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Local Spectral Asymptotics and Heat Kernel Bounds for Dirac and Laplace Operators

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Doctoral Thesis
submitted in partial fulfillment of the requirements for the award of
Doctor of Philosophy of Loughborough University

September, 2016

Abstract

In this dissertation we study non-negative self-adjoint Laplace type operators acting on smooth sections of a vector bundle. First, we assume base manifolds are compact, boundaryless, and Riemannian. We start from the Fourier integral operator representation of half-wave operators, continue with spectral zeta functions, heat and resolvent trace asymptotic expansions, and end with the quantitative Wodzicki residue method. In particular, all of the asymptotic coefficients of the microlocalized spectral counting function can be explicitly given and clearly interpreted. With the auxiliary pseudo-differential operators ranging all smooth endomorphisms of the given bundle, we obtain certain asymptotic estimates about the integral kernel of heat operators. As applications, we study spectral asymptotics of Dirac type operators such as characterizing those for which the second coefficient vanishes. Next, we assume vector bundles are trivial and base manifolds are Euclidean domains, and study non-negative self-adjoint extensions of the Laplace operator which acts component-wise on compactly supported smooth functions. Using finite propagation speed estimates for wave equations and explicit Fourier Tauberian theorems obtained by Yuri Safarov, we establish the principle of not feeling the boundary estimates for the heat kernel of these operators. In particular, the implied constants are independent of self-adjoint extensions. As a by-product, we affirmatively answer a question about upper estimate for the Neumann heat kernel. Finally, we study some specific values of the spectral zeta function of two-dimensional Dirichlet Laplacians such as spectral determinant and Casimir energy. For numerical purposes we substantially improve the short-time Dirichlet heat trace asymptotics for polygons. This could be used to measure the spectral determinant and Casimir energy of polygons whenever the first several hundred or one thousand Dirichlet eigenvalues are known with high precision by other means.

Acknowledgments

First and foremost, I would like to thank my supervisor Dr. Alexander Strohmaier for giving me the opportunity to undertake this project from various viewpoints, as well as his dedicated guidance.

I am wholeheartedly grateful to my wife Chunrong for her unreserved support and huge help in both my academic and personal life.

My thanks also go to Prof. Huaizhong Zhao for his extensive support since my move to the United Kingdom several years ago.

Finally, I acknowledge the financial support and excellent facilities provided by Loughborough University.

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Chapter 1

Introduction

1.1 Historical context

Weyl's law in its simplest version is a statement on the asymptotic growth of the Dirichlet eigenvalues for bounded Euclidean domains. This was obtained in February 1911 by Hermann Weyl (1885–1955), who was a 26-year-old student of David Hilbert (1862–1943). Weyl's law was motivated by Sommerfeld's problem proposed in September 1910 on the asymptotic behaviour of the Dirichlet, Neumann, and Robin eigenvalues, and the Lorentz-Jeans conjecture proposed one month later on the asymptotic behaviour of the eigenvalues of the electromagnetic cavity. Hilbert once predicted that the Lorentz-Jeans conjecture would not be solved during his lifetime, but he was wrong by many years. Letting $U \subset \mathbb{R}^d$ be a bounded domain, and letting $N(\lambda)$ count the number of Dirichlet eigenvalues for U which are less than λ, Weyl's law says that

$$N(\lambda) = \frac{|U|}{(4\pi)^{d/2}\Gamma(\frac{d+2}{2})}\lambda^{d/2} + o(\lambda^{d/2}) \quad (\lambda \to \infty), \tag{1.1}$$

where $|U|$ denotes the volume of U, and $\Gamma(\cdot)$ denotes the gamma function. This implies that one can deduce the volume of a bounded Euclidean domain from its Dirichlet spectrum. Weyl also conjectured the second asymptotic term which obeys

$$N(\lambda) = \frac{|U|}{(4\pi)^{d/2}\Gamma(\frac{d+2}{2})}\lambda^{d/2} - \frac{|\partial U|}{4(4\pi)^{(d-1)/2}\Gamma(\frac{d+1}{2})}\lambda^{(d-1)/2} + o(\lambda^{(d-1)/2}) \quad (\lambda \to \infty), \tag{1.2}$$

where $|\partial U|$ denotes the surface area of the boundary ∂U of U. This means in particular that one can deduce the surface area of a bounded Euclidean domain from its Dirichlet spectrum. It was justified under certain conditions by Victor Ivrii [83] and Richard Melrose [109] in 1980.

According to Weyl's law, the spectral zeta function of the Dirichlet Laplacian defined by

$$\zeta_U(s) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s}, \tag{1.3}$$

is analytic in $\mathrm{Re}(s) > \frac{d}{2}$, where the Dirichlet eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$ for U are listed in non-decreasing order. For example, the classical Riemann zeta function is $\zeta_{U_0}(\frac{s}{2})$, where U_0 is an arbitrary one-dimensional open interval of length π. It is well known that the Riemann zeta

function is meromorphic on the complex plane $\mathbb{C}$ whose singularity is the only simple pole at $s = 1$ with residue 1. Letting $\{u_n\}_{n=1}^{\infty}$ denote the associated real-valued eigenfunctions so that they form an orthonormal basis for the Hilbert space $L^2(U)$, one can similarly define

$$\zeta_U(s;x) = \sum_{n=1}^{\infty} \frac{u_n(x)^2}{\lambda_n^s} \tag{1.4}$$

for $x \in U$ and $\mathrm{Re}(s) > \frac{d}{2}$. Torsten Carleman (1892–1949) was the first person to attack the more difficult asymptotic behaviour of eigenfunctions by studying (1.4) for two-dimensional bounded domains in 1934. A breakthrough was achieved by Subbaramiah Minakshisundaram (1913–1968) and Carleman's student Åke Pleijel (1913–1989), as they showed in [113] in 1949 that $\zeta_U(s;x)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $\frac{d-k}{2}$ $(k = 0, 1, 2, \ldots)$ for each fixed $x \in U$. Coming back to spectral zeta function, we see that $\zeta_U(s)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $\frac{d-k}{2}$ $(k = 0, 1, 2, \ldots)$. The corresponding residues are determined only by U, so in principle they could carry certain geometric information about the domain itself. Minakshisundaram and Pleijel can also deduce the volume of a bounded Euclidean domain from its Dirichlet spectrum, and studied the Neumann and closed eigenvalue problems in a similar way. Here to be clear, for the Neumann boundary problems, they assumed that boundaries are sufficiently smooth.

The technique developed by Minakshisundaram and Pleijel is very important because they derived complete asymptotic expansion of the heat kernels. Let M be a closed Riemannian manifold, and let Δ_M denote the associated Laplace-Beltrami operator. The integral kernel of $e^{t\Delta_M}$ $(t > 0)$, denoted by $K_M(x, y; t)$ and also called the heat kernel for M, is the fundamental solution of the heat equation

$$\frac{\partial u}{\partial t} = \Delta_M u \quad (t > 0). \tag{1.5}$$

They showed that there exist smooth functions $\{a_k\}_{k=0}^{\infty}$ on M such that

$$K_M(x, x; t) \sim (4\pi t)^{-d/2} \sum_{k=0}^{\infty} a_k(x) t^k \quad (t \to 0^+). \tag{1.6}$$

The short-time heat kernel expansion (1.6) inspired enormous later works, as one can extend scalar Laplacians to vector-valued ones or other elliptic operators as well as study similar problems for manifolds with boundary. For example, not long after their seminal work, people could deduce the surface area of a bounded smooth Euclidean domain from its Dirichlet or Neumann spectrum, the number of holes of a two-dimensional closed Riemannian manifold from its spectrum, and so on. An influential paper [88] by Mark Kac (1914–1984) in 1966 asked whether or not one can hear the shape of a drum, although he himself believed the answer would be no. To be clear, Kac asked whether or not a bounded Euclidean domain is determined by its Dirichlet spectrum up to isometry. A couple of years before Kac's article, John Milnor [112] had constructed two non-congruent higher-dimensional tori whose Laplace-Beltrami operators share the same eigenvalues. Later in 1992, Carolyn Gordon, David Webb and Scott Wolpert [60] gave a negative answer to Kac's question. Nowadays, it is still an open problem in spectral geometry whether or not a bounded convex Euclidean domain is determined by its Dirichlet spectrum up to isometry.

The theory of pseudo-differential operators was systematically developed by Joseph J. Kohn and Louis Nirenberg [90], and Lars Hörmander (1931–2012) [74, 75] in the mid-sixties. Since its appearance, it has been very essential to modern analysis and mathematical physics. Pseudo-differential operators are of great importance in the study of elliptic equations. Some of the simplest operations, such as taking the inverse or the square root, lead out of the class of elliptic differential operators but preserve the class of pseudo-differential operators. In this way, pseudo-differential operators serve as a powerful and natural tool for the study of elliptic (and hypoelliptic) partial differential operators (e.g. [75, 76]).

A natural generalization of the theory of pseudo-differential operators is that of Fourier integral operators, which was systematically developed by Hörmander [77, 78] in the late sixties and early seventies. Johannes J. Duistermaat (1942–2010) also made important contributions as he improved with Hörmander [41] the global theory of Fourier integral operators, and mathematically justified [39] Victor P. Maslov's earlier formulation [106]. A typical example of a Fourier integral operator is the solution operator of the Cauchy problem for a hyperbolic equation. In this way, Fourier integral operators play the same role in the study of hyperbolic equations as pseudo-differential operators do in the theory of elliptic equations.

A significant area for applications of pseudo-differential and Fourier integral operators is the spectral theory of elliptic operators. As the main topics of the thesis lie in this field, let us address two classical applications with each one showcasing one of the two theories.

First, let A be an invertible classical elliptic pseudo-differential operator of positive order m acting on smooth sections of a vector bundle over a closed manifold M, such that A has a ray of minimal growth. An application of functional calculus allows us to define

$$A^s = \frac{\mathrm{i}}{2\pi} \int_\gamma \lambda^s (A - \lambda)^{-1} d\lambda. \tag{1.7}$$

Here γ is a contour in $\mathbb{C}$ from ∞ to a point near the origin along the minimal ray, clockwise about the origin for a full circle, and back to ∞ along the minimal ray. Robert T. Seeley [138] showed, first for small $\mathrm{Re}(s)$ then for all $s \in \mathbb{C}$, that A^s is a classical pseudo-differential operator of order $m\mathrm{Re}(s)$. More importantly, he extended the previous work of Minakshisundaram and Pleijel to invertible classical elliptic vector-valued pseudo-differential operators of positive order. To be clear, he proved that the integral kernel of A^s at any given (x, x) is a meromorphic matrix of smooth functions whose only singularities are simple poles at countably many points. Once again, the residues at these poles carry lots of information about the operator A.

Second, let P be a positive elliptic differential operator of order m on a closed manifold. Hörmander [77] showed that a parametrix for the hyperbolic equation $\mathrm{i}\partial_t + P^{1/m}$, which formally is $\exp(\mathrm{i}tP^{1/m})$, can be realized as a Fourier integral operator. As a consequence he then established the best possible estimates for the remainder term in the asymptotic formula for the spectral function of an arbitrary elliptic differential operator. Later on, Duistermaat and Victor W. Guillemin [40] studied the asymptotic behaviour of the wave kernel $\exp(\mathrm{i}tQ)$ for an arbitrary first order positive elliptic classical pseudo-differential operator Q, say for example, $Q = P^{1/m}$.

Apart from asymptotic expansions of the aforementioned spectral zeta functions, heat and wave kernels, there are other ways to recover local or global geometric information about a manifold or operator. For example, the Riesz mean [50, 77, 114, 129] is one of such methods.

