasi-momentum $k$ |
| $\lambda_j(k)$ | $j$th eigenvalue for the operator $H(k)$ |
| $k_j$ | see (3.3) |
| $\sigma_j$ | image of $\lambda_j$ |
| $\mu_j$, $\nu_j$ | minimum and maximum of $\sigma_j$, respectively |
| $S$ | genuine spectral band: a connected component of $\sigma(H)$ |
| $n_S$ | number of bands $\sigma_j$ contained in $S$ |
| $j_S$ | index of the band $\sigma_{j_S}$ whose bottom coincides with the bottom of $S$ |
| $\kappa_S$ | $k_{j_S}$ |
| $\Lambda^S(k)$ | analytic family of Bloch eigenvalues corresponding to the genuine spectral band $S$, see (3.11) |
| $\Phi^S(x,k)$ | analytic family of Bloch eigenfunctions corresponding to the genuine spectral band $S$, see Proposition 3.6 |
| $E^S(x,k)$ | periodic part of the function $\Phi^S(x,k)$, see (3.20) |
| $P^S(k)$ | analytic family of one-dimensional projections corresponding to the genuine band $S$ |
| $P_\mu[S]$ | spectral projection for the interval $S \cap (-\infty, \mu)$ |
| $\Pi_\mu$ | see (4.7) |
| $B_{L,\mu}$ | $\chi_{(-L,L)} P_\mu \chi_{(-L,L)}$ |
| $A_{L,\mu}$ | $B_{L,\mu}(\mathbb{1} - B_{L,\mu})$ |
| $A^{\pm}_{L,\mu}$ | see (4.39) |
| $D^{\pm}_L$ | see (4.42) |
| $K^{\pm}_{L,n}$ | see (4.44) |

CHAPTER 1

# Introduction

Translation-invariant linear operators are omnipresent in the research area of mathematical analysis, not least because of their occurrence in the description of many physical systems. When examining spectral properties of these operators, their symmetry properties are the key to a thorough analysis. In this thesis, we deal with spatial truncations of operators with discrete or continuous translational symmetry. The truncation breaks the symmetry and, therefore, complicates the spectral analysis of such operators. However, one can obtain interesting results on their spectral asymptotics in the regime when the truncation set becomes large. These findings are also motivated by applications in statistical physics and quantum information theory.

As a starting point, let us look at a translation-invariant bounded linear operator $\mathscr{L}$ on $\mathrm{l}^2(\mathbb{Z})$. Here, the translation invariance means that $\mathscr{L}$ commutes with all finite shifts on $\mathrm{l}^2(\mathbb{Z})$, i.e. the doubly-infinite matrix representation of $\mathscr{L}$ (with respect to the canonical basis) has constant entries along each diagonal. Such a matrix is called *Laurent matrix* and it is not difficult to see that its entries are the Fourier coefficients of a bounded, complex-valued function $\varphi$ on the unit circle $\partial\mathbb{D} := \{z \in \mathbb{C} : \ |z| = 1\}$, see [12, Thm. 1.1]. In other words, one has that

$$\mathscr{L}_{kl} = \varphi_{k-l}, \ k, l \in \mathbb{Z},$$

with

$$\varphi_k := (2\pi)^{-1} \int_0^{2\pi} d\theta \, \varphi(e^{i\theta}) e^{-ik\theta},$$

and via the discrete Fourier transform the operator $\mathscr{L} = \mathscr{L}(\varphi)$ is unitarily equivalent to multiplication by the function $\varphi$ on $\mathrm{L}^2(\partial\mathbb{D})$. One naturally refers to the function $\varphi$ as the *symbol* or *generating function* for the Laurent matrix (or the operator $\mathscr{L}$). Clearly, all spectral properties of the operator $\mathscr{L}$ are encoded within the function $\varphi$; in particular, the spectrum of $\mathscr{L}$ is given by $\operatorname{essran}(\varphi)$, the essential range of the function $\varphi$.

The spectral analysis becomes much harder if one instead looks at the *Toeplitz matrices*,

$$T_n(\varphi) := \big(\varphi_{k-l}\big)_{0\le k,l\le n-1},$$

$n = 1, 2, \ldots$, which are finite sections of the Laurent matrix $\mathscr{L}(\varphi)$. We refer to [12, 13] for an introduction to Toeplitz matrices. While a precise spectral description for a Toeplitz matrix of fixed size is out of reach, one often looks at the spectral asymptotics for $T_n(\varphi)$ as $n \to \infty$. Here, a powerful tool is to study the asymptotics of the Toeplitz determinant $\det T_n(\varphi)$. Notice at this point that the matrix $T_n(\varphi) - \lambda I_n$ (with $I_n$ being the identity matrix and $\lambda \in \mathbb{C}$) is again a Toeplitz matrix, so that the study of Toeplitz determinants includes the spectral determinants. The first results on the asymptotics of Toeplitz determinants date back to the year 1915, when Szegő verified a conjecture by Pólya: in [71] he proved that, for positive and continuous generating functions $\varphi$, we have

$$\lim_{n\to\infty} \sqrt[n]{\det T_n(\varphi)} = G[\varphi], \tag{1.1}$$

where

$$G[\varphi] := \exp\big[(\log\varphi)_0\big] = \exp\Big[(2\pi)^{-1}\int_0^{2\pi} d\theta \log\varphi(e^{i\theta})\Big] \tag{1.2}$$

denotes the geometric mean of $\varphi$. Szegő extended this result in [72] to trace asymptotics for continuous functions of hermitian Toeplitz matrices: if the symbol $\varphi$ is real-valued and continuous, and $h$ is a continuous function on the range of $\varphi$, then the formula

$$\lim_{n\to\infty} \frac{\operatorname{tr} h(T_n(\varphi))}{n} = (h\circ\varphi)_0 = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, (h\circ\varphi)(e^{i\theta}), \tag{1.3}$$

holds. In this context, the function $h$ is sometimes called *test function* as one can get information on the spetral asymptotics of $T_n(\varphi)$ (for a fixed symbol $\varphi$) by evaluating its trace asymptotics for assorted functions $h$. Namely, the formula (1.3) shows that, as $n \to \infty$, the eigenvalues of a hermitian Toeplitz matrix $T_n(\varphi)$ densely accumulate and equidistribute in the range of $\varphi$. While this does not need to be the case for non-hermitian Toeplitz matrices, the spectrum of $T_n(\varphi)$ is always contained in the convex hull of $\operatorname{essran}(\varphi)$, see [12].

Further work on the asymptotics of Toeplitz determinants was stimulated by applications in statistical mechanics: Kaufman and Onsager related in [36] the two-spin correlation functions in the two-dimensional Ising model to Toeplitz determinants, see [22] for a review and further references. In this simple model for a ferromagnet, the large distance behaviour of the two-spin correlations indicate the existence of a long-range order at a fixed temperature. However, formula (1.1) is not sufficient to determine their limiting behaviour: for the relevant Toeplitz determinants the leading order vanishes so that second order asymptotics are required. This motivated Szegő to establish his famous strong limit theorem for Toeplitz determinants in 1952, see [73]. Assuming that $\varphi > 0$ and $\varphi \in \mathrm{C}^{1,\gamma}(\partial\mathbb{D})$ is continuously differentiable with $\gamma$-Hölder continuous derivative, he proved the two-term asymptotic formula

$$\det T_n(\varphi) = G[\varphi]^n E[\varphi](1 + o(1)), \tag{1.4}$$

as $n \to \infty$, with $G[\varphi]$ defined in (1.2) and

$$E[\varphi] := \exp\big[\sum_{k=1}^{\infty} k|(\log\varphi)_k|^2\big].$$

Taking logarithms, this formula becomes

$$\log(\det T_n(\varphi)) = \mathrm{tr}(\log T_n(\varphi)) = n(\log\varphi)_0 + \sum_{k=1}^{\infty} k|(\log\varphi)_k|^2 + o(1), \tag{1.5}$$

as $n \to \infty$, which extends (1.3) for $h(t) = \log(t)$. Over time, the conditions on the symbol $\varphi$ in the strong limit theorem have been weakened significantly, see [61] and references therein. Nevertheless, looking at the definition of $E[\varphi]$, it becomes clear that some regularity of $\varphi$ is strictly necessary for the two-term formulae (1.4), (1.5) to hold. In fact, for the Ising model, Szegő's strong limit theorem only allows one to determine the limiting behaviour of spin correlations at small temperatures. Namely, at the critical temperature — where the long-range order breaks down — the computation of the correlation functions includes Toeplitz determinants with symbols that have a jump discontinuity on the unit circle. This discontinuity causes a slow decay ($\sim 1/|k|$) of the Fourier coefficients $(\log\varphi)_k$ so that the series in (1.5) no longer converges. In this framework, Fisher and Hartwig established a two-term asymptotic formula for a special case of such Toeplitz determinants and conjectured the formula for general symbols with discontinuities, see [30]. Ever since, determinant asymptotics for symbols with combinations of root-type singularities and jump discontinuities, now called Fisher-Hartwig singularities, have been the subject of indepth research, see [2, 3, 5, 6, 8, 10, 11, 18, 20, 23, 27, 28, 43, 78, 79]; for a general review we point towards [39]. To summarise the results for symbols with jump discontinuities, let us mention the trace asymptotics proved in [4]: for a piecewise $C^2$-symbol $\varphi : \partial\mathbb{D} \to \mathbb{C}$ and a test function $h$ that is analytic on a disc containing the range of $\varphi$, the asymptotic expansion

$$\operatorname{tr} h(T_n(\varphi)) = n(h \circ \varphi)_0 + \log(n) a_{\log}(h, \varphi) + a_0(h, \varphi) + o(1) \tag{1.6}$$

holds, as $n \to \infty$, with explicitly computable constants $a_{\log}(h, \varphi)$ and $a_0(h, \varphi)$. Here, the coefficient $a_{\log}(h, \varphi)$ depends on $\varphi$ only via its jump discontinuities, with each jump contributing individually. In particular, one has that $a_{\log}(h, \varphi) = 0$ if $\varphi$ is sufficiently regular, say, $\varphi \in C^2(\partial\mathbb{D})$. Thus, jump discontinuities of $\varphi$ create an additional term of logarithmic order in (1.6). If one, in addition, requires the symbol to be real-valued, then the works [41] and [81] suggest that one can close the asymptotics (1.6) up to sub-leading order for (sufficiently) smooth functions $h$. As a consequence, an evaluation of the coefficient $a_{\log}(h, \varphi)$ shows that in the hermitian case $\sim \log(n)$ of the $n$ eigenvalues of $T_n(\varphi)$ accumulate on the line segments joining the jumps of $\varphi$. These eigenvalues are more sparsely distributed than the $\sim n$ eigenvalues inside the range of $\varphi$ that contribute to the leading order term in (1.6). Further analysis with the help of lower order asymptotics for Toeplitz determinants is conducted in [21], see also references therein. To conclude this short review on asymptotic formulae for Toeplitz matrices let us remark that multi-dimensional analogues of Szegő's strong limit theorem have been obtained as well, see [17, 26, 34, 46, 57, 60, 76].

In this thesis, our interest is closer to the continuous analogue of Toeplitz matrices, which we introduce in the following. Consider now a bounded and (infinitesimally) translation-invariant operator $A$ on $L^2(\mathbb{R}^d)$, $d \geq 1$. In other words, let $A$ be a Fourier multiplier

$$A = A(a) := \mathcal{F}^* a \mathcal{F}$$

with a bounded and complex-valued *symbol* $a \in L^\infty(\mathbb{R}^d)$. Here, the Fourier transform $\mathcal{F}$ is chosen to be unitary on $L^2(\mathbb{R}^d)$, i.e.

$$(\mathcal{F}f)(\xi) := (2\pi)^{-d/2} \int dx \, e^{-ix\cdot\xi} f(x), \ \xi \in \mathbb{R}^d,$$

for Schwartz functions $f \in \mathcal{S}(\mathbb{R}^d)$. For any measurable set $\Omega \subseteq \mathbb{R}^d$, introduce the spatial restriction of the operator $A$ onto $\Omega$,

$$A_\Omega = A_\Omega(a) := \chi_\Omega \mathcal{F}^* a \mathcal{F} \chi_\Omega,$$

where $\chi_\Omega$ denotes the characteristic function for the set $\Omega$ and both $\chi_\Omega$ and $a$ are interpreted as multiplication operators on $\mathrm{L}^2(\mathbb{R}^d)$. Throughout this thesis, the variable $L \geq 1$ is used as a scaling parameter and

$$\Omega_L := L \cdot \Omega$$

denotes the scaled version of the set $\Omega$. If $d = 1$ and $\Omega = I \subset \mathbb{R}$ is a finite interval, then the operator $A_{I_L}$ is the continuous analogue of a one-dimensional Toeplitz matrix, where the scaling of the interval $I$ corresponds to increasing the size $n$ of the Toeplitz matrix. Such an operator $A_{I_L}$ is sometimes called *truncated Wiener–Hopf operator* because of its close relation to the Wiener–Hopf operator

$$W(a) := A_{[0,\infty)}(a) = \chi_{[0,\infty)} \mathcal{F}^* a \mathcal{F} \chi_{[0,\infty)}. \tag{1.7}$$

It is not difficult to prove that the operator $A_{\Omega_L}$ is trace class if the set $\Omega \subset \mathbb{R}^d$ is bounded and the symbol $a$ is integrable, see Lemma 2.9. This property transfers to operators $h(A_{\Omega_L})$ if the function $h$ is sufficiently regular and satisfies $h(0) = 0$.

Determinant and trace asymptotics for truncated Wiener–Hopf operators come with no surprises with the knowledge about the results in the discrete case. Again, the exact form of the asymptotic formulae depends on the regularity of the symbol. A continuous version of Szegő's strong limit theorem for one-dimensional truncated Wiener–Hopf operators was first established by Kac in [33]. Using different methods, Widom later proved a two-term trace formula for Wiener-Hopf operators with sufficiently regular symbols: for the sake of discussion, assume that the symbol $a$ is smooth and integrable and the test function $h : \mathbb{C} \to \mathbb{C}$ is entire with $h(0) = 0$. Then [82] contains the asymptotics

$$\operatorname{tr} h(A_{I_L}(a)) = L|I|\mathcal{B}_1(h, a) + \mathcal{B}_0(h, a) + o(1), \tag{1.8}$$

as $L \to \infty$. Here, the leading-order coefficient is

$$\mathcal{B}_1(h, a) := \frac{1}{2\pi} \int d\xi (h \circ a)(\xi),$$

and the constant

$$\mathcal{B}_0(h,a) := 2\,\mathrm{tr}\left[h(W(a)) - W(h\circ a)\right]$$

is given in terms of Wiener–Hopf operators on the half-line, but also has an explicit integral representation. Clearly, the formula (1.8) is the exact continuous analogue of (1.6) for smooth symbols, compare, in particular, the leading order coefficients. Again, if one assumes that the symbol $a$ is real-valued, and hence $A_{I_L}$ is self-adjoint, the asymptotics (1.8) extend to sufficiently regular test functions $h : \mathbb{R} \to \mathbb{C}$. As in the Toeplitz case, jump discontinuities of the symbol $a$ create an additional term of logarithmic order in the trace asymptotics. Let, for instance, $a = \chi_J$ be the characteristic function for a finite interval $J \subset \mathbb{R}$, and suppose that the test-function $h$ is (piecewise) continuous on $[0,1]$, differentiable at $t = 0$ and $t = 1$, and satisfies $h(0) = 0$. Then the results of [41] and [81] imply the asymptotic formula

$$\mathrm{tr}\,h(A_{I_L}(\chi_J)) = \frac{L}{2\pi}h(1)|I||J| + \log(L)\mathcal{W}(h) + o(\log(L)),\ L\to\infty, \tag{1.9}$$

with the coefficient

$$\mathcal{W}(h) := \frac{1}{\pi^2}\int_0^1 dt\,\frac{[h(t) - th(1)]}{t(1-t)}, \tag{1.10}$$

which is independent of the intervals $I$ and $J$. Notice that in this case the symbol of $A$ is supported on the set $\{0,1\}$ and, thus, the spectrum of $A_{I_L}(\chi_J)$ is contained in the interval $[0,1]$. Looking at (1.9), the leading order term captures the $\sim L$ eigenvalues of $A_{I_L}(\chi_J)$ close to 1, whereas the sub-leading order term describes the distribution of the $\sim\log(L)$ eigenvalues in every interval $(\epsilon, 1-\epsilon)$ for $\epsilon > 0$. The eigenvalues close to 0 do not show up in the asymptotics since we require $h(0) = 0$ to gain a trace class operator $h(A_{I_L}(\chi_J))$. Note also that $\mathcal{B}_1(h,\chi_J) = \frac{h(1)}{2\pi}|J|$, i.e. the leading order term in (1.9) is the same as in (1.8).

The trace asymptotics (1.8) and (1.9) have extensions to dimensions $d \geq 2$, in which the geometry of the truncation set starts to play an essential role. Let us first describe the results in the case of a smooth symbol. For simplicity, assume that $a$ belongs to the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ and $h$ is an entire function with $h(0) = 0$. If $\Omega \subset \mathbb{R}^d$ is a set with smooth boundary $\partial\Omega$, then [83] provides a complete asymptotic expansion for

$$\mathrm{tr}\,h(A_{\Omega_L}) \tag{1.11}$$

as $L \to \infty$, see also [15]. More precisely, for any $K \geq -d$ there exist constants $\mathcal{B}_j = \mathcal{B}_j(\Omega, h, a)$ such that

$$\operatorname{tr} h(A_{\Omega_L}) = \sum_{j=-K}^{d} L^j \mathcal{B}_j + o(L^{-K}), \tag{1.12}$$

as $L \to \infty$. While

$$\mathcal{B}_d = \frac{|\Omega|}{(2\pi)^d} \int_{\mathbb{R}^d} d\xi \, (h \circ a)(\xi) \tag{1.13}$$

only depends on $\Omega$ through its volume $|\Omega|$, the coefficients $\mathcal{B}_j$ for $j \leq d-1$ contain geometric information on the boundary $\partial\Omega$: $\mathcal{B}_{d-1}$ arises from a hyperplane approximation at each point of $\partial\Omega$ and $\mathcal{B}_{d-2}$ contains the curvature and the second fundamental form of $\partial\Omega$, see also [58]. As a general principle, the coefficient $\mathcal{B}_{d-k}$ depends on $C^k$-attributes of $\partial\Omega$; more precise formulae in terms of the geometric content are collected in [59]. On the other hand, if the symbol $a$ has jump discontinuities, for instance $a = \chi_\Lambda$ for some bounded set $\Lambda \subset \mathbb{R}^d$ with sufficiently smooth boundary, then only a two-term asymptotic formula for the trace (1.11) is known, where again the leading order term remains unchanged and the subleading order term gets enhanced to order $L^{d-1}\log(L)$. This result has been obtained quite recently, see [63, 64]; further extension to non-smooth functions $h$ was done in [44, 66, 67].

The increased recent interest in trace asymptotics for (multi-dimensional) Wiener–Hopf operators with possibly non-smooth test functions $h$ is partly due to their connection with the study of the *bipartite entanglement entropy (EE)*, see e.g. [31, 32, 44, 45]. The (bipartite) EE is a quantifier for the non-classical correlations between two subsystems of a quantum system. We refer to the general reviews [1, 16, 19, 40, 42] on the importance of the EE in the study of black holes, condensed matter systems and quantum information theory. For a gas of free fermions, the EE with respect to a bipartition of position space may be calculated via the corresponding one-particle Hamiltonian $H$. In the following, we will always assume $H$ to be a self-adjoint operator on $\mathrm{L}^2(\mathbb{R}^d)$, which corresponds to considering the Fermi gas in the thermodynamic limit. At zero temperature, the *Von Neumann* EE with respect to the bipartition into the set $\Omega_L \subset \mathbb{R}^d$ and its complement is given by

$$\operatorname{tr} \eta_1\big(\chi_{\Omega_L} \chi_{(-\infty,\mu]}(H) \chi_{\Omega_L}\big), \tag{1.14}$$

where $\mu \in \mathbb{R}$ denotes the *Fermi energy* and

$$\eta_1(t) := -t\log t - (1-t)\log(1-t),\ t \in [0,1], \tag{1.15}$$

see [31, 38]. If the one-particle Hamiltonian $H$ is (formally) a function of the momentum operator, the trace (1.14) may be rewritten in terms of truncated Wiener–Hopf operators. In particular, for $H = -\Delta$, the Von Neumann EE is given by

$$\operatorname{tr} \eta_1\big(A_{\Omega_L}(\chi_\Lambda)\big), \tag{1.16}$$

with $\Lambda \subset \mathbb{R}^d$ denoting the *Fermi sea* $\Lambda = \Lambda(\mu) = \{\xi \in \mathbb{R}^d : |\xi|^2 \le \mu\}$. Notice that the function $\eta_1$ is smooth on $(0,1)$ but not differentiable at the endpoints of the interval $[0,1]$. Moreover, let us mention that $\eta_1$ is just one representative of the family

$$\eta_\gamma(t) := \frac{1}{1-\gamma}\log\left[t^\gamma + (1-t)^\gamma\right],\ t \in [0,1], \tag{1.17}$$

with $\gamma > 0$, where $\eta_1$ is defined as the point-wise limit of $\eta_\gamma$ as $\gamma \to 1$, $\gamma \neq 1$. Replacing $\eta_1$ by $\eta_\gamma$ in (1.14) or (1.16) one obtains the more general $\gamma$-*Rényi* EE, see e.g. [44]. Since $\eta_\gamma \circ \chi_\Lambda \equiv 0$, the leading order coefficient in the asymptotics of (1.16) vanishes, see (1.13) for its definition. Thus, the EE (for $H = -\Delta$ and $\mu > 0$) behaves — because of the discontinuous symbol $\chi_\Lambda$ — like $L^{d-1}\log(L)$, as $L \to \infty$. If one instead looks at a free Fermi gas at positive temperature $T$, again with one-particle Hamiltonian $H = -\Delta$, then the symbol $\chi_\Lambda$ in (1.16) is replaced by the smooth function

$$a(\xi) = \left[1 + \exp\Big(\frac{|\xi|^2 - \mu}{T}\Big)\right]^{-1},$$

see [38, 45]. Thus, the asymptotics of the type (1.12) apply, see [68] for their extension to non-smooth test functions.

In accordance with the above, it is justified to call an asymptotic trace formula a *formula of Szegő type* if it describes the scaling asymptotics of

$$\operatorname{tr} h\big(A_{\Omega_L}\big) \tag{1.18}$$

or

$$\operatorname{tr} h\big(\chi_{\Omega_L} a(H) \chi_{\Omega_L}\big), \tag{1.19}$$

for a fixed class of test-functions $h$, a bounded function $a \in \mathrm{L}^\infty(\mathbb{R})$, a set $\Omega \subset \mathbb{R}^d$, and a self-adjoint operator $H$ on $\mathrm{L}^2(\mathbb{R}^d)$. In the context of the EE, the asymptotics of (1.19) have been studied especially for (random) ergodic Hamiltonians $H$, see

[25, 29, 37, 51, 52]. Here, the authors mostly worked in the spectrally localised regime, which corresponds to a fast decaying kernel of the spectral projection $\chi_{(-\infty,\mu]}(H)$. In this sense, the operator $\chi_{(-\infty,\mu]}(H)$ behaves similarly to a Fourier multiplier with smooth symbol even though it has less symmetries. As a consequence, the bipartite EE for fermions in a disordered $d$-dimensional medium obeys (when averaged over the randomness) an *area law* at zero temperature, see [29]. This means that the EE behaves to leading order like $L^{d-1}$ (the area of $\partial\Omega_L$). In contrast, in the homogeneous case $H = -\Delta$, the area law is violated: the EE at zero temperature is proportional to $L^{d-1}\log L$, as it was mentioned above.

In this thesis, we consider two problems related to Szegő-type trace asymptotics. As a first topic, we are interested in trace asymptotics for truncated Wiener–Hopf operators, i.e. the asymptotics of (1.18), for smooth symbols $a$ but for a set $\Omega$ with non-smooth boundary. Let us give a review on the known results in this specific context. As before, assume that $a \in \mathcal{S}(\mathbb{R}^d)$ and that $h$ is an entire function with $h(0) = 0$. In [77], the author dealt with polytopes $\Omega$ and proved a two-term asymptotic expansion of the trace (1.18). Recently, this result was extended to a larger class of domains, see [68]. Namely, let $\Omega$ be a bounded Lipschitz region with piecewise $\mathrm{C}^1$-boundary. Then [68] contains the asymptotics

$$\operatorname{tr} h(A_{\Omega_L}) = L^d \mathcal{B}_d + L^{d-1}\mathcal{B}_{d-1} + o(L^{d-1}), \tag{1.20}$$

as $L \to \infty$, where the coefficients $\mathcal{B}_j = \mathcal{B}_j(\Omega, h, a)$, $j = d, d-1$, are given via the same formulae as in the smooth boundary case. The coefficient $\mathcal{B}_d$ agrees with (1.13) and a formula for $\mathcal{B}_{d-1}$ can be found, for instance, in [58, Thm. 1.1]. In particular, one observes that the edges (or if $d = 2$ the corners) of $\Omega$ do not enter the trace asymptotics up to order $L^{d-1}$. In the special case of cubes $\Omega$, [25, Thm. 2.2] actually implies complete asymptotics for (1.18), consisting of $d + 1$ terms. However, the latter result is established in the more general framework of $\mathbb{Z}^d$-ergodic operators. This entails an exclusively abstract formulation of the asymptotic coefficients, which makes it difficult to relate them to the smooth boundary case. In addition, [25, Thm. 2.2] makes for the Wiener–Hopf case unnecessary symmetry assumptions; for instance, it is applicable to radially symmetric symbols $a$. Within the context of our discussion, let us also mention the works [48, 49], which identify the limits of norms of inverses and the limits of pseudospectra for Wiener–Hopf operators on convex polytopes $\Omega_L$ as $L \to \infty$.

Similar results have been obtained in the discrete setting, where $A_{\Omega_L}$ is replaced by the $d$-dimensional Toeplitz matrix $T_{\Lambda_L}$, which is the restriction of a $d$-dimensional Laurent matrix to the scaled lattice subset $\Lambda_L \subset \mathbb{Z}^d$. For polytopes $\Lambda$, the work [26] provides a two-term asymptotic formula for $\operatorname{tr} h(T_{\Lambda_L})$, analogous to the result in [77]. When $\Lambda$ is a cuboid, the authors of [60] and [76] proved a $(d+1)$-term asymptotic formula for $\operatorname{tr} h(T_{\Lambda_L})$, under the additional assumption that the symbol of the Toeplitz matrix allows for a specific factorisation. In [34] these results were recovered and further insights were given on the inverses of Toeplitz matrices on convex polytopes. Moreover, the recent work [57] treats triangles $\Lambda \subset \mathbb{Z}^2$ and provides a two-term asymptotic formula for $\operatorname{tr} L_\Lambda^{-1}$ with a new formula for the sub-leading coefficient.

The objective of the first part of this thesis, which is based on the paper [53], is to investigate further the term of order $L^{d-2}$ in (1.20). To this end, we restrict ourselves to dimension $d = 2$ and deal with the case when $\Omega = \mathscr{P} \subset \mathbb{R}^2$ is the interior of a polygon. By the latter we mean that $\mathscr{P}$ is bounded and $\partial\mathscr{P}$ is the finite disjoint union of piecewise linear, closed curves; we do not require $\mathscr{P}$ to be (simply) connected or convex. In particular, and in contrast to all previous works on the complete asymptotics of (1.18), we deal with corners of any angle. For a smooth, sufficiently decaying symbol $a$ and entire test functions $h$, we obtain complete asymptotics for the trace $\operatorname{tr} h(A_{\mathscr{P}_L})$, consisting of three terms, see Theorem 2.1. More precisely, we provide constants $\mathrm{c}_j = \mathrm{c}_j(\mathscr{P}, h, a)$ such that

$$\operatorname{tr} h(A_{\mathscr{P}_L}) = L^2 \mathrm{c}_2 + L \mathrm{c}_1 + \mathrm{c}_0 + \mathcal{O}(L^{-\infty}), \tag{1.21}$$

as $L \to \infty$. As it can be inferred from formula (1.20), the coefficient $\mathrm{c}_2$ incorporates the area of the polygon $\mathscr{P}$ and $\mathrm{c}_1$ depends on the lengths of its edges and their directions. However, our main focus is the constant order coefficient $\mathrm{c}_0$, which contains contributions from each corner of the polygon. In Theorem 2.1 we provide a formula for $\mathrm{c}_0$ given in terms of abstract traces, similarly to [25, Thm. 2.2]. Yet, in the polygon case $\mathrm{c}_0$ includes additional terms due to the presence of non-parallel edges. Furthermore, we compute $\mathrm{c}_0$ explicitly as a function of the polygon's interior angles for radially symmetric symbols $a$ and quadratic test functions $h$, see Theorem 2.5. As a consequence, one can compare $\mathrm{c}_0$ with the corresponding coefficient in the smooth boundary case and we obtain the following result: for a two-dimensional domain $\Omega$, one can determine from the constant order term of the trace asymptotics (1.20) whether $\Omega$ has a smooth boundary or it is a polygon, see Corollary 2.7. In addition, the coefficient $\mathrm{c}_0$ for the polygon $\mathscr{P}$ can not be obtained from (1.12) via approximation of $\mathscr{P}$ by domains with smooth boundary. This anomaly resembles the analogous result for the constant order term in the heat trace asymptotics for the Dirichlet Laplacian on a two-dimensional domain with corners, see [50].

In the second part of the thesis, we present formulae of Szegő type for the periodic Schrödinger operator in dimension one. This part is based on the paper [54], which emerged from a collaboration with Alexander V. Sobolev. For the sequel, set

$$H := -\frac{d^2}{dx^2} + V(x), \ \mathrm{dom}(H) = \mathrm{H}^2(\mathbb{R}), \tag{1.22}$$

where $V$ is a real-valued periodic $\mathrm{L}^2_{\mathrm{loc}}$- function, so that the operator $H$ is self-adjoint on $\mathrm{H}^2(\mathbb{R})$. Without loss of generality, we will assume that the period equals $2\pi$. The spectrum $\sigma(H)$ of the operator $H$ is known to be absolutely continuous. Moreover, it is the union of infinitely many spectral bands (closed intervals), and, generically, it has infinitely many gaps, see e.g. [55]. We introduce the notation $P_\mu := \chi_{(-\infty,\mu)}(H) = \chi_{(-\infty,\mu]}(H)$ for the spectral projection of $H$ associated with the interval $(-\infty, \mu)$. Referring to (1.19), obtaining Szegő-type trace asymptotics for the operator $H$ amounts to studying the trace of operators

$$h\big(\chi_{I_L} a(H) \chi_{I_L}\big),$$

where $I \subset \mathbb{R}$ is, say, a finite interval and $a$, $h$ are suitably chosen functions. Having the application to the EE in mind, we focus on the case $a = \chi_{(-\infty,\mu)}$, compare with (1.14). Moreover, we choose without loss of generality a symmetric interval $I = (-1, 1)$, i.e. we obtain an asymptotic formula for the trace

$$\operatorname{tr} h(B_{L,\mu}), \ B_{L,\mu} := \chi_{(-L,L)} P_\mu \chi_{(-L,L)}, \tag{1.23}$$

as $L \to \infty$. We only require the test-function $h : [0, 1] \to \mathbb{C}$ to be piecewise continuous and Hölder continuous at the points 0 and 1, which allows us to deal with functions like $\eta_1$ and $\eta_\gamma$, see (1.15), (1.17). Moreover, we assume that the potential $V$ is smooth, even though this condition may be relaxed up to $\mathrm{L}^2_{\mathrm{loc}}$ by requiring slightly more regularity for $h$. Under these assumptions, the asymptotic formula for (1.23) crucially depends on the position of the parameter $\mu$ with respect to the spectrum of $H$. If $\mu \in \big(\sigma(H)\big)^\circ$, we prove that

$$\operatorname{tr} h(B_{L,\mu}) = 2Lh(1)N(\mu, H) + \log(L)\mathcal{W}(h) + o(\log(L)), \tag{1.24}$$

as $L \to \infty$, where $N(\mu, H)$ denotes the integrated density of states for the operator $H$ and $\mathcal{W}(h)$ is defined in (1.10). In the special case $V \equiv 0$, formula (1.24) reduces to (1.9) with $J = (-\sqrt{\mu}, \sqrt{\mu})$. In this sense, (1.24) can be seen as an extension of (1.9). Remarkably, the sub-leading order term in (1.24) is actually independent of the potential $V$ and $\mu$, as long as $\mu$ remains an interior point of the spectrum. In contrast, the leading order term in (1.24) depends on both the potential $V$ and the parameter $\mu$. In other words, for $\mu \in \big(\sigma(H)\big)^\circ$ the number of eigenvalues of $B_{L,\mu}$ close to 1 depends crucially on the potential, while the eigenvalue distribution on an interval $(\epsilon, 1-\epsilon)$ for $\epsilon > 0$ is to leading order independent of $V$. If $\mu \notin \big(\sigma(H)\big)^\circ$, then we prove the formula

$$\operatorname{tr} h(B_{L,\mu}) = 2Lh(1)N(\mu, H) + \mathcal{O}(1), \tag{1.25}$$

as $L \to \infty$. Thus, in this case the sub-leading order remains bounded. These two different behaviours depending on the placement of $\mu$ are due to the respective spatial decay of the kernel of the spectral projection $P_\mu$. While the decay is slow when $\mu \in \big(\sigma(H)\big)^\circ$, the kernel of $P_\mu$ decays super-polynomially away from the diagonal when $\mu \notin \big(\sigma(H)\big)^\circ$. In the first case, the operator $P_\mu$ is somewhat comparable to a Fourier multiplier with discontinuous symbol, while in the second case we are in a similar regime as in the works [25, 29, 37, 52] mentioned before.