Finally in this section, we pay special attention to wave equation methods, which can be used to study the spectral theory of elliptic operators quite effectively. As early as 1952, Boris M. Levitan (1914–2004) [97] studied the asymptotic behavior of the spectral function of a positive self-adjoint differential operator P of order $m = 2$ by considering its cosine transform $\cos(t\sqrt{P})$, also called the half-wave operator [146]. Note $(\frac{\partial^2}{\partial t^2} + P)\cos(t\sqrt{P}) = 0$, so the half-wave operator is closely related to the fundamental solution of the hyperbolic operator $\frac{\partial^2}{\partial t^2} + P$. According to Hörmander [77], the reason why Levitan's methods had not been applied to operators of order $m > 2$ seemed to be that the differential equation

$$(\mathrm{i}^m \frac{\partial^m}{\partial t^m} - P)e^{-\mathrm{i}tP^{1/m}} = 0 \tag{1.8}$$

is not hyperbolic. But as explained earlier, Hörmander avoided this obstacle by constructing a Fourier integral operator parametrix for the equation

$$(\mathrm{i}\frac{\partial}{\partial t} - P^{1/m})e^{-\mathrm{i}tP^{1/m}} = 0. \tag{1.9}$$

Letting $m = 2$, Jeff Cheeger, Mikhail Gromov and Michael Taylor [28] studied the integral kernel of operators of the form

$$f(\sqrt{P}) = \frac{1}{2\pi}\int_{\mathbb{R}} (\mathscr{F}f)(s)\cos(s\sqrt{P})ds. \tag{1.10}$$

For example, letting f be Gaussian functions implies that the heat operator e^{-tP} $(t > 0)$ can be written as

$$e^{-tP} = \frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}} \cos(s\sqrt{P})e^{-\frac{s^2}{4t}}ds, \tag{1.11}$$

where the main contributions come from small s. Therefore, one can use wave equation methods such as finite propagation speed estimates to study heat kernels.

1.2 Motivation

Let E be a vector bundle over a d-dimensional closed Riemannian manifold M. Let Q be a first order non-negative self-adjoint classical elliptic pseudo-differential operator acting on smooth sections of E. Let $\{\lambda_j, \phi_j\}_{j=1}^{\infty}$ denote the discrete spectral resolution of Q, that is, $Q\phi_j = \lambda_j\phi_j$ for all j. It is known [138] that the eigenvalue counting function $N(\lambda)$ of Q still obeys Weyl's law, but a two-term asymptotic expansion

$$N(\lambda) = c_0\lambda^d + c_1\lambda^{d-1} + o(\lambda^{d-1}) \quad (\lambda \to \infty)$$

does not exist in general. Even so, Duistermaat and Guillemin [40] showed for scalar functions and Victor Ivrii [84] showed for vector-valued systems that

$$(\chi * N')(\lambda) = \sum_{j=1}^{\infty}\chi(\lambda - \lambda_j) \sim \sum_{k=0}^{\infty} a_k\lambda^{d-1-k} \quad (\lambda \to \infty), \tag{1.12}$$

where $\chi \in \mathscr{S}(\mathbb{R})$ is a Schwartz function such that its Fourier transform $\mathscr{F}\chi$ equals 1 near the origin and $\mathrm{supp}(\mathscr{F}\chi) \subset (-\delta, \delta)$ for some sufficiently small δ. Until now, it is still not clear

how to explicitly determine the second coefficient a_1 in terms of the invariantly-defined principal and sub-principal symbols of vector-valued operators Q. Actually, according to the bibliographic review in [30], there were quite a few flawed attempts at this problem. In this thesis we set Q to be the square root of a non-negative self-adjoint Laplace type operator, and introduce an auxiliary classical pseudo-differential operator A. Similar to (1.12), the following microlocalized spectral counting function satisfies

$$\sum_{j=1}^{\infty}\langle A\phi_j,\phi_j\rangle\chi(\lambda-\lambda_j)\sim\sum_{k=0}^{\infty}\mathscr{A}_k(A,Q)\lambda^{d+m-k-1}\quad(\lambda\to\infty),\tag{1.13}$$

where m denotes the order of A. For example, letting the Laplacian be the square of a self-adjoint Dirac type operator D, Sandoval [133] explicitly obtained $\mathscr{A}_1(D,Q)$, while Branson and Gilkey [22] can equivalently determine $\mathscr{A}_1(fD,Q)$ for smooth functions f on M. Note Chervova, Downes and Vassiliev [30, 31] were also able to derive $\mathscr{A}_1(D,Q)$, but only for a small class of Dirac type operators.

The first purpose of the thesis is to give a nice interpretation of $\mathscr{A}_k(A,Q)$ for all $k\geq 0$ in terms of Wodzicki residues. However, we should mention that in equivalent forms the Wodzicki residue representation of the coefficients $\mathscr{A}_k(A,Q)$ is a known result [91, 137]. Linking it with the spectral asymptotics of Dirac type operators may appear first in this thesis.

The second motivation of the thesis is to use the aforementioned wave equation methods to study the heat kernel of an arbitrary vector-valued non-negative self-adjoint Laplacian on Euclidean domains. Note that some results of Dirichlet boundary problems have not been found or do not have counterparts for some other boundary problems. For example, the Dirichlet heat kernel has full domain monotonicity, but the Neumann heat kernel was proven not to have such a property [8]. Note also M. Van den Berg's sharp estimates [10] on Kac's principle of not feeling the boundary for Dirichlet problems have not found the Neumann counterparts yet.

Our method is simple as follows. Let P_1,P_2 be two non-negative self-adjoint extensions of the (negative) Laplacian

$$-\Delta: C_c^\infty(U;\mathbb{C}^N)\to C_c^\infty(U;\mathbb{C}^N),\tag{1.14}$$

acting component-wise on the Hilbert space $L^2(U;\mathbb{C}^N)$. According to (1.11) we have

$$e^{-tP_i}=\frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}}\cos(s\sqrt{P_i})e^{-\frac{s^2}{4t}}ds.\tag{1.15}$$

It is known that if $|s|$ is small, then there is no difference at all between the diagonal kernels of $\cos(s\sqrt{P_1})$ and $\cos(s\sqrt{P_2})$ at certain points of the given domain because of finite propagation speed estimates for the wave equation. Considering the contributions made from those not too small s, we will show later on that the small-time heat kernels for P_1 and P_2 actually have no obvious difference. This means in particular that if one of them is completely known or under good control, then the heat kernel for the other is also under good control. In other words, the choice of possible boundary conditions brings no obvious difference for the small-time heat kernels. In this way we can study for the first time bilateral optimal estimates for the Neumann heat kernel without imposing any convex condition except smoothness.

The third motivation of the thesis is to develop an algorithm that can be used to calculate some specific values of two-dimensional Dirichlet spectral zeta functions on planar polygons

with high precision. So far this is doable only when all of the eigenvalues are explicitly known. A crucial technical difficulty that allows us to study squares only as examples in Chapter 6 is that there were no rigorous and effective completeness tests for sequences of computed eigenvalues generated by computer programs when this thesis was submitted for viva examination in May, 2016.

We are happy to announce that this issue has been solved quite effectively in a recent preprint [17] by Michael Bironneau, Alexander Strohmaier and the author. With this thesis available, the preprint depends crucially on our improvement of short-time heat trace asymptotic expansions for polygons. We would therefore like to recommend Chapter 6 and [17] to the reader. By the way, the close connection between the second and third motivations will be explained in detail at the beginning of Chapter 5.

1.3 Conclusions

The author should clearly state that Chapters 3 and 4 are based on paper [98] entitled “The local counting function of operators of Dirac and Laplace type”, and Chapter 5 is based on paper [99] entitled “Heat kernel estimates for general boundary problems”. Both papers have been published jointly by the author and his supervisor.

In Chapter 3 we provide a nearly self-contained description of five different approaches to the microlocalized spectral counting function of non-negative self-adjoint operators of Laplace type, except the connecting formula (2.22) between heat expansions and Wodzicki residues. With the auxiliary pseudo-differential operators ranging all smooth endomorphisms of the given vector bundle, we recover the short-time asymptotics of the diagonal integral kernel of certain operators (Theorem 3.6.1). As applications, we study the spectral asymptotics of self-adjoint operators of Dirac type (Theorems 4.1.1, 4.1.3 and 4.2.1), and characterized those for which the second coefficient vanishes in Chapter 4 (Theorem 4.3.1).

In Chapter 5 we show that the principle of not feeling the boundary estimates for heat kernels holds for any non-negative self-adjoint extension of the classical Laplace operator acting on vector-valued compactly supported smooth functions on a Euclidean domain (Theorems 5.3.1 and 5.4.3). They are valid for any choice of boundary condition and the implied constants can be chosen independent of the self-adjoint extension. As a by-product, we answer affirmatively a question about an upper estimate for the Neumann heat kernel (Theorem 5.6.2).

In Chapter 6 we substantially improve the short-time Dirichlet heat trace asymptotics for polygonal regions (Theorem 6.3.2). This could be used to measure the spectral determinant and Casimir energy of polygons whenever in general the first several hundred or one thousand Dirichlet eigenvalues are known with high precision by other means.

Chapter 2

Background

In this chapter we mainly review some invariant concepts relating to classical pseudo-differential operators such as principal and sub-principal symbols, and Wodzicki's residue. We also discuss the local representation of a class of Fourier integral operators and finite propagation speed estimates for wave equations.

2.1 Partial differential operators

2.1.1 Partial differential operators on Euclidean domains

Let U be an open subset of $\mathbb{R}^d$, and let

$$P = \sum_{|\alpha|\leq m} P_\alpha(x) D_x^\alpha = \sum_{|\alpha|\leq m} P_\alpha(x)(-\mathrm{i}\frac{\partial}{\partial x_1})^{\alpha_1}\cdots(-\mathrm{i}\frac{\partial}{\partial x_d})^{\alpha_d}$$

be a partial differential operator on U of order at most m. Here $\alpha = (\alpha_1, \ldots, \alpha_d) \in (\mathbb{N}\cup\{0\})^d$ denotes a multiple index, and $|\alpha|$ is short for the length of α, that is, $|\alpha| = \alpha_1 + \cdots + \alpha_d$. For simplicity we assume throughout the thesis that all of the coefficients P_α are smooth functions on U. The full and principal symbols of P, denoted by $\sigma_{\mathrm{Full}}(P)$ and $\sigma_m(P)$ respectively, are complex-valued functions on $U \times \mathbb{R}^d$ defined by

$$\begin{aligned}\sigma_{\mathrm{Full}}(P)(x,\xi) &= \sum_{|\alpha|\leq m} P_\alpha(x)\xi^\alpha = \sum_{|\alpha|\leq m} P_\alpha(x)\xi_1^{\alpha_1}\cdots\xi_d^{\alpha_d},\\ \sigma_m(P)(x,\xi) &= \sum_{|\alpha|=m} P_\alpha(x)\xi^\alpha.\end{aligned}$$

If $\sigma_m(P)$ is not identically equal to zero, we say that P is of order m. For example, the Laplace operator is a second order partial differential operator whose full and principal symbols are the same as $-|\xi|^2$. Via Fourier analysis we see that

$$Pu = \mathscr{F}^{-1}(\sigma_{\mathrm{Full}}(P)(x,\xi)\mathscr{F}u(\xi)) \quad (u \in C_c^\infty(U)),$$

where $\mathscr{F}$ denotes the Fourier transform on $\mathbb{R}^d$. Based on this formula one can similarly define matrix-valued full and principal symbols for vector-valued partial differential operators.