Formulae (1.24) and (1.25) imply the following behaviour of the bipartite EE for a one-dimensional free Fermi gas in a periodic external field at zero temperature. Let us, for instance, consider the Von Neumann EE with respect to the splitting $\mathbb{R} = (-L, L) \cup \big(\mathbb{R} \setminus (-L, L)\big)$. For $h = \eta_1$, see (1.15), the leading order term in (1.24) and (1.25) vanishes as usual. Thus, if $\mu \notin \big(\sigma(H)\big)^\circ$, then the EE remains bounded, as $L \to \infty$, i.e the EE satisfies an area law. However, if $\mu \in \big(\sigma(H)\big)^\circ$, then the EE grows logarithmically, like in the unperturbed case $V \equiv 0$. To the author's knowledge, this is the first instance where a violation of the area law could be proved when the one-particle Hamiltonian is a Schrödinger operator with non-trivial potential.

A few remarks on the structure of this thesis are in order. The first part concerns the Szegő-type trace asymptotics for truncated Wiener–Hopf operators on polygons, see Chapter 2. We start by formulating our main results: Theorems 2.1 and 2.3 state the asymptotics (1.21) with various formulae for the coefficients $\mathrm{c}_j$ and Theorem 2.5 deals with the radially symmetric case. The trace norm estimates that enter the proofs of Theorems 2.1 and 2.3 are collected in Section 2.2. In Section 2.3 we apply these trace norm bounds to extract the leading order term of the asymptotics (1.21). Moreover, we reduce the remaining part to individual corner contributions, which only depend on the corner angle and the lengths and directions of the enclosing edges. The trace asymptotics corresponding to a single corner of the polygon are provided in Section 2.4, which completes the proof of Theorem 2.1. The proofs of Theorems 2.3 and 2.5 can be found in Sections 2.5 and 2.6.

In the second part of the thesis, we deal with the proof of the formulae of Szegő type (1.24) and (1.25) for the periodic Schrödinger operator in dimension one. In Chapter 3 we introduce fundamental properties of such Schrödinger operators and develop a convenient formalism for Bloch eigenvalues and eigenfunctions. This allows us to write out the kernel of the spectral projection, see Section 3.2. Chapter 4 contains the actual proof of our results, which are summarised in Theorem 4.2. To begin with, an approximation of the kernel of the spectral projection $P_\mu$ in terms of Bloch eigenfunctions corresponding to the Fermi energy $\mu$ is given in Section 4.3. Section 4.4 contains some elementary trace class estimates, similar to the ones obtained in [41]. Here we also introduce an averaging procedure for integral operators that involve almost-periodic functions, see Subsection 4.4.3. For the logarithmic term in the trace asymptotic, this can be used to average out the precise dependence on the Bloch eigenfunctions at the Fermi energy $\mu$. As a consequence, we are able to prove Theorem 4.2 for polynomial functions $h$, see Section 4.6. The extension to non-smooth functions calls for more advanced bounds in Schatten-von Neumann classes, which are collected in Section 4.5. Finally, the closure of the asymptotics from the polynomial $h$, is implemented in Section 4.7.

To conclude the introduction, let us fix some general notation that will be applied throughout the thesis. 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 will always be independent of the scaling parameter $L$, but it may depend on the test function $h$, the symbol $a$, the geometry of the polygon $\mathscr{P}$, and the periodic potential $V$. To avoid confusion we will comment on its explicit dependence whenever necessary. We make use of the standard notation for Schatten-von Neumann classes $\mathfrak{S}_p$ for $p > 0$, see e.g. [7], [62]. A compact operator $T$ is an element of $\mathfrak{S}_p$ if and only if its singular values $\{s_k(T)\}_{k=1}^{\infty}$ are $p$-summable, that is

$$\|T\|_p^p := \sum_{k=1}^{\infty} s_k(T)^p < \infty. \tag{1.26}$$

For a set $\Omega \subset \mathbb{R}^d$, we denote by $\Omega^\circ$ the set of interior points, by $|\Omega|$ the ($d$-dimensional) Lebesgue measure, and by $\sharp\Omega$ the cardinality. For $x, y \in \mathbb{R}^d$, we use the notation $\langle x \rangle := (1 + |x|^2)^{1/2}$, where $|\cdot|$ is the standard Euclidean norm, and we write $x \cdot y$ for the scalar product of the vectors $x$ and $y$. Moreover, $Q_x$ denotes the (closed) unit cube centred at $x$ and $B_r(x)$ is the (closed) ball of radius $r > 0$ around $x$ (with respect to $|\cdot|$). In many situation (e.g. for the intervals $I$, $J$, $K$ in Section 4.4) it will not matter whether the considered intervals are open, semi-open or closed. Whenever this is the case, we shall use open intervals only.

CHAPTER 2

# A Szegő Limit Theorem for Translation-invariant Operators on Polygons

Let $\mathscr{P} \subset \mathbb{R}^2$ be (the interior of) a polygon as specified in the introduction and consider a (bounded) Fourier multiplier $A = \mathcal{F}^* a \mathcal{F}$ on $\mathrm{L}^2(\mathbb{R}^2)$. In this chapter, we obtain full trace asymptotics for the operator $h\big(A_{\mathscr{P}_L}\big)$ for a smooth, sufficiently decaying symbol $a : \mathbb{R}^2 \to \mathbb{C}$ and entire test functions $h : \mathbb{C} \to \mathbb{C}$ with $h(0) = 0$. As it was mentioned in the introduction, this chapter is in many parts identical with the publication [53]. We start by formulating our main results, that is the formula (1.21) with various formulae for the coefficients $\mathrm{c}_j = \mathrm{c}_j(\mathscr{P}, h, a)$.

## 2.1. Results

Let $h : \mathbb{C} \to \mathbb{C}$ be an entire function with $h(0) = 0$ and consider a symbol $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$, see (2.30) for the definition. In order to write out the formulae for the coefficients in (1.21) we need to fix some notation for the polygon $\mathscr{P}$.

**2.1.1. Notation for the polygon $\mathscr{P}$ and coefficients in the asymptotics.** Let $\Xi(\mathscr{P}) \subset \mathbb{R}^2$ denote the set of vertices of $\mathscr{P}$ and $\mathcal{E}(\mathscr{P})$ the set of edges of $\mathscr{P}$. In the following, we specify the contribution of each edge $E \in \mathcal{E}(\mathscr{P})$ and each corner at $X \in \Xi(\mathscr{P})$ to the asymptotics (1.21).

First, fix an edge $E \in \mathcal{E}(\mathscr{P})$. Let $\nu_E$ be its inward pointing unit normal vector, and let $\tau_E$ be the unit tangent vector such that the frame $(\tau_E, \nu_E)$ has the standard orientation in $\mathbb{R}^2$. This induces an orientation on $\partial\mathscr{P}$. Introduce the half-space

$$\mathscr{H}_E := \{y \in \mathbb{R}^2 : y \cdot \nu_E \geq 0\}, \tag{2.1}$$

and the semi-infinite strip of unit width,

$$S_E := \{t\tau_E + \xi\nu_E : (t, \xi) \in [0,1] \times [0, \infty)\} \subset \mathscr{H}_E. \tag{2.2}$$

We label the interior angles between $E$ and its adjacent edges by $\gamma_E^{(1)}$ and $\gamma_E^{(2)}$. For definiteness, the enumeration is chosen in accordance with the orientation of $\partial\mathscr{P}$.

However, the latter is not of much relevance as we will mainly be interested in a symmetric function of the angles, $F : \mathcal{E}(\mathscr{P}) \to \mathbb{R}$,

$$F(E) := -\cot(\gamma_E^{(1)}) - \cot(\gamma_E^{(2)}). \tag{2.3}$$

Note that $F(E) = 0$ if and only if $\gamma_E^{(1)} + \gamma_E^{(2)} \in \{\pi, 2\pi, 3\pi\}$, i.e. if and only if the edges adjacent to $E$ are parallel. Define also the function

$$h_1(z) := h(z) - zh'(0). \tag{2.4}$$

Then we introduce the following coefficients corresponding to the edge $E$, which are finite under our assumptions on $h$ and $a$, see also Theorem 2.1. We set

$$\mathrm{a}_1(\nu_E) := \operatorname{tr}\big(\chi_{S_E}\big[h_1(A_{\mathscr{H}_E}) - h_1(A)\big]\big), \tag{2.5}$$

with $S_E$ and $\mathscr{H}_E$ as in (2.1), (2.2). Note that the strip $S_E$ on the right-hand side of (2.5) may actually be shifted along the edge $E$, leaving the value of $\mathrm{a}_1(\nu_E)$ unchanged since the operator $h_1(A_{\mathscr{H}_E}) - h_1(A)$ is translation-invariant in the direction $\tau_E$. Similarly, we define the coefficient

$$\mathrm{a}_0(\nu_E) := \operatorname{tr}\big(\chi_{S_E} M(x \cdot \nu_E)\big[h_1(A_{\mathscr{H}_E}) - h_1(A)\big]\big), \tag{2.6}$$

where $M(x \cdot \nu_E)$ is the multiplication operator

$$[M(x \cdot \nu_E) f](x) := (x \cdot \nu_E) f(x),$$

for any function $f : \mathbb{R} \to \mathbb{C}$. Clearly, also the operator $M(x \cdot \nu_E)\big[h_1(A_{\mathscr{H}_E}) - h_1(A)\big]$ is invariant with respect to translations along the edge $E$.

Fix now a vertex $X \in \Xi(\mathscr{P})$. Its adjacent edges are named $E^{(1)}(X)$ and $E^{(2)}(X)$, where the enumeration is again chosen according to the orientation of $\partial\mathscr{P}$. Corresponding to the vertex $X$ we have the two half-spaces

$$\mathscr{H}^{(j)}(X) := \mathscr{H}_{E^{(j)}(X)},\ j = 1, 2, \tag{2.7}$$

compare with (2.1). Moreover, let $\gamma_X \in (0, \pi) \cup (\pi, 2\pi)$ denote the interior angle at $X$. In the following, we distinguish convex and concave corners of the polygon, employing the notation

$$\Xi_{\lessgtr}(\mathscr{P}) := \{X \in \Xi(\mathscr{P}) : \gamma_X \lessgtr \pi\}.$$

Define the semi-infinite sector that models the corner at $X \in \Xi(\mathscr{P})$ by

$$\mathscr{C}(X) := \begin{cases} \mathscr{H}^{(1)}(X) \cap \mathscr{H}^{(2)}(X), & X \in \Xi_<(\mathscr{P}), \\ \mathscr{H}^{(1)}(X) \cup \mathscr{H}^{(2)}(X), & X \in \Xi_>(\mathscr{P}). \end{cases} \tag{2.8}$$

If $X \in \Xi_<(\mathscr{P})$, the corner at $X \in \Xi(\mathscr{P})$ or equivalently the sector $\mathscr{C}(X)$ is *convex*, otherwise we call it *concave*. We are now ready to introduce coefficients corresponding to vertices $X \in \Xi(\mathscr{P})$.

If $X \in \Xi_<(\mathscr{P})$, we define

$$\mathrm{b}_0(X) := \operatorname{tr}\left(\chi_{\mathscr{C}(X)}\left[h_1(A_{\mathscr{C}(X)}) - h_1(A_{\mathscr{H}^{(1)}(X)}) - h_1(A_{\mathscr{H}^{(2)}(X)}) + h_1(A)\right]\right), \tag{2.9}$$

with $\mathscr{C}(X)$ and $\mathscr{H}^{(j)}(X)$, $j = 1, 2$, defined in (2.8) and (2.7), respectively.

If $X \in \Xi_>(\mathscr{P})$, we set

$$\begin{aligned} \mathrm{b}_0(X) := \operatorname{tr}&\left(\chi_{\mathscr{H}^{(1)}(X)\cap\mathscr{H}^{(2)}(X)}\left[h_1(A_{\mathscr{C}(X)}) - h_1(A)\right]\right) \\ &+ \operatorname{tr}\left(\chi_{\mathscr{C}(X)\setminus\mathscr{H}^{(1)}(X)}\left[h_1(A_{\mathscr{C}(X)}) - h_1(A_{\mathscr{H}^{(2)}(X)})\right]\right) \\ &+ \operatorname{tr}\left(\chi_{\mathscr{C}(X)\setminus\mathscr{H}^{(2)}(X)}\left[h_1(A_{\mathscr{C}(X)}) - h_1(A_{\mathscr{H}^{(1)}(X)})\right]\right). \end{aligned} \tag{2.10}$$

**2.1.2. Main result.** Our first and main theorem of this chapter provides a complete asymptotic expansion of $\operatorname{tr} h(A_{\mathscr{P}_L})$ and contains formulae for all the coefficients in (1.21).

**Theorem 2.1.** *Assume that $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$, see (2.30), and let $h : \mathbb{C} \to \mathbb{C}$ be an entire function with $h(0) = 0$. Then we have the asymptotic formula*

$$\operatorname{tr} h(A_{\mathscr{P}_L}) = L^2 \mathrm{c}_2 + L\mathrm{c}_1 + \mathrm{c}_0 + \mathcal{O}(L^{-\infty}), \tag{2.11}$$

*as $L \to \infty$, with coefficients*

$$\begin{aligned} \mathrm{c}_2 &= \frac{|\mathscr{P}|}{4\pi^2} \int_{\mathbb{R}^2} d\xi\, (h \circ a)(\xi) \\ \mathrm{c}_1 &= \sum_{E \in \mathcal{E}(\mathscr{P})} |E|\, \mathrm{a}_1(\nu_E), \\ \mathrm{c}_0 &= \sum_{E \in \mathcal{E}(\mathscr{P})} F(E)\, \mathrm{a}_0(\nu_E) + \sum_{X \in \Xi(\mathscr{P})} \mathrm{b}_0(X). \end{aligned}$$

*In particular, for all $E \in \mathcal{E}(\mathscr{P})$ and $X \in \Xi(\mathscr{P})$, the coefficients $\mathrm{a}_1(\nu_E)$, $\mathrm{a}_0(\nu_E)$, and $\mathrm{b}_0(X)$ are well-defined, see Subsection 2.1.1 for their definition.*

**Remark 2.2.** (1) The super-polynomial error in formula (2.11) is a consequence of both the smoothness of the symbol $a$ and the piecewise-straight boundary of $\mathscr{P}$. That a smooth symbol leads to the absence of all but two terms in the trace asymptotics for one-dimensional truncated Wiener–Hopf or Toeplitz operators has been known for a long time, see [9, p. 120].

(2) Formula (1.20) implies that the corners of the polygon do not affect the two leading coefficients in the asymptotics compared to the smooth boundary case. However, the above formula for $\mathrm{c}_0$ shows that the corners do enter the trace asymptotics at the constant order.

(3) An edge $E \in \mathcal{E}(\mathscr{P})$ does not contribute to the coefficient $\mathrm{c}_0$ if $F(E) = 0$, i.e. if the edges adjacent to $E$ are parallel, see also (2.3). In particular, all contributions from the edges to $\mathrm{c}_0$ vanish if, for instance, $\mathscr{P}$ is a parallelogram. As it becomes clear from the proof of the theorem, the edge contributions to $\mathrm{c}_0$ are in fact aggregated local contributions from corners of $\mathscr{P}$.

(4) We emphasise that the coefficients $\mathrm{b}_0(X)$ are defined by the two distinct formulae (2.9) and (2.10), depending on the type of the corner at $X \in \Xi(\mathscr{P})$.

The coefficients $\mathrm{a}_1(\nu_E)$ and $\mathrm{a}_0(\nu_E)$, which only depend on the half-space operators $h(A_{\mathscr{H}_E})$ and the full-space operator $h(A)$, may be rewritten in terms of one-dimensional Wiener–Hopf operators. This is the content of the next theorem. Here, we recall the notation

$$W(a) = A_{[0,\infty)}(a),$$

for $a \in \mathrm{L}^\infty(\mathbb{R})$, see (1.7). As anticipated, the formula (2.15) for $\mathrm{c}_1$ reduces the corresponding formula from the smooth boundary case, see [80, Thm.].

**Theorem 2.3.** *Let $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ and let $h : \mathbb{C} \to \mathbb{C}$ be an entire function with $h(0) = 0$. Define, for $E \in \mathcal{E}(\mathscr{P})$ and $t \in \mathbb{R}$, the family of one-dimensional symbols*

$$\mathbb{R} \ni \xi \mapsto a_{E,t}(\xi) := a(t\tau_E + \xi\nu_E). \tag{2.12}$$

*Then, for all $E \in \mathcal{E}(\mathscr{P})$, the coefficients* $\mathrm{a}_1(\nu_E)$ *and* $\mathrm{a}_0(\nu_E)$ *in Theorem 2.1 may be rewritten as*

$$\mathrm{a}_1(\nu_E) = \frac{1}{2\pi} \int_{\mathbb{R}} dt \; \mathrm{tr}\, \big[h\big\{W(a_{E,t})\big\} - W(h \circ a_{E,t})\big], \tag{2.13}$$

$$\mathrm{a}_0(\nu_E) = \frac{1}{2\pi} \int_{\mathbb{R}} dt \; \mathrm{tr}\, \big(M(x)\big[h\{W(a_{E,t})\} - W(h \circ a_{E,t})\big]\big), \tag{2.14}$$

*where $M(x)$ denotes multiplication by $x$ on* $\mathrm{L}^2(\mathbb{R})$*. In particular, we have that*

$$\mathrm{c}_1 = \sum_{E \in \mathcal{E}(\mathscr{P})} \frac{|E|}{2\pi} \int_{\mathbb{R}} dt \; \mathrm{tr}\, \big[h\big\{W(a_{E,t})\big\} - W(h \circ a_{E,t})\big]. \tag{2.15}$$

**Remark 2.4.** The advantage of formulae (2.13) and (2.14) lies in the fact that explicit formulae for the traces of one-dimensional Wiener–Hopf operators are known. Assuming for simplicity that $a \in \mathcal{S}(\mathbb{R}^2)$, [83, Prop. 5.4] implies that

$$\mathrm{a}_1(\nu_E) = \frac{1}{8\pi^3} \int_{\mathbb{R}} dt \int_{\mathbb{R}} d\xi_1 \int_{\mathbb{R}} d\xi_2 \, \frac{h(a_{E,t}(\xi_1)) - h(a_{E,t}(\xi_2))}{a_{E,t}(\xi_1) - a_{E,t}(\xi_2)} \frac{a'_{E,t}(\xi_2)}{\xi_2 - \xi_1},$$

where the integral over $\xi_2$ is interpreted as a Cauchy principal value. Referring to the same proposition, one similarly gets that

$$\begin{aligned} \mathrm{a}_0(\nu_E) = &- \frac{1}{64\pi^2} \int_{\mathbb{R}} dt \int_{\mathbb{R}} d\xi \, h''(a_{E,t}(\xi)) a'_{E,t}(\xi)^2 \\ &- \frac{1}{32\pi^4} \int_{\mathbb{R}} dt \int_{\mathbb{R}} d\xi_1 \int_{\mathbb{R}} d\xi_2 \int_{\mathbb{R}} d\xi_3 \left\{ \sum_{k=1}^{3} \frac{h(a(\xi_k))}{\prod_{j \neq k} [a(\xi_k) - a(\xi_j)]} \right\} \frac{a'_{E,t}(\xi_2)}{\xi_2 - \xi_1} \frac{a'_{E,t}(\xi_3)}{\xi_3 - \xi_1}. \end{aligned}$$

**2.1.3. The radially symmetric case.** In contrast to the above, the coefficients $\mathrm{b}_0(X)$, see (2.9) and (2.10), can naturally not be transformed into integrals over traces of one-dimensional fibre operators since they incorporate the truly two-dimensional sector operators $h(A_{\mathscr{C}(X)})$. This makes their explicit calculation rather involved. However, we manage to compute the coefficients $\mathrm{b}_0(X)$ in the special case when $h$ is a quadratic polynomial and the symbol $a$ is radially symmetric. By the latter we mean that, for any orthogonal matrix $O \in \mathbb{R}^{2\times 2}$ and for all $\xi \in \mathbb{R}^2$,

$$a(\xi) = a(O\xi).$$

Define

$$\check{f}(x) := (2\pi)^{-d/2} (\mathcal{F}^* f)(x) = (2\pi)^{-d} \int_{\mathbb{R}^d} d\xi \, e^{i\xi\cdot x} f(\xi), \tag{2.16}$$

for functions $f \in \mathrm{L}^1(\mathbb{R}^d)$, so that the operator $A$ has the difference kernel

$$A(x,y) = \check{a}(x-y),\ x,y \in \mathbb{R}^d.$$

If $a$ is radially symmetric, so is $\check{a}$ and we shall write, slightly abusing notation,

$$a(|\xi|) = a(\xi),\ \check{a}(|x|) = \check{a}(x),$$

for all $x, \xi \in \mathbb{R}^2$. In the following theorem, all coefficients $\mathrm{c}_j$ in the asymptotics (1.21) are computed explicitly for such symbols $a$ and quadratic test functions $h$. Again, our focus lies on the coefficient $\mathrm{c}_0$ since the formulae for $\mathrm{c}_2$ and $\mathrm{c}_1$ are known to be the same as in the smooth boundary case.

**Theorem 2.5.** *Suppose that $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ is radially symmetric and let $h(z) = z^2 + dz$ for some $d \in \mathbb{C}$. Then we have that*

$$\operatorname{tr} h(A_{\mathscr{P}_L}) = L^2 \mathrm{c}_2 + L \mathrm{c}_1 + \mathrm{c}_0 + \mathcal{O}(L^{-\infty}),$$

*as $L \to \infty$, with*

$$\mathrm{c}_2 = \frac{|\mathscr{P}|}{2\pi} \int_0^\infty dR\, R\, (h \circ a)(R),$$

$$\mathrm{c}_1 = -2\, |\partial \mathscr{P}| \int_0^\infty dr\, r^2 \check{a}(r)^2,$$

$$\mathrm{c}_0 = \sum_{X \in \Xi(\mathscr{P})} \tfrac{1}{2}\big[1 + (\pi - \gamma_X) \cot \gamma_X\big] \int_0^\infty dr\, r^3 \check{a}(r)^2.$$

**Remark 2.6.**
(1) As in Theorem 2.1, the coefficients $\mathrm{c}_1$ and $\mathrm{c}_0$ only depend on the test function $h$ via the function $h_1(z) = z^2$.
(2) Notice that, due to the radial symmetry of $a$, the dependence of the coefficients $\mathrm{c}_j$, $j = 0,1,2$, on the geometry of $\mathscr{P}$ separates from their dependence on the symbol $a$.
(3) Interestingly, the contribution of convex corners and concave corners to $\mathrm{c}_0$ are obtained via the same formula, in contrast to the two distinct formulae (2.9), (2.10).

The explicit formula for the coefficient $\mathrm{c}_0$ given in Theorem 2.5 allows us to compare it with the corresponding coefficient $\mathcal{B}_0$ from the smooth boundary case, see (1.12). As in the theorem, let $h$ be a quadratic test function and assume that

$a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ is radially symmetric. Applying [58, Thm. 1.1], one gets that, for any bounded $\Omega \subset \mathbb{R}^2$ with smooth boundary,

$$\mathcal{B}_0 = \mathcal{B}_0(\Omega, h, a) = 0. \tag{2.17}$$

To our knowledge, this surprising fact has not been noted explicitly before and it even holds without the radial symmetry of $a$. For the reader's convenience we provide a proof of (2.17) in the appendix to this thesis, see Lemma A.1. In contrast to the above, the function

$$f(\gamma) := 1 + (\pi - \gamma)\cot(\gamma) \tag{2.18}$$

is positive on $(0, \pi) \cup (\pi, 2\pi)$. This yields the following corollary.

**Corollary 2.7.** *Let $h(z) = z^2 + dz$ and suppose that the symbol $0 \neq a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ is real-valued and radially symmetric. Moreover, assume that $\mathcal{P}$ is a polygon and $\Omega \subset \mathbb{R}^2$ is a bounded set with smooth boundary. Then one has that*

$$\mathrm{c}_0(\mathcal{P}, h, a) > 0,$$

*while*

$$\mathcal{B}_0(\Omega, h, a) = 0,$$

*where $\mathrm{c}_0$ and $\mathcal{B}_0$ are the constant order coefficients from* (1.21) *and* (1.12).

**Remark 2.8.** The corollary implies the following: consider a bounded set $\Lambda \subset \mathbb{R}^2$ with either smooth or piecewise linear boundary. Then the type of the boundary can be determined from the spectral asymptotics of $A_{\Lambda_L}$, as $L \to \infty$.

As a consequence of Corollary 2.7, the constant order coefficient in the trace asymptotics exhibits an anomaly, similarly to the heat trace asymptotics for the Dirichlet Laplacian on two-dimensional domains with corners, see e.g. [47, 50]. Any approximation of a polygon $\mathcal{P}$ by a sequence of smooth domains $\{\Omega_n\}$ can not recover the coefficient $\mathrm{c}_0$: for functions $h$ and $a$ as in the corollary, one gets that

$$\mathcal{B}_0(\Omega_n, h, a) = 0 \nrightarrow \mathrm{c}_0(\mathcal{P}, h, a),$$

as $n \to \infty$. On the other hand, the approximation of domains with smooth boundary by polygons works fine. As a simple but representative example consider a disc $\Omega$

and let $\{\mathscr{P}_n\}$ be a sequence of inscribed regular $n$-gons, approximating $\Omega$. Since the function $f$, see (2.18), vanishes to second order at $\gamma = \pi$, one easily checks that

$$\mathrm{c}_0(\mathscr{P}_n, h, a) \to 0 = \mathcal{B}_0(\Omega, h, a),$$

as $n \to \infty$.

We also point out that one may apply Theorem 2.5 to compute the particle number fluctuation (PNF) of an infinitely extended free Fermi gas (in dimension $d = 2$) with respect to the spatial bipartition $\mathbb{R}^2 = \mathscr{P}_L \dot\cup \mathbb{R}^2 \setminus \mathscr{P}_L$ at positive temperature. The PNF is a basic measure for quantum correlations: it constitutes a lower bound for the entanglement entropy, but the PNF is easier to compute. If the one-particle Hamiltonian is the unperturbed two-dimensional Laplacian $-\Delta$, the PNF is given by

$$\operatorname{tr} h(A_{\mathscr{P}_L}),$$

with

$$h(x) = x(1-x),\ a(\xi) = \Big[1 + \exp\Big(\frac{|\xi|^2 - \mu}{T}\Big)\Big]^{-1},$$

see [38]. Here, $\mu \in \mathbb{R}$ is the chemical potential and $T > 0$ denotes temperature. Corollary 2.7 allows us to compare the PNF for a scaled polygon $\mathscr{P}_L$ with the PNF for a scaled set $\Omega_L$ with smooth boundary: if $\mathscr{P}$ and $\Omega$ have the same area and perimeter, then the PNF for the polygon $\mathscr{P}_L$ is strictly larger than the PNF for $\Omega_L$, as $L \to \infty$.

**2.1.4. Strategy of the proofs.** Let us comment on the basic ideas for the proofs of Theorems 2.1, 2.3, and 2.5.

The strategy of the proof of Theorem 2.1 is as follows. The leading order term in the asymptotics originates from approximating the operator $h(A_{\mathscr{P}_L})$ by its bulk approximation $\chi_{\mathscr{P}_L} h(A) \chi_{\mathscr{P}_L}$, which is a very familiar idea. Indeed, one easily computes that

$$\operatorname{tr}\big(\chi_{\mathscr{P}_L} h(A) \chi_{\mathscr{P}_L}\big) = \int_{\mathscr{P}_L} dx\, h(A)(x,x) = |\mathscr{P}_L| (h \circ a)^{\vee}(0) = L^2 \mathrm{c}_2. \tag{2.19}$$

Subtracting the latter from $\operatorname{tr} h(A_{\mathscr{P}_L})$ leaves a remainder that is independent of the linear part of $h$, hence we may replace $h$ by the function $h_1(z) = h(z) - z h'(0)$:

$$\operatorname{tr}\big(\chi_{\mathscr{P}_L} \big[h(A_{\mathscr{P}_L}) - h(A)\big] \chi_{\mathscr{P}_L}\big) = \operatorname{tr}\big(\chi_{\mathscr{P}_L} \big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big] \chi_{\mathscr{P}_L}\big). \tag{2.20}$$

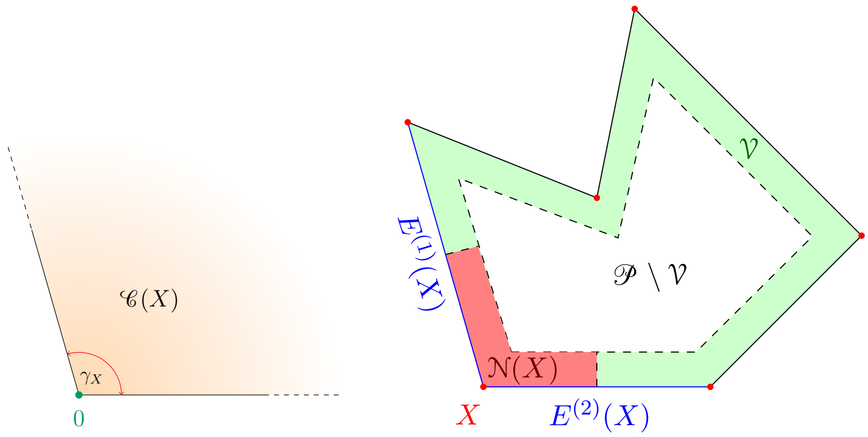


FIGURE 1. The sector $\mathscr{C}(X)$, the one-sided boundary neighbourhood $\mathcal{V}$, and the corner neighbourhood $\mathcal{N}(X)$

For the following steps we mainly rely on the locality of the operator $A$: due to the assumptions on the symbol $a$, the kernel $A(x,y) = \check{a}(x-y)$ decays super-polynomially away from the diagonal, see Lemma 2.10. As a first consequence, we can prove that the operator $\chi_{\mathscr{P}_L}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\chi_{\mathscr{P}_L}$ is concentrated on the boundary $\partial\mathscr{P}_L$. More precisely, defining for small but fixed $\epsilon > 0$ the (unscaled) one-sided $\epsilon$-neighbourhood of $\partial\mathscr{P}$,

$$\mathcal{V} := \mathcal{V}^{(\epsilon)} := \{y \in \mathscr{P} \cup \partial\mathscr{P} : \operatorname{dist}(y, \partial\mathscr{P}) \leq \epsilon\}, \tag{2.21}$$

we show that

$$\operatorname{tr}\big(\chi_{\mathscr{P}_L}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\big) = \operatorname{tr}\big(\chi_{\mathcal{V}_L}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\big) + \mathcal{O}(L^{-\infty}), \tag{2.22}$$

as $L \to \infty$. It is convenient to partition $\mathcal{V}$ into corner neighbourhoods $\mathcal{N}(X)$, $X \in \Xi(\mathscr{P})$, that extend along half of the edges $E^{(1)}(X)$ and $E^{(2)}(X)$, see Figure 1 above. This reduces the problem to computing the asymptotics of

$$\operatorname{tr}\big(\chi_{\mathcal{N}_L(X)}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\big), \tag{2.23}$$

for a fixed vertex $X \in \Xi(\mathscr{P})$. In view of the translation-invariance of $A$, we may assume that $X = 0$, hence the sector $\mathscr{C}(X)$ models the corner at $X \in \Xi(\mathscr{P})$, see (2.8) and Figure 1. Again the locality of the operator $A$ implies that one can replace the operator $h_1(A_{\mathscr{P}_L})$ in (2.23) by the $L$-independent sector operator $h_1(A_{\mathscr{C}(X)})$:

$$\operatorname{tr}\big(\chi_{\mathcal{N}_L(X)}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\big) = \operatorname{tr}\big(\chi_{\mathcal{N}_L(X)}\big[h_1(A_{\mathscr{C}(X)}) - h_1(A)\big]\big) + \mathcal{O}(L^{-\infty}). \tag{2.24}$$

Thus, we have completely localised the problem to the corner at $X \in \Xi(\mathscr{P})$. It remains to prove that the right-hand side of (2.24) exhibits a two-term asymptotic expansion with super-polynomial error: the leading order term, linear in $L$, results from the parts of $\mathcal{N}(X)$ near an edge $E^{(1)}(X)$ or $E^{(2)}(X)$, whereas its constant order correction is solely produced by the fraction of $\mathcal{N}(X)$ close to the vertex $X$. In order to extract these two terms, we provide a trace-class regularisation of the operator $h_1(A_{\mathscr{C}(X)})$, see Proposition 2.18. This part of the proof shows some commonalities with the analysis in [25] for the case of cubes. Summing up the contributions from all $X \in \Xi(\mathscr{P})$ finishes the proof of Theorem 2.1.

Theorem 2.3 is deduced from Theorem 2.1. Here, the key observation is that, for a fixed edge $E \in \mathcal{E}(\mathscr{P})$, the operator $h(A_{\mathscr{H}_E}) - h(A)$ is invariant with respect to translations along $E$. As a consequence, it is unitarily equivalent to a direct integral over one-dimensional fibre operators that are parametrised by the tangential coordinate. Not surprisingly, these fibre operators can be rewritten in terms of one-dimensional Wiener–Hopf operators, which results in the formulae (2.13) and (2.14) for the coefficients $\mathrm{a}_1(\nu_E)$ and $\mathrm{a}_0(\nu_E)$.

The proof of Theorem 2.5 requires the evaluation of all the coefficients $\mathrm{c}_j$, $j = 0, 1, 2$, from Theorem 2.1. To compute $\mathrm{a}_1(\nu_E)$ and $\mathrm{a}_0(\nu_E)$ for all $E \in \mathcal{E}(\mathscr{P})$ we apply Theorem 2.3. Moreover, the specific choice of the function $h$ allows us to evaluate $\mathrm{b}_0(X)$ for each $X \in \Xi(\mathscr{P})$ via a straightforward calculation. Here, the radial symmetry of the symbol $a$ is essential to extract the dependence of $\mathrm{b}_0(X)$ on the interior angle $\gamma_X$.

## 2.2. Trace Norm Estimates

In this section, we collect the trace norm estimates that will be sufficient to prove Theorems 2.1 and 2.3. For the notation regarding Schatten-von Neumann classes and Schatten (quasi)norms we refer to the end of the introduction, in particular (1.26). We shall often utilise Hölder's inequality

$$\|T_1 T_2\|_1 \le \|T_1\|_p \|T_2\|_q, \tag{2.25}$$

for $T_1 \in \mathfrak{S}_p, T_2 \in \mathfrak{S}_q$, and $p, q > 0$ such that $\frac{1}{p} + \frac{1}{q} = 1$. Notice also the interpolation inequality

$$\|T\|_p^p \le \|T\|^{p-q} \|T\|_q^q, \tag{2.26}$$

which holds if $T \in \mathfrak{S}_q$, $0 < q < p$.

**2.2.1. Finite volume truncations of the operator *A*.** We recall the notation

$$A = A(a) = \mathcal{F}^* a \mathcal{F},$$

and

$$A_\Omega = A_\Omega(a) = \chi_\Omega \mathcal{F}^* a \mathcal{F} \chi_\Omega,$$

where $\Omega \subseteq \mathbb{R}^d$ is a measurable subset and $a : \mathbb{R}^d \to \mathbb{C}$ is the symbol of the operator $A$, acting on $\mathrm{L}^2(\mathbb{R}^d)$. The dependence of $A$ on $a$ will be mostly suppressed, unless we consider the dimension-reduced symbol as in Section 2.5. Let us also remind the reader of the following general notation, which was introduced in the introduction: If $f, g$ are non-negative functions, we write $f \lesssim g$ or $g \gtrsim f$ if $f \le Cg$ for some constant $C > 0$. This constant will always be independent of the scaling parameter $L$, but it might depend on the test function $h$, the symbol $a$, and the geometry of the polygon $\mathscr{P}$.

The next lemma shows that, under mild assumptions on the symbol $a$, the operator $A_\Omega$ is trace class if $\Omega \subset \mathbb{R}^d$ is bounded. Even though this is well-known, see [13, Subsec. 10.83] for the one-dimensional case, we provide a proof for the reader's convenience. Having the application to the polygon $\mathscr{P}$ in mind, one deduces from (2.28) below the trace norm bound

$$\|h(A_{\mathscr{P}_L})\|_1 \lesssim L^2 |\mathscr{P}|,$$

if $a \in \mathrm{L}^1(\mathbb{R}^2) \cap \mathrm{L}^\infty(\mathbb{R}^2)$, and $h : \mathbb{C} \to \mathbb{C}$ is an entire function such that $h(0) = 0$. Here, the implied constant depends on $h$ and $a$.

**Lemma 2.9.** *Let $a \in \mathrm{L}^1(\mathbb{R}^d)$ and assume that $\Omega, \Lambda \subset \mathbb{R}^d$ are bounded sets. Then one has the bound*

$$\|\chi_\Lambda A \chi_\Omega\|_1 \le (2\pi)^{-d} |\Lambda|^{1/2} |\Omega|^{1/2} \|a\|_{\mathrm{L}^1(\mathbb{R}^d)}. \tag{2.27}$$

*If in addition $a \in \mathrm{L}^\infty(\mathbb{R}^d)$ and $h : \mathbb{C} \to \mathbb{C}$ is an entire function with $h(0) = 0$, then also the estimate*

$$\|h(A_\Omega)\|_1 \lesssim |\Omega| \tag{2.28}$$

*holds, with implied constant only depending on $h$ and $a$.*

PROOF. We start by proving the estimate (2.27). Without loss of generality, we may assume that $a \geq 0$ since the symbol can be decomposed as $a = a_1 - a_2 + i(a_3 - a_4)$ for suitable functions $a_j \geq 0$. We have that

$$\chi_\Lambda A \chi_\Omega = B_1 B_2,$$

where $B_1$ and $B_2$ are the operators on $\mathrm{L}^2(\mathbb{R}^d)$ with kernels

$$B_1(x, \xi) := (2\pi)^{-d/2} \chi_\Lambda(x) e^{ix\cdot\xi} \sqrt{a(\xi)}$$
$$B_2(\xi, y) := (2\pi)^{-d/2} \sqrt{a(\xi)} e^{-iy\cdot\xi} \chi_\Omega(y).$$

Hence, (2.25) yields

$$\|\chi_\Lambda A \chi_\Omega\|_1 \leq \|B_1\|_2 \|B_2\|_2 = (2\pi)^{-d} |\Lambda|^{1/2} |\Omega|^{1/2} \|a\|_{\mathrm{L}^1(\mathbb{R}^d)},$$

which proves (2.27).

Let us now assume that $a \in \mathrm{L}^1(\mathbb{R}^d) \cap \mathrm{L}^\infty(\mathbb{R}^d)$ and that $h$ is as in the formulation of the lemma. The boundedness of $a$ implies the (uniform) operator norm bound

$$\|A_\Omega\| \leq \|A\| \leq \|a\|_{\mathrm{L}^\infty(\mathbb{R}^d)}.$$

It follows that

$$\|h(A_\Omega)\|_1 \lesssim \|A_\Omega\|_1,$$

with implied constant depending only on $h$ and $\|a\|_{\mathrm{L}^\infty(\mathbb{R}^d)}$. In view of (2.27), this finishes the proof of the lemma. □

**2.2.2. Symbol estimates.** Introduce, for $N \geq 0$, the Sobolev spaces

$$\mathrm{W}^{N,1}(\mathbb{R}^d) := \{f \in \mathrm{L}^1(\mathbb{R}^d) : \ \partial^\alpha f \in \mathrm{L}^1(\mathbb{R}^d) \text{ for all } \alpha \in \mathbb{N}_0^d, \ |\alpha| \leq N\},$$

with corresponding norms

$$|f|_N := \sum_{|\alpha| \leq N} \|\partial^\alpha f\|_{\mathrm{L}^1(\mathbb{R}^d)}. \tag{2.29}$$

Moreover, set

$$\mathrm{W}^{\infty,1}(\mathbb{R}^d) := \bigcap_{N=0}^{\infty} \mathrm{W}^{N,1}(\mathbb{R}^d).$$

In view of [24, Thm. 2.31(2)] we note that

$$\mathrm{W}^{\infty,1}(\mathbb{R}^d) \subset \mathrm{C}^\infty(\mathbb{R}^d),$$

i.e.

$$\mathrm{W}^{\infty,1}(\mathbb{R}^d) = \{f \in \mathrm{C}^\infty(\mathbb{R}^d) : \partial^\alpha f \in \mathrm{L}^1(\mathbb{R}^d) \text{ for all } \alpha \in \mathbb{N}_0^d\}. \tag{2.30}$$

The next lemma recalls the standard fact that, for a symbol $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^d)$, its (inverse) Fourier transform $\check{a}$, see (2.16), decays super-polynomially at infinity. Moreover, it provides some information on the dimension-reduced symbol, which will be useful when proving Theorem 2.3.

**Lemma 2.10.** *Let $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^d)$. Then the following statements hold true.*

*(i) For all $N \in \mathbb{N}_0$, one has the bound*

$$|\check{a}(x)| \lesssim |a|_N \langle x \rangle^{-N},$$

*with implied constants only depending on $N$.*

*(ii) Assume that $d \geq 2$ and define, for $t \in \mathbb{R}$, the reduced symbol*

$$\mathbb{R}^{d-1} \ni \xi \mapsto a_t(\xi) := a(t, \xi).$$

*Then we have that $a_t \in \mathrm{W}^{\infty,1}(\mathbb{R}^{d-1})$, for all $t \in \mathbb{R}$. Moreover, for every $N \in \mathbb{N}_0$, it holds that $(t \mapsto a_t) \in \mathrm{L}^1\big(\mathbb{R}, \mathrm{W}^{N,1}(\mathbb{R}^{d-1})\big) \cap \mathrm{C}\big(\mathbb{R}, \mathrm{W}^{N,1}(\mathbb{R}^{d-1})\big)$.*

Proof. Using the fact that $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^d)$ and integrating by parts, we get that

$$\begin{aligned}
|\check{a}(x)| &\lesssim \Big| \int d\xi\, e^{ix\cdot\xi} a(\xi) \Big| \\
&= \Big| \int d\xi\, a(\xi) \Big[\frac{1 - ix \cdot \nabla_\xi}{1 + x^2}\Big]^N e^{ix\cdot\xi} \Big| \\
&= \Big| \int d\xi\, e^{ix\cdot\xi} \Big[\frac{1 + ix \cdot \nabla_\xi}{1 + x^2}\Big]^N a(\xi) \Big| \\
&\lesssim |a|_N \langle x \rangle^{-N},
\end{aligned}$$

where the implied constants only depend on $N$. For the proof of the second part of the statement notice that, since $a \in \mathrm{L}^1(\mathbb{R}^d)$, there is some $t_0 \in \mathbb{R}$ such that $a_{t_0} \in \mathrm{L}^1(\mathbb{R}^{d-1})$. This in turn implies that

$$\begin{aligned}
\sup_{t\in\mathbb{R}} \|a_t\|_{\mathrm{L}^1(\mathbb{R}^{d-1})} \leq \|\sup_{t\in\mathbb{R}} |a_t|\|_{\mathrm{L}^1(\mathbb{R}^{d-1})} &= \int_{\mathbb{R}^{d-1}} d\xi \sup_{t\in\mathbb{R}} \Big| a_{t_0}(\xi) + \int_{t_0}^{t} ds\, \partial_s a_s(\xi) \Big| \\
&\leq \|a_{t_0}\|_{\mathrm{L}^1(\mathbb{R}^{d-1})} + \|\partial_t a\|_{\mathrm{L}^1(\mathbb{R}^d)} < \infty,
\end{aligned} \tag{2.31}$$

i.e. $a_t \in \mathrm{L}^1(\mathbb{R}^{d-1})$ for all $t$. Moreover, the fact that $a \in \mathrm{L}^1(\mathbb{R}^d) \cap \mathrm{C}(\mathbb{R}^d)$ and the uniform bound (2.31) ensure that $(t \mapsto a_t) \in \mathrm{L}^1\big(\mathbb{R}, \mathrm{L}^1(\mathbb{R}^{d-1})\big) \cap \mathrm{C}\big(\mathbb{R}, \mathrm{L}^1(\mathbb{R}^{d-1})\big)$. The analogous statements for derivatives of $a_t$ follow along the same lines. This finishes the proof of the lemma. □

For $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^d)$, the off-diagonal decay of the kernel $A(x,y) = \check{a}(x-y)$, see Lemma 2.10, and the continuity of $\check{a}$ imply the following lemma. Its proof is not difficult but technical and can be found in Appendix A.2.

**Lemma 2.11.** *Let $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^d)$ and let $h : \mathbb{C} \to \mathbb{C}$ be an entire function with $h(0) = 0$. Then for any open set $G \subseteq \mathbb{R}^d$ the operator kernel*

$$(x,y) \mapsto h(A_G)(x,y)$$

*is a continuous function on $G \times G$.*

**2.2.3. Localisation estimates.** Throughout this subsection, let $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^d)$ and let $h : \mathbb{C} \to \mathbb{C}$ be an entire function that vanishes to second order at $z = 0$. One of the main tools for proving Theorem 2.1 is the next proposition. It is of similar spirit as [25, Thm. 2.5], which was recently established in the context of ergodic Schrödinger operators.

**Proposition 2.12.** *Suppose that $\Lambda \subseteq \Omega \subseteq \mathbb{R}^d$ and let $v, w \in \mathbb{R}^d$. Then, for any $N \in \mathbb{N}$, there exists a constant $C_{h,a,N} \geq 0$ such that*

$$\begin{aligned} \|\chi_{Q_v \cap \Lambda}\big[h(A_\Lambda) - h(A_\Omega)\big]\chi_{Q_w}\|_1 \leq C_{h,a,N} &\langle \operatorname{dist}(v, \Omega \setminus \Lambda)\rangle^{-N} \\ &\times \langle \operatorname{dist}(w, \Omega \setminus \Lambda)\rangle^{-N} \langle v - w\rangle^{-N}. \end{aligned} \tag{2.32}$$

*More precisely, if $h$ is given by the power series $h(z) = \sum_{k=2}^{\infty} d_k z^k$, then the constant $C_{h,a,N}$ may be bounded as*

$$C_{h,a,N} \lesssim \sum_{k=2}^{\infty} k|d_k|\big[C_N |a|_{2N+2d+2}\big]^k, \tag{2.33}$$

*for some constant $C_N \geq 0$ and implied constant only depending on $N$.*

**Remark 2.13.** (1) Unlike in [25, Thm. 2.5], we do not require convexity of the set $\Omega$.

(2) In [25] the author deduced their result with the help of an a-priori Schatten quasi-norm bound in $\mathfrak{S}_q$ for some $q < 1$, see [25, Eq. (2.3)]. In the special case of Wiener–Hopf-operators, this a-priori bound reduces to

$$\sup_{v,w \in \mathbb{R}^d} \|\chi_{Q_v} A \chi_{Q_w}\|_q < \infty. \tag{2.34}$$

This estimate holds if, in addition to $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$, we suppose that $a \in \mathrm{L}^p(\mathbb{R}^2)$ for some $p \in (0,q)$, see [7, Ch. 11, Thm. 13]. However, we prefer not to assume any additional decay on $a$. Instead, we exploit the basic Hilbert Schmidt bound (2.35) on unit cubes from Lemma 2.14 below.

(3) The mild decay assumptions on the symbol $a$ are compensated by assuming that the test function $h$ vanishes to second order at $z=0$. This assumption is sufficient to prove Theorem 2.1: we will exclusively apply Proposition 2.12 to the function $h_1$, see (2.4).

Proposition 2.12 follows from approximation of the test function $h$ by polynomials and the next lemma.

**Lemma 2.14.** *Let $v, w \in \mathbb{R}^d$. Then, for all $N \in \mathbb{N}$, there exist constants $c_N \geq \tilde{c}_N \geq 0$ such that*

$$\|\chi_{Q_v} A \chi_{Q_w}\| \leq \|\chi_{Q_v} A \chi_{Q_w}\|_2 \leq \tilde{c}_N |a|_N \langle v-w\rangle^{-N}, \tag{2.35}$$

*and such that, for all $k \in \mathbb{N} \setminus \{1\}$, $p \in \{1,2\}$,*

$$\sup_{G \subseteq \mathbb{R}^d} \|\chi_{Q_v} [A_G]^k \chi_{Q_w}\|_p \leq \big[c_N |a|_{N+d+1}\big]^k \langle v-w\rangle^{-N}. \tag{2.36}$$

Proof. The estimate (2.35) is a direct consequence of Lemma 2.10. To prove (2.36) define, for all $N \geq 1$, the constants

$$\tilde{c}_{N,a} := \tilde{c}_N |a|_N,$$

and set

$$c'_d := \sup_{|x| \leq 1} \sum_{y \in \mathbb{Z}^d} \langle y + x\rangle^{-d-1} < \infty. \tag{2.37}$$

Let $N \in \mathbb{N}$, $k \geq 2$, $G \subseteq \mathbb{R}^d$, and $M := N+d+1$. Then (2.35) implies that, for $p \in \{1,2\}$ and for all $v, w \in \mathbb{R}^d$,

$$\begin{aligned}
\|\chi_{Q_v}[A_G]^k \chi_{Q_w}\|_p &\leq \sum_{y_1,\ldots,y_{k-1} \in \mathbb{Z}^d} \|\chi_{Q_v} A \chi_{Q_{y_1}}\|_2 \Big(\prod_{j=1}^{k-2} \|\chi_{Q_{y_j}} A \chi_{Q_{y_{j+1}}}\|\Big) \|\chi_{Q_{y_{k-1}}} A \chi_{Q_w}\|_2 \\
&\leq \tilde{c}_{M,a}^k \sum_{y_1,\ldots,y_{k-1} \in \mathbb{Z}^d} \langle v - y_1\rangle^{-M} \Big(\prod_{j=1}^{k-2} \langle y_j - y_{j+1}\rangle^{-M}\Big) \langle y_{k-1} - w\rangle^{-M} \\
&\leq \tilde{c}_{M,a}^k \big[2^{N/2} c'_d\big]^{k-1} \langle v-w\rangle^{-N}. \qquad (2.38)
\end{aligned}$$

Here we have used Peetre's inequality,

$$\langle x-y\rangle^N \langle y-z\rangle^N \geq 2^{-N/2}\langle x-z\rangle^N, \text{ for } x,y,z\in\mathbb{R}^d, \tag{2.39}$$

and the definition of $c'_d$, see (2.37). Setting

$$c_N := \tilde{c}_M 2^{N/2} c'_d,$$

(2.36) follows and the proof of the lemma is complete. □

PROOF OF PROPOSITION 2.12. Let $h$ be an entire function of the form $h(z) = \sum_{k=2}^{\infty} d_k z^k$. Then Lemma 2.14 implies that

$$\|\chi_{Q_v\cap\Lambda}\big[h(A_\Lambda)-h(A_\Omega)\big]\chi_{Q_w}\|_1 \leq C'_{h,a,N}\langle v-w\rangle^{-N}, \tag{2.40}$$

where

$$C'_{h,a,N} := 2\sum_{k\geq 2}|d_k|\big[c_N|a|_{N+d+1}\big]^k,$$

and $c_N$ is the constant in Lemma 2.14. As we may interpolate with (2.40), it suffices to show that

$$\|\chi_{Q_v\cap\Lambda}\big[h(A_\Lambda)-h(A_\Omega)\big]\chi_{Q_w}\|_1 \leq C''_{h,a,N}\langle \operatorname{dist}(v,\Omega\setminus\Lambda)\rangle^{-N}\langle \operatorname{dist}(w,\Omega\setminus\Lambda)\rangle^{-N}, \tag{2.41}$$

for an appropriate constant $C''_{h,a,N}$. Again, we first prove (2.41) for monomials $h(z) = z^k$, $k\geq 2$. Defining for $m,n\in\mathbb{N}_0$ the operators

$$\tau_{mn} := \chi_{Q_v}[A_\Lambda]^m\chi_\Lambda A\chi_{\Omega\setminus\Lambda}[A_\Omega]^n\chi_{Q_w},$$

one gets that

$$\begin{aligned}\chi_{Q_v\cap\Lambda}\big([A_\Lambda]^k-[A_\Omega]^k\big)\chi_{Q_w} &= \sum_{l=0}^{k-1}\chi_{Q_v\cap\Lambda}[A_\Lambda]^{k-l-1}(A_\Lambda-A_\Omega)[A_\Omega]^l\chi_{Q_w}\\ &= -\chi_\Lambda\sum_{l=0}^{k-1}\tau_{k-l-1,l}.\end{aligned} \tag{2.42}$$

Fix the numbers $M$ and $M'$, depending on $N$ and $d$:

$$M := N+d+1,\ M' := N+2d+2 = M+d+1.$$

Moreover, define for any set $G\subseteq\mathbb{R}^d$ the corresponding lattice point neighbourhood

$$G_+ := \{y\in\mathbb{Z}^d : Q_y\cap G\neq\emptyset\}. \tag{2.43}$$

We apply Lemma 2.14 and estimate as in (2.38) to deduce that, for $m, n \in \mathbb{N}$,

$$\begin{aligned}
\|\tau_{mn}\|_1 &\le \sum_{\substack{x\in\Lambda_+ \\ y\in(\Omega\setminus\Lambda)_+}} \|\chi_{Q_v}[A_\Lambda]^m\chi_{Q_x}\|_2\|\chi_{Q_x}A\chi_{Q_y}\|\|\chi_{Q_y}[A_\Omega]^n\chi_{Q_w}\|_2 \\
&\le \sum_{\substack{x\in\Lambda_+ \\ y\in(\Omega\setminus\Lambda)_+}} \big[c_M|a|_{M'}\big]^{n+m+1}\langle v-x\rangle^{-M}\langle x-y\rangle^{-M}\langle y-w\rangle^{-M} \\
&\lesssim \big[c_M|a|_{M'}\big]^{n+m+1}\langle \operatorname{dist}(v,\Omega\setminus\Lambda)\rangle^{-N}\langle \operatorname{dist}(w,\Omega\setminus\Lambda)\rangle^{-N}. \qquad (2.44)
\end{aligned}$$

Here, the implied constants only depend on $N$. Similarly, we estimate for $n \ge 1$,

$$\begin{aligned}
\|\tau_{0n}\|_1 &\le \sum_{y\in(\Omega\setminus\Lambda)_+} \|\chi_{Q_v}A\chi_{Q_y}\|_2\|\chi_{Q_y}[A_\Omega]^n\chi_{Q_w}\|_2 \\
&\le \sum_{y\in(\Omega\setminus\Lambda)_+} \big[c_M|a|_{M'}\big]^{n+1}\langle v-y\rangle^{-M}\langle y-w\rangle^{-M} \\
&\lesssim \big[c_M|a|_{M'}\big]^{n+1}\langle \operatorname{dist}(v,\Omega\setminus\Lambda)\rangle^{-N}\langle \operatorname{dist}(w,\Omega\setminus\Lambda)\rangle^{-N}. \qquad (2.45)
\end{aligned}$$

In case $Q_w \cap \Omega \setminus \Lambda = \emptyset$, one has that $\tau_{m0} = 0$, hence combining (2.42), (2.44), and (2.45) gives

$$\begin{aligned}
\|\chi_{Q_v\cap\Lambda}\big([A_\Omega]^k - [A_\Lambda]^k\big)\chi_{Q_w}\|_1 \lesssim k\big[c_M|a|_{M'}\big]^k&\langle \operatorname{dist}(v,\Omega\setminus\Lambda)\rangle^{-N} \\
&\times \langle \operatorname{dist}(w,\Omega\setminus\Lambda)\rangle^{-N}, \qquad (2.46)
\end{aligned}$$

with implied constants only depending on $N$. If $Q_w \cap \Omega \setminus \Lambda \neq \emptyset$, we estimate

$$\begin{aligned}
\|\tau_{m0}\|_1 &\le \|\chi_{Q_v}[A_\Lambda]^m\chi_\Lambda A\chi_{Q_w}\|_1 \\
&\le \sum_{x\in\Lambda_+} \|\chi_{Q_v}[A_\Lambda]^m\chi_{Q_x}\|_2\|\chi_{Q_x}A\chi_{Q_w}\|_2 \\
&\le \sum_{x\in\Lambda_+} \big[c_M|a|_{M'}\big]^{m+1}\langle v-x\rangle^{-M}\langle x-w\rangle^{-M} \\
&\lesssim \big[c_M|a|_{M'}\big]^{m+1}\langle \operatorname{dist}(v,\Omega\setminus\Lambda)\rangle^{-N},
\end{aligned}$$

which together with (2.42), (2.44), and (2.45) again implies (2.46). The extension of Estimate (2.46) to entire functions $h$ of the form $h(z) = \sum_{k=2}^{\infty} d_k z^k$, and an interpolation with (2.40) finishes the proof of the proposition. □

Proposition 2.12 implies two corollaries, which will be useful in applications. For example, it follows from Corollary 2.15 that the coefficient $\mathrm{a}_1(\nu_E)$, see (2.5), is well-defined.

**Corollary 2.15.** *Suppose that the sets* $\mathsf{M}$, $\Lambda$, $\Omega \subseteq \mathbb{R}^d$ *satisfy*

$$\mathsf{M} \subseteq \Lambda \cap \Omega.$$

*Moreover, assume that there exists* $\beta \geq 0$ *and a constant* $C_\beta \geq 0$ *such that, for all* $r > 0$,

$$\sharp\{x \in \mathsf{M}_+ : \ \operatorname{dist}(x, \Lambda \triangle \Omega) \leq r\} \leq C_\beta \langle r \rangle^\beta, \tag{2.47}$$

*where the set* $\mathsf{M}_+ \subseteq \mathbb{Z}^d$ *is defined in* (2.43).
*Then we have that*

$$\chi_{\mathsf{M}}\big[h(A_\Lambda) - h(A_\Omega)\big] \in \mathfrak{S}_1.$$

Proof. An application of the triangle inequality shows that we may restrict ourselves to the case that $\Lambda \subseteq \Omega$. Applying Proposition 2.12 for $N = d + \beta + 1$ and the assumption $\mathsf{M} \subseteq \Lambda$, one gets that

$$\begin{aligned}
\big\|\chi_{\mathsf{M}}\big[h(A_\Lambda) - h(A_\Omega)\big]\big\|_1 &\leq \sum_{\substack{v \in \mathsf{M}_+ \\ w \in \mathbb{Z}^d}} \big\|\chi_{Q_v \cap \Lambda}\big[h(A_\Lambda) - h(A_\Omega)\big]\chi_{Q_w}\big\|_1 \\
&\lesssim \sum_{\substack{v \in \mathsf{M}_+ \\ w \in \mathbb{Z}^d}} \langle \operatorname{dist}(v, \Omega \setminus \Lambda)\rangle^{-d-\beta-1} \langle v - w\rangle^{-d-\beta-1} \\
&\lesssim \sum_{v \in \mathsf{M}_+} \langle \operatorname{dist}(v, \Omega \setminus \Lambda)\rangle^{-d-\beta-1} \\
&\leq \sum_{k=0}^{\infty} \sum_{\substack{v \in \mathsf{M}_+ \\ k \leq \operatorname{dist}(v, \Omega\setminus\Lambda) \leq k+1}} \langle k \rangle^{-d-\beta-1} \\
&\lesssim \sum_{k=0}^{\infty} C_\beta \langle k+1\rangle^\beta \langle k \rangle^{-d-\beta-1} < \infty,
\end{aligned} \tag{2.48}$$

where the implied constants depend on $\beta$, $h$, and $a$. This finishes the proof of the corollary. □

The next corollary treats $L$-dependent sets $\mathsf{M}$, $\Lambda$, and $\Omega$. Here, the dependence on $L$ does not need to be linear, unlike for scaled sets. The corollary gives sufficient conditions under which the spatial restriction of the operator $h(A_\Lambda)$ to $\mathsf{M}$ may be replaced by the corresponding restriction of $h(A_\Omega)$, with a super-polynomially small error in trace norm, as $L \to \infty$.

**Corollary 2.16.** *Let* $\mathsf{M}, \Lambda, \Omega \subseteq \mathbb{R}^d$ *be sets that all possibly depend on the parameter* $L \geq 1$*. Suppose that*

$$\mathsf{M} \subseteq \Lambda \cap \Omega \quad \textit{and} \quad \operatorname{dist}(\mathsf{M}, \Lambda \triangle \Omega) \gtrsim L. \tag{2.49}$$

*Moreover, assume that there exists some* $\beta \geq 0$ *and a constant* $C_\beta \geq 0$*, independent of* $L$*, such that at least one of the following conditions is satisfied:*

*(i)* $\sharp \mathsf{M}_+ \leq C_\beta L^\beta$.
*(ii) Estimate* (2.47) *holds.*

*Then one has that*

$$\big\| \chi_{\mathsf{M}} \big[ h(A_\Lambda) - h(A_\Omega) \big] \big\|_1 = \mathcal{O}(L^{-\infty}),$$

*as* $L \to \infty$.