2.1.2 Partial differential operators on manifolds

Let M be a smooth manifold of dimension d. A local linear map $P : C^\infty(M) \to C^\infty(M)$ is called a partial differential operator of order at most m, if for every coordinate chart $V \xrightarrow{\varphi} U \subset \mathbb{R}^d$, the operator P_φ induced by the following diagram

$$\begin{array}{ccc} C^\infty(V) & \xleftarrow{\varphi_*^{-1}} & C^\infty(U) \\ {\scriptstyle P|_V}\downarrow & & \downarrow{\scriptstyle P_\varphi} \\ C^\infty(V) & \xrightarrow{\varphi_*} & C^\infty(U) \end{array}$$

is a standard partial differential operator on the Euclidean domain U of order at most m. Here φ_* denotes the push-forward operation sending function u on V to $u \circ \varphi^{-1}$ on U, and P is called a local operator if $\mathrm{Supp}(Pu) \subset \mathrm{Supp}(u)$ for all $u \in C^\infty(M)$. Obviously, the restriction $P|_V$ of P onto $C^\infty(V)$ is well-defined. P is said to be of order m if for some coordinate chart the induced operator has this property.

Next, we explain how to define the principal symbol of P. If $M = V$ is a Euclidean domain, then for any smooth diffeomorphism $V \xrightarrow{\varphi} U$ one can deduce from the chain rule that (e.g. [3, I.7.1], [48, Thm. 8.58], [62, (3.7)], [75, Thm. 2.16], [102, Prop. 13, Chap. 5] [128, Prop. 2.5.25], [139, Cor. 4.1], [146, Cor. 3.2.2] [153, Thm. 5.1, Chap. 1], [155, Page 33])

$$\sigma_m(P_\varphi)(y, \xi) = \sigma_m(P)(\varphi^{-1}(y), J_\varphi(\varphi^{-1}(y))^T \xi),$$

where J_φ denotes the Jacobian matrix of φ. Generally, one can collaborate the transformation rule for covectors at any given point of M with the above relation to invariantly define the principal symbol of P as a smooth function on the cotangent bundle T^*M of M. Alternatively, one can set (e.g. [14, 74, 75])

$$\sigma_m(P)(\xi) = \lim_{t \to 0^+} t^{-m} e^{-\mathrm{i}t\phi(p)} (P e^{\mathrm{i}t\phi})(x) \quad (\xi \in T_x^* M),$$

where ϕ is any real-valued smooth function on M with $(d\phi)_x = \xi$.

2.1.3 Partial differential operators on vector bundles

Let E be a complex vector bundle of rank r over a smooth manifold M of dimension d. Let $C^\infty(M; E)$ denote the space of smooth sections of E. In the event that $E = M \times \mathbb{C}^r$ is a trivial bundle, we also let $C^\infty(M; \mathbb{C}^r)$ be short for $C^\infty(M; E)$. Similar to the previous discussion, a local linear map $P : C^\infty(M; E) \to C^\infty(M; E)$ is called a partial differential operator of order at most m if, for every coordinate chart $V \xrightarrow{\varphi} U \subset \mathbb{R}^d$ and every bundle trivialization $E_V \xrightarrow{\Phi} V \times \mathbb{C}^r$, the operator $\widetilde{P}$ induced by the following diagram

$$\begin{array}{ccccc} C^\infty(V; E_V) & \longleftarrow & C^\infty(V; \mathbb{C}^r) & \longleftarrow & C^\infty(U; \mathbb{C}^r) \\ {\scriptstyle P|_V}\downarrow & & & & \downarrow{\scriptstyle \widetilde{P}} \\ C^\infty(V; E_V) & \longrightarrow & C^\infty(V; \mathbb{C}^r) & \longrightarrow & C^\infty(U; \mathbb{C}^r) \end{array}$$

is a standard vector-valued partial differential operator on the Euclidean domain U of order at most m. Here each unlabelled arrow in the diagram can be naturally interpreted. As usual, P is said to be of order m if some induced local operator is of this property. The principal symbol of P, denoted by $\sigma_m(P)$ or σ_P, can be similarly defined as a map on T^*M sending $\xi \in T_x^*M$ to some unique element in the space $\mathrm{End}(E_x)$ of endomorphisms of the fiber E_x of E at x. For details we refer the reader to the books [14, 94, 102].

The principal symbol can also be defined for partial differential operators mapping between sections of two bundles over the same base manifold. For example, on differential forms the Lie derivative, exterior product, interior product, codifferential, Hodge star, and Laplace-Beltrami operators all are partial differential operators, and it is a good exercise to explicitly determine the corresponding principal symbols.

A foundational result due to Peetre claims that any local linear map acting on $C^\infty(M)$ must be a partial differential operator. This implies that any local linear map between smooth sections of two bundles over the same base manifold is locally a partial differential operator. As an application, we see that if X is a non-vanishing smooth vector field on M and ∇ is a connection on E, then the covariant derivative $\nabla_X : C^\infty(M;E) \to C^\infty(M;E)$ in the direction of X is globally a partial differential operator of first order. In general, letting $X_1, \ldots, X_m$ be smooth vector fields on M and letting F be a smooth bundle endomorphism of E, we see that

$$F\nabla_{X_m} \cdots \nabla_{X_1}$$

is a partial differential operator of order at most m.

2.1.4 Laplace type operators

Let M be a smooth manifold admitting a Riemannian metric g. As before, E denotes a smooth complex vector bundle over M. Given a connection ∇ on E, let Δ^∇ denote the connection Laplacian generated by ∇. Some authors call this operator the Bochner or reduced Laplacian. Locally, Δ^∇ is of the form $-g^{ij}(\nabla_i\nabla_j - \Gamma_{ij}^k\nabla_k)$, where we have used Einstein's sum convention, $g^{ij} = g(dx^i, dx^j)$, $\nabla_k = \nabla_{\partial_k}$, Γ_{ij}^k denotes the Christoffel symbols of the Riemannian connection on TM, that is, $\nabla_{\partial_i}\partial_j = \Gamma_{ij}^k\partial_k$. The principal symbol of the connection Laplacian, however, is independent of the choice of connections on E. Actually, $\sigma_{\Delta^\nabla}(\xi) = g_x(\xi,\xi)\mathrm{id}_{E_x}$ for all covectors $\xi \in T_x^*M$. A second order partial differential operator P acting on $C^\infty(M;E)$ is said to be of Laplace type if its principal symbol agrees with that of a connection Laplacian. In local coordinates this means that P is of the form $-g^{ij}(x)\partial_i\partial_j + a^k(x)\partial_k + b(x)$, where a^k, b are smooth matrix-valued functions. Given such an operator P, the Bochner-Weitzenböck technique (e.g. [54, 57, 94]) guarantees that there exists a unique connection ∇ on E and a unique bundle endomorphism $F \in C^\infty(M;\mathrm{End}(E))$ such that $P = \Delta^\nabla + F$.

2.1.5 Dirac type operators

A first order partial differential operator $D : C^\infty(M;E) \to C^\infty(M;E)$ is said to be of Dirac type if its square is of Laplace type. The main purpose of this part is to recall the representation structure as well as study the Bochner-Weitzenböck technique for such operators.

First of all, let us provide some concrete examples. Let (M, g) be a parallelizable Riemannian manifold of dimension d, and let $E = M \times \mathbb{C}^r$ be a trivial bundle over M of rank $r = 2^{\lfloor \frac{d}{2} \rfloor}$. Since M is parallelizable, there exist smooth real vector fields $\{X_k\}_{k=1}^d$ on M such that $\{X_k(x)\}_{k=1}^d$ is an orthonormal basis for (T_xM, g_x) at each $x \in M$. According to the Clifford algebra theory (e.g. [49, 52]), one can set $\{R_k\}_{k=1}^d$ to be complex matrices of size $r \times r$ such that $R_jR_k + R_kR_j = -2\delta_{jk}$ for all j, k. Obviously, each R_k can be naturally regarded as a partial differential operator of order zero on $C^\infty(M; E)$. According to the discussion in the last paragraph of §2.1.3, each ∇_{X_k} is a partial differential operator of first order on $C^\infty(M; E)$, where ∇ is any prescribed connection on E. Then it is easy to check that $D = R_k\nabla_{X_k}$ is a Dirac type operator. For example, if $M = \mathbb{R}^3$, $E = \mathbb{R}^3 \times \mathbb{C}^2$, ∇_X means the ordinary derivative in the direction X, and if

$$R_1 = \begin{pmatrix} 0 & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}, \quad R_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad R_3 = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix},$$

then $D = R_k\nabla_{X_k}$ is just the operator named after P. A. M. Dirac.

Let $\mathrm{Cl}(TM)$ be the universal unital complex algebra bundle generated by the tangent bundle TM subject to the commutation relation $X*Y+Y*X = -2g(X, Y)$, where $X, Y \in C^\infty(M; TM)$ and $*$ denotes the algebra operation. A Clifford module structure on E is just a unital algebra morphism $\gamma : \mathrm{Cl}(TM) \to \mathrm{End}(E)$. Given any connection $\widehat{\nabla}$ on the Clifford module $E = (E, \gamma)$, $\gamma\widehat{\nabla} \triangleq \gamma(e_k)\widehat{\nabla}_{e_k}$ is a well-defined first order partial differential operator acting on $C^\infty(M; E)$, where $\{e_k\}_{k=1}^d$ denotes any orthonormal basis of T_xM at each point $x \in M$. To see this let ϕ be a smooth section of E. Then the value of $(\gamma\widehat{\nabla})\phi$ at an arbitrary point $x \in M$ is just the trace of the following bilinear map, acting from the twofold sum of the inner-product space (T_xM, g_x) to the fiber E_x, defined by sending $(X, Y) \in T_xM \times T_xM$ to $\gamma(X)\widehat{\nabla}_Y\phi \in E_x$. On the other hand, one can naturally extend the Riemannian metric g and connection ∇ on TM to $\mathrm{Cl}(TM)$ with the properties that: the extended connection also denoted by ∇ preserves the extended metric, and

$$\nabla_X(\alpha * \beta) = (\nabla_X\alpha) * \beta + \alpha * (\nabla_X\beta) \tag{2.1}$$

for all $X \in C^\infty(M; TM)$, $\alpha, \beta \in C^\infty(M; \mathrm{Cl}(TM))$. Among plenty of connections on the Clifford module (E, γ), we call a connection $\widetilde{\nabla}$ compatible with γ if

$$\widetilde{\nabla}_X(\gamma(\alpha)\phi) = \gamma(\nabla_X\alpha)\phi + \gamma(\alpha)(\widetilde{\nabla}_X\phi) \tag{2.2}$$

for all $X \in C^\infty(M; TM)$, $\alpha \in C^\infty(M; \mathrm{Cl}(TM))$, $\phi \in C^\infty(M; E)$. It is well known [22] that on a Clifford module there always exists a compatible connection. Such a triple $(E, \gamma, \widetilde{\nabla})$ is called a Dirac bundle. It is easy to see that any operator D of Dirac type can always be written as $D = \gamma\widetilde{\nabla} + \psi$, where $(E, \gamma, \widetilde{\nabla})$ is some Dirac bundle with its Clifford module structure γ uniquely determined by the principal symbol of D, $\psi \in C^\infty(M; \mathrm{End}(E))$. We call ψ the potential of D associated with the Dirac bundle $(E, \gamma, \widetilde{\nabla})$.

To help understand the concept of Dirac bundle, we construct such a bundle associated with the Dirac type operators studied earlier on trivial bundles over parallelizable Riemannian manifolds. All the relevant notations are followed. It is easy to verify that $\gamma : TM \to \mathrm{End}(E)$, defined by $\gamma(X) = g(X, X_k)R_k$, is a Clifford module structure on E. Define $L : TM \to \mathrm{End}(E)$ by $L(X) = \frac{R_k\gamma(\nabla_X X_k)}{4}$, and put a flat connection $\widehat{\nabla}$ on E by

$$\widehat{\nabla}_X\phi = \widehat{\nabla}_X \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_r \end{pmatrix} = \begin{pmatrix} X\phi_1 \\ \vdots \\ X\phi_r \end{pmatrix}.$$

Following Branson-Gilkey [22], we claim $\widetilde{\nabla} \triangleq \widehat{\nabla} + L$ is a compatible connection on (E, γ). To this end we first note $\alpha \in C^\infty(M; TM)$ is of the form $\alpha = \alpha_k X_k$ for some $\alpha_k \in C^\infty(M)$. Thus

$$\begin{aligned}\widetilde{\nabla}_X(\gamma(\alpha)\phi) &= \widetilde{\nabla}_X(\alpha_k R_k\phi) = \widehat{\nabla}_X(\alpha_k R_k\phi) + L(X)\gamma(\alpha)\phi \\ &= (X\alpha_k)(R_k\phi) + \gamma(\alpha)\widehat{\nabla}_X\phi + L(X)\gamma(\alpha)\phi,\end{aligned}$$

and

$$\begin{aligned}\gamma(\nabla_X\alpha)\phi + \gamma(\alpha)\widetilde{\nabla}_X\phi &= \gamma((X\alpha_k)X_k + \alpha_k\nabla_X X_k)\phi + \gamma(\alpha)\widehat{\nabla}_X\phi + \gamma(\alpha)L(X)\phi \\ &= (X\alpha_k)(R_k\phi) + \alpha_k\gamma(\nabla_X X_k)\phi + \gamma(\alpha)\widehat{\nabla}_X\phi + \gamma(\alpha)L(X)\phi.\end{aligned}$$

Hence to prove the compatibility condition (2.2) currently for $\alpha \in C^\infty(M; TM)$, it suffices to show $[L(X), \gamma(\alpha)] = g(\alpha, X_k)\gamma(\nabla_X X_k)$, which is obviously equivalent to

$$[L(X_i), \gamma(X_j)] = g(X_j, X_k)\gamma(\nabla_{X_i} X_k) \quad (1 \le i, j \le d). \tag{2.3}$$

Denoting $\nabla_{X_i} X_j = \Gamma_{ij}^k X_k$ and considering $\Gamma_{ij}^k = -\Gamma_{ik}^j$, we have

$$\begin{aligned}[L(X_i), \gamma(X_j)] &= \frac{1}{4}\big(R_k\gamma(\nabla_{X_i} X_k)R_j - R_j R_k\gamma(\nabla_{X_i} X_k)\big) \\ &= \frac{1}{4}\big(R_k\Gamma_{ik}^n R_n R_j - R_j R_k\Gamma_{ik}^n R_n\big) \\ &= \frac{1}{4}\big(-2R_k\Gamma_{ik}^n\delta_{nj} - R_k\Gamma_{ik}^n R_j R_n - R_j R_k\Gamma_{ik}^n R_n\big) \\ &= \frac{1}{2}(-R_k\Gamma_{ik}^j + \Gamma_{ij}^n R_n) = \Gamma_{ij}^n R_n \\ &= \gamma(\nabla_{X_i} X_j) = g(X_j, X_k)\gamma(\nabla_{X_i} X_k),\end{aligned}$$

which proves (2.3). Generally, if $\alpha \in C^\infty(M; \mathrm{Cl}(TM))$ is of the form $\alpha = \alpha^{(1)} * \alpha^{(2)} * \cdots * \alpha^{(n)}$ where $\alpha^{(k)} \in C^\infty(M; TM)$ $(1 \le k \le n)$, then according to (2.1),

$$\begin{aligned}\widetilde{\nabla}_X(\gamma(\alpha)\phi) &= \widetilde{\nabla}_X\big(\gamma(\alpha^{(1)})\big[\gamma(\alpha^{(2)})\cdots\gamma(\alpha^{(n)})\phi\big]\big) \\ &= \gamma(\nabla_X\alpha^{(1)})\big[\gamma(\alpha^{(2)})\cdots\gamma(\alpha^{(n)})\phi\big] + \gamma(\alpha^{(1)})\widetilde{\nabla}_X\big[\gamma(\alpha^{(2)})\cdots\gamma(\alpha^{(n)})\phi\big] \\ &= \cdots \\ &= \sum_{k=1}^n \gamma(\alpha^{(1)})\cdots\gamma(\alpha^{(k-1)})\gamma(\nabla_X\alpha^{(k)})\gamma(\alpha^{(k+1)})\cdots\gamma(\alpha^{(n)})\phi + \gamma(\alpha)\widetilde{\nabla}_X\phi \\ &= \gamma(\nabla_X\alpha)\phi + \gamma(\alpha)\widetilde{\nabla}_X\phi,\end{aligned}$$

which suffices to claim (2.2) for arbitrary $\alpha \in C^\infty(M; \mathrm{Cl}(TM))$ by linearity. Thus $(E, \gamma, \widetilde{\nabla})$ is a Dirac bundle. Note $\gamma\widetilde{\nabla} = \gamma\widehat{\nabla} + \psi$ where

$$\psi = \frac{R_i R_j\gamma(\nabla_{X_i} X_j)}{4}.$$

This means that $-\psi$ is the potential of $\gamma\widehat{\nabla}$ associated with the Dirac bundle $(E, \gamma, \widetilde{\nabla})$.

Next, we study the Bochner-Weitzenböck technique for Dirac type operators. Let D be a Dirac type operator acting on $C^\infty(M;E)$. The Bochner-Weitzenböck technique for Laplace type operators, discussed in §2.1.4, ensures that there exist a unique connection $\widehat{\nabla}$ on E, and a unique bundle endomorphism $\psi_2 \in C^\infty(M;\mathrm{End}(E))$ such that $P = \Delta^{\widehat{\nabla}} + \psi_2$. In a series of papers by P. Gilkey and his collaborators (e.g. [22, 54, 57, 58]), the potential ψ_2 is always written as a function explicitly depending on $\widehat{\nabla}$ and a few others. But note that there exists a Dirac bundle $(E, \gamma, \widetilde{\nabla})$ such that $D = \gamma\widetilde{\nabla} + \psi$ for some potential ψ. Our purpose below is to express ψ_2 as a function of γ, $\widetilde{\nabla}$, ψ for later use. To the best of the author's knowledge, there does not exist such an explicit formula in the literature unless $\psi = 0$ (e.g. [63, 94]).

To this end we first fix a few notations. Given Dirac bundle $(E, \gamma, \widetilde{\nabla})$, define a connection $\overline{\nabla}$ on $\mathrm{End}(E)$ by

$$(\overline{\nabla}_X\omega)(\phi) = \widetilde{\nabla}_X(\omega(\phi)) - \omega(\widetilde{\nabla}_X\phi) \tag{2.4}$$

for all $X \in C^\infty(M;TM)$, $\omega \in C^\infty(M;\mathrm{End}(E))$, $\phi \in C^\infty(M;E)$. Then $\overline{\nabla}$ is compatible with γ in the following sense:

$$(\overline{\nabla}_X)(\omega\gamma(Y)) = (\overline{\nabla}_X\omega)\gamma(Y) + \omega\gamma(\nabla_X Y), \tag{2.5}$$

$$(\overline{\nabla}_X)(\gamma(Y)\omega) = \gamma(Y)(\overline{\nabla}_X\omega) + \gamma(\nabla_X Y)\omega, \tag{2.6}$$

where X, ω, ϕ remain the same meanings as before, $Y \in C^\infty(M;TM)$. The curvature tensor of any connection $\widehat{\nabla}$ on E is denoted by $R^{\widehat{\nabla}}$, that is,

$$R^{\widehat{\nabla}}_{XY} = [\widehat{\nabla}_X, \widehat{\nabla}_Y] - \widehat{\nabla}_{[X,Y]}.$$

We use the metric tensor to identify the tangent and cotangent bundles $TM = T^*M$, which means locally $dx^j \equiv g^{ij}\partial_i$. Denote $G^{i_1,\dots,i_n} = G(dx^{i_1},\dots,dx^{i_n})$, $G_{i_1,\dots,i_n} = G(\partial_{i_1},\dots,\partial_{i_n})$ for any map G defined on the n-fold product of TM. Recall that Γ^k_{ij} denotes the Christoffel symbols of the Riemannian metric, that is, $\nabla_{\partial_i}\partial_j = \Gamma^k_{ij}\partial_k$ where ∇ denotes the Riemannian connection.

Proposition 2.1.1. *Let D be a Dirac type operator of potential ψ associated with the Dirac bundle $(E, \gamma, \widetilde{\nabla})$. Let $L : TM \to \mathrm{End}(E)$ denote the map defined by*

$$L(X) = \frac{\gamma(X)\psi + \psi\gamma(X)}{2}.$$

Then $\nabla_\psi \triangleq \widetilde{\nabla} - L$ is a connection on E and $\psi_2 \triangleq P - \Delta^{\nabla_\psi} \in C^\infty(M;\mathrm{End}(E))$. Locally

$$\psi_2 = \frac{1}{2}\gamma^i\gamma^j R^{\widetilde{\nabla}}_{ij} + \frac{1}{2}[\gamma^i, \overline{\nabla}_i\psi] + L^iL_i + \psi^2.$$

Proof. Let L be naturally identified with $C^\infty(M;TM) \times C^\infty(M;E) \xrightarrow{L} C^\infty(M;E)$, which is $C^\infty(M)$-linear in both variables. Thus $\widehat{\nabla} \triangleq \widetilde{\nabla} - L$ is a connection on E. By (2.4) we get

$$\begin{aligned}
\triangle^{\widetilde{\nabla}} - \triangle^{\widehat{\nabla}} &= -g^{ij}(\widetilde{\nabla}_i\widetilde{\nabla}_j - \widetilde{\nabla}_i\widehat{\nabla}_j + \widetilde{\nabla}_i\widehat{\nabla}_j - \widehat{\nabla}_i\widehat{\nabla}_j) + g^{ij}\Gamma^k_{ij}(\widetilde{\nabla}_k - \widehat{\nabla}_k) \\
&= -g^{ij}\widetilde{\nabla}_i L_j - g^{ij}L_i\widehat{\nabla}_j + g^{ij}\Gamma^k_{ij}L_k \\
&= -g^{ij}((\overline{\nabla}_i L_j) + L_j\widetilde{\nabla}_i) - g^{ij}L_i(\widetilde{\nabla}_j - L_j) + g^{ij}\Gamma^k_{ij}L_k \\
&= -2L^i\widetilde{\nabla}_i - g^{ij}(\overline{\nabla}_i L_j) + L^iL_i + g^{ij}\Gamma^k_{ij}L_k.
\end{aligned}$$

On the other hand, according to (2.2) and (2.4) we have

$$\begin{aligned}
P &= (\gamma^i\widetilde{\nabla}_i + \psi)(\gamma^j\widetilde{\nabla}_j + \psi) \\
&= \gamma^i\gamma^j\widetilde{\nabla}_i\widetilde{\nabla}_j - \Gamma^j_{ik}\gamma^i\gamma^k\widetilde{\nabla}_j + \gamma^i(\overline{\nabla}_i\psi) + \gamma^i\psi\widetilde{\nabla}_i + \psi\gamma^j\widetilde{\nabla}_j + \psi^2 \\
&= \gamma^i\gamma^j\frac{\widetilde{\nabla}_i\widetilde{\nabla}_j + \widetilde{\nabla}_j\widetilde{\nabla}_i}{2} + \gamma^i\gamma^j\frac{R^{\widetilde{\nabla}}_{ij}}{2} + \Gamma^j_{ik}g^{ik}\widetilde{\nabla}_j + \gamma^i(\overline{\nabla}_i\psi) + (\gamma^i\psi + \psi\gamma^i)\widetilde{\nabla}_i + \psi^2 \\
&= -g^{ij}\widetilde{\nabla}_i\widetilde{\nabla}_j + g^{ij}\Gamma^k_{ij}\widetilde{\nabla}_k + \gamma^i\gamma^j\frac{R^{\widetilde{\nabla}}_{ij}}{2} + \gamma^i(\overline{\nabla}_i\psi) + (\gamma^i\psi + \psi\gamma^i)\widetilde{\nabla}_i + \psi^2 \\
&= \triangle^{\widetilde{\nabla}} + (\gamma^i\psi + \psi\gamma^i)\widetilde{\nabla}_i + \gamma^i\gamma^j\frac{R^{\widetilde{\nabla}}_{ij}}{2} + \gamma^i(\overline{\nabla}_i\psi) + \psi^2.
\end{aligned}$$