Proof. As in the proof of Corollary 2.15, we may assume that $\Lambda \subseteq \Omega$. Moreover, similarly as in (2.48), an application of Proposition 2.12 yields

$$\big\| \chi_{\mathsf{M}} \big[ h(A_\Lambda) - h(A_\Omega) \big] \big\|_1 \lesssim \sum_{v \in \mathsf{M}_+} \langle \operatorname{dist}(v, \Omega \setminus \Lambda) \rangle^{-N},$$

with implied constant depending on $h$, $a$, and $N \geq d + 1$. If the estimate (i) holds, then one easily concludes with (2.49) that

$$\big\| \chi_{\mathsf{M}} \big[ h(A_\Lambda) - h(A_\Omega) \big] \big\|_1 \lesssim L^{\beta - N},$$

with implied constant depending on $\beta, N, h$, and $a$. Assuming (ii) instead, we obtain as in the proof of Corollary 2.15 that

$$\begin{aligned} \big\| \chi_{\mathsf{M}} \big[ h(A_\Lambda) - h(A_\Omega) \big] \big\|_1 &\lesssim L^{-N/2} \sum_{v \in \mathsf{M}_+} \langle \operatorname{dist}(v, \Omega \setminus \Lambda) \rangle^{-N/2} \\ &\lesssim L^{-N/2}, \end{aligned}$$

where we chose $N \geq 2(d + \beta + 1)$ and the implied constants depend on $N$, $\beta$, $h$, $a$, and the constant in (2.47). This finishes the proof of the corollary. □

## 2.3. Proof of Theorem 2.1: Localisation to the Corners of $\mathscr{P}$

Fix $\epsilon > 0$ to be chosen later and recall the definition (2.21) of $\mathcal{V} = \mathcal{V}^{(\epsilon)}$, the one-sided $\epsilon$–neighbourhood of $\partial\mathscr{P}$. As indicated in Subsection 2.1.4, we split $\mathcal{V}$ into (almost) disjoint sets $\mathcal{N}(X)$, $X \in \Xi(\mathscr{P})$, such that $\mathcal{N}(X)$ contains the part of $\mathcal{V}$ close to the vertex $X$, see Figure 1 on page 41. This induces a corresponding partition of $\mathcal{V}_L = L \cdot \mathcal{V}$.

**2.3.1. Partition of $\mathcal{V}_L$.** Fix a vertex $X \in \Xi(\mathscr{P})$ and recall that its adjacent edges are named $E^{(1)}(X)$ and $E^{(2)}(X)$, see Subsection 2.1.1. It will be convenient to introduce the following two choices for the unit normal and the unit tangent vector at $X$:

$$\begin{aligned} (\tau_X^{(1)}, \nu_X^{(1)}) &:= (-\tau_{E^{(1)}(X)}, \nu_{E^{(1)}(X)}), \\ (\tau_X^{(2)}, \nu_X^{(2)}) &:= (\tau_{E^{(2)}(X)}, \nu_{E^{(2)}(X)}). \end{aligned} \tag{2.50}$$

This definition ensures that $\tau_X^{(1)}$ and $\tau_X^{(2)}$, considered as vectors at $X$, point into the direction of the edges $E^{(1)}(X)$ and $E^{(2)}(X)$, respectively. For $j = 1, 2$, define the tubes

$$\mathsf{T}^{(j)}(X) : = \{t\tau_X^{(j)} + \xi\nu_X^{(j)} : \ (t, \xi) \in [0, \tfrac{|E^{(j)}(X)|}{2}] \times [0, \epsilon]\}, \tag{2.51}$$

and set

$$\mathsf{N}(X) := \big[\mathsf{T}^{(1)}(X) \cup \mathsf{T}^{(2)}(X) \cup B_\epsilon(0)\big] \cap \mathscr{C}(X), \tag{2.52}$$

see Figure 2. Then $\mathsf{N}(X)$ is a corner-neighbourhood of $0 \in \Xi(\mathscr{P} - X)$ and we define the corresponding neighbourhood at $X \in \Xi(\mathscr{P})$ by

$$\mathcal{N}(X) := X + \mathsf{N}(X). \tag{2.53}$$

Combining the scaled neighbourhoods $\mathcal{N}_L(X) = L \cdot \mathcal{N}(X)$, we arrive at the partition

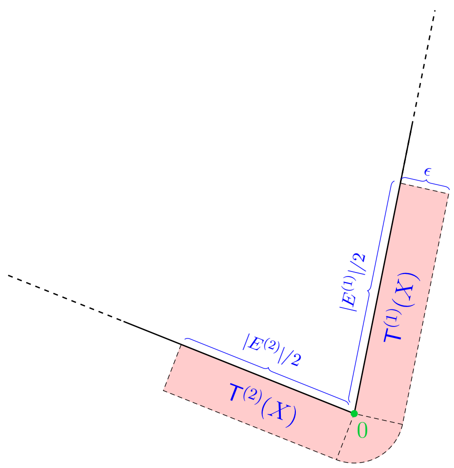


FIGURE 2. The neighbourhood $\mathsf{N}(X)$ for a vertex $X \in \Xi_>(\mathscr{P})$

$$\mathcal{V}_L = \bigcup_{X \in \Xi(\mathscr{P})} \mathcal{N}_L(X). \tag{2.54}$$

At this point we choose $\epsilon > 0$ small enough such that the union (2.54) is disjoint up to sets of zero two-dimensional Lebesgue measure.

**2.3.2. Reduction to individual corner contributions.** As in the formulation of Theorem 2.1, let $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ and assume that $h$ is an entire function with $h(0) = 0$. Notice that due to Lemma 2.9 the operators $h(A_{\mathscr{P}_L})$ and $\chi_{\mathscr{P}_L} h(A) \chi_{\mathscr{P}_L}$ are trace class, the trace of the latter operator being computed in (2.19). This gives us the leading order term in the asymptotics (2.11):

$$\operatorname{tr} h(A_{\mathscr{P}_L}) = L^2 \mathrm{c}_2 + \operatorname{tr}\big(\chi_{\mathscr{P}_L}\big[h(A_{\mathscr{P}_L}) - h(A)\big]\chi_{\mathscr{P}_L}\big). \tag{2.55}$$

Moreover, it follows from Corollary 2.15 that

$$\chi_{\mathscr{P}_L}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big] \in \mathfrak{S}_1,$$

where we recall the definition of the function $h_1(z) = h(z) - zh'(0)$. By construction, we have that

$$\operatorname{dist}(\mathscr{P}_L \setminus \mathcal{V}_L \,,\, \mathbb{R}^2 \setminus \mathscr{P}_L) \gtrsim L,$$

hence Corollary 2.16 with Assumption (i) implies that

$$\begin{aligned} \operatorname{tr}\big(\chi_{\mathscr{P}_L}\big[h(A_{\mathscr{P}_L}) - h(A)\big]\chi_{\mathscr{P}_L}\big) &= \operatorname{tr}\big(\chi_{\mathscr{P}_L}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\big) \\ &= \operatorname{tr}\big(\chi_{\mathcal{V}_L}\big[h_1(A_{\mathscr{P}_L}) - h_1(A)\big]\big) + \mathcal{O}(L^{-\infty}). \end{aligned}$$

In particular, we may from now on assume that $h$ vanishes to second order at $z = 0$, such that $h_1 = h$. Also, we have reduced the proof of Theorem 2.1 to computing the asymptotics of

$$\operatorname{tr}\big(\chi_{\mathcal{V}_L}\big[h(A_{\mathscr{P}_L}) - h(A)\big]\big) = \sum_{X \in \Xi(\mathscr{P})} \operatorname{tr}\big(\chi_{\mathcal{N}_L(X)}\big[h(A_{\mathscr{P}_L}) - h(A)\big]\big),$$

employing (2.54) for the latter equality. For fixed $X \in \Xi(\mathscr{P})$, the translation-invariance of the operator $A$ implies that

$$\operatorname{tr}\big(\chi_{\mathcal{N}_L(X)}\big[h(A_{\mathscr{P}_L}) - h(A)\big]\big) = \operatorname{tr}\big(\chi_{\mathsf{N}_L(X)}\big[h(A_{(\mathscr{P}-X)_L}) - h(A)\big]\big),$$

with $\mathsf{N}(X) = \mathcal{N}(X) - X$, see (2.53). Moreover, it is not difficult to see that

$$\operatorname{dist}\big(\mathsf{N}_L(X)\,,\, \mathscr{C}(X) \triangle (\mathscr{P} - X)_L\big) \gtrsim L.$$

Hence, Corollary 2.16 with Assumption (i) yields that

$$\operatorname{tr}\left(\chi_{\mathsf{N}_L(X)}\left[h(A_{(\mathscr{P}-X)_L})-h(A)\right]\right)=\operatorname{tr}\left(\chi_{\mathsf{N}_L(X)}\left[h(A_{\mathscr{C}(X)})-h(A)\right]\right)+\mathcal{O}(L^{-\infty}).$$

We emphasise that the trace

$$\operatorname{tr}\left(\chi_{\mathsf{N}_L(X)}\left[h(A_{\mathscr{C}(X)})-h(A)\right]\right) \tag{2.56}$$

depends on the polygon $\mathscr{P}$ only via the directions $\tau_X^{(j)}$, $j=1,2$, and the length of the edges adjacent to $X$. To compute its asymptotics for each $X\in\Xi(\mathscr{P})$ is the object of the next section.

## 2.4. Proof of Theorem 2.1: Asymptotics for a Fixed Corner of $\mathscr{P}$

Throughout this section, we fix a vertex $X\in\Xi(\mathscr{P})$. In particular, we shall omit all arguments, sub- and superscripts "$(X)$"; for instance, we will write $\mathscr{C}=\mathscr{C}(X)$ and $\mathsf{N}_L=\mathsf{N}_L(X)$. As before, let $a\in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ and assume that $h=h_1$ is an entire function that vanishes to second order at $z=0$. The main purpose of this section is to obtain an asymptotic formula for (2.56), which will complete the proof of Theorem 2.1.

**2.4.1. The $L$-term in the asymptotics.** In the smooth boundary case, the sub-leading order term in the asymptotics (1.12) is (at least morally) obtained via approximation of the operator $h(A_{\Omega_L})$ by half-space operators: around $x\in\partial\Omega_L$, the operator $h(A_{\Omega_L})$ is replaced by $h(A_{\mathscr{H}_x})$ where $\mathscr{H}_x$ is the half-space approximation of $\Omega_L$ at $x$. Similarly, the half-spaces $\mathscr{H}^{(1)}$ and $\mathscr{H}^{(2)}$, see (2.7), locally model the sector $\mathscr{C}$ in (2.56), as long as one stays away from the apex of the sector. Thus, to get a first-order approximation to (2.56), the strategy is to replace the sector $\mathscr{C}$ by the half-space $\mathscr{H}^{(j)}$, $j=1,2$, on the part of $\mathsf{N}_L$ close to $\partial\mathscr{H}^{(j)}\cap\partial\mathscr{C}$. This philosophy was used for right-angled cones in [76] and [25]. In the course of this section, we will thus prove that

$$\operatorname{tr}\left(\chi_{\mathsf{N}_L}\left[h(A_{\mathscr{C}})-h(A)\right]\right)=\sum_{j=1}^{2}\operatorname{tr}\left(\chi_{\mathsf{T}_L^{(j)}}\left[h(A_{\mathscr{H}^{(j)}})-h(A)\right]\right)+\mathcal{O}(1), \tag{2.57}$$

as $L\to\infty$, see (2.51) and Figure 2 above for the definition of $\mathsf{T}^{(j)}$. Here, the $\mathcal{O}(1)$-term contains the corner contribution at $X$ to the coefficient $\mathrm{c}_0$ and a super-polynomial error in $L$. The approximation (2.57) is useful since the invariance of the operator $h(A_{\mathscr{H}^{(j)}})-h(A)$ with respect to translations along the edge $E^{(j)}$ can be applied to scale out the length of the tube $\mathsf{T}_L^{(j)}$. This is demonstrated in the next lemma, which hence provides the $L$-term in the asymptotics of (2.56).

**Lemma 2.17.** *Let $j \in \{1,2\}$ and set $S^{(j)} := S_{E^{(j)}}$, compare with* (2.2). *Then one has that*

$$\operatorname{tr}\big(\chi_{\mathsf{T}_L^{(j)}}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big) = L^{\frac{|E^{(j)}|}{2}} \operatorname{tr}\big(\chi_{S^{(j)}}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big) + \mathcal{O}(L^{-\infty}).$$

Proof. Fix $j \in \{1,2\}$ and omit the superscript "$(j)$" for the duration of the proof. Moreover, we may assume after a suitable rotation that $\mathscr{H} = \mathbb{R} \times [0,\infty)$ and $S = [0,1] \times [0,\infty)$. Then it follows from Corollary 2.16 that

$$\operatorname{tr}\big(\chi_{\mathsf{T}_L}\big[h(A_{\mathscr{H}}) - h(A)\big]\big) = \operatorname{tr}\big(\chi_{L^{\frac{|E|}{2}} \cdot S}\big[h(A_{\mathscr{H}}) - h(A)\big]\big) + \mathcal{O}(L^{-\infty}).$$

Here, the trace on the right-hand side is well-defined due to Corollary 2.15. Also, the invariance of the operator $h(A_{\mathscr{H}}) - h(A)$ with respect to translations in the $x_1$-direction implies that, for all $x = (x_1, x_2) \in \mathbb{R}^2$,

$$(h(A_{\mathscr{H}}) - h(A))(x_1, x_2; x_1, x_2) = (h(A_{\mathscr{H}}) - h(A))(0, x_2; 0, x_2).$$

Thus, a change of coordinates in the $x_1$-variable finishes the proof of the lemma. □

**2.4.2. Regularisation of sector operators.** The key to finding the constant order term in the asymptotics of (2.56) is a trace-class regularisation of the sector operator $h(A_{\mathscr{C}})$ with the help of the half-space operators $h(A_{\mathscr{H}^{(j)}})$, $j = 1, 2$, and the full-space operator $h(A)$. This regularisation is given in the next proposition. For its proof we consider spatial restrictions of $h(A_{\mathscr{C}})$ to different parts of the sector $\mathscr{C}$ and then compare these to the operators $h(A_{\mathscr{H}^{(j)}})$, $j = 1, 2$, or $h(A)$, depending on which part of the sector we localise to. In that respect we follow the ideas of [25]. However, instead of only looking at a right-angled convex cone, we tackle sectors of any angle; in particular, we also deal with concave sectors. Moreover, our regularisation for convex sectors $\mathscr{C}$, see (2.58), does not require a partition of $\mathscr{C}$. At the same time, it is independent of the scaling parameter $L$, in contrast to the ones given in [25, Thm. 2.2].

**Proposition 2.18.** *Let $L \geq 1$. If $X \in \Xi_{<}(\mathscr{P})$, then the operator*

$$Z := \chi_{\mathscr{C}}\big[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}}) - h(A_{\mathscr{H}^{(2)}}) + h(A)\big] \tag{2.58}$$

*is trace class with*

$$\|\chi_{\mathbb{R}^2\setminus B_L(0)} Z\|_1 = \mathcal{O}(L^{-\infty}), \tag{2.59}$$

*as* $L \to \infty$.

*If* $X \in \Xi_>(\mathcal{P})$, *then the operators*

$$Z_1 := \chi_{\mathcal{H}^{(1)} \cap \mathcal{H}^{(2)}} \big[h(A_{\mathcal{C}}) - h(A)\big],$$
$$Z_2 := \chi_{\mathcal{C}\setminus\mathcal{H}^{(1)}} \big[h(A_{\mathcal{C}}) - h(A_{\mathcal{H}^{(2)}})\big],$$
$$Z_3 := \chi_{\mathcal{C}\setminus\mathcal{H}^{(2)}} \big[h(A_{\mathcal{C}}) - h(A_{\mathcal{H}^{(1)}})\big],$$

*are trace class and, for every* $j = 1, 2, 3$, *one has that*

$$\|\chi_{\mathbb{R}^2\setminus B_L(0)} Z_j\|_1 = \mathcal{O}(L^{-\infty}),$$

*as* $L \to \infty$.

Proof. As in the statement of the proposition we treat convex and concave corners separately.

*Convex corners, i.e.* $X \in \Xi_<(\mathcal{P})$: we divide the semi-infinite sector $\mathcal{C}$ into two halves,

$$\mathcal{C}_l := \{y \in \mathcal{C} : y \cdot (\nu^{(2)} - \nu^{(1)}) \geq 0\},$$
$$\mathcal{C}_r := \{y \in \mathcal{C} : y \cdot (\nu^{(1)} - \nu^{(2)}) \geq 0\},$$

where we recall the definition (2.50) for $\nu^{(j)} = \nu_X^{(j)}$. Then one can write

$$Z = \chi_{\mathcal{C}_l} \big[h(A_{\mathcal{C}}) - h(A_{\mathcal{H}^{(1)}})\big] + \chi_{\mathcal{C}_r} \big[h(A_{\mathcal{C}}) - h(A_{\mathcal{H}^{(2)}})\big]$$
$$+ \chi_{\mathcal{C}_l} \big[h(A) - h(A_{\mathcal{H}^{(2)}})\big] + \chi_{\mathcal{C}_r} \big[h(A) - h(A_{\mathcal{H}^{(1)}})\big].$$

Thus, Corollary 2.15 implies that the operator $Z$ is trace class since the estimate (2.47) with $\beta = 1$ is easily checked for all involved sets. Moreover, applying the same splitting for $Z$, the bound (2.59) follows from Corollary 2.16.

*Concave corners, i.e.* $X \in \Xi_>(\mathcal{P})$: in the concave case we may directly apply Corollaries 2.15 and 2.16 to the operators $Z_j$, $j = 1, 2, 3$; no further partition is required. The claim follows as in the convex case, which finishes the proof of the proposition. □

**2.4.3. Contributions from non-right-angled corners.** In the next subsection we will apply the regularisation for the sector operator $h(A_{\mathscr{C}})$ from Proposition 2.18 to find the asymptotics of the trace (2.56). As it turns out during this process, non-perpendicular edges $E^{(1)}$ and $E^{(2)}$ generate an extra term of constant order. Technically, this relies on the fact that the tubes $\mathsf{T}^{(j)}$, which are responsible for the $L$-term in the asymptotics, see Lemma 2.17, are rectangles. In this sense, they are not compatible with interior angles $\gamma \notin \{\frac{\pi}{2}, \frac{3\pi}{2}\}$.

For the fixed vertex $X \in \Xi(\mathscr{P})$, introduce the following sectors, which depend on $j \in \{1, 2\}$, see Figure 3 below:

$$\Gamma^{(j)} := \begin{cases} \{t\tau^{(j)} + \xi\nu^{(j)} : \ 0 \le t < \cot(\gamma)\xi\}, & \gamma \in (0, \frac{\pi}{2}] \cup (\pi, \frac{3\pi}{2}], \\ \{t\tau^{(j)} + \xi\nu^{(j)} : \ \cot(\gamma)\xi < t \le 0\}, & \gamma \in [\frac{\pi}{2}, \pi) \cup [\frac{3\pi}{2}, 2\pi). \end{cases} \tag{2.60}$$

We will see in Subsection 2.4.4 that non-perpendicular edges $E^{(1)}$ and $E^{(2)}$ contribute the constants

$$\operatorname{tr}\left(\chi_{\Gamma^{(j)}}\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right), \ j = 1, 2, \tag{2.61}$$

to the asymptotics of (2.56). These traces are well-defined in view of Corollary 2.15 and the following lemma provides an alternative characterisation of (2.61).

**Lemma 2.19.** *Let $X \in \Xi(\mathscr{P})$ be a vertex of $\mathscr{P}$ and let $\Gamma^{(j)}$, $j = 1, 2$, be the sectors introduced in* (2.60)*. Moreover, let $S^{(j)}$ be the strip of unit width defined in Lemma 2.17. Then we have that, for $j = 1, 2$,*

$$\operatorname{tr}\left(\chi_{\Gamma^{(j)}}\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right) = |\cot(\gamma)| \operatorname{tr}\left(\chi_{S^{(j)}} M(x \cdot \nu_{\mathscr{H}^{(j)}})\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right).$$

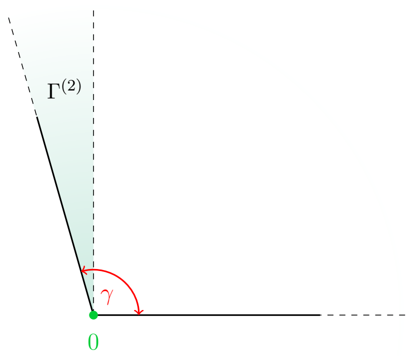


FIGURE 3. The sector $\Gamma^{(2)}$ for $\gamma \in (\frac{\pi}{2}, \pi)$

Proof. Fix $X \in \Xi(\mathscr{P})$. Without loss of generality suppose that $\gamma \in (0, \pi/2]$ and $j = 2$, and, for the matter of readability, omit the superscript "(2)". The other cases can be reduced to this one via a symmetry argument. After a suitable rotation we may also assume that $\mathscr{H} = \mathbb{R} \times [0, \infty)$, $\Gamma = \{(x_1, x_2) \in \mathscr{H} : 0 \leq x_1 \leq \cot(\gamma)x_2\}$, and $S = [0, 1] \times [0, \infty)$. Splitting the strip $S$ into unit cubes, one easily gets from Proposition 2.12 that the operator

$$\chi_S M(x_2)\big[h(A_{\mathscr{H}}) - h(A)\big]$$

is trace-class. In view of Corollary 2.15, we likewise have that

$$\chi_\Gamma \big[h(A_{\mathscr{H}}) - h(A)\big] \in \mathfrak{S}_1. \tag{2.62}$$

Furthermore, as in the proof of Lemma 2.17, the invariance of the operator $h(A_{\mathscr{H}}) - h(A)$ with respect to translations in the $x_1$-direction implies that, for all $x = (x_1, x_2) \in \mathbb{R}^2$,

$$(h(A_{\mathscr{H}}) - h(A))(x_1, x_2; x_1, x_2) = (h(A_{\mathscr{H}}) - h(A))(0, x_2; 0, x_2).$$

By Lemma 2.11 this kernel is continuous on $\Gamma \times \Gamma \subset \mathscr{H} \times \mathscr{H}$, so [14, Thm. 3.5] and (2.62) ensure that it is integrable on $\Gamma \times \Gamma$. Hence, we may apply Fubini's theorem to arrive at

$$\begin{aligned}
\operatorname{tr}\big(\chi_\Gamma\big[h(A_{\mathscr{H}}) - h(A)\big]\big) &= \int_\Gamma dx_1 dx_2\, (h(A_{\mathscr{H}}) - h(A))(0, x_2; 0, x_2) \\
&= \int_0^\infty dx_2 \int_0^{\cot(\gamma)x_2} dx_1\, (h(A_{\mathscr{H}}) - h(A))(0, x_2; 0, x_2) \\
&= \cot(\gamma) \int_0^\infty dx_2\, x_2\, (h(A_{\mathscr{H}}) - h(A))(0, x_2; 0, x_2) \\
&= \cot(\gamma) \int_0^1 dx_1 \int_0^\infty dx_2\, x_2\, (h(A_{\mathscr{H}}) - h(A))(0, x_2; 0, x_2) \\
&= \cot(\gamma) \operatorname{tr}\big(\chi_S M(x_2)\big[h(A_{\mathscr{H}}) - h(A)\big]\big).
\end{aligned}$$

This finishes the proof of the lemma. □

**2.4.4. Complete asymptotics.** Equipped with Proposition 2.18 and Lemmas 2.17 and 2.19, we are now ready to extract the asymptotics from (2.56). As the regularisation for the sector operators in Proposition 2.18 depends on the type of the sector, we naturally have to distinguish convex and concave corners of the polygon $\mathscr{P}_L$. Propositions 2.20 and 2.21 contain the respective results.

**Proposition 2.20** (Convex corners). *Let $X \in \Xi_<(\mathscr{P})$. Then we have that*

$$\begin{aligned}\operatorname{tr}\big(\chi_{\mathsf{N}_L}[h(A_{\mathscr{C}}) - h(A)]\big) &= L\sum_{j=1}^{2} \tfrac{|E^{(j)}|}{2} \operatorname{tr}\big(\chi_{S^{(j)}}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big)\\ &\quad + \operatorname{tr}\big(\chi_{\mathscr{C}}\big[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}}) - h(A_{\mathscr{H}^{(2)}}) + h(A)\big]\big)\\ &\quad - \cot(\gamma)\sum_{j=1}^{2}\operatorname{tr}\big(\chi_{S^{(j)}}M(x\cdot\nu_{\mathscr{H}^{(j)}})\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big) + \mathcal{O}(L^{-\infty}),\end{aligned}$$

*as $L \to \infty$.*

Proof. We write

$$\begin{aligned}\operatorname{tr}\big(\chi_{\mathsf{N}_L}\big[h(A_{\mathscr{C}}) - h(A)\big]\big) &= \operatorname{tr}\big(\chi_{\mathsf{N}_L}\big[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}}) - h(A_{\mathscr{H}^{(2)}}) + h(A)\big]\big)\\ &\quad + \sum_{j=1}^{2}\operatorname{tr}\big(\chi_{\mathsf{N}_L}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big). \qquad (2.63)\end{aligned}$$

Proposition 2.18 implies that the operator

$$\chi_{\mathscr{C}}\big[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}}) - h(A_{\mathscr{H}^{(2)}}) + h(A)\big]$$

is trace class with

$$\operatorname{tr}\big(\chi_{\mathscr{C}\setminus\mathsf{N}_L}\big[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}}) - h(A_{\mathscr{H}^{(2)}}) + h(A)\big]\big) = \mathcal{O}(L^{-\infty}),$$

since $\operatorname{dist}(0, \mathscr{C}\setminus\mathsf{N}_L) \gtrsim L$. Thus it remains to find the asymptotics for

$$\operatorname{tr}\big(\chi_{\mathsf{N}_L}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big),\ j = 1, 2.$$

Recall the definition (2.60) of the sectors $\Gamma^{(j)}$ and define its finite sections

$$\Gamma^{(j)}[r] := \{y \in \Gamma^{(j)} : y\cdot\nu^{(j)} \le r\},\ j = 1, 2,\ r \ge 0.$$

Applying the definition of $\mathsf{N}$, see (2.52), and Corollary 2.16, we get that

$$\begin{aligned}\operatorname{tr}\big(\chi_{\mathsf{N}_L}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big) &= \operatorname{tr}\big(\chi_{\mathsf{T}_L^{(j)}}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big)\\ &\quad + \operatorname{sgn}(\gamma - \tfrac{\pi}{2})\operatorname{tr}\big(\chi_{\Gamma^{(j)}[\epsilon L]}\big[h(A_{\mathscr{H}^{(j)}}) - h(A)\big]\big) + \mathcal{O}(L^{-\infty}).\end{aligned}$$

Furthermore, Lemma 2.17 and another application of Corollary 2.16 yield that

$$\operatorname{tr}\left(\chi_{\mathsf{N}_L}\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right) = \tfrac{L|E^{(j)}|}{2}\operatorname{tr}\left(\chi_{S^{(j)}}\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right)$$
$$+ \operatorname{sgn}(\gamma - \tfrac{\pi}{2})\operatorname{tr}\left(\chi_{\Gamma^{(j)}}\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right) + \mathcal{O}(L^{-\infty}).$$

Hence, the claim follows from Lemma 2.19 and (2.63). □

**Proposition 2.21** (Concave corners)**.** *Let $X \in \Xi_>(\mathscr{P}_L)$. Then we have that*

$$\operatorname{tr}\left(\chi_{\mathsf{N}_L}[h(A_{\mathscr{C}}) - h(A)]\right) = L\sum_{j=1}^{2}\tfrac{|E^{(j)}|}{2}\operatorname{tr}\left(\chi_{S^{(j)}}\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]\right)$$
$$+ \operatorname{tr}\left(\chi_{\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}}\left[h(A_{\mathscr{C}}) - h(A)\right]\right)$$
$$+ \operatorname{tr}\left(\chi_{\mathscr{C}\setminus\mathscr{H}^{(1)}}\left[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(2)}}\right]\right)$$
$$+ \operatorname{tr}\left(\chi_{\mathscr{C}\setminus\mathscr{H}^{(2)}}\left[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}}\right]\right)$$
$$- \cot(\gamma)\sum_{j=1}^{2}\operatorname{tr}(\chi_{S^{(j)}}M(x\cdot\nu_{\mathscr{H}^{(j)}})\left[h(A_{\mathscr{H}^{(j)}}) - h(A)\right]) + \mathcal{O}(L^{-\infty}).$$

*as $L \to \infty$.*

Proof. The proof is analogous to the convex case. We write

$$\operatorname{tr}\left(\chi_{\mathsf{N}_L}[h(A_{\mathscr{C}}) - h(A)]\right) = \eta_1(L) + \eta_2(L),$$

with

$$\eta_1(L) := \operatorname{tr}\left(\chi_{\mathsf{N}_L\cap\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}}\left[h(A_{\mathscr{C}}) - h(A)\right]\right) + \operatorname{tr}\left(\chi_{\mathsf{N}_L\cap\mathscr{C}\setminus\mathscr{H}^{(1)}}\left[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(2)}})\right]\right)$$
$$+ \operatorname{tr}\left(\chi_{\mathsf{N}_L\cap\mathscr{C}\setminus\mathscr{H}^{(2)}}\left[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}})\right]\right),$$

and

$$\eta_2(L) := \operatorname{tr}\left(\chi_{\mathsf{N}_L\cap\mathscr{C}\setminus\mathscr{H}^{(1)}}\left[h(A_{\mathscr{H}^{(2)}}) - h(A)\right]\right) + \operatorname{tr}\left(\chi_{\mathsf{N}_L\cap\mathscr{C}\setminus\mathscr{H}^{(2)}}\left[h(A_{\mathscr{H}^{(1)}}) - h(A)\right]\right).$$

Proposition (2.18) implies that

$$\eta_1(L) = \operatorname{tr}\left(\chi_{\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}}\left[h(A_{\mathscr{C}}) - h(A)\right]\right) + \operatorname{tr}\left(\chi_{\mathscr{C}\setminus\mathscr{H}^{(1)}}\left[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(2)}})\right]\right)$$
$$+ \operatorname{tr}\left(\chi_{\mathscr{C}\setminus\mathscr{H}^{(2)}}\left[h(A_{\mathscr{C}}) - h(A_{\mathscr{H}^{(1)}})\right]\right) + \mathcal{O}(L^{-\infty}).$$

Moreover, we notice that the sectors $\mathscr{C}\setminus\mathscr{H}^{(j)}$, $j = 1, 2$, have an interior angle of $\gamma-\pi \in (0, \pi)$. This and the fact that $\cot(\gamma-\pi) = \cot(\gamma)$ explains why the contribution of $\eta_2(L)$ to the asymptotics is the same as in the convex case. Alternatively, one easily gets that, for instance,

$$\begin{aligned}\operatorname{tr}\big(\chi_{\mathsf{N}_L\cap\mathscr{C}\setminus\mathscr{H}^{(1)}}\big[h(A_{\mathscr{H}^{(2)}})-h(A)\big]\big) &= \operatorname{tr}\big(\chi_{\mathsf{T}_L^{(2)}}\big[h(A_{\mathscr{H}^{(2)}})-h(A)\big]\big)\\ &\quad+\operatorname{sgn}(\gamma-\tfrac{3\pi}{2})\operatorname{tr}\big(\chi_{\mathsf{N}_L\cap\Gamma^{(2)}}\big[h(A_{\mathscr{H}^{(2)}})-h(A)\big]\big).\end{aligned}$$

Thus, as in the convex case the claim follows from Corollaries 2.15 and 2.16, and Lemmas 2.17 and 2.19. □

The proof of Theorem 2.1 is now complete:

PROOF OF THEOREM 2.1. Subsection 2.3.2 implies that for $h = h_1$,

$$\operatorname{tr}\big(\chi_{\mathscr{P}_L}\big[h(A_{\mathscr{P}_L})-h(A)\big]\chi_{\mathscr{P}_L}\big) = \sum_{X\in\Xi(\mathscr{P})}\operatorname{tr}\big(\chi_{\mathsf{N}_L(X)}\big[h(A_{\mathscr{C}(X)})-h(A)\big]\big)+\mathcal{O}(L^{-\infty}).$$

Hence, it follows from Propositions 2.20 and 2.21 that

$$\operatorname{tr}\big(\chi_{\mathscr{P}_L}\big[h(A_{\mathscr{P}_L})-h(A)\big]\chi_{\mathscr{P}_L}\big) = L\mathrm{c}_1+\mathrm{c}_0+\mathcal{O}(L^{-\infty}).$$

In view of (2.55), this finishes the proof of the theorem. □

## 2.5. Proof of Theorem 2.3

Fix an edge $E\in\mathcal{E}(\mathscr{P})$. It suffices to prove the theorem for test functions $h$ of the form $h(z)=\sum_{k=2}^{\infty} d_k z^k$ since both sides of (2.13) and (2.14) vanish for linear functions $h$. Moreover, we may assume after a suitable rotation that $\mathscr{H}_E=\mathscr{H}=\mathbb{R}\times[0,\infty)$, i.e. $S_E=S=[0,1]\times[0,\infty)$. Thus, we have that

$$a_{E,t}(\xi)=a(t,\xi)=:a_t(\xi),\ (t,\xi)\in\mathbb{R}^2.$$

Define, for $\alpha\in\{0,1\}$ and fixed $t\in\mathbb{R}$, the operator

$$B_\alpha(t):=M(x^\alpha)\big[h\{W(a_t)\}-W(h\circ a_t)\big],$$

which acts on $\mathrm{L}^2(\mathbb{R})$. Proposition 2.12 implies that, for $\alpha \in \{0,1\}$ and $t \in \mathbb{R}$,

$$\begin{aligned}\big\|B_\alpha(t)\big\|_1 &\le \sum_{n=1}^{\infty} \big\|M(x^\alpha)\chi_{[n-1,n]}\big[h\{A_{[0,\infty)}(a_t)\} - h\{A(a_t)\}\big]\chi_{[0,\infty)}\big\|_1 \\ &\le \sum_{n=1}^{\infty} \big\|M(x^\alpha)\chi_{[n-1,n]}\big\|\big\|\chi_{[n-1,n]}\big[h\{A_{[0,\infty)}(a_t)\} - h\{A(a_t)\}\big]\big\|_1 \\ &\lesssim \sum_{n=1}^{\infty} n^\alpha \langle n-1\rangle^{-3} \sum_{k=2}^{\infty} k|d_k|\big[C_3|a_t|_{12}\big]^k \\ &\lesssim \sum_{k=2}^{\infty} k|d_k|\big[C_3|a_t|_{12}\big]^k < \infty.\end{aligned}$$

Hence, in view of Lemma 2.10 we have that $(t \mapsto \|B_\alpha(t)\|_1) \in \mathrm{L}^1(\mathbb{R}) \cap \mathrm{L}^\infty(\mathbb{R})$. In particular, the right-hand sides of (2.13) and (2.14) are well-defined under our assumptions on $h$ and $a$.