Consequently, combining the above calculations yields

$$P = \triangle^{\widehat{\nabla}} + \gamma^i\gamma^j\frac{R^{\widetilde{\nabla}}_{ij}}{2} + \gamma^i(\overline{\nabla}_i\psi) + \psi^2 - g^{ij}(\overline{\nabla}_i L_j) + L^i L_i + g^{ij}\Gamma^k_{ij}L_k \triangleq \triangle^{\widehat{\nabla}} + \psi_2.$$

Next let us simplify the expression of ψ_2. According to (2.5) and (2.6) we have

$$\begin{aligned}
-g^{ij}(\overline{\nabla}_i L_j) &= -g^{ij}\frac{\gamma_j(\overline{\nabla}_i\psi) + \Gamma^k_{ij}\gamma_k\psi + (\overline{\nabla}_i\psi)\gamma_j + \Gamma^k_{ij}\psi\gamma_k}{2} \\
&= -g^{ij}\frac{\gamma_j(\overline{\nabla}_i\psi) + (\overline{\nabla}_i\psi)\gamma_j}{2} - g^{ij}\Gamma^k_{ij}L_k \\
&= -\frac{\gamma^i(\overline{\nabla}_i\psi) + (\overline{\nabla}_i\psi)\gamma^i}{2} - g^{ij}\Gamma^k_{ij}L_k,
\end{aligned}$$

which implies

$$\begin{aligned}
\psi_2 &= \gamma^i\gamma^j\frac{R^{\widetilde{\nabla}}_{ij}}{2} + \gamma^i(\overline{\nabla}_i\psi) + \psi^2 - \frac{\gamma^i(\overline{\nabla}_i\psi) + (\overline{\nabla}_i\psi)\gamma^i}{2} + L^i L_i \\
&= \gamma^i\gamma^j\frac{R^{\widetilde{\nabla}}_{ij}}{2} + \frac{1}{2}[\gamma^i, \overline{\nabla}_i\psi] + \psi^2 + L^i L_i.
\end{aligned}$$

This finishes the proof of Proposition 2.1.1. □

2.2 Pseudo-differential operators

Based on the theory of singular integral operators, Kohn and Nirenberg [90] and Hörmander [74, 75] systematically introduced the theory of pseudo-differential operators, which has proved to be extremely useful to the study of elliptic equations since its appearance. In this section we start by defining pseudo-differential operators on Euclidean domains and manifolds, continue with extending the concept of sub-principal symbol from manifolds to vector bundles, and end with discussing the concept of Wodzicki residue and Seeley's construction of complex powers of an elliptic operator. All these ingredients are essential to our later study of operators of Dirac and Laplace type.

2.2.1 Pseudo-differential operators on Euclidean spaces

Let $\mathscr{S}(\mathbb{R}^d)$ denote the Schwartz space of smooth functions that are rapidly decreasing at infinity, and let $\mathscr{S}'(\mathbb{R}^d)$ denote the dual space of $\mathscr{S}(\mathbb{R}^d)$. The Fourier transform $\mathscr{F} : \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ is defined by

$$(\mathscr{F}f)(\xi) = \mathscr{F}f(\xi) = \widehat{f}(\xi) = (\mathscr{F}_x f)(\xi) = \int_{\mathbb{R}^d} e^{-\mathrm{i}x\cdot\xi} f(x)dx.$$

Let $m \in \mathbb{R}$ and let $P(x,\xi)$ be a smooth complex-valued function on $\mathbb{R}^d \times \mathbb{R}^d$. We say (e.g. [80, 94, 102, 124, 128, 146, 149, 155, 161]) that P is a symbol of order m, or more succinctly $P \in S^m$, if for all multi-indices α, β,

$$\Big|(\frac{\partial}{\partial x})^\alpha(\frac{\partial}{\partial \xi})^\beta P(x,\xi)\Big| \le C_{\alpha\beta}\langle\xi\rangle^{m-|\beta|} \quad (x \in \mathbb{R}^d,\ \xi \in \mathbb{R}^d),$$

where $\langle\xi\rangle \triangleq \sqrt{1+|\xi|^2}$. To a given symbol $P \in S^m$ we associate the operator

$$\begin{aligned}\Big[P(x,D)u\Big](x) &= \Big[\mathscr{F}_\xi^{-1}\big(P(x,\xi)\cdot\widehat{u}(\xi)\big)\Big](x) \qquad\qquad (u \in \mathscr{S}(\mathbb{R}^d))\\ &= (2\pi)^{-d}\int_{\mathbb{R}^d} e^{\mathrm{i}x\cdot\xi}P(x,\xi)\widehat{u}(\xi)d\xi\\ &= (2\pi)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{\mathrm{i}(x-y)\cdot\xi}P(x,\xi)u(y)dyd\xi \quad \text{(repeated integral)},\end{aligned}$$

which is called the pseudo-differential operator (on $\mathbb{R}^d$) with symbol $P(x,\xi)$. The order of the symbol $P(x,\xi)$ is also called the order of $P(x,D)$. It is easy to show that $P(x,D)$ maps $\mathscr{S}(\mathbb{R}^d)$ to $\mathscr{S}(\mathbb{R}^d)$ and is a continuous linear map. The basic theory of pseudo-differential operators answers affirmatively the following three questions.

QUESTION 1: Is the operator $P(x,D)$ uniquely determined by its symbol $P(x,\xi)$?

QUESTION 2: Suppose $P, Q \in S^\infty = \cup_{m\in\mathbb{R}} S^m$. Note $Q(x,D)\circ P(x,D)$ is a continuous linear map from $\mathscr{S}(\mathbb{R}^d)$ to $\mathscr{S}(\mathbb{R}^d)$. Does there exist an $R \in S^\infty$ such that $R(x,D) = Q(x,D)\circ P(x,D)$?

QUESTION 3: Suppose $P \in S^m$. The (formal) adjoint of $P(x,D)$, denoted by P^*, exists in the following sense

$$\langle P(x,D)u, v\rangle = \langle u, P^*v\rangle \quad (u, v \in \mathscr{S}(\mathbb{R}^d)), \tag{2.7}$$

where $\langle\cdot,\cdot\rangle$ denotes the inner-product on $L^2(\mathbb{R}^d)$. Does there exist an $S \in S^m$ such that $P^* = S(x,D)$?

To deal with these questions we will frequently encounter the technical issue of changing the order of integration. To this end the following lemma [128, Prop. 2.1.10] is quite useful. As applications, to study Questions 2 and 3 one can first assume that the symbols of P, Q are compactly supported in $\mathbb{R}^d \times \mathbb{R}^d$, then apply this lemma to reach their full generality.

Lemma 2.2.1. *Suppose we have a sequence of symbols $\{P_k \in S^m\}_{k=0}^\infty$ which satisfies the uniform symbolic estimates*

$$\Big|(\frac{\partial}{\partial x})^\alpha(\frac{\partial}{\partial \xi})^\beta P_k(x,\xi)\Big| \le C_{\alpha\beta}\langle\xi\rangle^{m-|\beta|} \quad (x \in \mathbb{R}^d,\ \xi \in \mathbb{R}^d)$$

for all multi-indices α, β. Suppose $P_k(x,\xi)$ and all of its derivatives converge to $P_0(x,\xi)$ and its derivatives, respectively, pointwise as $k \to \infty$. Let $\{u_k\}_{k=0}^\infty$ be a sequence of Schwartz functions such that $u_k \overset{\mathscr{S}(\mathbb{R}^d)}{\longrightarrow} u_0$ as $k \to \infty$. Then $P_k(x,D)u_k \overset{\mathscr{S}(\mathbb{R}^d)}{\longrightarrow} P_0(x,D)u_0$ as $k \to \infty$.

In the following we study in detail the first question and sketch solutions to the other two. According to (2.7), it is easy to show that P^* maps $\mathscr{S}(\mathbb{R}^d)$ to $\mathscr{S}(\mathbb{R}^d)$ and is a continuous linear map. Thus one can extend $P(x,D)$ as a continuous linear map from $\mathscr{S}'(\mathbb{R}^d)$ to $\mathscr{S}'(\mathbb{R}^d)$ via (2.7) by defining

$$\Big[P(x,D)u\Big](v) = u\Big(\overline{P(x,D)^*\overline{v}}\Big) \qquad (u \in \mathscr{S}'(\mathbb{R}^d),\ v \in \mathscr{S}(\mathbb{R}^d)). \tag{2.8}$$

Let $\xi \in \mathbb{R}^d$ be a fixed element, and note $e_\xi(x) = e^{\mathrm{i}x\cdot\xi}$ is an element of $\mathscr{S}'(\mathbb{R}^d)$. We are going to explicitly relate $P(x,D)e_\xi \in \mathscr{S}'(\mathbb{R}^d)$ to the symbol of P, and thus derive the answer to Question 1. According to (2.7), (2.8) and Lemma 2.2.1, one can show for any $v \in \mathscr{S}(\mathbb{R}^d)$ that

$$\Big[P(x,D)e_\xi\Big](v) = (2\pi)^{-d}\int\int\int e^{\mathrm{i}x\cdot\xi}\cdot\frac{e^{\mathrm{i}(y-x)\cdot\eta}}{\langle\eta\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\eta)\cdot v(y)\Big]dyd\eta dx \text{ (repeated integral)},$$

where N is an arbitrary integer with $2N > m+d$, m denotes as usual the order of P, $\mathscr{L} = 1-\Delta$. Let $\gamma \in C_c^\infty(\mathbb{R}^d)$ be a fixed function such that $\gamma = 1$ in a neighborhood of the origin. Then

$$\begin{aligned}
(2\pi)^d\Big[P(x,D)e_\xi\Big](v) &= \lim_{k\to\infty}\int\int\int e^{\mathrm{i}x\cdot\xi}\cdot\gamma(\frac{x}{k})\cdot\frac{e^{\mathrm{i}(y-x)\cdot\eta}}{\langle\eta\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\eta)\cdot v(y)\Big]dyd\eta dx\\
&= \lim_{k\to\infty}\int\int\int e^{\mathrm{i}x\cdot(\xi-\eta)}\cdot\gamma(\frac{x}{k})\cdot\frac{e^{\mathrm{i}y\cdot\eta}}{\langle\eta\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\eta)\cdot v(y)\Big]dxdyd\eta\\
&= \lim_{k\to\infty}\int\int k^n\cdot\widehat{\gamma}(k(\eta-\xi))\cdot\frac{e^{\mathrm{i}y\cdot\eta}}{\langle\eta\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\eta)\cdot v(y)\Big]dyd\eta\\
&= \lim_{k\to\infty}\int\int\widehat{\gamma}(\theta)\cdot\frac{e^{\mathrm{i}y\cdot(\xi+\frac{\theta}{k})}}{\langle\xi+\frac{\theta}{k}\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\xi+\frac{\theta}{k})\cdot v(y)\Big]d\theta dy\\
&= \int\int\widehat{\gamma}(\theta)\cdot\frac{e^{\mathrm{i}y\cdot\xi}}{\langle\xi\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\xi)\cdot v(y)\Big]d\theta dy\\
&= (2\pi)^d\int\frac{e^{\mathrm{i}y\cdot\xi}}{\langle\xi\rangle^{2N}}\cdot\mathscr{L}_y^N\Big[P(y,\xi)\cdot v(y)\Big]dy \quad \text{(Fourier inversion formula)}\\
&= (2\pi)^d\int e^{\mathrm{i}y\cdot\xi}\cdot P(y,\xi)\cdot v(y)dy.
\end{aligned}$$

Equivalently,

$$\Big[P(x,D)e_\xi\Big](v) = \int_{\mathbb{R}^d} e^{\mathrm{i}x\cdot\xi}P(x,\xi)\cdot v(x)dx.$$

This implies that, as tempered distributions

$$P(x,D)e_\xi = e_\xi P(\cdot,\xi)$$

or

$$e_{-\xi}\big[P(x,D)e_\xi\big] = P(\cdot,\xi).$$

Together, the above discussions can be summarized in the following proposition, answering Question 1 affirmatively.