Introduce the unitary (identification) map

$$J : \mathrm{L}^2(\mathbb{R}^2) \to \mathrm{L}^2\big(\mathbb{R}, \mathrm{L}^2(\mathbb{R})\big), \ (Jf)(t) := f(t, \cdot).$$

Moreover, define the partial Fourier transforms $\mathcal{F}_1$, $\mathcal{F}_2$ on $\mathrm{L}^2(\mathbb{R}^2)$ that only act on the first and second variable, respectively. To obtain the identities (2.13) and (2.14), we first prove that

$$M(x_2^\alpha)\big[h(A_{\mathcal{H}}) - \chi_{\mathcal{H}} h(A)\chi_{\mathcal{H}}\big] = \mathcal{F}_1^* J^* B_\alpha J \mathcal{F}_1, \tag{2.64}$$

where $B_\alpha := \int_{\mathbb{R}}^{\oplus} dt\, B_\alpha(t)$ acts on $\mathrm{L}^2\big(\mathbb{R}, \mathrm{L}^2(\mathbb{R})\big)$. For an introduction to direct integral operators see for example [55]. To verify (2.64), notice that

$$\mathcal{F}_1 \chi_{\mathcal{H}} = \chi_{\mathcal{H}} \mathcal{F}_1,$$

hence

$$A_{\mathcal{H}} = \chi_{\mathcal{H}} \mathcal{F}_1^* \mathcal{F}_2^* a \mathcal{F}_2 \mathcal{F}_1 \chi_{\mathcal{H}} = \mathcal{F}_1^* \chi_{\mathcal{H}} \mathcal{F}_2^* a \mathcal{F}_2 \chi_{\mathcal{H}} \mathcal{F}_1.$$

Moreover, the definition of $J$ yields that

$$\chi_{\mathcal{H}} \mathcal{F}_2^* a \mathcal{F}_2 \chi_{\mathcal{H}} = J^* \int_{\mathbb{R}}^{\oplus} dt\, W(a_t)\, J,$$

implying that

$$h(A_{\mathcal{H}}) = \mathcal{F}_1^* J^* h\Big(\int_{\mathbb{R}}^{\oplus} dt\, W(a_t)\Big) J \mathcal{F}_1 = \mathcal{F}_1^* J^* \int_{\mathbb{R}}^{\oplus} dt\, h\{W(a_t)\} J \mathcal{F}_1. \tag{2.65}$$

Similarly, one gets that

$$\chi_{\mathscr{H}} h(A) \chi_{\mathscr{H}} = A_{\mathscr{H}}(h \circ a) = \mathcal{F}_1^* J^* \int_{\mathbb{R}}^{\oplus} dt\, W(h \circ a_t)\, J \mathcal{F}_1. \tag{2.66}$$

Thus, combining (2.65) and (2.66) gives

$$M(x_2^\alpha) \chi_{\mathscr{H}} \big[h(A_{\mathscr{H}}) - h(A)\big] \chi_{\mathscr{H}} = M(x_2^\alpha) \mathcal{F}_1^* J^* \int_{\mathbb{R}}^{\oplus} dt\, B_0(t) J \mathcal{F}_1 = \mathcal{F}_1^* J^* \int_{\mathbb{R}}^{\oplus} dt\, B_\alpha(t)\, J \mathcal{F}_1,$$

which proves (2.64).

As a consequence of (2.64), the coefficients $\mathrm{a}_1(\nu_E)$ and $\mathrm{a}_0(\nu_E)$ are given by the traces of the operators $\chi_S \tilde{B}_\alpha \chi_S$, $\alpha = 0, 1$, where

$$\tilde{B}_\alpha := \mathcal{F}_1^* J^* B_\alpha J \mathcal{F}_1.$$

In order to calculate these traces, we evaluate the quadratic form of $\tilde{B}_\alpha$ on product states. Namely, for $\phi, \psi \in \mathrm{L}^2(\mathbb{R})$, we have that

$$\begin{aligned} \big\langle \phi \otimes \psi, \tilde{B}_\alpha(\phi \otimes \psi) \big\rangle_{\mathrm{L}^2(\mathbb{R}^2)} &= \big\langle J((\mathcal{F}\phi) \otimes \psi), B_\alpha J((\mathcal{F}\phi) \otimes \psi) \big\rangle_{\mathrm{L}^2(\mathbb{R}, \mathrm{L}^2(\mathbb{R}))} \\ &= \int_{\mathbb{R}} dt\, \big\langle (\mathcal{F}\phi)(t)\psi, (\mathcal{F}\phi)(t) B_\alpha(t)\psi \big\rangle_{\mathrm{L}^2(\mathbb{R})} \\ &= \int_{\mathbb{R}} dt\, |(\mathcal{F}\phi)(t)|^2 \langle \psi, B_\alpha(t)\psi \rangle_{\mathrm{L}^2(\mathbb{R})}. \end{aligned} \tag{2.67}$$

Choose now an orthonormal basis $\{\psi_n\}_{n \in \mathbb{N}}$ of $\mathrm{L}^2(\mathbb{R})$, so that $\{\psi_n \otimes \psi_m\}_{n,m \in \mathbb{N}}$ is an orthonormal basis of $\mathrm{L}^2(\mathbb{R}^2)$. Then (2.67) implies that

$$\begin{aligned} \operatorname{tr}\big(\chi_S \tilde{B}_\alpha \chi_S\big) &= \sum_{n,m \in \mathbb{N}} \langle \psi_n \otimes \psi_m, \chi_S \tilde{B}_\alpha \chi_S \psi_n \otimes \psi_m \rangle_{\mathrm{L}^2(\mathbb{R}^2)} \\ &= \sum_{n,m \in \mathbb{N}} \int_{\mathbb{R}} dt\, |\mathcal{F}(\chi_{[0,1]}\psi_n)(t)|^2 \langle \psi_m, B_\alpha(t)\psi_m \rangle_{\mathrm{L}^2(\mathbb{R})}. \end{aligned}$$

As we have the estimate

$$\sum_{m \in \mathbb{N}} \big| \langle \psi_m, B(t)\psi_m \rangle_{\mathrm{L}^2(\mathbb{R})} \big| \le \|B_\alpha(t)\|_1 \in \mathrm{L}^\infty(\mathbb{R}),$$

we may apply Fubini's theorem to get that

$$\begin{aligned} \operatorname{tr}(\chi_S \tilde{B}_\alpha \chi_S) &= \sum_{n \in \mathbb{N}} \int_{\mathbb{R}} dt\, |\mathcal{F}(\chi_{[0,1]}\psi_n)(t)|^2 \operatorname{tr} B_\alpha(t) \\ &= \sum_{n \in \mathbb{N}} \langle \psi_n, \chi_{[0,1]} \mathcal{F}^* \operatorname{tr} B_\alpha(\,\cdot\,) \mathcal{F} \chi_{[0,1]} \psi_n \rangle_{\mathrm{L}^2(\mathbb{R})}. \end{aligned}$$

Hence, employing the fact that $\operatorname{tr} B_\alpha(\,\cdot\,) \in \mathrm{L}^1(\mathbb{R})$, we arrive at

$$\operatorname{tr}(\chi_S \tilde{B}_\alpha \chi_S) = \operatorname{tr}\big(\chi_{[0,1]}\mathcal{F}^* \operatorname{tr} B_\alpha(\,\cdot\,)\mathcal{F}\chi_{[0,1]}\big) = (\operatorname{tr} B_\alpha)\check{}(0) = \frac{1}{2\pi}\int_{\mathbb{R}} dt\ \operatorname{tr} B_\alpha(t).$$

This finishes the proof of Theorem 2.3.

## 2.6. Radially Symmetric Symbols – Proof of Theorem 2.5

As in the statement of Theorem 2.5, assume that the symbol $a$ is radially symmetric and the test function $h$ is a quadratic polynomial, i.e. $h(z) = z^2 + dz$ for some $d \in \mathbb{C}$. The coefficient $\mathrm{c}_2 = \mathrm{c}_2(\mathcal{P}, h, a)$ is easily computed from Theorem 2.1. Recall also that the linear part of $h$ does not contribute to the coefficients $\mathrm{c}_1$ and $\mathrm{c}_0$, so we may assume in the following that $h(z) = z^2$. To compute $\mathrm{c}_1$ and $\mathrm{a}_0(\nu_E)$, $E \in \mathcal{E}(\mathcal{P})$, we apply Theorem 2.3. This is done in the next lemma.

**Lemma 2.22.** *Let $h(z) = z^2$ and assume that $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ is radially symmetric. Then the coefficients $\mathrm{c}_1$, $\mathrm{a}_0(\nu_E)$ in Theorem 2.1 satisfy the equations*

$$\mathrm{c}_1 = -2\,|\partial\mathcal{P}| \int_0^\infty dr\, r^2 \check{a}(r)^2,$$

$$\sum_{E\in\mathcal{E}(\mathcal{P})} F(E)\,\mathrm{a}_0(\nu_E) = \sum_{X\in\Xi(\mathcal{P})} \frac{\pi}{2}\cot(\gamma_X) \int_0^\infty dr\, r^3 \check{a}(r)^2.$$

Proof. We first notice that the radial symmetry of the symbol implies that $a_{E,t}(\xi) = a(t,\xi) = a_t(\xi)$ for all $E \in \mathcal{E}(\mathcal{P})$, and $t, \xi \in \mathbb{R}$. Furthermore, we make use of the formulae (2.13) and (2.14) in Theorem 2.3. Similarly as in [82], one calculates that, for $\alpha \in \{0,1\}$, $t \in \mathbb{R}$,

$$\begin{aligned}
-\operatorname{tr}\big(M(x^\alpha)\big[W(a_t)^2 - W(a_t^2)\big]\big) &= \int_0^\infty dx\, x^\alpha \int_{-\infty}^0 dy\, \check{a}_t(x-y)\check{a}_t(y-x)\\
&= \int_0^\infty dx\, x^\alpha \int_x^\infty dy\, \check{a}_t(y)\check{a}_t(-y)\\
&= \int_0^\infty dy\, \check{a}_t(y)\check{a}_t(-y) \int_0^y dx\, x^\alpha\\
&= \frac{1}{2}\int_{-\infty}^\infty dy\, \frac{|y|^{\alpha+1}}{\alpha+1}\check{a}_t(y)\check{a}_t(-y).
\end{aligned}$$

Parseval's identity in the $t$-variable and the radial symmetry of $\check{a}$ imply that

$$\begin{aligned}
-\frac{1}{2\pi}\int_{\mathbb{R}} dt\ \mathrm{tr}\left(M(x^\alpha)\left[W(a_t)^2 - W(a_t^2)\right]\right) &= \frac{1}{4\pi}\int_{\mathbb{R}} dt \int_{\mathbb{R}} dy\, \frac{|y|^{\alpha+1}}{\alpha+1}\check{a}_t(y)\check{a}_t(-y) \\
&= \frac{1}{2}\int_{\mathbb{R}} dy_1 \int_{\mathbb{R}} dy_2 \frac{|y_2|^{\alpha+1}}{\alpha+1}\check{a}(-y_1,y_2)\check{a}(y_1,-y_2) \\
&= \frac{1}{2}\int_0^\infty dr\, r \int_0^{2\pi} d\theta \frac{|r\sin(\theta)|^{\alpha+1}}{\alpha+1}\check{a}(r)^2 \\
&= \begin{cases} 2\int_0^\infty dr\, r^2\check{a}(r)^2, & \alpha = 0, \\ \frac{\pi}{4}\int_0^\infty dr\, r^3\check{a}(r)^2, & \alpha = 1. \end{cases}
\end{aligned}$$

Hence, the claim follows from Theorem 2.3 and the definition of $F(E)$, see (2.3). □

It remains to compute the coefficients $\mathrm{b}_0(X)$, $X \in \Xi(\mathscr{P})$, from formulae (2.9) and (2.10). This calculation is performed in the next lemma.

**Lemma 2.23.** *Let $h(z) = z^2$ and assume that the symbol $a \in \mathrm{W}^{\infty,1}(\mathbb{R}^2)$ is radially symmetric.*
*Then for every $X \in \Xi(\mathscr{P})$ the formula*

$$\mathrm{b}_0(X) = \frac{1-\gamma_X\cot(\gamma_X)}{2}\int_0^\infty dr\, r^3\check{a}(r)^2 \tag{2.68}$$

*holds.*

Proof. Fix $X \in \Xi(\mathscr{P})$ and omit the subscript or argument "$(X)$" for the duration of the proof. As usual, we treat the cases of convex and concave corners separately.

First, let $X \in \Xi_<(\mathscr{P})$. Then, due to the radial symmetry of $a$, we may assume that

$$\mathscr{C} = \{(r\cos(\theta), r\sin(\theta)) :\ r \geq 0,\ \theta \in [0,\gamma]\}, \tag{2.69}$$

with $\gamma \in (0,\pi)$. From (2.9) one gets that

$$\mathrm{b}_0 = \mathrm{tr}\left[\chi_{\mathscr{C}}\left([A_{\mathscr{C}}]^2 - [A_{\mathscr{H}(1)}]^2 - [A_{\mathscr{H}(2)}]^2 + A^2\right)\right] = \mathrm{tr}\left(\chi_{\mathscr{C}}A\chi_{-\mathscr{C}}A\chi_{\mathscr{C}}\right), \tag{2.70}$$

and evaluating the trace gives

$$\mathrm{b}_0 = \int_{\mathscr{C}} dx \int_{-\mathscr{C}} dy\, \check{a}(x-y)^2 = \int_{\mathscr{C}} dx \int_{x+\mathscr{C}} dy\, \check{a}(y)^2 = \int_{\mathscr{C}} dy\, \check{a}(y)^2\, |(y-\mathscr{C})\cap\mathscr{C}|\,.$$

For the last equality we have used the fact that $x \in \mathscr{C}$ and $y \in x+\mathscr{C}$ is equivalent to $y \in \mathscr{C}$ and $x \in (y-\mathscr{C})\cap\mathscr{C}$. Applying (2.69) and the assumption that $\gamma \in (0,\pi)$, one easily computes that, for $y \in \mathscr{C}$,

$$|(y-\mathscr{C})\cap\mathscr{C}| = y_1 y_2 - \cot(\gamma) y_2^2.$$

Hence, the radial symmetry of $a$ yields

$$\begin{aligned}\int_{\mathscr{C}} dy\, \check{a}(y)^2\, |(y-\mathscr{C})\cap\mathscr{C}| &= \int_0^\infty dr\, r^3 \check{a}(r)^2 \int_0^\gamma d\theta\, \cos(\theta)\sin(\theta) - \cot(\gamma)\sin^2(\theta) \\ &= \frac{1-\gamma\cot(\gamma)}{2} \int_0^\infty dr\, r^3 \check{a}(r)^2,\end{aligned}$$

and the claim follows for $X \in \Xi_<(\mathscr{P})$.

Secondly, let $X \in \Xi_>(\mathscr{P})$. Then we get from (2.10) that

$$\begin{aligned}\mathrm{b}_0 &= \mathrm{tr}\left[\chi_{\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}}\big([A_{\mathscr{C}}]^2 - A^2\big)\right] + \mathrm{tr}\left[\chi_{\mathscr{C}\setminus\mathscr{H}^{(1)}}\big([A_{\mathscr{C}}]^2 - [A_{\mathscr{H}^{(2)}}]^2\big)\right] \\ &\quad + \mathrm{tr}\left[\chi_{\mathscr{C}\setminus\mathscr{H}^{(2)}}\big([A_{\mathscr{C}}]^2 - [A_{\mathscr{H}^{(1)}}]^2\big)\right] \\ &= -\,\mathrm{tr}\left(\chi_{\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}} A \chi_{-\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}} A \chi_{\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}}\right) \\ &\quad + \sum_{j=1}^{2} \mathrm{tr}\left(\chi_{\mathscr{C}\setminus\mathscr{H}^{(j)}} A \chi_{-\mathscr{C}\setminus\mathscr{H}^{(j)}} A \chi_{\mathscr{C}\setminus\mathscr{H}^{(j)}}\right).\end{aligned}$$

Note that $\mathscr{H}^{(1)}\cap\mathscr{H}^{(2)}$ and $\mathscr{C}\setminus\mathscr{H}^{(j)}$, $j=1,2$, are convex sectors with interior angles $2\pi-\gamma$ and $\gamma-\pi$, respectively. Thus, the formulae (2.70) and (2.68) for $X \in \Xi_<(\mathscr{P})$ yield

$$\begin{aligned}\mathrm{b}_0 &= \Big[-\frac{1-(2\pi-\gamma)\cot(2\pi-\gamma)}{2} + 1 - (\gamma-\pi)\cot(\gamma-\pi)\Big] \int_0^\infty dr\, r^3 \check{a}(r)^2 \\ &= \frac{1-\gamma\cot(\gamma)}{2} \int_0^\infty dr\, r^3 \check{a}(r)^2.\end{aligned}$$

This finishes the proof of the lemma. □

Theorem 2.5 follows now from combining Lemmas 2.22 and 2.23.

CHAPTER 3

# One-Dimensional Periodic Schrödinger Operators

Throughout this chapter, we give an introduction to periodic Schrödinger operators in dimension one. This builds the foundation for Chapter 4, where we obtain formulae of Szegő type for these operators. Essentially, the present chapter expands [54, Sec. 2], which is part of joint work with Alexander V. Sobolev. However, we give here a gentler introduction to the material and carry out the proofs in more details.

Let $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R})$ be a real-valued and $2\pi$-periodic function. As in (1.22), we consider the periodic Schrödinger operator

$$H := -\frac{d^2}{dx^2} + V(x),\ \operatorname{dom}(H) = \mathrm{H}^2(\mathbb{R}) \subset \mathrm{L}^2(\mathbb{R}),$$

in dimension one, which constitutes a densely defined operator on $\mathrm{L}^2(\mathbb{R})$. Treating $H$ as a perturbation of the free Laplacian $H_0 := -\frac{d^2}{dx^2}$, which is self-adjoint on $\mathrm{H}^2(\mathbb{R})$, it follows from the Kato-Rellich theorem that $H$ is self-adjoint on the same domain: indeed, $V$ is $H_0$-bounded with relative bound 0, see e.g. [74, Lem. 9.33]. In particular, $H$ is bounded from below. The characteristic properties of the operator $H$ result from its (discrete) translation symmetry, i.e. the fact that $H$ commutes with the shift operator

$$(T_{2\pi}\psi)(x) := \psi(x + 2\pi),\ \psi \in \mathrm{L}^2(\mathbb{R}).$$

The latter suggests that the operators $H$ and $T_{2\pi}$ admit a common basis of generalised eigenfunctions. These can indeed be constructed and will be labelled by the *quasi-momentum* $k \in \mathbb{T} := \mathbb{R}/\mathbb{Z}$, which indicates the corresponding (generalised) eigenvalue $e^{2\pi ik}$ of the operator $T_{2\pi}$. A detailed spectral analysis of $H$ with the help of Floquet-Bloch theory is presented in the next section.

## 3.1. Floquet-Bloch Theory

Throughout this section, we follow the standard references [55, Sec. XIII.16], [75, Sec. 5.6]. However, while the potential $V$ in [55] and [75] is assumed to be piecewise continuous with finite jumps, we stick to the milder assumption $V \in \mathrm{L}^2_{\mathrm{loc}}$. We remark at this point that the proofs of the cited results from [55] all remain valid, replacing the boundedness of $V$ by its relative boundedness with respect to $H_0$. Also the standard ODE theory holds for our class of potentials, see [74, Thm. 9.1].

Define the Floquet-Bloch-Gelfand transform

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

given by

$$(U\psi)(x, k) := \sum_{\gamma \in 2\pi\mathbb{Z}} e^{-ik\gamma}\psi(x + \gamma),\ k \in \mathbb{T},\ x \in [0, 2\pi],$$

for Schwartz class functions or $\mathrm{L}^2(\mathbb{R})$-function with compact support. The operator $U$ is easily checked to extend as a unitary operator to the entire $\mathrm{L}^2(\mathbb{R})$, see [55, Lem., p. 289]. Moreover, the following proposition shows that $U$ decomposes the operator $H$ into operators $H(k)$ corresponding to each quasi-momentum channel $k$.

**Proposition 3.1** ([55, Thm. XIII.88])**.** *Under $U$ the periodic Schrödinger operator $H$ transforms into the direct integral*

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

*with self-adjoint fibres*

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

$$\operatorname{dom}\big(H(k)\big) = \{f \in \mathrm{H}^2(0, 2\pi) : f(2\pi) = e^{2\pi ik}f(0),\ f'(2\pi) = e^{2\pi ik}f'(0)\}, \tag{3.1}$$

*that are well-defined for $k \in \mathbb{T}$.*

**Remark 3.2.** The operator $\int_{\mathbb{T}}^{\oplus} dk\, H(k)$ acts on $g \in \mathrm{L}^2(\mathbb{T}, \mathrm{L}^2(0, 2\pi))$ with $g(k) := g(\,\cdot\,, k) \in \operatorname{dom}(H(k))$ by

$$\Big(\int_{\mathbb{T}}^{\oplus} dk\, H(k)g\Big)(k) = H(k)g(k),\ k \in \mathbb{T}.$$

For an introduction to direct integral operators see [55, pp. 280-287].

The fibre operators $H(k)$ contain all the spectral information for the operator $H$. To begin with, a direct computation shows that, if $V \equiv 0$, the operator $H(k)$ has compact resolvent for each $k \in \mathbb{T}$. Moreover, this resolvent is analytic in $k$ so that $k \mapsto H(k)$ extends to an analytic family in a neighbourhood of $\mathbb{T}$, see [55, Lem.,

p. 292]. These properties carry over to the case $V \not\equiv 0$ using the relative boundedness of $V$ with respect to the unperturbed operator. Consequently, each operator $H(k)$ has a discrete spectrum that consists of eigenvalues

$$\lambda_1(k) \le \lambda_2(k) \le \ldots, \tag{3.2}$$

labelled in ascending order counting multiplicity. Moreover, the standard analytic perturbation theory is applicable to the family of operators $k \mapsto H(k)$. In the following, we will make an extensive analysis of the eigenvalues $\lambda_j(\,\cdot\,)$ and the corresponding eigenspaces. This ultimately leads to the following well-known result, for whose proof we refer to [55].

**Proposition 3.3** ([55, Thm. XIII.90])**.** *The spectrum $\sigma(H)$ of the operator $H$ is purely absolutely continuous. Moreover, let*

$$k_j := \begin{cases} 0, & j \text{ odd}, \\ \frac{1}{2}, & j \text{ even}. \end{cases} \tag{3.3}$$

*and*

$$\mu_j := \lambda_j(k_j),\ \nu_j := \lambda_j\big(k_j + \tfrac{1}{2}\big), \qquad \sigma_j := [\mu_j, \nu_j],\ j = 1, 2, \ldots.$$

*Then $\sigma(H)$ is represented as the union of the spectral bands $\sigma_j$:*

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

*with non-degenerate intervals $\sigma_j$, i.e. $|\sigma_j| > 0$ for every $j = 1, 2, \ldots$.*

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

$$\mathbb{T}_0 := \mathbb{T} \setminus \big(\{0\} \cup \{\tfrac{1}{2}\}\big).$$

**Proposition 3.4.** *Let $H(k)$, $k \in \mathbb{T}$, be as defined above. Then*

*(i) For every $k \in \mathbb{T}$, the operators $H(k)$ and $H(-k)$ are anti-unitarily equivalent under complex conjugation. In particular, one has that $\lambda_j(-k) = \lambda_j(k)$ for all $k \in \mathbb{T}$.*

*(ii) The eigenvalues $\lambda_j(k)$ are continuous functions of $k \in \mathbb{T}$. Moreover, they are simple and analytic on $\mathbb{T}_0$.*

*(iii) For $j$ odd (resp. even), each $\lambda_j(\,\cdot\,)$ is strictly increasing (resp. decreasing) on $(0, \frac{1}{2})$.*

*(iv) If for some $j$ we have that $\lambda_{j-1}(k_j) = \lambda_j(k_j)$, then it holds that*

$$\lambda_l'(k_j\pm) \neq 0, \;\; l = j-1, j. \tag{3.4}$$

*In particular, in a neighbourhood of $k_j$, the eigenvalues $\lambda_{j-1}$ and $\lambda_j$ are analytic continuations of each other.*

**Remark 3.5.** As a consequence of (i)–(iii), we have in Proposition 3.3 that $\nu_j \leq \mu_{j+1}$, $j = 1, 2, \ldots$, and the bands $\sigma_j$ can not overlap, but at most touch. If $\sigma_{j-1}$ and $\sigma_j$ touch, as in (iv), then the analytic continuation of $\lambda_{j-1}$ through $k_j$ is $\lambda_{j+1}$.

Proof. Let us comment on the main ingredients for the proof of the proposition. Properties (i)–(iii) are standard facts, which are proved, for instance, in [55, Thm. XIII.89]. Property (iv) is less well-known; to the author's knowledge, it has not been mentioned in the literature before. As a basis for the proof of (iv) we also paraphrase the ideas for the proofs of (i)–(iii), mainly following [55].

The anti-unitary equivalence (i) follows directly from the definition of $H(k)$ and it implies that the eigenvalues $\lambda_j(k)$, $j = 1, 2, \ldots$, are even functions of $k$.

These eigenvalues can have multiplicity at most 2 since, for every fixed $E \in \mathbb{C}$, the space of solutions to the ODE

$$-u'' + Vu = Eu \tag{3.5}$$

is two-dimensional, see [74, Thm. 9.1]. Besides, the antiunitary equivalence (i) implies that the eigenvalues of $H(k)$ are simple as long as $k \in \mathbb{T}_0$: if $E$ is an eigenvalue for $H(k)$ for some $k \in \mathbb{T}_0$, then it is also an eigenvalue for $H(-k)$ and corresponding eigenfunctions are linearly independent since they satisfy distinct boundary conditions. As mentioned above, $k \mapsto H(k)$ constitutes an analytic family in a neighbourhood of the real axis. Thus, Rellich's theorem, see [56, Satz 2], implies that – away from potential branching points – the eigenvalues of $H(k)$ can be described by analytic functions of $k$. In fact, the self-adjointness of $H(k)$ ensures that no such branching points exist for $k \in \mathbb{T}$, see [35, Ch. II, Thm. 1.10]. In particular, the eigenvalues $\lambda_j(\,\cdot\,)$, $j = 1, 2, \ldots$, are analytic on $\mathbb{T}_0$ since they are simple there. In addition, every eigenvalue $\lambda_j(\,\cdot\,)$ must have analytic continuations through $k = 0$ and $k = \frac{1}{2}$, where it potentially crosses the eigenvalues $\lambda_{j-1}$ or $\lambda_{j+1}$. Looking at $k = k_j$, this

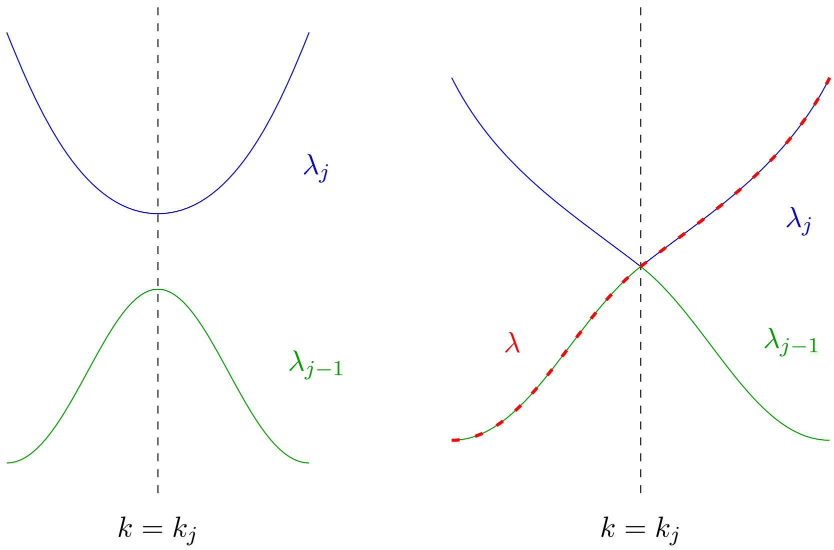


FIGURE 4. Eigenvalues $\lambda_{j-1}$ and $\lambda_j$ around $k = k_j$. If there is a gap between the bands $\sigma_{j-1}$ and $\sigma_j$ (as on the left), then the eigenvalues are analytic at $k = k_j$ with $\lambda_l'(k_j) = 0$ for $l = j-1, j$. However, if the bands $\sigma_{j-1}$ and $\sigma_j$ touch, then $\lambda_l'(k_j\pm) \neq 0$, $l = j-1, j$, and the eigenvalues $\lambda_{j-1}$ and $\lambda_j$ are not analytic at $k_j$, but they are analytic continuations of each other at this point. For instance, the function $\lambda$ (dashed curve) is analytic.

continuation is undoubtedly $\lambda_j$ if $\lambda_j(k_j)$ is simple. However, it might also be $\lambda_{j-1}$ in case $\lambda_{j-1}(k_j) = \lambda_j(k_j)$. In the following, we shall see that the latter is actually the only possible analytic continuation when $\lambda_j(k_j)$ is a double eigenvalue, see also Figure 4. In any case, the functions $\lambda_j(\,\cdot\,)$ are continuous on $\mathbb{T}$, which finishes the proof of (ii).