Proposition 2.2.2. *A continuous linear map $T : \mathscr{S}'(\mathbb{R}^d) \to \mathscr{S}'(\mathbb{R}^d)$ is a pseudo-differential operator of order m if and only if $e^{-\mathrm{i}x\cdot\xi}\big[T_x(e^{\mathrm{i}x\cdot\xi})\big]$ is a symbol of order m. Suppose this is the case, then the symbol of T is $e^{-\mathrm{i}x\cdot\xi}\big[T_x(e^{\mathrm{i}x\cdot\xi})\big]$.*

Next, we first study the third question. For simplicity we assume that $P \in S^m$ is of compact support in $\mathbb{R}^d \times \mathbb{R}^d$. It is straightforward to induce a precise definition of $P^* e_\xi \in \mathscr{S}'(\mathbb{R}^d)$ from (2.7) for any parameter $\xi \in \mathbb{R}^d$, and prove that

$$e_{-\xi}\big[P^* e_\xi\big] = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{\mathrm{i}x\cdot\eta} (\mathscr{F}_1 \overline{P})(\eta, \eta+\xi) d\eta, \tag{2.9}$$

where $\mathscr{F}_1$ denotes the Fourier transform with respect to the first variable. By Proposition 2.2.2 we need to show that the right-hand side belongs to S^m. In general, one can use integration by parts to get

$$\Big|\Big[\partial_\xi^\beta (\mathscr{F}_1 \overline{P})\Big](\eta, \xi)\Big| \le C_{z,\beta,P} \langle \eta \rangle^{-z} \langle \xi \rangle^{m-|\beta|},$$

where z can be any positive integer. Peetre's inequality claims for any $\eta, \xi \in \mathbb{R}^d$ that

$$\langle \eta + \xi \rangle^s \le c_s \langle \eta \rangle^{|s|} \langle \xi \rangle^s,$$

where c_s is a positive constant depending only on $s \in \mathbb{R}$. Combining the above three formulae together easily shows that P^* is a pseudo-differential operator of order m.

As to the second question, it is straightforward to show that

$$e_{-\xi}\big[Q(x,D) \circ P(x,D) e_\xi\big] = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{\mathrm{i}x\cdot\eta} Q(x, \xi+\eta) (\mathscr{F}_1 P)(\eta, \xi) d\eta, \tag{2.10}$$

where $P \in S^{m_1}$, $Q \in S^{m_2}$ are assumed to be compactly supported in $\mathbb{R}^d \times \mathbb{R}^d$. Similar to the above discussion, $(\mathscr{F}_1 P)(\eta, \xi)$ and its derivatives with respect to the second variable are under good control, while $Q(x, \xi+\eta)$ and its derivatives with respect to x and ξ are governed by Peetre's inequality as well as the assumption $Q \in S^{m_2}$. This easily proves that $Q(x,D) \circ P(x,D)$ is a pseudo-differential operator of order $m_1 + m_2$.

For full details about how to drop the compactness assumption on the symbols in the last two questions, we refer the reader to [128].

Lemma 2.2.3. *Let $\{P_k \in S^{m_k}\}_{k=1}^\infty$ be a sequence of symbols such that $m_k \to -\infty$ as $k \to \infty$. Then there exists a symbol P of order $\max m_k$ such that for any positive integer N,*

$$P - \sum_{k=1}^N P_k \in S^{\alpha_N},$$

where $\alpha_N \triangleq \max_{k>N} m_k$.

This lemma was established by Hörmander. For convenience we call P an asymptotic sum of $\{P_k\}_{k=1}^\infty$, and denote $P \sim \sum_{k=1}^\infty P_k$. We also let $P \sim Q$ to mean that P, Q are asymptotically equivalent, that is, $P - Q \in S^{-\infty} = \cap_{m\in\mathbb{R}} S^m$.

As applications, one can show that the symbol of P^* is asymptotically equivalent to

$$\sum_\alpha \frac{1}{\alpha!} \cdot D_\xi^\alpha \partial_x^\alpha \overline{P}, \tag{2.11}$$

and that of $Q(x,D) \circ P(x,D)$ is asymptotically equivalent to

$$\sum_\alpha \frac{1}{\alpha!} \cdot D_\xi^\alpha Q \cdot \partial_x^\alpha P. \tag{2.12}$$

2.2.2 Pseudo-differential operators on manifolds

In this part we discuss various definitions of pseudo-differential operators on a manifold. For simplicity, assume that M denotes a smooth closed manifold of dimension d. Let Ψ^m denote the space of pseudo-differential operators on $\mathbb{R}^d$ of order m. Let $A : C^\infty(M) \to C^\infty(M)$ denote a continuous linear map.

METHOD 1 (via standard pseudo-differential operators): For any coordinate chart $M \supset V \xrightarrow{\varphi} U \subset \mathbb{R}^d$, and any two functions ψ_1, ψ_2 in $C_c^\infty(V)$, define $A_{\psi_1,\psi_2} : \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ as the following composition map

$$\mathscr{S}(\mathbb{R}^d) \xrightarrow{r_U} C^\infty(U) \xrightarrow{\varphi_*^{-1}} C^\infty(V) \xrightarrow{M_{\psi_1}} C_c^\infty(V) \hookrightarrow C^\infty(M)$$

$$\xrightarrow{A} C^\infty(M) \xrightarrow{M_{\psi_2}} C_c^\infty(V) \xrightarrow{\varphi_*} C_c^\infty(U) \hookrightarrow \mathscr{S}(\mathbb{R}^d),$$

where r_U denotes the restriction operator onto U, and M_{ψ_i} is the multiplication operator by ψ_i.

Definition 2.2.4. *A continuous linear map $A : C^\infty(M) \to C^\infty(M)$ is called a pseudo-differential operator of order m if, for any coordinate chart $V \xrightarrow{\varphi} U$ and any functions ψ_1, ψ_2 in $C_c^\infty(V)$, $A_{\psi_1,\psi_2} \in \Psi^m$.*

Some authors (e.g. Alinhac-Gérard [3, §I.7], Hörmander [80, Defn. 18.1.20], Sogge [146, §3.3]) adopt the above definition.

METHOD 2 (via symbols on open subsets): Let U be an open subset of $\mathbb{R}^d$. A smooth complex-valued function P on $U \times \mathbb{R}^d$ is called a symbol of order m on U (e.g. [3, 48, 62, 139, 154]), or more succinctly $P \in S^m(U \times \mathbb{R}^d)$, if for all compact subsets K of U and all multi-indices α, β,

$$\left|(\frac{\partial}{\partial x})^\alpha(\frac{\partial}{\partial \xi})^\beta P(x,\xi)\right| \le C_{\alpha\beta K}\langle\xi\rangle^{m-|\beta|} \quad (x \in K,\ \xi \in \mathbb{R}^d).$$

Given $P \in S^m(U \times \mathbb{R}^n)$, one can define a continuous linear map $T_P : \mathscr{S}(\mathbb{R}^d) \to C^\infty(U)$ by

$$(T_P u)(x) = (2\pi)^{-d}\int_{\mathbb{R}^d} e^{\mathrm{i}x\cdot\xi}\cdot P(x,\xi)\cdot\widehat{u}(\xi)d\xi \quad (u \in \mathscr{S}(\mathbb{R}^d),\ x \in U).$$

Since $C_c^\infty(U)$ can be naturally regarded as a subset of $\mathscr{S}(\mathbb{R}^d)$, one can induce a continuous linear map $T : C_c^\infty(U) \to C^\infty(U)$ by defining

$$T : C_c^\infty(U) \hookrightarrow \mathscr{S}(\mathbb{R}^d) \xrightarrow{T_P} C^\infty(U).$$

The set of all maps of the above form is denoted by $\Psi^m(U)$.

Now for any coordinate chart $M \supset V \xrightarrow{\varphi} U \subset \mathbb{R}^d$, define $A|_V : C_c^\infty(V) \to C^\infty(V)$ as the following composition map

$$A|_V : C_c^\infty(V) \hookrightarrow C^\infty(M) \xrightarrow{A} C^\infty(M) \xrightarrow{r_V} C^\infty(V),$$

which naturally induces a map $A_U : C_c^\infty(U) \to C^\infty(U)$ by the pull-back and push-forward operations φ_*^{-1}, φ_*. Some authors (e.g. Shubin [139, §4.3]) adopt the following definition.

Definition 2.2.5. *A continuous linear map $A : C^\infty(M) \to C^\infty(M)$ is called a pseudo-differential operator of order m if for any coordinate chart $V \xrightarrow{\varphi} U$, $A_U \in \Psi^m(U)$.*

METHOD 3 (combined with operator kernel): Both of the above definitions have the same shortcoming as we are not aware of any non-local information for such operators. So some authors (e.g. Taylor [153, 155]) call A a pseudo-differential operator by imposing on either definition an additional assumption that the operator kernel of A is smooth off the diagonal. Equivalently, this additional assumption means that (e.g. Grigis-Sjöstrand [62, Exer. 3.4]) for any $\phi, \psi \in C^\infty(M)$ with disjoint supports, $M_\phi \circ A \circ M_\psi$ is of smooth kernel in $M \times M$.

Obviously, a pseudo-differential operator in the sense of Definition 2.2.5 is a pseudo-differential operator in the sense of Definition 2.2.4. The next proposition shows that the converse is almost true if operators with smooth kernel are negligible. Based on this reason we choose the third method as the right definition for pseudo-differential operators on manifolds. Let $\Psi^m(M)$ denote the set of pseudo-differential operators of order m on M, and let $\Psi^\infty(M) = \cup_{m\in\mathbb{R}}\Psi^m(M)$.

Proposition 2.2.6. *Let $X_1, X_2 \subset \mathbb{R}^d$ be two open sets, and let $T : C_c^\infty(X_1) \to C^\infty(X_2)$ be a continuous linear map. Suppose for any $\psi_i \in C_c^\infty(X_i)$, $M_{\psi_2} \circ T \circ M_{\psi_1} \in \Psi^m$. Here $M_{\psi_2} \circ T \circ M_{\psi_1}$ means exactly the following composition map*

$$\mathscr{S}(\mathbb{R}^d) \xrightarrow{M_{\psi_1}} C_c^\infty(X_1) \xrightarrow{T} C^\infty(X_2) \xrightarrow{M_{\psi_2}} C_c^\infty(X_2) \hookrightarrow \mathscr{S}(\mathbb{R}^d).$$

Then there exists an operator $S \in \Psi^m(X_1, X_2)$ such that $K_T - K_S \in C^\infty(X_1 \times X_2)$. Here S is uniquely determined modulo $S^{-\infty}(X_2 \times \mathbb{R}^d)$.

Here K_T denotes the Schwartz kernel of T (see §2.5 or [79] for details). Proposition 2.2.6 follows from Propositions 18.1.19 and 18.1.22 in [80] (or Propositions 6.2 and 6.3 in [3]) with straightforward modification. We omit the details of the proof.

Lemma 2.2.7. *Let $A, B : C^\infty(M) \to C^\infty(M)$ be continuous linear maps. If one of A, B is of smooth kernel in $M \times M$, then AB is also of smooth kernel in $M \times M$.*

This lemma is an immediate consequence of [79, Thm. 5.2.6]. As an application, one can show that the product of two pseudo-differential operators is also a pseudo-differential operator.

Similar to the partial differential operator case, one can define the principal symbol for pseudo-differential operators as a function on T^*M. But we should note that operators with smooth kernel are regarded as negligible; the principal symbol at small ξ is thus of no importance.

In this thesis, we will be mainly interested in so-called classical pseudo-differential operators. To be precise, $A \in \Psi^m(M)$ is called classical if in every local coordinate system,

$$\sigma_A(x, \xi) \sim \sum_{k=0}^{\infty} \sigma_A^{(k)}(x, \xi),$$

where σ_A denotes the local full symbol of A, each $\sigma_A^{(k)}$ is homogeneous of degree $m-k$ in large enough ξ. When this happens, we shall write $A \in \Psi^m_{\mathrm{cl}}(M)$. The principal symbol of $A \in \Psi^m_{\mathrm{cl}}(M)$ can be either regarded as a homogeneous map of degree m on $T^*M\backslash 0$, or simply a smooth function on the unit cotangent bundle T_1^*M of M provided M admits a Riemannian metric g.

We end this section with discussion on how to construct pseudo-differential operators with prescribed principal symbols.

We begin with two simple facts. Previously we defined $\Psi^m(M)$ for closed manifolds M. In the case that V is an open subset of a closed manifold M, one can similarly define $\Psi^m(V)$ as the set of pseudo-differentials of order m on V. In particular, $A|_V : C_c^\infty(V) \to C^\infty(V)$ belongs to $\Psi^m(V)$ for any $A \in \Psi^m(M)$. On the other hand, if $B \in \Psi^m(V)$, then

$$M_\phi \circ B \circ M_\psi : C^\infty(M) \to C^\infty(M)$$

belongs to $\Psi^m(M)$ for any $\phi, \psi \in C_c^\infty(V)$.

Let $\{V_i\}$ be a fixed finite open cover of M. Assume that $\{B_i \in \Psi^m(V_i)\}$ are some locally defined pseudo-differential operators of the same order m, such that there exists an $l < m$ satisfying

$$B_i|_{V_i \cap V_j} - B_j|_{V_i \cap V_j} \in \Psi^l(V_i \cap V_j)$$

for all i, j. This implies that, when restricted to $V_i \cap V_j$, B_i and B_j must have the same principal symbol. For example, if given in advance an operator $A \in \Psi^m_{\mathrm{cl}}(M)$, then $\{B_i = A|_{V_i}\}$ satisfy the above assumption for $l = m-1$. In the following we will construct an operator $A \in \Psi^m(M)$ such that $A|_{V_i} - B_i \in \Psi^l(V_i)$ for each i. This implies that the principal symbol of A locally must agree with that of some local operator.

Let $\{\psi_j\}_{j=1}^N$ be a partition of unity associated with the open cover $\{V_i\}$ of M, that is, $\sum \psi_j = 1$ and each ψ_j belongs to some $C_c^\infty(V_{i_j})$. Let $\phi_j \in C_c^\infty(V_{i_j})$ be such that $\phi_j = 1$ in a neighborhood of the support of ψ_j. Define

$$A = \sum_{j=1}^N M_{\psi_j} \circ B_{i_j} \circ M_{\phi_j},$$

which obviously is an element of $\Psi^m(M)$. To study the local behaviour of A, we fix a point $p \in M$. Let $\psi_{j_1}, \ldots, \psi_{j_n}$ be all of the functions such that p lies in the supports of these functions. Without loss of generality we may assume that $j_1 = 1, \ldots, j_n = n$. Obviously, there exists a small open neighborhood $V = V_p$ of p such that

(1) V is contained in $\{x \in M : \phi_j(x) = 1\}$ for each $j = 1, \ldots, n$,

(2) V is disjoint with the support of ψ_j for each $j = n+1, \ldots, N$,

(3) $B_{i_j}|_V - B_{i_k}|_V \in \Psi^l(V)$ for all $1 \le j, k \le n$.

Now for any $\phi, \psi \in C_c^\infty(V)$, we have

$$\begin{aligned} M_\phi \circ A \circ M_\psi &= \sum_{j=1}^N M_\phi \circ M_{\psi_j} \circ B_{i_j} \circ M_{\phi_j} \circ M_\psi \\ &= \sum_{j=1}^s M_{\psi_j} \circ M_\phi \circ B_{i_j} \circ M_\psi \quad ((1)+(2)) \\ &= M_\phi \circ B_{i_1} \circ M_\psi + T, \qquad ((2)+(3)) \end{aligned}$$

where T belongs to $\Psi^l(M)$. This suffices to conclude that $A|_{V_i} - B_i \in \Psi^l(V_i)$ for each i.

With the above construction available, one can freely construct many new pseudo-differential operators. As applications, it is not hard to prove the following three corollaries (e.g. [3]):

Corollary 2.2.8. *Let $\{A_k \in \Psi^{m_k}(M)\}_{k=1}^{\infty}$ be a sequence of pseudo-differential operators such that $\{m_k\}$ decreases monotonically to $-\infty$. Then there exists an operator $A \in \Psi^{m_1}(M)$ such that $A \sim \sum_{k=1}^{\infty} A_k$, that is, $A - \sum_{k=1}^{N-1} A_k \in \Psi^{m_N}(M)$ for any positive integer N.*

Corollary 2.2.9. *Let σ be a smooth function on T^*M such that σ is homogeneous of degree m in large enough $\xi \in T^*M$. Then there exists an operator $A \in \Psi^m(M)$ such that $\sigma_m(A) = \sigma$.*

Corollary 2.2.10. *Let $A \in \Psi^m_{\mathrm{cl}}(M)$ be a classical pseudo-differential operator such that its principal symbol is nowhere zero in $T^*M\backslash 0$. Then there exists an operator $B \in \Psi^{-m}(M)$ such that $AB \equiv BA \equiv I$ modulo operators in $\Psi^{-\infty}(M)$.*

2.2.3 Sub-principal symbols

In this part we discuss the sub-principal symbol concept for pseudo-differential operators that was first introduced by Duistermaat and Hörmander in the classical paper [41]. Let M always denote a smooth closed manifold of dimension d.

Let $A \in \Psi^m_{\mathrm{cl}}(M)$ be a classical pseudo-differential operator of order m. In local coordinates the full symbol of A admits an asymptotic expansion of the following form

$$\sigma_A(x,\xi) \sim \sum_{k=0}^{\infty} \sigma_A^{(k)}(x,\xi),$$

where each $\sigma_A^{(k)}$ is homogeneous of degree $m-k$ in large enough ξ. We know in §2.2.2 that the local principal symbol $\sigma_A^{(0)}$ can be extended as a locally invariantly defined map on $T^*M\backslash 0$. A natural question is: can we do so for $\sigma_A^{(1)}$? The answer is no. To see this one can study the Laplace-Beltrami operator on the round sphere $\mathbb{S}^2$.

To overcome this barrier Duistermaat and Hörmander identified operator $A \in \Psi^m_{\mathrm{cl}}(M)$ with operator $\widetilde{A}$ acting on smooth half-densities. It is not a surprise that the local full symbol of $\widetilde{A}$ admits an asymptotic expansion of a similar form

$$\sigma_{\widetilde{A}}(x,\xi) \sim \sum_{k=0}^{\infty} \sigma_{\widetilde{A}}^{(k)}(x,\xi),$$

and the principal symbol of $\widetilde{A}$ can be similarly invariantly defined as a map on $T^*M\backslash 0$. But quite unexpectedly, they invariantly defined another map on $T^*M\backslash 0$, called the sub-principal symbol of $\widetilde{A}$, locally in terms of both $\sigma_{\widetilde{A}}^{(0)}$ and $\sigma_{\widetilde{A}}^{(1)}$. One can define the sub-principal symbol of A simply as that of $\widetilde{A}$, but we should note that its local expressions depend not only on $\sigma_A^{(0)}$, $\sigma_A^{(1)}$, but also on the identification between functions and half-densities.

A new question comes: can we invariantly define on the cotangent bundle a “sub-sub-principal symbol” and so on for pseudo-differential operators? Logically it is very hard to exclude such a possibility.

In later sections we will see that the concept of Wodzicki residue provides an excellent way to study the above question. The basic viewpoint is, the Wodzicki residue of a classical pseudo-differential operator is no longer some invariantly defined concept on the cotangent bundle, but a density over the base manifold.

Now we present the details of the definition of the sub-principal symbol of a classical pseudo-differential operator. Some preliminary facts about the concept of density are needed.

1) Assume at the moment that M is further orientable. This means in particular that there exists a nowhere vanishing d-form μ on M. Such a d-form is also called a volume form on M. People like to use $\int_M f$ ($f \in C^\infty(M)$) to be short for $\int_M f\mu$ provided the volume form μ is known in the context. For example, it is well known that one can endow M with a Riemannian metric g. The Riemannian volume form μ_g is the unique smooth orientation d-form satisfying $\mu_g(X_1, \ldots, X_d) = 1$ for every local oriented orthonormal frame $\{X_i\}$ for M. In any oriented smooth coordinates $\{x^i\}$, the Riemannian volume form has the local coordinate expression

$$\mu_g = \sqrt{\det(g_{ij})}dx^1 \wedge \cdots \wedge dx^d,$$

where g_{ij} are the components of g in these coordinates. Let $\Omega^d(M)$ denote the space of d-forms on M. A continuous linear map $B : \Omega^d(M) \to \Omega^d(M)$ is called a pseudo-differential operator of order m if for some volume form μ the following composition map, denoted by A_μ,

$$C^\infty(M) \xrightarrow{M_\mu} \Omega^d(M) \xrightarrow{B} \Omega^d(M) \xrightarrow{M_\mu^{-1}} C^\infty(M),$$

is of such a property, where M_μ denotes the map sending f to $f\mu$. Although as operators B and A_μ have no essential difference, the corresponding local full symbols do have. For example, in the same local coordinates, the full symbol of A_μ depends on μ but that of B does not.

2) From now on we no longer assume that M is orientable. The following method [51] is a very simple way to define the integration of functions over M. Let $\{(V_i, \varphi_i)\}$ be an atlas for the smooth structure on M. Assume that, on each open subset $\varphi_i(V_i)$ of $\mathbb{R}^d$, there exists a measure μ_i that is absolutely continuous and has strictly positive density with respect to the Lebesgue measure, and for any continuous function f on M with $\mathrm{supp}(f) \subset V_i \cap V_j$ we have the compatibility condition

$$\int_{\varphi_i(V_i)} f \circ \varphi_i^{-1} d\mu_i = \int_{\varphi_j(V_j)} (f \circ \varphi_j^{-1})|J(\varphi_i \circ \varphi_j^{-1})|d\mu_j.$$

The data of the measures $\{\mu_i\}$, also called a density on M, play the role of volume forms as one can first introduce a subordinate partition of unity $\{\phi_i\}$, then define

$$\int_M f = \sum_i \int_{\varphi_i(V_i)} (\phi_i f) \circ \varphi_i^{-1} d\mu_i. \tag{2.13}$$

For example, in the case that M admits a Riemannian metric g, one can set a canonical measure of (M, g) by defining

$$\mu_k = \sqrt{\det(g_{ij}^{(k)})}L_d, \tag{2.14}$$

where $\sum_{ij} g_{ij}^{(k)} dx^i dx^j$ denotes the local expression of g in a local chart (V_k, φ_k), L_d denotes the d-dimensional Lebesgue measure on $\mathbb{R}^d$. As it seems a little bit inconvenient to define pseudo-differential operators on densities of the above form, we try to first capture a pointwise concept of density, then introduce a global density bundle in the next step.