Property (iii) is more subtle: that $\lambda_1(0)$ constitutes the minimum of the spectrum of $H$ is a consequence of the semi-group $e^{-tH(0)}$, $t > 0$, being positivity improving, which can be proved as in [74, Thm. 10.12]. The monotonicity of the functions $\lambda_j(\cdot)$ then follows from carefully studying the Floquet discriminant for the ODE (3.5), see (3.6).

Assume now that $\lambda_{j-1}(k_j) = \lambda_j(k_j)$ for some $j$, i.e. that $\lambda_j(k_j)$ is a double eigenvalue of $H(k_j)$. By previous arguments, this double eigenvalue is the intersection point of two analytic eigenvalue functions around $k_j$. Let $\lambda = \lambda(k)$ be the analytic eigenvalue on $(k_j - \frac{1}{2}, k_j + \frac{1}{2})$ that coincides with $\lambda_{j-1}$ on $(k_j - \frac{1}{2}, k_j)$.

In order to prove that $\lambda(k) = \lambda_j(k)$ for $k \in (k_j, k_j + \frac{1}{2})$ it suffices to show that $\lambda'(k_j) \neq 0$. For if $\lambda_{j-1}$ was analytic at $k_j$ its axis symmetry around $k_j$ would imply that $0 = \lambda'_{j-1}(k_j) = \lambda'(k_j)$. Let $u_1(x) = u_1(E, x)$, $u_2(x) = u_2(E, x)$ be the unique solutions of (3.5) with $u_1(0) = 1$, $u_1'(0) = 0$, and $u_2(0) = 0$, $u_2'(0) = 1$, respectively. Then the Floquet discriminant for (3.5), defined by

$$D(E) := \operatorname{tr} \begin{pmatrix} u_1(E, 2\pi) & u_2(E, 2\pi) \\ u_1'(E, 2\pi) & u_2'(E, 2\pi) \end{pmatrix} = u_1(E, 2\pi) + u_2'(E, 2\pi), \tag{3.6}$$

is an entire function of $E$, see again [74, Thm. 9.1], and satisfies the relation

$$D(\lambda(k)) = 2\cos(2\pi k) \tag{3.7}$$

in a neighbourhood of $k = k_j$, as well as

$$D(\lambda(k_j)) \in \{-2, 2\}, \; D'(\lambda(k_j)) = 0,$$

see [55, p. 296]. Differentiating (3.7) twice gives

$$D''(\lambda(k))[\lambda'(k)]^2 + D'(\lambda(k))\lambda''(k) = -4\pi^2 D(\lambda(k)),$$

thus at $k = k_j$ one has that

$$D''(\lambda(k_j))[\lambda'(k_j)]^2 = -4\pi^2 D(\lambda(k_j)) \in \{\pm 8\pi^2\}.$$

Consequently, we arrive at

$$[\lambda'(k_j)]^2 = \frac{-4\pi^2 D(\lambda(k_j))}{D''(\lambda(k_j))} \neq 0,$$

hence the analytic continuation of $\lambda_{j-1}$ through $k_j$ is indeed $\lambda_j$ and (3.4) is proved. ☐

It is natural to split the spectrum of $H$ into its connected components, which we will call *genuine (spectral) bands*. Every genuine spectral band $S \subset \sigma(H)$ is a closed interval formed by the finite or infinite union of bands $\sigma_j$, see Proposition 3.3 and Remark 3.5. For a fixed genuine band $S$, define

$$\begin{aligned} j_S :&= \min\{j : \sigma_j \subset S\} \\ n_S :&= \sharp\{j : \sigma_j \subset S\}, \end{aligned} \tag{3.8}$$

so that $S$ is of the form

$$S = \bigcup_{l=0}^{n_S - 1} \sigma_{j_S + l}. \tag{3.9}$$

Note that we have that $\sigma_{j_S-1} \cap \sigma_{j_S} = \emptyset$ (if $j_S \geq 2$) and $\sigma_{j_S+n_S-1} \cap \sigma_{j_S+n_S} = \emptyset$ (if $n_S < \infty$). With the help of Proposition 3.4, we can somewhat simplify the spectral structure of $H$ inside $S$. Indeed, set

$$\kappa = \kappa_S := k_{j_S}, \tag{3.10}$$

see (3.3), and define on $[\kappa_S - n_S/2, \kappa_S + n_S/2]$ the real-valued function $\Lambda(k) = \Lambda^S(k)$ by

$$\begin{aligned} &\Lambda(k) := \lambda_{j_S+l}(k),\ k \in \left[\kappa_S + \frac{l}{2}, \kappa_S + \frac{l+1}{2}\right],\ l = 0, 1, \ldots, n_S - 1, \\ &\Lambda(k) := \Lambda(2\kappa_S - k),\ k \in \left[\kappa_S - \frac{n_S}{2}, \kappa_S\right]. \end{aligned} \tag{3.11}$$

Note that $k \in \mathbb{R}$ is identified here (and in the following) with its fractional part in $\mathbb{T}$ when we evaluate the functions $\lambda_j(\,\cdot\,)$, $j = 0, 1, 2, \ldots,$ or $H(\,\cdot\,)$. According to Proposition 3.4, see also Remark 3.5, the function $\Lambda = \Lambda^S$ is $n_S$-periodic and analytic on the circle $n_S\mathbb{T} = \mathbb{R}/n_S\mathbb{Z}$. Moreover, it is monotonically increasing in $k \in [\kappa_S, \kappa_S + n_S/2]$, and symmetric in $k = \kappa_S$. Here, we use the convention that $\infty\mathbb{T} = \mathbb{R}$ and some of the closed intervals need to be replaced by semi-closed intervals when $n_S = \infty$.

For the fixed genuine band $S$, let us also consider the family of one-dimensional projections $P(k) = P^S(k)$ on $\mathrm{L}^2(0, 2\pi)$ that is analytic on $n_S\mathbb{T}$ and coincides with the eigenprojection for the simple eigenvalue $\Lambda(k)$ of $H(k)$ for $k \in n_S\mathbb{T} \setminus \{\kappa_S \pm \frac{l}{2},\ l = 1, 2, \ldots n_S - 1\}$. This family of projections exists by [35, Thm. 1.10]. The following proposition constructs a corresponding analytic family of normalised eigenfunctions, which has convenient symmetry properties.

**Proposition 3.6.** *Let $S \subset \sigma(H)$ be a genuine spectral band and let $\Lambda = \Lambda^S$ be defined as in* (3.11)*. Consider the analytic family of one-dimensional projections $P(k) = P^S(k)$ from above. Then there exists a corresponding family of eigenfunctions $\Phi(k) = \Phi^S(k) \in \operatorname{ran} P(k)$,*

$$H(k)\Phi(k) = \Lambda(k)\Phi(k),\ k \in n_S\mathbb{T}, \tag{3.12}$$

*such that*

*(i)* $k \mapsto \Phi(k)$ *is $n_S$-periodic in $k$ and analytic as a function $n_S\mathbb{T} \to \mathrm{L}^2(0, 2\pi)$,*

*(ii)* $\Phi(k) \in \operatorname{dom}(H(k))$ *is normalised on $\mathrm{L}^2(0, 2\pi)$,*

*(iii) for all* $k \in n_S\mathbb{T}$*,*

$$\Phi(\kappa_S - k) = \overline{\Phi(\kappa_S + k)}. \tag{3.13}$$

*In particular,* $\Phi(\kappa_S)$ *and (if* $n_S < \infty$*)* $\Phi(\kappa_S + \frac{n_S}{2})$ *are real-valued.*

*Furthermore, we have that, for* $l = 1, 2, \ldots, n_S - 1$*,*

$$\int_0^{2\pi} dx\, \Phi(x, \kappa_S \pm l/2)^2 = 0. \tag{3.14}$$

**Remark 3.7.** (1) To avoid any ambiguity we fix in the following one analytic family of eigenfunctions $\Phi^S(k)$ with the properties stated in Proposition 3.6 for each genuine spectral band $S \subset \sigma(H)$.

(2) In view of (3.11) and Proposition 3.4, for any $l = 1, 2, \ldots, n_S - 1$, the eigenvalue $\Lambda^S(\kappa_S + l/2) = \Lambda^S(\kappa_S - l/2)$ is a double eigenvalue of $H(\kappa_S + l/2)$. Corresponding eigenfunctions are $\Phi^S(\kappa_S + l/2)$ and $\Phi^S(\kappa_S - l/2) = \overline{\Phi^S(\kappa_S + l/2)}$, which form an orthonormal basis of the eigenspace for $\Lambda(\kappa + l/2)$, due to (3.14). Away from these points, the eigenvalues $\Lambda^S(k)$ are simple eigenvalues of $H(k)$ and their eigenspace is spanned by $\Phi^S(k)$.

Proof. Fix a genuine band $S$ and omit the super- and subscripts "$S$" (except for $\kappa_S$) for the duration of the proof. We deal only with the case $n < \infty$; the proof for $n = \infty$ is considerably easier. Since the family of projections $k \mapsto P(k)$ is analytic in a neighbourhood of the real line, [55, Thm. XII.12] implies that there exists an analytic family $\mathcal{U}(k)$ of invertible operators, unitary for $k \in \mathbb{R}$, such that

$$P(\kappa_S + k) = \mathcal{U}(k) P(\kappa_S) \mathcal{U}(k)^{-1}. \tag{3.15}$$

Moreover, one infers from the proof of [55, Thm. XII.12] that the operator $\mathcal{U}(k)$ can be chosen as the unique (analytic) solution of the differential equation

$$\begin{aligned} \mathcal{U}'(k) &= [P'(\kappa_S + k), P(\kappa_S + k)]\mathcal{U}(k), \\ \mathcal{U}(0) &= \mathbb{1}_{\mathrm{L}^2(0,2\pi)}, \end{aligned} \tag{3.16}$$

in a neighbourhood of the real axis. As $k \mapsto P(k)$ is $n$-periodic on $\mathbb{R}$, one has that

$$\mathcal{U}(k + n) = \mathcal{U}(k)\mathcal{U}(n), k \in \mathbb{R}, \tag{3.17}$$

since both sides of (3.17) satisfy (3.16) with initial condition $\mathcal{U}(n)$. In view of Proposition 3.4(i), one has that

$$P(\kappa_S - k) = CP(\kappa_S + k)C,\ \ k \in n\mathbb{T}, \tag{3.18}$$

where $C$ denotes complex conjugation on $\mathrm{L}^2(0, 2\pi)$. In particular, we can choose a real-valued and normalised eigenfunction $\Phi_0(\kappa_S)$ from the one-dimensional space $\operatorname{ran} P(\kappa_S) = \overline{\operatorname{ran} P(\kappa_S)}$. Define

$$\Phi_0(\kappa_S + k) := \mathcal{U}(k)\Phi_0(\kappa_S),\ \ k \in \mathbb{R}$$

so that, due to (3.15), $\Phi_0(k) \in \operatorname{ran} P(k)$ for all $k \in n\mathbb{T}$. Thus, $\Phi_0(k)$ is a normalised eigenfunction of $H(k)$, which satisfies (3.12). Notice also that $\Phi_0(\kappa_S + n) \in \operatorname{ran} P(\kappa_S + n) = \operatorname{ran} P(\kappa_S)$ so that $\Phi_0(\kappa_S + n) = e^{i\theta}\Phi_0(\kappa_S)$ for some $\theta \in [0, 2\pi)$. Hence setting

$$\Phi(\kappa_S + k) := e^{-ik\theta/n}\Phi_0(\kappa_S + k),$$

we get from (3.17) that for all $k \in \mathbb{R}$,

$$\begin{aligned}\Phi(\kappa_S + k + n) &= e^{-i(k+n)\theta/n}\mathcal{U}(k)\mathcal{U}(n)\Phi_0(\kappa_S) = e^{-i(k+n)\theta/n}\mathcal{U}(k)\Phi_0(\kappa_S + n)\\ &= e^{-ik\theta/n}\mathcal{U}(k)\Phi_0(\kappa_S) = \Phi(\kappa_S + k).\end{aligned}$$

So, we have constructed an $n$-periodic analytic family of eigenfunctions $k \mapsto \Phi(k)$ that satisfies (3.12), (i), and (ii). For its symmetry properties notice first that (3.18) and unique analytic continuation imply that

$$P(\kappa_S - k) = CP(\kappa_S + \bar{k})C,$$

for $k$ in a neighbourhood of the real axis. From this we also get that

$$\mathcal{U}(-k) = C\mathcal{U}(\bar{k})C, \tag{3.19}$$

in a neighbourhood of $\mathbb{R}$ since, due to (3.16), both sides of (3.19) solve the differential equation

$$\begin{aligned}&\mathcal{V}'(k) = -[P'(\kappa_S - k), P(\kappa_S - k)]\mathcal{V}(k),\\ &\mathcal{V}(0) = \mathbb{1}_{\mathrm{L}^2(0,2\pi)}.\end{aligned}$$

This equation has again a unique analytic solution $\mathcal{V}(k)$ in a neighbourhood of the real axis, see [55, Lem., p. 23]. Hence, for $k \in \mathbb{R}$, we arrive at

$$\overline{\Phi_0(\kappa_S + k)} = C\mathcal{U}(k)\Phi_0(\kappa_S) = C\mathcal{U}(k)C\Phi_0(\kappa_S) = \mathcal{U}(-k)\Phi_0(\kappa_S) = \Phi_0(\kappa_S - k),$$

and $\overline{\Phi(\kappa_S + k)} = \Phi(\kappa_S - k)$ follows.

Finally, fix $l \in \{1, 2, \dots, n-1\}$ and let $\epsilon \in (0, \frac{1}{2})$. Then one has that

$$\Lambda(\kappa_S + \tfrac{l}{2} - \epsilon) = \lambda_{j+l-1}(\kappa_S + \tfrac{l}{2} - \epsilon)$$

and

$$\Lambda(\kappa_S - \tfrac{l}{2} - \epsilon) = \Lambda(\kappa_S + \tfrac{l}{2} + \epsilon) = \lambda_{j+l}(\kappa_S + \tfrac{l}{2} + \epsilon) = \lambda_{j+l}(\kappa_S + \tfrac{l}{2} - \epsilon),$$

where we used for the last equality that $\lambda_{j+l}$ is a 1-periodic, even function. Thus, the eigenspaces $\operatorname{ran} P(\kappa_S + \frac{l}{2} - \epsilon)$ and $\operatorname{ran} P(\kappa_S - \frac{l}{2} - \epsilon)$ correspond to distinct eigenvalues of $H(\kappa_S + \frac{l}{2} - \epsilon) = H(\kappa_S - \frac{l}{2} - \epsilon)$ and are, therefore, orthogonal to each other. Consequently, we get that

$$0 = \big\langle \Phi(\kappa_S - \tfrac{l}{2} - \epsilon), \Phi(\kappa_S + \tfrac{l}{2} - \epsilon) \big\rangle_{\mathrm{L}^2(0,2\pi)} = \int_0^{2\pi} dx\, \Phi(x, \kappa_S + \tfrac{l}{2} + \epsilon)\Phi(x, \kappa_S + \tfrac{l}{2} - \epsilon),$$

which, together with (3.13), yields (3.14) in the limit $\epsilon \searrow 0$. This finishes the proof of the proposition. □

It will be useful to extend the Bloch eigenfunctions $\Phi(k) = \Phi^S(k) \in \mathrm{H}^2(0, 2\pi)$ from Proposition 3.6 to functions on the whole real line. For this purpose, we introduce the functions

$$E(x, k) = E^S(x, k) := e^{-ixk}\Phi^S(x, k), \tag{3.20}$$

for $x \in [0, 2\pi]$ and $k \in n_S\mathbb{T}$, which have the same regularity properties as the Bloch eigenfunctions. As for fixed $k$, $\Phi^S(k) \in \operatorname{dom}(H(k)) \subset \mathrm{C}^1[0, 2\pi]$, it follows from the imposed boundary conditions that the functions $E^S(k) := E^S(\,\cdot\,, k)$, $k \in n_S\mathbb{T}$, extend to $2\pi$-periodic $\mathrm{C}^1$-functions on the real line. This induces a corresponding extension of the functions $\Phi^S(k)$. Slightly abusing notation, these extensions are again denoted by $E^S(k)$ and $\Phi^S(k)$, respectively. The following technical lemma will be useful in Chapter 4. It provides further information on the regularity of the functions $E^S$ and $\Phi^S$, also depending on the regularity of the potential $V$.

**Lemma 3.8.** *Let $S \subset \sigma(H)$ be a genuine spectral band. Then the functions*

$$(x, k) \mapsto \Phi^S(x, k) \quad \text{and} \quad (x, k) \mapsto \partial_k^m E^S(x, k),$$

*$m = 0, 1, 2, \dots,$ are continuous and infinitely differentiable with respect to the $k$-variable as functions $\mathbb{R} \times n_S\mathbb{T} \to \mathbb{C}$. They are uniformly bounded on $\mathbb{R} \times K$ for*

*any compact subset $K \subseteq n_S\mathbb{T}$. Moreover, if $V \in \mathrm{C}^\infty(\mathbb{R})$, then we have that $E^S$, $\Phi^S \in \mathrm{C}^\infty(\mathbb{R} \times n_S\mathbb{T})$.*

Proof. Let us again fix the genuine band $S$ and omit all super- and subscripts "$S$" during this proof. Also, we restrict ourselves to the case $n < \infty$; otherwise replace in the following $n\mathbb{T}$ by a compact subset $K \subset \mathbb{R}$. As the functions $E(k)$, $k \in n\mathbb{T}$, are $2\pi$-periodic and continuously differentiable, we can expand them into a uniformly convergent Fourier series

$$E(x,k) = \frac{1}{2\pi} \sum_{l \in \mathbb{Z}} a_l(k) e^{ilx}, \tag{3.21}$$

$(x,k) \in \mathbb{R} \times n\mathbb{T}$, with

$$a_l(k) = \int_0^{2\pi} dx\, e^{-ilx} E(x,k).$$

In view of Proposition 3.6(i), the coefficients $a_l(k)$ are analytic functions of $k$. Moreover, integrating by parts twice, we get that

$$\begin{aligned} a_l(k) &= \int_0^{2\pi} dx\, e^{-i(k+l)x} \Phi(x,k) \\ &= \frac{1}{i(k+l)} \int_0^{2\pi} dx\, e^{-i(k+l)x} \partial_x \Phi(x,k) \\ &= \frac{-1}{(k+l)^2} \int_0^{2\pi} dx\, e^{-i(k+l)x} \partial_x^2 \Phi(x,k), \end{aligned}$$

for $l \neq -k$. Here, the boundary terms vanish since $\partial_x^r \Phi(x+2\pi,k) = e^{2\pi k i} \partial_x^r \Phi(x,k)$, $r = 0,1$, for all $x,k$. Due to the eigenvalue equation (3.12), the coefficients $a_l(k)$ may be rewritten as

$$a_l(k) = \frac{1}{(k+l)^2} \int_0^{2\pi} dx\, e^{-i(l+k)x} \big[\Lambda(k) - V(x)\big] \Phi(x,k). \tag{3.22}$$

This yields the bounds

$$|\partial_k^m a_l(k)| \lesssim \langle l \rangle^{-2},\ m = 0,1,2,\ldots, \tag{3.23}$$

with implied constants continuously depending on $m$, $\|V\|_{\mathrm{L}^2(0,2\pi)}$, the derivatives $\partial_k^r \Lambda(k)$, and the norms $\|\partial_k^r \Phi(k)\|_{\mathrm{L}^2(0,2\pi)}$, for $r = 0, \ldots m$. In particular, the estimate (3.23) is uniform on $n\mathbb{T}$. Together with the representation (3.21) this implies the (classical) infinite differentiability of $E^S$ and $\Phi^S$ with respect to the $k$-variable as well as the (joint) continuity of $\partial_k^m E$ and $\partial_k^m \Phi$, $m = 0, 1, 2, \dots$. Furthermore, the uniform boundedness of the functions $\partial_k^m E$, $m = 0, 1, 2, \dots$, follows from their periodicity in $x$. This, in turn, implies the uniform boundedness of the function $\Phi$. If the potential $V$ is smooth, then one can continue integrating by parts in (3.22) to prove super-polynomial $l$-decay of the coefficients $a_l(k)$, locally uniformly in $k$. An estimate of similar nature can be obtained for their $k$-derivatives. Thus, the function $(x, k) \mapsto E(x, k)$ is smooth in this case, finishing the proof of the lemma. □

**3.1.1. Mean values of Bloch eigenfunctions.** As the functions $E^S(k)$, $k \in n_S\mathbb{T}$, have uniformly convergent Fourier series, the functions $\Phi^S(k)$, $k \in n_S\mathbb{T}$, belong to the algebra CAP($\mathbb{R}$) of uniformly almost-periodic functions on $\mathbb{R}$. These are defined as the closure of the span of exponentials $e^{ix\xi}$, $\xi \in \mathbb{R}$, in the $\mathrm{L}^\infty$-norm. We refer to [70] or [69] for an introduction to almost periodic functions and their properties. For any $f \in \mathrm{CAP}(\mathbb{R})$, the *almost-periodic mean*

$$\mathcal{M}(f) := \lim_{T\to\infty} (2T)^{-1} \int_{-T}^{T} dt\, f(t) \tag{3.24}$$

is well-defined. For future use we need to evaluate some means for the eigenfunctions $\Phi^S(k)$.

**Lemma 3.9.** *Let $k \mapsto \Phi(k) = \Phi^S(k)$ be the family of eigenfunctions associated with a genuine band $S \subset \sigma(H)$, see Proposition 3.6. Then one has that*

$$\mathcal{M}(|\Phi(k)|^2) = \frac{1}{2\pi}, \ \forall k \in n_S\mathbb{T}, \tag{3.25}$$

*and*

$$\mathcal{M}(\Phi^2(k)) = 0, \ \forall k \neq \kappa_S, k \neq \kappa_S + n_S/2. \tag{3.26}$$

Proof. We again omit super- and subscripts "$S$". In view of Proposition 3.6(ii), the functions $\Phi(k)$, $k \in n\mathbb{T}$, are normalised in $\mathrm{L}^2(0, 2\pi)$, whence $\mathcal{M}(|\Phi|^2) = (2\pi)^{-1}$, as claimed in (3.25).

To prove (3.26), suppose first that $2k \not\equiv 0 \mod \mathbb{Z}$, so that $k \neq \kappa \pm l/2$, $l = 0, 1, \dots, n$. We use the representation (3.20), so

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

The function $w = E(k)^2$ is again continuously differentiable and $2\pi$-periodic, thus its Fourier series is uniformly convergent. Hence, picking an $\varepsilon > 0$, we can approximate $w$ by a trigonometric polynomial

$$p(x) = \sum_{s=-N}^{N} p_s e^{isx},$$

so that $|w - p| < \epsilon$. Let us find the mean for each component of the polynomial $p$ separately:

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

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

$$|\mathcal{M}(\Phi^2(k))| = |\mathcal{M}(e^{2ikx}(w-p))| \le \varepsilon.$$

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

Finally, the equality $\mathcal{M}(\Phi^2(k)) = 0$ at the points $k = \kappa \pm l/2$, $l = 1, 2, \dots, (n-1)$ follows from (3.14). This leads to (3.26) again and finishes the proof of the lemma. □

**3.1.2. The integrated density of states.** 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:*

$$N(\mu; H) := \frac{1}{2\pi}\int_{\mathbb{T}} dk\, N(\mu, k). \tag{3.27}$$

In view of Proposition 3.4(iii), the function $\mu \mapsto N(\mu; H)$ is continuous. The definition (3.27) 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. [70, Thm. 4.2] or [55, Ch. XIII]. Moreover, with the eigenvalues $\Lambda^S(k)$, see (3.11), we may rewrite (3.27) as

$$N(\mu; H) = \frac{1}{2\pi}\sum_{\substack{S \subset \sigma(H)\\ \text{genuine}}} \big|\{k \in n_S\mathbb{T} : \Lambda^S(k) < \mu\}\big|. \tag{3.28}$$

## 3.2. The Kernel of the Spectral Projection

Using the eigenfunctions $\Phi^S(k)$ for each genuine band $S$, we can write out the kernel $P_\mu(x,y)$ of the spectral projection $P_\mu = \chi_{(-\infty,\mu)}(H)$.

**Lemma 3.10.** *Let $\mu \in \mathbb{R}$. Moreover, let $P_\mu[S] := \chi_{(-\infty,\mu)\cap S}(H)$ be the spectral projection corresponding to each genuine band $S \subset \sigma(H)$. Then the operator $P_\mu$ has the integral kernel*

$$P_\mu(x,y) = \sum_{\substack{S\subset\sigma(H)\\ \text{genuine}}} P_\mu[S](x,y)$$

*with*

$$P_\mu[S](x,y) = \int\limits_{k\in n_S\mathbb{T}:\Lambda^S(k)<\mu} dk\ \Phi^S(x,k)\overline{\Phi^S(y,k)}, \tag{3.29}$$

*and the functions $\Phi^S$ as constructed in Proposition 3.6.*

Proof. It suffices to check formula (3.29) for a fixed genuine band $S$. To this end, we compute the quadratic form of $P_\mu[S]$ for compactly supported functions $f, g \in \mathrm{L}^2(\mathbb{R})$. As before, let $U$ denote the Floquet-Bloch-Gelfand transform, set $S_\mu := S \cap (-\infty,\mu)$, and note that

$$P_\mu[S] = U^*\chi_{S_\mu}(UHU^*)U = U^*\Big(\int_{\mathbb{T}}^{\oplus} dk\,\chi_{S_\mu}(H(k))\Big)U,$$

by the functional calculus for direct integral operators, see [55, Thm. XIII.85]. In view of Proposition 3.6, we have that, for all $k \in \mathbb{T}$,

$$\chi_{S_\mu}(H(k)) = \sum_{l=0}^{n_S-1} \chi_{(-\infty,\mu)}(\Lambda^S(k+l))P^S(k+l),$$

where $P^S(k+l)$ is the one-dimensional orthogonal projection onto $\Phi^S(k+l)$. Thus, one gets that

$$\begin{aligned}\langle f, P_\mu[S]g\rangle_{\mathrm{L}^2(\mathbb{R})} &= \Big\langle Uf, \Big(\int_{\mathbb{T}}^{\oplus} dk\,\chi_{S_\mu}(H(k))\Big)Ug\Big\rangle_{\mathrm{L}^2(\mathbb{T},\mathrm{L}^2(0,2\pi))}\\ &= \sum_{l=0}^{n_S-1}\int_{\mathbb{T}} dk\,\chi_{(-\infty,\mu)}(\Lambda^S(k+l))\big\langle (Uf)(k), P^S(k+l)(Ug)(k)\big\rangle_{\mathrm{L}^2(0,2\pi)}\\ &= \int_{n_S\mathbb{T}} dk\,\chi_{(-\infty,\mu)}(\Lambda^S(k))\big\langle (Uf)(k), P^S(k)(Ug)(k)\big\rangle_{\mathrm{L}^2(0,2\pi)}.\end{aligned} \tag{3.30}$$

Furthermore, note that

$$\big\langle (Uf)(k), P^S(k)(Ug)(k)\big\rangle_{\mathrm{L}^2(0,2\pi)} = \big\langle (Uf)(k), \Phi^S(k)\rangle_{\mathrm{L}^2(0,2\pi)} \times \langle \Phi^S(k), (Ug)(k)\big\rangle_{\mathrm{L}^2(0,2\pi)}, \tag{3.31}$$

with

$$\begin{aligned}\big\langle \Phi^S(k), (Ug)(k)\big\rangle_{\mathrm{L}^2(0,2\pi)} &= \int_0^{2\pi} dx\, \overline{\Phi^S(x,k)} \sum_{\gamma\in 2\pi\mathbb{Z}} e^{-ik\gamma} g(x+\gamma) \\ &= \sum_{\gamma\in 2\pi\mathbb{Z}} \int_0^{2\pi} dx\, \overline{\Phi^S(x+\gamma,k)} g(x+\gamma) \\ &= \langle \Phi^S(k), g\rangle_{\mathrm{L}^2(\mathbb{R})}.\end{aligned} \tag{3.32}$$

Due to Lemma 3.8, the function $(x,k)\mapsto \Phi^S(x,k)$ is uniformly bounded on $\mathbb{R}\times \big(\Lambda^S\big)^{-1}\big((-\infty,\mu]\big)$, thus combining (3.30), (3.31), and (3.32) and an application of Fubini's theorem yields (3.29). □

CHAPTER 4

# Formulae of Szegő Type for the Periodic Schrödinger Operator

The purpose of this chapter is to obtain the asymptotic trace formulae (1.24) and (1.25) for the periodic Schrödinger operator in dimension one. In doing so, we will extensively rely on the Floquet-Bloch theory introduced in Chapter 3. Most of the present chapter coincides with parts of the paper [54], which is joint work with A.V. Sobolev. We start by formulating the main results in all details.

## 4.1. Main Result

Let $H = -\frac{d^2}{dx^2} + V$ be the periodic Schrödinger operator defined in (1.22). Moreover, recall the notation $P_\mu$ for its spectral projection as well as the abbreviation $B_{L,\mu} = \chi_{(-L,L)} P_\mu \chi_{(-L,L)}$ for the spatial truncation of $P_\mu$. Notice that, as both $P_\mu$ and $\chi_{(-L,L)}$ are projections, one has that $0 \leq B_{L,\mu} \leq 1$. We prove trace asymptotics for the operators $h\big(B_{L,\mu}\big)$ with test functions $h$ that satisfy the following condition.

**Condition 4.1.** *The function $h : [0,1] \mapsto \mathbb{C}$ is piecewise continuous, it is Hölder continuous at $t = 0$ and $1$, and $h(0) = 0$.*

For such functions $h$, the integral

$$\mathcal{W}(h) = \frac{1}{\pi^2} \int_0^1 dt \, \frac{[h(t) - th(1)]}{t(1-t)}, \tag{4.1}$$

see also (1.10), is well-defined. The next theorem is the main result of this chapter.

**Theorem 4.2.** *Let $H$ be the operator defined in (1.22) and suppose that $V \in \mathrm{C}^\infty(\mathbb{R})$. Assume that the function $h$ satisfies Condition 4.1. Then for any $\mu \in \big(\sigma(H)\big)^\circ$, we have the asymptotic formula*

$$\operatorname{tr}[h(B_{L,\mu})] = 2Lh(1)N(\mu, H) + \log(L)\mathcal{W}(h) + o(\log(L)), \ \text{as } L \to \infty. \tag{4.2}$$

*If* $\mu \notin \big(\sigma(H)\big)^\circ$*, then*

$$\operatorname{tr}[h(B_{L,\mu})] = 2Lh(1)N(\mu, H) + \mathcal{O}(1), \ \text{as } L \to \infty. \tag{4.3}$$

*Here,* $\big(\sigma(H)\big)^\circ$ *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* (3.27)*.*

**Remark 4.3.** (1) To emphasize the dependence of the asymptotics on the spectral parameter $\mu$ consider a test function $h$ such that $h(0) = h(1) = 0$. Then $\operatorname{tr} h(B_{L,\mu})$ remains bounded if $\mu$ is in a spectral gap. If however, $\mu$ is inside a spectral band, then the asymptotics are exactly as in the case $V \equiv 0$, described by the formula (1.9).

(2) Notice that the coefficient $\mathcal{W}(h)$ in (4.2) vanishes for test functions $h$ that are point-symmetric around $t = 1/2$, i.e. satisfy $h(t) = -h(1-t)$. Thus, for $\mu \in \sigma(H)^\circ$ the spectrum of the operator $B_{L,\mu}$ (in every interval $(\epsilon, 1-\epsilon)$, for fixed $\epsilon > 0$) is to leading order symmetric around $1/2$, as $L$ tends to infinity.

(3) We point out that the function $h$ in Theorem 4.2 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 $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R})$. This can be observed at the first step of Section 4.7, where we take the closure of the asymptotics, starting from polynomial test functions $h$. The increased smoothness of $V$, i.e. the condition $V \in \mathrm{C}^\infty(\mathbb{R})$, is required to handle functions $h$ that are only Hölder-continuous at $t = 0, 1$. To be precise, a finite smoothness of $V$, depending on the Hölder exponent, would be sufficient, but we do not go into these details to avoid excessive technicalities.

Let us describe the strategy of the proof of Theorem 4.2, focusing on the case where $\mu \in \big(\sigma(H)\big)^\circ$. The proof of (4.3) is considerably easier, and we do not comment on it now.

To prove formula (4.2) we proceed in three steps. First we represent the function $h$ as the sum

$$h(t) = th(1) + h_0(t) \tag{4.4}$$

so that the function $h_0$ satisfies Condition 4.1 and, in addition, $h_0(1) = 0$. The function $th(1)$ is responsible for the first term in (4.2) and the trace asymptotics for this function are found easily, see Section 4.2.

The analysis of the asymptotic behaviour of $\operatorname{tr} h_0(B_{L,\mu})$, which yields the logarithmic correction in (4.2), is the second and main part of the proof. Here, we follow the strategy of [41], where the asymptotics (1.9) were derived. As in [41], we focus first on polynomial functions $h_0$, 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 [41] is not directly applicable since the kernel of the operator $B_{L,\mu}$ contains the Bloch eigenfunctions of $H$ instead of plain waves. One of the central points of our proof is to show that, at the cost of constant order errors in trace norm, for the operators $p_n(B_{L,\mu})$ one can replace terms involving Bloch eigenfunctions by their mean values. This reduces the problem to the case $V \equiv 0$, and enables us to use the known formula (1.9) 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 [41], the reflection symmetry and translation invariance of $H$, which were essential for [41], are not available in our problem.

At the final stage of the proof we extend the asymptotics to functions $h_0$ satisfying Condition 4.1. To this end, we approximate $h_0$ 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 $o(\log(L))$ with the help of bounds for pseudo-differential operators in Schatten-von Neumann classes obtained in [65]. The required extension of the bounds from [65] to the periodic setting is relatively straightforward. This finishes the proof.

## 4.2. The Leading Order Term in the Trace Asymptotics

Having established Lemma 3.10 for the kernel of the spectral projection $P_\mu$, we can already prove Theorem 4.2 for the special case $h(t) = t$. Via the decomposition (4.4) this gives the main term in the trace asymptotics (4.2), (4.3), as explained above. Indeed, according to Lemma 3.10,

$$\|B_{L,\mu}\|_{\mathfrak{S}_1} = \operatorname{tr} B_{L,\mu} = \sum_{\substack{S \subset \sigma(H) \\ \text{genuine}}} \operatorname{tr} \big(\chi_{(-L,L)} P_\mu[S] \chi_{(-L,L)}\big),$$

with

$$\operatorname{tr}\left(\chi_{(-L,L)}P_\mu[S]\chi_{(-L,L)}\right) = \int_{-L}^{L} dx \int_{n_S\mathbb{T}} dk\, \chi_{(-\infty,\mu)}(\Lambda^S(k))|\Phi^S(x,k)|^2.$$

Assume first that $L$ is a multiple of $2\pi$. Since the function $\Phi^S(k)$ is normalized on $(0, 2\pi)$, it follows from Fubini's theorem and (3.28) that

$$\operatorname{tr} B_{L,\mu} = \frac{L}{\pi} \sum_S \left|\{k \in n_S\mathbb{T} : \Lambda^S(k) < \mu\}\right| = 2LN(\mu, H).$$

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

$$4\pi \left\lfloor \frac{L}{2\pi} \right\rfloor N(\mu, H) \le \operatorname{tr} B_{L,\mu} \le 4\pi \left\lceil \frac{L}{2\pi} \right\rceil N(\mu, H), \ \forall L > 1. \tag{4.5}$$

Consequently, we conclude that

$$\operatorname{tr} B_{L,\mu} = 2LN(\mu, H) + \mathcal{O}(1), \text{ as } L \to \infty.$$

The study of $\operatorname{tr} h_0(B_{L,\mu})$ is much more difficult, and the rest of Chapter 4 is focused on this task.

## 4.3. An Expansion of the Integral Kernel of the Spectral Projection

Let us from now on assume that $\mu \in \sigma(H)$. Namely, if $\mu < \min \sigma(H)$, then Theorem 4.2 becomes trivial, and if $\mu$ lies in a spectral gap we can simply replace it by the maximum of the band below $\mu$. So, let $S$ be the genuine band (i.e. the connected component) of $\sigma(H)$ that contains $\mu$. Inspecting the formula (3.11), we observe that the set $\{k \in n_S\mathbb{T} : \Lambda^S(k) < \mu\}$ is the interval $(2\kappa_S - \delta, \delta)$ where $\delta = \delta(\mu) \in [\kappa_S, \kappa_S + n_S/2]$ is the uniquely defined value such that $\Lambda^S(\delta) = \mu$. The following lemma provides a convenient expansion of the kernel $P_\mu[S](x, y)$, see (3.29), in powers of $|x - y|^{-1}$.

**Lemma 4.4.** *Let $\mu \in S \subset \sigma(H)$, where $S$ is a genuine spectral band, and let $\delta = \delta(\mu)$ be as defined above. Then for all $x$, $y \in \mathbb{R}$, we have*

$$P_\mu[S](x, y) = \Pi_\mu(x, y) + R_\mu[S](x, y), \tag{4.6}$$

*where*

$$\Pi_\mu(x, y) := \frac{\Phi^S(x,\delta)\overline{\Phi^S(y,\delta)} - \overline{\Phi^S(x,\delta)}\Phi^S(y,\delta)}{i(x-y)}, \tag{4.7}$$

*and*

$$R_\mu[S](x,y) = \mathcal{O}\big((1+|x-y|^2)^{-1}\big), \ \forall x,y \in \mathbb{R}. \tag{4.8}$$

*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*

$$|P_\mu[S](x,y)| + |\Pi_\mu(x,y)| = \mathcal{O}\big((1+|x-y|)^{-1}\big), \ \forall x,y \in \mathbb{R}. \tag{4.9}$$

*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*

$$P_\mu[S](x,y) = \mathcal{O}\big((1+|x-y|^2)^{-1}\big), \ \forall x,y \in \mathbb{R}. \tag{4.10}$$

**Remark 4.5.** If $\mu \notin S^\circ$, then $P_\mu[S](x,y)$ actually decays super-polynomially, as $|x-y| \to \infty$. This is easily deduced from formula (3.29), the fact that $k \mapsto \Phi^S(k)$ is analytic on $n_S\mathbb{T}$, and successive integration by parts as in the proof of the lemma. However, the bound (4.10) suffices for our purposes.

Proof. Let us deduce Estimate (4.10) first. Observe that if $\mu \notin S^\circ$, then either $\mu = \min S$ and $P_\mu[S] = 0$, or $\mu = \max S < \infty$ and $\delta(\mu) = \kappa_S + n_S/2$. In the first case, the bound (4.10) is trivial. In the second case, the function $\Phi^S(\delta)$ is real-valued, see Proposition 3.6(iii). Hence, $\Pi_\mu(x,y) = 0$, and the bound (4.10) follows from (4.6) and (4.8).

It remains to prove the continuity and the bounds (4.8) and (4.9) for $\mu \in S$. Note that the kernel $P_\mu[S](x,y)$ (see (3.29)) is continuous and uniformly bounded in $x,y$ since, due to Lemma 3.8, the function $(x,k) \mapsto \Phi^S(x,k)$ is uniformly bounded on $\mathbb{R} \times (2\kappa_S - \delta, \delta)$ and continuous. For the same reason, the kernel (4.7) is continuous and bounded by $|x-y|^{-1}$ for all $x,y : |x-y| \geq 1$. Due to the continuity of both $\Phi^S(\delta)$ and $\partial_x\Phi^S(\delta)$, the kernel (4.7) is also continuous and uniformly bounded for $|x-y| < 1$. As a consequence, the kernel $\Pi_\mu(x,y)$ satisfies (4.9), and the remainder $R_\mu[S](x,y)$ is continuous and uniformly bounded. Thus it remains to prove (4.9) for $P_\mu[S](x,y)$ and the bound (4.8), both when $|x-y| \geq 1$.

Using (3.20), we rewrite

$$P_\mu[S](x,y) = \int\limits_{2\kappa_S-\delta}^{\delta} dk\, e^{ik(x-y)} E^S(x,k)\overline{E^S(y,k)}, \tag{4.11}$$

and, for $|x-y|\ge 1$, integrate by parts to arrive at

$$P_\mu[S](x,y) = \frac{e^{i\delta(x-y)}}{i(x-y)} E^S(x,\delta)\overline{E^S(y,\delta)} - \frac{e^{i(2\kappa_S-\delta)(x-y)}}{i(x-y)} E^S(x,2\kappa_S-\delta)\overline{E^S(y,2\kappa_S-\delta)} + R_\mu[S](x,y)$$

with

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

Due to (3.20) and the symmetry property (3.13), one obtains the representation (4.6). Another integration by parts for $R_\mu[S]$ gives

$$R_\mu[S](x,y) = \left.\frac{e^{ik(x-y)}\partial_k\big(E^S(x,k)\overline{E^S(y,k)}\big)}{(x-y)^2}\right|_{2\kappa_S-\delta}^{\delta} - \int_{2\kappa_S-\delta}^{\delta} dk\, \frac{e^{ik(x-y)}}{(x-y)^2}\partial_k^2\big(E^S(x,k)\overline{E^S(y,k)}\big).$$

Hence, the estimate (4.8) follows from the fact that the functions $E^S$, $\partial_k E^S$, and $\partial_k^2 E^S$ are uniformly bounded on $\mathbb{R}\times(2\kappa_S-\delta,\delta)$, see Lemma 3.8. □

Now, Lemma 4.4 may be used for each genuine spectral band separately to get the corresponding expansion of the kernel $P_\mu(x,y)$.

**Lemma 4.6.** *Let $\mu\in S\subset\sigma(H)$, where $S$ is a genuine spectral band, and let $\delta=\delta(\mu)$ be as defined above. Then for all $x$, $y\in\mathbb{R}$ we have*

$$P_\mu(x,y) = \Pi_\mu(x,y) + R_\mu(x,y), \tag{4.12}$$

*where $\Pi_\mu$ is as defined in (4.7), and*

$$R_\mu(x,y) = \mathcal{O}\big((1+|x-y|^2)^{-1}\big),\ \forall x,y\in\mathbb{R}. \tag{4.13}$$

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

$$|P_\mu(x,y)| + |\Pi_\mu(x,y)| = \mathcal{O}\big((1+|x-y|)^{-1}\big),\ \forall x,y\in\mathbb{R}. \tag{4.14}$$

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

$$P_\mu(x,y) = \mathcal{O}\big((1+|x-y|^2)^{-1}\big),\ \forall x,y\in\mathbb{R}. \tag{4.15}$$

**Remark 4.7.** Again, the decay in (4.15) is actually super-polynomial away from the diagonal.

Proof. The continuity of the kernel $P_\mu(x,y)$ follows immediately from the previous lemma. Moreover, if $\mu \notin \big(\sigma(H)\big)^\circ$, then (4.15) follows directly from (4.10).

Assume now that $\mu \in S \subset \sigma(H)$. Let $S_1, S_2, \dots, S_N$, be genuine spectral bands lying below the band $S$. With the notation of Lemma 4.4 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 4.4, the kernel $R_\mu[S]$ and each term $P_\mu[S_l] = P_{\max S_l}[S_l]$, $l = 1, 2, \dots, N$ satisfy (4.13), whence (4.12). The bound (4.14) for the kernel $P_\mu[S](x,y)$ follows from (4.9). □

## 4.4. Elementary Trace Norm Estimates

Throughout the proof of Theorem 4.2 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 [41]. 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

$$\chi_I P_\mu \chi_J P_\mu \chi_K, \tag{4.16}$$

where $I, J, K \subset \mathbb{R}$ are some intervals that may depend on the parameter $L > 0$. While in this section we limit ourselves to estimates in the trace class $\mathfrak{S}_1$, Section 4.5 treats operators in the classes $\mathfrak{S}_q$ for $q \in (0,1]$.

The next basic trace class estimate (see [41, Eq. (12)]) plays a central role in this section. We provide a proof for the reader's convenience.

**Lemma 4.8.** *Let* $\mathsf{M} \subset \mathbb{R}$ *be a Borel-measurable set. Consider (weakly) measurable mappings* $f, g : \mathsf{M} \mapsto \mathrm{L}^2(\mathbb{R})$*, such that*

$$\int\limits_{\mathsf{M}} dz \, \|f(z)\|_{\mathrm{L}^2} \|g(z)\|_{\mathrm{L}^2} < \infty.$$

*Then the operator* $A : \mathrm{L}^2(\mathbb{R}) \to \mathrm{L}^2(\mathbb{R})$ *which is defined via the form*

$$\langle u, Av \rangle_{\mathrm{L}^2} := \int\limits_{\mathsf{M}} dz \, \langle u, f(z) \rangle_{\mathrm{L}^2} \langle g(z), v \rangle_{\mathrm{L}^2}, \; u, v \in \mathrm{L}^2(\mathbb{R}),$$

*is of trace class with*

$$\|A\|_1 \leq \int\limits_{\mathsf{M}} dz \, \|f(z)\|_{\mathrm{L}^2} \|g(z)\|_{\mathrm{L}^2}.$$

Proof. Let $(d_n)_n$ and $(e_n)_n$ be orthonormal bases (ONB's) of $\mathrm{L}^2(\mathbb{R})$ and denote by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ the scalar product and the norm on $\mathrm{L}^2(\mathbb{R})$, respectively. Then we have that

$$\begin{aligned} \sum_n \big| \langle d_n, A e_n \rangle \big| &\leq \sum_n \int_{\mathsf{M}} dz \, \big| \langle d_n, f(z) \rangle \langle g(z), e_n \rangle \big| \\ &= \int_{\mathsf{M}} dz \sum_n \big| \langle d_n, f(z) \rangle \langle g(z), e_n \rangle \big|. \end{aligned}$$

Moreover, the Cauchy-Schwartz inequality and Parseval's identity yield

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

implying that

$$\sum_n \big| \langle d_n, A e_n \rangle \big| \leq \int\limits_{\mathsf{M}} dz \, \|f(z)\| \, \|g(z)\|.$$

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

Equipped with this basic trace norm estimate, we can start now our investigation of the operator (4.16).

**4.4.1. Replacing the Spectral Projection by its Approximation.** Let us recall the following general notation, which was introduced in the introduction. If $f$, $g$ are real-valued functions we write $|f| \lesssim |g|$ if and only if $|f| \le C|g|$ for some constant $C > 0$ which might depend on the potential $V$ but does not depend on the dilation parameter $L$. The following lemma provides a condition under which one can replace the spectral projection $P_\mu$ in the operator (4.16) by its approximation $\Pi_\mu$, see Lemma 4.4, leading to a constant order error in trace norm.

**Lemma 4.9.** *Let $I$, $J$, $K \subset \mathbb{R}$ be intervals, possibly depending on the scaling parameter $L$, such that $I \cap J = \varnothing$ and $K \cap J = \varnothing$. Then we have that*

$$\big\|\chi_I P_\mu \chi_J P_\mu \chi_K - \chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K\big\|_1 \lesssim 1, \tag{4.17}$$

*where the integral kernel of* $\Pi_\mu$ *is defined in* (4.7).

Proof. With the notation of Lemma 4.6, 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

$$(x,y) \mapsto \chi_I(x)\chi_K(y) \int_J dz\, R_\mu(x,z) P_\mu(z,y).$$

We apply Lemma 4.8 with

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

leading to

$$\|\chi_I R_\mu \chi_J P_\mu \chi_K\|_1 \le \int_J dz\, \|R_\mu(\cdot,z)\|_{\mathrm{L}^2(I)} \|P_\mu(\cdot,z)\|_{\mathrm{L}^2(K)}.$$

Thus, Estimates (4.13) and (4.14) yield

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

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

**4.4.2. Uniform trace norm bounds.** Under particular assumptions on the intervals $I$, $J$, and $K$, the operator (4.16) is of trace class with uniformly bounded trace norm. We list some of these conditions in the following proposition.

**Proposition 4.10.** *Let $I$, $J$, $K \subset \mathbb{R}$ be intervals, possibly depending on $L$, such that one of the following conditions holds:*

*(i)* $|J| \lesssim 1$,

*(ii) Either*

*(a)* $|J| \lesssim \max\{\mathrm{dist}(I,J),\ \mathrm{dist}(J,K)\}$, *or*

*(b)* $|K| \lesssim \mathrm{dist}(J,K)$, $|I| \lesssim \mathrm{dist}(I,J)$, *or*

*(c)* $|K| \lesssim \mathrm{dist}(J,K)$, $|J| \lesssim \mathrm{dist}(I,J)$.

*(iii) $J$ is finite, and $I$ and $K$ lie on opposite sides of $J$, i.e.*

$$x \le y \le z \text{ or } \ z \le y \le x, \quad \text{for all } (x,y,z) \in I \times J \times K. \tag{4.18}$$

*(iv)* $|I| \lesssim 1$ *and* $I \cap J = \varnothing, K \cap J = \varnothing$.

*Then the operator $\chi_I P_\mu \chi_J P_\mu \chi_K$ is uniformly bounded (independently of $L$) in trace norm, i.e.*

$$\|\chi_I P_\mu \chi_J P_\mu \chi_K\|_1 \lesssim 1. \tag{4.19}$$

**Remark 4.11.** In the unperturbed case, that is for $V \equiv 0$, Proposition 4.10 with assumptions similar to (i) and (iii) has been obtained in [41, Lem.].

Proof of Proposition 4.10. According to Lemma 4.8 and bound (4.14), one has that

$$\|\chi_I P_\mu \chi_J P_\mu \chi_K\|_{\mathfrak{S}_1} \lesssim \int_J dz \left[\int_I dx\,(1+|z-x|)^{-2}\right]^{\frac12} \left[\int_K dy\,(1+|z-y|)^{-2}\right]^{\frac12}. \tag{4.20}$$

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

Assume Condition (i), i.e. $|J| \lesssim 1$. Then both integrals inside (4.20) 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 (4.20) by

$$\left[\int_J dz \int_I dx\,(1+|z-x|)^{-2}\right]^{\frac12} \left[\int_J dz \int_K dy\,(1+|z-y|)^{-2}\right]^{\frac12}.$$

The first integral is bounded by

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

and the second integral is bounded by

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

Thus, under any of the conditions (ii), the right-hand side of (4.20) is uniformly bounded, as required.

Assume that the first of the conditions (4.18) holds (for the second one look at the adjoint operator). Let

$$I = (s_1, t_1), J = (s_2, t_2), K = (s_3, t_3) \tag{4.21}$$

with

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

Using (4.20), we get the bound

$$\begin{aligned}
\|\chi_I P_\mu \chi_J P_\mu \chi_K\|_1 &\lesssim \int_{s_2}^{t_2} dz \left[\int_{s_1}^{t_1} dx\, |z-x|^{-2}\right]^{\frac12} \left[\int_{s_3}^{t_3} dy\, |z-y|^{-2}\right]^{\frac12} \\
&\lesssim \int_{s_2}^{t_2} dz\, (z-t_1)^{-\frac12}(s_3-z)^{-\frac12} \\
&\le \int_{s_2}^{t_2} dz\, (z-s_2)^{-\frac12}(t_2-z)^{-\frac12} = \int_0^s dz\, z^{-\frac12}(s-z)^{-\frac12},
\end{aligned}$$

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

$$\int_0^1 dz\, z^{-\frac12}(1-z)^{-\frac12} \lesssim 1,$$

which leads to (4.19) again.

Finally, assume that (iv) holds. Then the right-hand side of (4.20) is bounded by

$$\begin{aligned}
&|I|^{\frac12} \int_J dz\, \big(1+\mathrm{dist}(z,I)\big)^{-1}\big(1+\mathrm{dist}(z,K)\big)^{-\frac12} \\
&\qquad\lesssim \int_J dz\, \big(1+\mathrm{dist}(z,I)\big)^{-\frac32} + \int_J dz\, \big(1+\mathrm{dist}(z,K)\big)^{-\frac32} \lesssim 1.
\end{aligned}$$

Thus, the proof is complete. □

**4.4.3. Replacing almost periodic functions by their mean value.** Looking at formula (4.7), we see that the kernel of $\chi_I \Pi_\mu \chi_J \Pi_\mu \chi_K$ contains kernels of the form

$$S_{I,J,K}(x,y;f) = \chi_I(x)\chi_K(y) \int_J dz \, \frac{f(z)}{(z-x)(z-y)}, \tag{4.22}$$

where $f$ is a product of functions such as $\Phi^S(\delta)$ and $\overline{\Phi^S(\delta)}$. 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, see (3.24), while the resulting error is uniformly bounded in trace norm.

**Lemma 4.12.** *Let $\Theta \subset \mathbb{R}$ be a countable set, and let $(a_\theta)_{\theta\in\Theta} \subset \mathbb{C}$ be such that*

$$\sum_{\substack{\theta\in\Theta \\ \theta\neq 0}} |a_\theta| \big(1 + |\theta|^{-1}\big) < \infty. \tag{4.23}$$

*Let the function $f \in \mathrm{CAP}(\mathbb{R})$ 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 $\operatorname{dist}(I,J)$, $\operatorname{dist}(J,K) \gtrsim 1$ and consider the operator $S_{I,J,K}(f)$ in $\mathrm{L}^2(\mathbb{R})$ with the integral kernel (4.22). Then one has that*

$$\| S_{I,J,K}(f) - S_{I,J,K}\big(\mathcal{M}(f)\big) \|_1 \lesssim 1. \tag{4.24}$$

Proof. Without loss of generality, we may assume that $\mathcal{M}(f) = 0$, i.e. $0 \notin \Theta$ (otherwise consider $f - \mathcal{M}(f)$). Introduce the primitive $F(x) := \int_0^x f(t)dt$ of $f$. Then the assumption (4.23) implies that $F$ is uniformly bounded:

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

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

$$\begin{aligned} S_{I,J,K}(x,y;f) = {} & \chi_I(x)\chi_K(y) \frac{F(z)}{(z-x)(z-y)} \bigg|_{z=s}^{t} \\ & + \chi_I(x)\chi_K(y) \int_J dz \left[ \frac{F(z)}{(z-x)^2(z-y)} + \frac{F(z)}{(z-x)(z-y)^2} \right]. \end{aligned} \tag{4.25}$$

The first term in formula (4.25) constitutes the kernel of a rank two operator, whose norm, and hence trace norm as well, is easily estimated by a constant times $\operatorname{dist}(I,J)^{-1/2} \operatorname{dist}(J,K)^{-1/2}$. The second term on the right-hand side of (4.25) is treated with the help of Lemma 4.8, as in the proof of Lemma 4.9. Thus (4.24) follows. □

## 4.5. 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 4.8. At the final stages of the proof of Theorem 4.2, 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 4.8 is no longer applicable, and we have to appeal to other results available in the literature.

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

$$\mathrm{Op}(p)u(x) := \frac{1}{2\pi} \iint d\xi dy\, e^{i\xi(x-y)} p(x,y,\xi) u(y). \tag{4.26}$$

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 lemma that implies Schatten-(quasi)norm estimates for the operator

$$A_{L,\mu} := B_{L,\mu}(\mathbb{1} - B_{L,\mu}), \tag{4.27}$$

see Corollary 4.15.

**Lemma 4.13.** *Let $I$, $\Omega \subset \mathbb{R}$ be bounded intervals, independent of $L$, and let $p \in \mathrm{C}^\infty(\mathbb{R}^3)$. Furthermore, assume that the function $p = p(x,y,\xi)$ is $2\pi$-periodic in $x$ and $y$, and there exists a constant $R > 0$ with $p(x,y,\xi) = 0$ for all $x,y \in \mathbb{R}$, and $|\xi| \geq R$. Denote*

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

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

$$\|\chi_{I_L} \mathrm{Op}(p)(\mathbb{1} - \chi_{I_L})\|_q \lesssim 1, \tag{4.28}$$

*and*

$$\|\chi_{I_L} \operatorname{Op}\big(p[\Omega]\big)(\mathbb{1} - \chi_{I_L})\|_q \lesssim (\log(L))^{\frac{1}{q}}. \tag{4.29}$$

*The implicit constants in* (4.28) *and* (4.29) *depend on the amplitude* $p$*, number* $R$*, and also on the intervals* $I$ *and* $\Omega$*.*

Our proof relies on similar results from [65]. We state these results in a form adjusted to our purposes. Namely, the next proposition is a direct consequence of [65, Cor. 4.4 and Thm. 4.6]. Let us emphasise at this point that the main focus of [65] is the *quasi-classical* asymptotics, whereas our objective here 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.

**Proposition 4.14.** *Let* $I$*,* $\Omega \subset \mathbb{R}$ *be bounded intervals, and let the function* $p = p(\xi)$ *be smooth and compactly supported. In particular, fix* $R > 0$ *such that* $p(\xi) = 0$ *for* $|\xi| \geq R$*. For* $q \in (0, 1]$ *denote*

$$N_q(p) := \max_{0 \leq m \leq \lfloor 2q^{-1} \rfloor + 1} \sup_{\xi} |p^{(m)}(\xi)| < \infty. \tag{4.30}$$

*Then*

$$\|\chi_{I_L} \operatorname{Op}(p)(\mathbb{1} - \chi_{I_L})\|_q \lesssim N_q(p), \tag{4.31}$$

*and*

$$\|\chi_{I_L} \operatorname{Op}\big(p[\Omega]\big)(\mathbb{1} - \chi_{I_L})\|_q \lesssim (\log(L))^{\frac{1}{q}} N_q(p). \tag{4.32}$$

*The implicit constants in* (4.31) *and* (4.32) *depend on the intervals* $I$*,* $\Omega$ *and number* $R$*, but are independent of the amplitude* $p$*.*

In order to prove Lemma 4.13, we need to extend Proposition 4.14 to amplitudes, that are periodic in $x$ and $y$.

Proof of Lemma 4.13. We only prove the bound (4.29); Estimate (4.28) can be derived in a similar way.

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

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

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

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

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 (4.30) for the definition of $N_q$). Consequently, the operator $\mathrm{Op}(p[\Omega])$ can be represented as

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

Using (4.32), we immediately obtain the bound

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

Furthermore, employing the $q$-triangle inequality for the ideals $\mathfrak{S}_q$ (see [7, p. 262]), we arrive at

$$\begin{aligned}\|\chi_{I_L}\,\mathrm{Op}\big(p[\Omega]\big)(\mathbb{1}-\chi_{I_L})\|_q^q &\le \sum_{n,l}\|\chi_{I_L}A_{nl}(\mathbb{1}-\chi_{I_L})\|_q^q\\ &\lesssim \log(L)\sum_{n,l}(1+|n|)^{-sq}(1+|l|)^{-tq}.\end{aligned}$$

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

**Corollary 4.15.** *Assume that $V\in\mathrm{C}^\infty(\mathbb{R})$ and let $A_{L,\mu}$ be defined as in* (4.27).

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

$$\|\chi_{I_L}P_\mu(\mathbb{1}-\chi_{I_L})\|_q^q \lesssim \log(L). \tag{4.33}$$

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

$$\|\chi_{I_L}P_\mu(\mathbb{1}-\chi_{I_L})\|_q^q \lesssim 1. \tag{4.34}$$

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

$$\|A_{L,\mu}\|_q^q \lesssim \begin{cases} 1, & \mu \notin (\sigma(H))^\circ, \\ \log(L), & \mu \in (\sigma(H))^\circ. \end{cases} \tag{4.35}$$

*Moreover, assume that* $h$ *satisfies Condition 4.1. Then* $h(B_{L,\mu})$ *is of trace class and*

$$\|h(B_{L,\mu})\|_1 \lesssim \begin{cases} L|h(1)| + 1, & \mu \notin (\sigma(H))^\circ, \\ L|h(1)| + \log(L), & \mu \in (\sigma(H))^\circ. \end{cases} \tag{4.36}$$

*(iii) If* $\mu \notin (\sigma(H))^\circ$, *then* (4.3) *holds.*

*The implicit constants in the inequalities* (4.33), (4.34), (4.35), *and* (4.36) *are independent of the scaling parameter* $L$.

PROOF. It suffices to prove (4.33) and (4.34) for the projections $P_\mu[S]$ under the conditions $\mu \in S^\circ$ and $\mu \notin S^\circ$ respectively, for any genuine spectral band $S$.

Suppose first that $\mu \in S^\circ$. By virtue of (4.11), the operator $P_\mu[S]$ has the form $\mathrm{Op}\big(p[\Omega]\big)$ with

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

where $\kappa_S$ is defined in (3.10), and $\delta \in (\kappa_S, \kappa_S + n_S/2)$ is the unique solution of the equation $\Lambda(\delta) = \mu$. The function $(x,\xi) \mapsto E^S(x,\xi)$ is $2\pi$-periodic in $x$, and infinitely smooth, due to the $\mathrm{C}^\infty$-smoothness of $V$, see Lemma 3.8. Thus, (4.33) follows from (4.29).

Suppose now that $\mu \notin S^\circ$. According to (3.29), either $P_\mu[S] = 0$, in which case (4.34) is trivial, or

$$P_\mu[S](x,y) = \int\limits_{n_S\mathbb{T}} dk\, \Phi^S(x,k)\overline{\Phi^S(y,k)},$$

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

$$p(x,y,\xi) = E^S(x,\xi)\overline{E^S(y,\xi)}\zeta(\xi), \ \zeta \in \mathrm{C}_0^\infty(\mathbb{R}).$$

Therefore, (4.34) is a consequence of (4.28).

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

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

and (4.35) follows from (4.34).

To prove (4.36) we use the representation (4.4): $h(t) = th(1) + h_0(t)$, so that $h_0(0) = h_0(1) = 0$ and $|h_0(t)| \lesssim t^q(1-t)^q$, where $q \in (0,1]$ is the Hölder exponent of the function $h$. The first term on the right-hand side of (4.36) results from the bound (4.5). For the second term, note that

$$\|h_0(B_{L,\mu})\|_1 \lesssim \|A^q_{L,\mu}\|_1 = \|A_{L,\mu}\|^q_q, \tag{4.37}$$

hence the required bounds follow from (4.35). Applying the splitting (4.4), estimates (4.37) and (4.35) also imply Part (iii) of the corollary. □

## 4.6. Proof of Theorem 4.2: Polynomial Test Functions

By virtue of Corollary 4.15(iii), formula (4.3) is already proved. Thus it remains to prove Theorem 4.2 for $\mu \in (\sigma(H))^\circ$. So, assume from now on that $\mu$ is an interior point of a (fixed) genuine band $S \subset \sigma(H)$. As before, let $\delta \in (\kappa_S, \kappa_S + n_S/2)$ be the solution of the equation $\Lambda^S(\delta) = \mu$. For simplicity, we abbreviate in the following $\Phi := \Phi^S(\delta)$.

**4.6.1. Polynomial classes.** We begin the proof of (4.2) with studying polynomial test functions. The following classes of polynomials on the interval $[0,1]$ will be relevant:

$$\begin{aligned} \mathfrak{P} &:= \{p : [0,1] \mapsto \mathbb{C},\ \text{polynomial}\}, \\ \mathfrak{P}_0 &:= \{p \in \mathfrak{P} : p(0) = p(1) = 0\}, \\ \mathfrak{P}_s &:= \{p \in \mathfrak{P} : p(t) = p(1-t) \text{ for all } t\}, \\ \mathfrak{P}_{s,0} &:= \mathfrak{P}_s \cap \mathfrak{P}_0. \end{aligned} \tag{4.38}$$

By virtue of Section 4.2 and the splitting (4.4), it remains to prove (4.2) for functions $h_0$ satisfying Condition 4.1, such that $h_0(0) = h_0(1) = 0$. 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 [41] we choose the basis

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

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

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

In so doing, we follow the strategy of [41], where the problem was analysed in the unperturbed case $V \equiv 0$. In fact, our objective is to reduce the calculations to the unperturbed case, by using Lemmas 3.9 and 4.12.

**4.6.2. Trace class calculus for the operator $A_{L,\mu}$.** Let us rewrite the operator $A_{L,\mu}$ in the form

$$A_{L,\mu} = A_{L,\mu}^- + A_{L,\mu}^+$$

with

$$\begin{cases} A_{L,\mu}^- &:= \chi_{(-L,L)} P_\mu \chi_{(-\infty,-L)} P_\mu \chi_{(-L,L)}, \\ A_{L,\mu}^+ &:= \chi_{(-L,L)} P_\mu \chi_{(L,\infty)} P_\mu \chi_{(-L,L)}. \end{cases} \tag{4.39}$$

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

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 $L$), $A \sim B$ implies $A^n \sim B^n$ for any $n = 1, 2, \dots$.

To begin with, by virtue of Proposition 4.10(i), one has that

$$A_{L,\mu}^+ \sim \chi_{(-L,L)} P_\mu \chi_{(L+1,\infty)} P_\mu \chi_{(-L,L)} \tag{4.40}$$

and

$$A_{L,\mu}^- \sim \chi_{(-L,L)} P_\mu \chi_{(-\infty,-L-1)} P_\mu \chi_{(-L,L)}. \tag{4.41}$$

4.6.2.1. *Operators $D_L^\pm$.* The next step is to replace $A_{L,\mu}^\pm$ with operators that do not contain any information on the Bloch eigenfunctions for $H$. These are the operators $D_L^\pm : \mathrm{L}^2(\mathbb{R}) \mapsto \mathrm{L}^2(\mathbb{R})$, defined via their integral kernels

$$D_L^+(x,y) := \frac{1}{4\pi^2}\chi_{(-L,L)}(x)\chi_{(-L,L)}(y)\int_{L+1}^{\infty} dz\,\frac{1}{(z-x)(z-y)},$$

$$D_L^-(x,y) := \frac{1}{4\pi^2}\chi_{(-L,L)}(x)\chi_{(-L,L)}(y)\int_{-\infty}^{-L-1} dz\,\frac{1}{(z-x)(z-y)}.$$

Note that $D_L^+$ and $D_L^-$ are unitarily equivalent via the change $x \mapsto -x$. The crucial fact is that the asymptotic formulae for the traces of powers $(D_L^\pm)^n$ can be easily deduced from the results of [41]:

**Lemma 4.17.** *Let $p_n(t) = t^n(1-t)^n$, $n = 1, 2, \ldots$. Then*

$$\mathrm{tr}(D_L^\pm)^n = \frac{1}{4}\log(L)\ \mathcal{W}(p_n) + o(\log(L)),\ \ L \to \infty, \tag{4.42}$$

*where $\mathcal{W}(\,\cdot\,)$ is as defined in* (4.1).

Proof. Since $D_L^+$ and $D_L^-$ are unitarily equivalent, we show (4.42) for $D_L := D_L^+$ only. By translation and reflection, the operator $D_L$ is unitarily equivalent to the operator with kernel

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

This is the kernel of the operator which is denoted by $K_c$ in [41, p. 476]. Thus the formula (4.42) immediately follows from [41, Eq. (19), p. 477]. □

A useful way to write $D_L^\pm$ is

$$D_L^\pm = (Z_L^\pm)^* Z_L^\pm,$$

where the operators $Z_L^\pm$ have the integral kernels

$$Z_L^+(x,y) := \frac{\chi_{(L+1,\infty)}(x)\chi_{(-L,L)}(y)}{2\pi(x-y)} \quad \text{and}$$
$$Z_L^-(x,y) := \frac{\chi_{(-\infty,-L-1)}(x)\chi_{(-L,L)}(y)}{2\pi(x-y)}, \tag{4.43}$$

respectively. In the following, we establish a few facts for the operators $D_L^\pm$ and $Z_L^\pm$. Recall that we abbreviate $\Phi = \Phi^S(\delta)$, $\delta = \delta(\mu)$, remembering that $\mu$ is strictly inside the band $S$.

**Lemma 4.18.** *Denote by $Y_L^\pm$ any of the two operators $Z_L^\pm$ or $(Z_L^\pm)^*$. With the notation as above, one has that*

$$Y_L^\pm|\Phi|^2(Y_L^\pm)^* \sim \frac{1}{2\pi}Y_L^\pm(Y_L^\pm)^* \quad \text{and} \quad Y_L^\pm\Phi^2(Y_L^\pm)^* \sim 0.$$

**Remark 4.19.** Taking adjoints, the second estimate in Lemma 4.18 also holds with $\Phi^2$ replaced by $\overline{\Phi}^2$.

PROOF. We prove the lemma for the "+" sign and for the case $Y_L^+ = Z_L^+$ only. The remaining cases are treated in the same way. For brevity, we omit the superscript "+" and write $Z_L$ instead of $Z_L^+$.

For $f = |\Phi|^2$ or $\Phi^2$, the operator $Z_L f Z_L^*$ coincides with the operator $\frac{1}{4\pi^2}S_{I,J,K}(f)$ with

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

see the definition (4.22). Thus, Lemma 4.12 implies that

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

In view of (3.25) and (3.26), $\mathcal{M}(|\Phi|^2) = (2\pi)^{-1}$ and $\mathcal{M}(\Phi^2) = 0$, whence the claimed result. □

**Corollary 4.20.** *Let*

$$K_{L,n}^\pm := 2\pi\big[\Phi(D_L^\pm)^n\overline{\Phi} + \overline{\Phi}(D_L^\pm)^n\Phi\big],\ \ n = 1, 2, \dots. \tag{4.44}$$

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

$$(K_{L,1}^\pm)^n \sim K_{L,n}^\pm, \tag{4.45}$$

*and*

$$(K_{L,1}^\pm)^n \approx 2(D_L^\pm)^n,\ \ \text{as } L \to \infty. \tag{4.46}$$

PROOF. For brevity, we omit the superscript "±" and write $K_{L,1}, D_L$ instead of $K_{L,1}^\pm, D_L^\pm$ etcetera. The powers of $K_{L,1}$ contain terms of the form

$$D_L f D_L = Z_L^* Z_L f Z_L^* Z_L,$$

with $f = |\Phi|^2,\ \Phi^2$ or $\overline{\Phi}^2$. Thus by Lemma 4.18,

$$K_{L,1}^n \sim (2\pi)^n\big[(\Phi D_L\overline{\Phi})^n + (\overline{\Phi}D_L\Phi)^n\big] \sim 2\pi\big[\Phi D_L^n\overline{\Phi} + \overline{\Phi}D_L^n\Phi\big] = K_{L,n},$$

as claimed.

In order to prove (4.46), we use the cyclicity of the trace. If $n = 1$, then, again by Lemma 4.18,

$$\Phi D_L \overline{\Phi} \approx Z_L |\Phi|^2 Z_L^* \sim \frac{1}{2\pi} Z_L Z_L^* \approx \frac{1}{2\pi} D_L.$$

If $n \geq 2$, we arrive in the same way at

$$\Phi D_L^n \overline{\Phi} \approx Z_L D_L^{n-2} Z_L^* Z_L |\Phi|^2 Z_L^* \sim \frac{1}{2\pi} Z_L D_L^{n-2} Z_L^* Z_L Z_L^* \approx \frac{1}{2\pi} D_L^n.$$

For the summand containing $\Phi$ and $\overline{\Phi}$ in the reversed order, one can proceed analogously. Thus, (4.46) follows and the proof of the lemma is complete. □

4.6.2.2. *Approximating operators $A_{L,\mu}^{\pm}$.* Let $\mu \in S^\circ$ and $\Phi = \Phi^S(\delta)$ as before and recall the definition of the operators $A_{L,\mu}^{\pm}$, see (4.39). The next lemma compares the operators $A_{L,\mu}^{\pm}$ with the operators $K_{L,1}^{\pm}$, which were defined in (4.44). In view of (4.46) from Corollary 4.20, this completes the procedure of averaging out the dependence on the Bloch eigenfunctions.

**Lemma 4.21.** *The trace norm bounds*

$$(A_{L,\mu}^{\pm})^n \sim (K_{L,1}^{\pm})^n \tag{4.47}$$

*and*

$$A_{L,\mu}^n \sim (A_{L,\mu}^{+})^n + (A_{L,\mu}^{-})^n \sim (K_{L,1}^{+})^n + (K_{L,1}^{-})^n \tag{4.48}$$

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

Proof. It suffices to prove (4.47) for $n = 1$ since the operator norm of $A_{L,\mu}^{\pm}$ is uniformly bounded with respect to $L$. As before, we consider $A_{L,\mu}^{+}$ only, omitting the superscript "+". From (4.40) and Lemma 4.9 it follows that

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

Moreover, the definitions (4.7) and (4.43) imply that

$$\begin{aligned}
\chi_{(L+1,\infty)} \Pi_\mu \chi_{(-L,L)} &= -2\pi i \big(\Phi Z_L \overline{\Phi} - \overline{\Phi} Z_L \Phi\big), \\
\chi_{(-L,L)} \Pi_\mu \chi_{(L+1,\infty)} &= 2\pi i \big(\Phi Z_L^* \overline{\Phi} - \overline{\Phi} Z_L^* \Phi\big),
\end{aligned}$$

so that

$$A_{L,\mu} \sim 4\pi^2\big(\Phi Z_L^* |\Phi|^2 Z_L \overline{\Phi} + \overline{\Phi} Z_L^* |\Phi|^2 Z_L \Phi\big) \\ - 4\pi^2\big(\Phi Z_L^* \overline{\Phi}^2 Z_L \Phi + \overline{\Phi} Z_L^* \Phi^2 Z_L \overline{\Phi}\big).$$

Consequently, Lemma 4.18 yields

$$A_{L,\mu} \sim 2\pi\big(\Phi Z_L^* Z_L \overline{\Phi} + \overline{\Phi} Z_L^* Z_L \Phi\big) = K_{L,1},$$

as required.

So, let us proceed with the proof of (4.48). By the definition (4.39),

$$A_{L,\mu}^- A_{L,\mu}^+ = \chi_{(-L,L)} P_\mu \Big(\chi_{(-\infty,-L)} P_\mu \chi_{(-L,L)} P_\mu \chi_{(L,\infty)}\Big) P_\mu \chi_{(-L,L)}.$$

In virtue of Proposition 4.10(iii), the trace norm of the operator in the middle is uniformly bounded, and hence $A_{L,\mu}^- A_{L,\mu}^+ \sim 0$. Taking adjoints, we also get that $A_{L,\mu}^+ A_{L,\mu}^- \sim 0$. Thus,

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

follows and (4.48) is now a consequence of (4.47). □

Equipped with Lemma 4.21, we are ready to prove Theorem 4.2 for $h = p_n$, $n = 1, 2, \dots$.

**4.6.3. Proof of Theorem 4.2 for symmetric polynomials.** Estimates (4.48), (4.46), and the asymptotics (4.42) imply that

$$\begin{aligned} \operatorname{tr} A_{L,\mu}^n &= \operatorname{tr}(K_{L,1}^+)^n + \operatorname{tr}(K_{L,1}^-)^n + \mathcal{O}(1) \\ &= 2\operatorname{tr}(D_L^+)^n + 2\operatorname{tr}(D_L^-)^n + \mathcal{O}(1) \\ &= \log(L)\mathcal{W}(p_n) + o(\log(L)),\ n = 1, 2, \dots. \end{aligned} \tag{4.49}$$

Hence, Theorem 4.2 for polynomials $p \in \mathfrak{P}_{s,0}$ follows from the identity $p_n(B_{L,\mu}) = A_{L,\mu}^n$. □

**4.6.4. Arbitrary polynomials.** As above, we assume that $\mu \in S^\circ$, where $S$ is a genuine spectral band. So far we have proved Theorem 4.2 for polynomials $p \in \mathfrak{P}_{s,0}$, see (4.38) for the 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 [41] for the unperturbed case, this is done by a symmetry argument that reduces $\operatorname{tr} q_n(B_{L,\mu}) = \operatorname{tr}\left[B_{L,\mu} A_{L,\mu}^n\right]$ to $\operatorname{tr} p_n(B_{L,\mu}) = \operatorname{tr} A_{L,\mu}^n$.

**Lemma 4.22.** *For every $n = 1, 2, \dots$, we have*

$$B_{L,\mu}\big(A_{L,\mu}\big)^n \approx \frac{1}{2} \operatorname{tr}\big(A_{L,\mu}\big)^n, \tag{4.50}$$

*as $L \to \infty$.*

**Remark 4.23.** The result of this lemma may be interpreted as follows: if $h$ is a polynomial, which is point-symmetric around $t = 1/2$ and vanishes at $t = 0$ (and $t = 1$), then $\operatorname{tr} h(B_{L,\mu})$ is of constant order. Namely, the functions $\{t \mapsto (t - \frac{1}{2})t^n(1 - t)^n;\ n = 1, 2, \dots\}$ form a basis for these polynomials. This ultimately leads to the logarithmic term vanishing in (4.2) for point-symmetric test functions (around $t = 1/2$).

Compared to [41], the proof of Lemma 4.22 requires some extra work. The main difference is that instead of the reflection symmetry used in [41], we exploit the periodicity of the spectral projection $P_\mu$. The operators $A_{L,\mu}^+$ and $A_{L,\mu}^-$(see (4.39)) are considered separately. Applying Proposition 4.10 (iib), we get

$$A_{L,\mu}^+ \sim \chi_{(-L,L)} P_\mu \chi_{(L,3L)} P_\mu \chi_{(-L,L)}. \tag{4.51}$$

Let $U_L^\pm$ be the unitary shift operators defined by

$$U_L^\pm f(x) := f(x \mp L_0),\ L_0 = 2\pi \left\lfloor \frac{L}{2\pi} \right\rfloor.$$

Then the equivalence (4.51) implies that

$$(U_L^+)^* A_{L,\mu}^+ U_L^+ \sim \chi_{(-2L,0)} P_\mu \chi_{(0,2L)} P_\mu \chi_{(-2L,0)}. \tag{4.52}$$

Indeed, (4.51) yields

$$(U_L^+)^* A_{L,\mu}^+ U_L^+ \sim \chi_{(-L-L_0,L-L_0)} P_\mu \chi_{(L-L_0,3L-L_0)} P_\mu \chi_{(-L-L_0,L-L_0)},$$

since $(U_L^+)^* P_\mu U_L^+ = P_\mu$. Now, to get (4.52), one needs to use Proposition 4.10(i), (iv) repeatedly. For the following, let us introduce the notation

$$\chi_L^+ := \chi_{(0,2L)}, \ \chi_L^- := \chi_{(-2L,0)},$$

and

$$T_{L,\mu}^\pm := \chi_L^\mp P_\mu \chi_L^\pm P_\mu \chi_L^\mp.$$

Thus, one can write

$$(U_L^\pm)^* A_{L,\mu}^\pm U_L^\pm \sim T_{L,\mu}^\pm. \tag{4.53}$$

This relation with the "+" sign coincides with (4.52), and for the "−" sign it is proved in the same way. The proof of Lemma 4.22 begins with the following observation.

**Lemma 4.24.** *For any $n = 1, 2, \dots,$ we have that*

$$P_\mu (T_{L,\mu}^\pm)^n \approx (\mathbb{1} - P_\mu)(T_{L,\mu}^\mp)^n, \ \text{as } L \to \infty. \tag{4.54}$$

PROOF. For brevity, we write $\chi^\pm = \chi_L^\pm$, $T^\pm = T_{L,\mu}^\pm$, $P = P_\mu$, and $Q = \mathbb{1} - P$. One has that

$$\begin{aligned} P(T^+)^n &= P\chi^- P\chi^+ P\chi^- (T^+)^{n-1} = -P\chi^- Q\chi^+ P\chi^- (T^+)^{n-1} \\ &= P(\mathbb{1} - \chi^-) Q\chi^+ P\chi^- (T^+)^{n-1} \\ &= P\chi^+ Q\chi^+ P\chi^- (T^+)^{n-1} + R_1 + R_2, \end{aligned} \tag{4.55}$$

with

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

Moreover, notice that $Q = \mathbb{1} - P$ can be replaced by $-P$ in $R_1$. By Proposition 4.10(iii),

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

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

$$\chi^+ P\chi^- (T^+)^{n-1} = (T^-)^{n-1} \chi^+ P\chi^-, \tag{4.56}$$

and hence, by cyclicity of the trace,

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

Applying again Proposition 4.10(iii) to the factor $\chi^+ P \chi^- P \chi_{(-\infty,-2L)}$, we infer that $R_2 \approx 0$.

Returning to (4.55), let us apply (4.56) to the first operator on the right-hand side and use again the cyclicity:

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

Together with (4.55) and $R_{1/2} \approx 0$, this yields (4.54) for the "+" sign. The relation (4.54) for the "−" sign is obtained in the same way. □

Proof of Lemma 4.22. We shall use the simplified notation as in the proof of Lemma 4.24 and, in addition, write $A = A_{L,\mu}$, $A^\pm = A^\pm_{L,\mu}$, and $B = B_{L,\mu}$. First, observe that $BA^n \approx PA^n$. Thus, it follows from (4.48) and (4.53) that

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

By Lemma 4.24,

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

so that

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

Hence, using (4.53) and (4.48) again, we arrive at

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

which leads to (4.50) and completes the proof of the lemma. □

As a consequence of Lemma 4.22, Theorem 4.2 can be proved for arbitrary $p \in \mathfrak{P}_0$.

Proof of Theorem 4.2 for arbitrary polynomials. It remains to validate the theorem for polynomials of the form $q_n(t) = tp_n(t)$, $n = 1, 2, \ldots$. From Lemma 4.22 and (4.49) we deduce that

$$\operatorname{tr}\left[B_{L,\mu}\big(A_{L,\mu}\big)^n\right] = \frac{1}{2}\log(L)\mathcal{W}(p_n) + o(\log(L)),\ L \to \infty. \tag{4.57}$$

Moreover, the function $q_n - \frac{1}{2}p_n$ is point-symmetric around $t = 1/2$ such that

$$\mathcal{W}(q_n - \tfrac{1}{2}p_n) = 0,$$

hence $\mathcal{W}(q_n) = \frac{1}{2}\mathcal{W}(p_n)$. Together with (4.57) this leads to Theorem 4.2 for the polynomials $q_n$ and, thus, the theorem is proved for arbitrary polynomials $p \in \mathfrak{P}_0$. $\square$

## 4.7. Proof of Theorem 4.2: Closure of the Asymptotics

Throughout this final section, we assume that $h$ satisfies Condition 4.1. We recall that, applying the splitting (4.4), we may, in addition, assume that $h(1) = 0$. Also, without loss of generality, suppose 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 $h$ that are differentiable at $t = 0$ and $t = 1$. The differentiability condition at $t = 0$ and $t = 1$ (together with $h(0) = h(1) = 0$) 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

$$h(t) \le t(1-t)(p(t) + \epsilon) = \tilde{p}(t) + \epsilon t(1-t), \tag{4.58}$$

and

$$h(t) \ge t(1-t)(p(t) - \epsilon) = \tilde{p}(t) - \epsilon t(1-t). \tag{4.59}$$

The monotonicity of the trace in combination with (4.58) gives

$$\operatorname{tr}\left[h(B_{L,\mu})\right] \le \operatorname{tr}\left[\tilde{p}(B_{L,\mu})\right] + \epsilon \operatorname{tr}\left[B_{L,\mu}(\mathbb{1} - B_{L,\mu})\right].$$

From Theorem 4.2 for polynomials from $\mathfrak{P}_0$, we get

$$\limsup_{L\to\infty} \frac{\operatorname{tr}\left[h(B_{L,\mu})\right]}{\log(L)} \le \mathcal{W}(\tilde{p}) + \epsilon\mathcal{W}(t(1-t)) = \mathcal{W}(\tilde{p}) + \frac{\epsilon}{\pi^2},$$

where we have used that $\mathcal{W}(t(1-t)) = \pi^{-2}$, see (4.1). Moreover, we notice that

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

and, hence,

$$\limsup_{L\to\infty} \frac{\operatorname{tr}\left[h(B_{L,\mu})\right]}{\log(L)} \le \mathcal{W}(h) + \frac{2\epsilon}{\pi^2}.$$

In the same way, (4.59) implies

$$\liminf_{L\to\infty} \frac{\operatorname{tr}\left[h(B_{L,\mu})\right]}{\log(L)} \ge \mathcal{W}(h) - \frac{2\epsilon}{\pi^2},$$

and as $\epsilon > 0$ was chosen arbitrarily we deduce formula (4.2) for our choice of $h$.

Step 2. Now, let $h$ be a continuous function that is Hölder-continuous at 0 and 1 with exponent $q \in (0,1]$ so that

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

Fix again $\epsilon > 0$ and choose a smooth function $\zeta_\epsilon$ such that $0 \le \zeta_\epsilon \le 1$ 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

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

we have

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

By Corollary 4.15, the right-hand side does not exceed $\log(L)$, $L \ge 2$. Consequently,

$$\frac{\left|\operatorname{tr}\left[(\zeta_\epsilon h)(B_{L,\mu})\right]\right|}{\log(L)} \lesssim \epsilon^r,\ L \ge 2. \tag{4.60}$$

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

$$\operatorname{tr}\left[h_\epsilon(B_{L,\mu})\right] = \log(L)\mathcal{W}(h_\epsilon) + o(\log(L)),\ L \to \infty. \tag{4.61}$$

It is clear that

$$\left|\mathcal{W}(h) - \mathcal{W}(h_\epsilon)\right| \lesssim \left(\int_0^\epsilon dt + \int_{1-\epsilon}^1 dt\right) t^{q-1}(1-t)^{q-1} \lesssim \epsilon^q, \tag{4.62}$$

hence, combining (4.60), (4.61), and (4.62) gives

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

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

Step 3. Suppose that $h$ satisfies Condition 4.1 and fix $\epsilon > 0$. Let $g_1, g_2$ be two continuous functions, such that

(i) $g_1(t) = g_2(t) = h(t)$ in a neighbourhood of the endpoints $t = 0, 1$,

(ii) $g_1(t) \le h(t) \le g_2(t)$, for all $t \in [0,1]$, and

(iii) $\|g_1 - g_2\|_{\mathrm{L}^1} < \epsilon$.

Applying the definition (4.1) of $\mathcal{W}$, this implies that

$$|\mathcal{W}(g_1) - \mathcal{W}(h)| \lesssim \epsilon, \ |\mathcal{W}(g_2) - \mathcal{W}(h)| \lesssim \epsilon.$$

Also, the monotonicity of the trace yields

$$\operatorname{tr} g_1(B_{L,\mu}) \leq \operatorname{tr} h(B_{L,\mu}) \leq \operatorname{tr} g_2(B_{L,\mu}),$$

thus, by Step 2,

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

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

This completes the proof of Theorem 4.2.

# Appendix

## A.1. A Remark on the Third Coefficient in the Trace Asymptotics for Wiener–Hopf Operators with Smooth Symbol

The purpose of this section is to provide a proof of the following result.

**Lemma A.1.** *Suppose that $d \geq 2$ and let $\Omega \subset \mathbb{R}^d$ be a bounded set with smooth boundary. Moreover, assume that $a \in \mathsf{W}^{\infty,1}(\mathbb{R}^d)$ and let $h(z) = z^2 + dz$ for some $d \in \mathbb{C}$. Then the coefficient $\mathcal{B}_{d-2} = \mathcal{B}_{d-2}(\Omega, h, a)$ in (1.12) vanishes:*

$$\mathcal{B}_{d-2}(\Omega, h, a) = 0.$$

For $a$ and $\Omega$ as in the lemma and (general) entire test functions $h$ with $h(0) = 0$, a formula for $\mathcal{B}_{d-2}$ is contained, for instance, in [58]. In order to write it down, we need to fix some notation. Let $d\Sigma$ denote the surface measure on $\partial\Omega$ and write $\nu_x$ for the inwards pointing unit normal vector at $x \in \partial\Omega$. Consider the canonical volume element $dX = d\Sigma d\overline{\xi}$ on $T^*(\partial\Omega)$ where $d\overline{\xi}$ is the Lebesgue measure on $\{\nu_x\}^\perp$. Moreover, let $\mathrm{I\!I}$ denote the second fundamental form on $\partial\Omega$ with respect to the unit normal $\nu$ and write $\mathrm{H}$ for $(d-1)$ times the mean curvature on $\partial\Omega$. Finally, introduce for a vector $w \in \mathbb{R}^d$ its orthogonal projection $w_{T_x} = w_{T_x(\partial\Omega)}$ onto $T_x(\partial\Omega) = \{\nu_x\}^\perp$.

In view of [58, Thm. 1.1], the coefficient $\mathcal{B}_{d-2} = \mathcal{B}_{d-2}(\Omega, h, a)$ is given by

$$\begin{aligned}
\mathcal{B}_{d-2} = &- \frac{1}{2(2\pi)^{d+2}} \int\limits_{T^*(\partial\Omega)} dX \int\limits_{\mathbb{R}} d\xi_1 \int\limits_{\mathbb{R}} \frac{d\xi_2}{\xi_1 - \xi_2} \int\limits_{\mathbb{R}} \frac{d\xi_3}{\xi_1 - \xi_3} \\
&\times \left\{ \sum_{k=1}^{3} \frac{h(a(\overline{\xi} + \xi_k \nu))}{\prod\limits_{j \neq k} [a(\overline{\xi} + \xi_k \nu) - a(\overline{\xi} + \xi_j \nu)]} \right\} \Bigg( \mathrm{I\!I}\Big[(\nabla a)_T(\overline{\xi} + \xi_2 \nu), (\nabla a)_T(\overline{\xi} + \xi_3 \nu)\Big] \\
&\qquad - \mathrm{H}\big[\nu \cdot (\nabla a)(\overline{\xi} + \xi_2 \nu)\big]\big[\nu \cdot (\nabla a)(\overline{\xi} + \xi_3 \nu)\big] \Bigg),
\end{aligned} \tag{A.1}$$

where the integrals over $\xi_2$ and $\xi_3$ are interpreted as Cauchy principal values. Armed with this formula, we are ready to prove the lemma.

Proof of Lemma A.1. Note that, for the given function $h$, one has that

$$\sum_{k=1}^{3} \frac{h(a(\overline{\xi}+\xi_k\nu))}{\prod\limits_{j\neq k}[a(\overline{\xi}+\xi_k\nu)-a(\overline{\xi}+\xi_j\nu)]}=1,$$

for all $\overline{\xi},\nu\in\mathbb{R}^d$ and $\xi_1,\xi_2,\xi_3\in\mathbb{R}$. Thus, as the Hilbert transform

$$\mathsf{C}^\infty(\mathbb{R})\cap\mathsf{L}^2(\mathbb{R})\ni f\mapsto\tilde{f};\quad \tilde{f}(t):=\frac{1}{\pi}\lim_{\epsilon\searrow 0}\int\limits_{|s-t|>\epsilon} ds\,\frac{f(s)}{t-s},$$

extends to a unitary operator on $\mathsf{L}^2(\mathbb{R})$, the formula (A.1) for $\mathcal{B}_{d-2}$ simplifies to

$$-\frac{1}{8(2\pi)^d}\int\limits_{T^*(\partial\Omega)} dX\int\limits_{\mathbb{R}} d\zeta\,\Big\{\mathrm{I\!I}\Big[(\nabla a)_T(\overline{\xi}+\zeta\nu),(\nabla a)_T(\overline{\xi}+\zeta\nu)\Big]-\mathrm{H}\big[\nu\cdot(\nabla a)(\overline{\xi}+\zeta\nu)\big]^2\Big\}.$$

To see that this expression vanishes identically we repeat an argument from [58, p. 600]. Writing out the volume element $dX=d\Sigma d\overline{\xi}$ and combining the $\overline{\xi}$- and $\zeta$-integration, one arrives at

$$\mathcal{B}_{d-2}=-\frac{1}{8(2\pi)^d}\int\limits_{\partial\Omega} d\Sigma(x)\int\limits_{\mathbb{R}^d} d\xi\,\Big\{\mathrm{I\!I}_x\big[(\nabla a)_{T_x}(\xi),(\nabla a)_{T_x}(\xi)\Big]-\mathrm{H}(x)\big[\nu_x\cdot(\nabla a)(\xi)\big]^2\Big\}.$$

Hence, the lemma follows from Fubini's theorem and the identity

$$\int\limits_{\partial\Omega} d\Sigma(x)\Big(\mathrm{I\!I}_x\big[w_{T_x},w_{T_x}\big]-\mathrm{H}(x)[\nu_x\cdot w]^2\Big)=0,$$

which holds for any $w\in\mathbb{R}^d$, see [58, Eq. (4.16)]. □

## A.2. Proof of Lemma 2.11

We first prove the lemma for monomials $h(z)=z^k$, $k=1,2,\ldots$. For $k=1$ the statement is trivial, so assume that $k\geq 2$. The operator $[A_G]^k$ has the kernel

$$[A_G]^k(x,y)=\chi_G(x)\int\limits_G dz_1\cdots\int\limits_G dz_{k-1}\,F_k(x,z_1,z_2,\ldots,z_{k-1},y)\chi_G(y)$$

with

$$F_k(x,z_1,z_2,\ldots,z_{k-1},y):=\check{a}(x-z_1)\check{a}(z_1-z_2)\cdots\check{a}(z_{k-2}-z_{k-1})\check{a}(z_{k-1}-y).$$

Due to Lemma 2.10, there exist a constant $C_{a,d}$, depending on the symbol $a$ and $d$, such that

$$|F_k(x,z_1,z_2,\ldots,z_{k-1},y)| \leq C_{a,d}^k\langle x-z_1\rangle^{-d-1}\langle z_1-z_2\rangle^{-d-1}\cdots\langle z_{k-2}-z_{k-1}\rangle^{-d-1}\langle z_{k-1}-y\rangle^{-d-1}. \quad \text{(A.2)}$$

Moreover, the function $F_k$ is continuous on $\left(\mathbb{R}^d\right)^{k+1}$. Fix $y_0 \in G$ and $\delta \in (0,1)$ such that $B_\delta(y_0) \subset G$. By Peetre's inequality, see (2.39), one has that, for $y \in B_\delta(y_0)$ and $z \in \mathbb{R}^d$,

$$\frac{\langle z-y\rangle^{-d-1}}{\langle z-y_0\rangle^{-d-1}} \leq 2^{(d+1)/2}\langle y-y_0\rangle^{d+1} \leq 2^{d+1}.$$

Together with (A.2), this yields the bound

$$\begin{aligned}\sup_{(x,y)\in G\times B_\delta(y_0)} & |F_k(x,z_1,z_2,\dots,z_{k-1},y)| \\ & \leq 2^{d+1}C_{a,d}^k\langle z_1-z_2\rangle^{-d-1}\cdots\langle z_{k-2}-z_{k-1}\rangle^{-d-1}\langle z_{k-1}-y_0\rangle^{-d-1},\end{aligned}$$

the right-hand side being integrable on $\left(\mathbb{R}^d\right)^{k-1} \supset G^{k-1}$. Thus, the kernel $A_G^k(x,y)$ is continuous on $G\times G$. Furthermore, one deduces from (A.2) that

$$|[A_G]^k(x,y)| \leq C_{a,d}^k\Big[\int_{\mathbb{R}^d} dz\,\langle z\rangle^{-d-1}\Big]^{k-1},$$

for all $x,y\in G$. Hence, by uniform convergence, the kernel $h(A_G)(x,y)$ is continuous on $G\times G$ for every entire function $h$ with $h(0)=0$. This finishes the proof of the lemma.

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