3) Let $\alpha \in [0,1]$, and let H denote a d-dimensional vector space over $\mathbb{R}$. An α-density on H is a map $\omega : H^d \to \mathbb{R}$ such that for any $S \in \mathrm{GL}(H)$, $\omega(Sh_1, \ldots, Sh_d) = |\det(S)|^\alpha \omega(h_1, \ldots, h_d)$. It is known that the space of α-densities, denoted by $\Omega_\alpha(H)$, is a one-dimensional vector space over $\mathbb{R}$ [95]. Given a linear basis $X_1, \ldots, X_d$ for H, also regarded as an orthonormal structure on H[1], one can define $\omega_{\alpha;X_1,\ldots,X_d}(h_1, \ldots, h_d)$ as the α-th power of the volume of the parallelepiped generated by $h_1, \ldots, h_d$. Obviously, $\omega_{\alpha;X_1,\ldots,X_d} \in \Omega_\alpha(H)$. Define the complex α-density bundle

$$\Omega_\alpha(M) = \coprod_{p \in M} \big(\mathbb{C} \otimes \Omega_\alpha(T_pM)\big).$$

Let $C^\infty(M;\Omega_\alpha)$ denote the space of smooth sections of $\Omega_\alpha(M)$. A continuous linear map $B : C^\infty(M;\Omega_\alpha) \to C^\infty(M;\Omega_\alpha)$ is called a pseudo-differential operator of order m, if for some nowhere vanishing smooth α-density $\mu = \mu^{(\alpha)}$, the following composition map, denoted by A_μ,

$$C^\infty(M) \xrightarrow{M_\mu} C^\infty(M;\Omega_\alpha) \xrightarrow{B} C^\infty(M;\Omega_\alpha) \xrightarrow{M_\mu^{-1}} C^\infty(M), \tag{2.15}$$

is of such a property. In the case that M admits a Riemannian metric g, there exists a unique smooth nowhere vanishing α-density, called the Riemannian α-density and denoted by $\mu_g^{(\alpha)}$, such that at each $p \in M$, $\mu_g^{(\alpha)}(p) = \omega_{\alpha;X_1,\ldots,X_d}$ for some orthonormal basis $\{X_i\}$ for (T_pM, g_p). We then always set $\mu = \mu_g^{(\alpha)}$ in (2.15) and thus have $B = M_\mu A_\mu M_\mu^{-1}$. Note in local coordinates, $\mu_g^{(\alpha)} = G^{\frac{\alpha}{2}} \omega_{\alpha;\partial_1,\ldots,\partial_d}$, which implies that M_μ is locally the multiplication operator by $G^{\frac{\alpha}{2}}$. Here $G = \det(g_{ij})$. In particular, B can be locally regarded as the product of three pseudo-differential operators.

Now we can start to define the sub-principal symbol of $A \in \Phi^m_{\mathrm{cl}}(M)$. In local coordinates we also let $\sigma_A^{(j)} = \sigma_A^{(j)}(x,\xi)$ ($j = 0, 1, 2, \ldots$) denote the homogeneous part of degree $m - j$ of the full symbol of A. Given a Riemannian metric g on M, define $B = M_\mu A M_\mu^{-1}$ which is a pseudo-differential operator acting on half-densities of order m, where $\mu = \mu_g^{(1/2)}$ is the Riemannian half-density. In local coordinates its full symbol admits an asymptotic expansion $\sum_{j=0}^\infty \sigma_B^{(j)}(x,\xi)$ with $\sigma_B^{(j)}$ homogeneous of degree $m - j$ in ξ. It is well known that the sub-principal symbol (e.g. [41, Section 5.2]) of B, defined in local coordinates by

$$\mathrm{Sub}(B) = \sigma_B^{(1)} + \frac{\mathrm{i}}{2} \cdot \frac{\partial^2 \sigma_B^{(0)}}{\partial x^k \partial \xi_k}, \tag{2.16}$$

transforms like a homogeneous smooth function of degree $m - 1$ on $T^*M \backslash 0$ under change of charts. Since $B = M_\mu A M_\mu^{-1}$ locally is the product of three pseudo-differential operators with corresponding full symbols $G(x)^{1/4}$, $\sum_{j=0}^\infty \sigma_A^{(j)}(x,\xi)$, $G(x)^{-1/4}$, one can deduce from the product rule (2.12) that

$$\mathrm{Sub}(B) = \sigma_A^{(1)} + \frac{\mathrm{i}}{2} \cdot \frac{\partial^2 \sigma_A^{(0)}}{\partial x^k \partial \xi_k} + \frac{\mathrm{i}}{2} \cdot \frac{\partial \sigma_A^{(0)}}{\partial \xi_k} \cdot \frac{\partial (\log \sqrt{G})}{\partial x^k}.$$

This implies the sub-principal symbol of A, locally defined by

$$\mathrm{Sub}(A) = \sigma_A^{(1)} + \frac{\mathrm{i}}{2} \cdot \frac{\partial^2 \sigma_A^{(0)}}{\partial x^k \partial \xi_k} + \frac{\mathrm{i}}{2} \cdot \frac{\partial \sigma_A^{(0)}}{\partial \xi_k} \cdot \frac{\partial (\log \sqrt{G})}{\partial x^k}, \tag{2.17}$$

is a homogeneous smooth function of degree $m - 1$ on $T^*M \backslash 0$.

[1] It does not matter whether or not there exists in advance an inner-product structure on H.

2.2.4 Pseudo-differential operators on vector bundles

Let $A : C^\infty(M;E) \to C^\infty(M;E)$ be a continuous linear map, where E is a complex vector bundle over a closed manifold M. Let $\{\psi_i\}$ be finitely many smooth functions on M such that $\sum_i \psi_i = 1$, and the support of each ψ_i is contained in the domain of some coordinate chart, say for example (V_i, φ_i). Then for each i, let $\phi_i \in C_c^\infty(V_i) \subset C^\infty(M)$ be such that $\phi_i = 1$ in a neighborhood of the support of ψ_i. Obviously,

$$A = \sum_i M_{\psi_i} A M_{\phi_i} + \sum_i M_{\psi_i} A(1 - M_{\phi_i}).$$

Similar to the discussion in 2.2.2, we call A a (classical) pseudo-differential operator of order at most m if, for each i, the local representation of $M_{\psi_i} A M_{\phi_i}$ is a matrix-valued (classical) pseudo-differential operator on some Euclidean domain of order at most m, and $M_{\psi_i} A(1 - M_{\phi_i})$ is of smooth integral kernel. The space of all classical pseudo-differential operators of order at most m is denoted by $\Psi^m_{\mathrm{cl}}(M;E)$.

We have yet to give a detailed definition of the integral kernel of an operator. Although this is not a problem for operators on Euclidean domains, we should exercise care for those acting on smooth sections. For example, let $B : C^\infty(M) \to C^\infty(M)$ be a continuous linear map such that

$$(Bf)(x) = \int_M K(x,y) f(y) d\mu(y),$$

where K is a function on $M \times M$, μ is a positive smooth density μ on M. We say K is the integral kernel of B with respect to μ. According to this definition, for any positive smooth function h on M, $K(x,y)h(y)$ is the integral kernel of B with respect to $\frac{\mu}{h}$. Thus the smoothness of the integral kernels of B is independent of the choice of positive smooth densities on M. In particular, in the case that M admits a Riemannian metric, the integral kernel of B is always taken with respect to the Riemannian density. Generally, let $A : C^\infty(M;E) \to C^\infty(M;E)$ be a continuous linear map such that

$$(A\phi)(x) = \int_M K(x,y) \phi(y) d\mu(y),$$

where $K(x,y) : E_y \to E_x$, μ is a positive smooth density on M. We say K is the integral kernel of A with respect to μ. Obviously, the naturally interpreted smoothness of the integral kernel of A is also independent of the choice of positive smooth densities on M.

We now define the sub-principal symbol for classical pseudo-differential operators (see also [86]). Suppose $A \in \Psi^m_{\mathrm{cl}}(M;E)$. For a fixed local bundle trivialization of E over a coordinate neighborhood V, one can naturally identify $A|_V : C_c^\infty(V;E) \to C^\infty(V;E)$, the restriction of A onto V, with a matrix $(A^V_{\mu\nu})_{1\le\mu,\nu\le r}$ of classical pseudo-differential operators $A^V_{\mu\nu} : C^\infty(M) \to C^\infty(M)$ of order m, where r denotes the rank of E. This implies that the sub-principal symbol of A defined by

$$\mathrm{Sub}(A) = (\mathrm{Sub}(A^V_{\mu\nu}))_{1\le\mu,\nu\le r} \tag{2.18}$$

is a homogeneous smooth $\mathrm{Mat}(r,\mathbb{C})$-valued function of degree $m-1$ on $T^*V\backslash 0$. Locally $\mathrm{Sub}(A)$ is still of the form (2.17). We should remember, however, that the definition of the sub-principal symbol depends on the choice of *local frames* for E and *Riemannian metrics* on M.

EXAMPLE 1: Let $P = \Delta^{\nabla}$ denote the connection Laplacian generated by the connection ∇ on a vector bundle E of rank r. For fixed local frame $\{s_\mu\}_{\mu=1}^r$ for $E|_V$ there exists a matrix $\omega = (\omega_{\mu\nu})_{1\leq\mu,\nu\leq r}$ of one-forms on V such that $\nabla s_\mu = \omega_{\mu\nu} \otimes s_\nu$. Recall in any local coordinates system $(x^1, \ldots, x^d)$ on V, $P = -g^{ij}(\nabla_i\nabla_j - \Gamma_{ij}^k\nabla_k)$. Letting $\nabla_j = \partial_j + b_j$ one can easily get $\sigma_P^{(0)} = g^{jk}(x)\xi_j\xi_k$, $\sigma_P^{(1)} = -2\mathrm{i}g^{jk}b_j\xi_k + \mathrm{i}g^{ln}\Gamma_{ln}^k\xi_k$. Considering $\frac{\partial(\log\sqrt{G})}{\partial x^k} = \Gamma_{kn}^n$ (e.g. [27, Prop. 2.8], [29, Sec. 2.5], [31, Sec. 6]) we have

$$\begin{aligned}
\mathrm{Sub}(P) &= \sigma_P^{(1)} + \frac{\mathrm{i}}{2}\cdot\frac{\partial^2\sigma_P^{(0)}}{\partial x^k\partial\xi_k} + \frac{\mathrm{i}}{2}\cdot\frac{\partial\sigma_P^{(0)}}{\partial\xi_k}\cdot\frac{\partial(\log\sqrt{G})}{\partial x^k}\\
&= \sigma_P^{(1)} + \mathrm{i}\cdot\frac{\partial g^{jk}}{\partial x^k}\cdot\xi_j + \mathrm{i}\cdot g^{jk}\xi_j\cdot\Gamma_{kn}^n\\
&= (-2\mathrm{i}g^{jk}b_j\xi_k + \mathrm{i}g^{ln}\Gamma_{ln}^k\xi_k) + \mathrm{i}\cdot(-\Gamma_{kn}^j g^{nk} - \Gamma_{kn}^k g^{nj})\cdot\xi_j + \mathrm{i}\cdot g^{jk}\xi_j\cdot\Gamma_{kn}^n\\
&= -2\mathrm{i}g^{jk}b_j\xi_k.
\end{aligned}$$

Also, it is easy to check that $b_j = \omega^T(\partial_j)$ where ω^T denotes the transpose of ω. Thus in an invariant manner, $\mathrm{Sub}(P)(x,\xi) = -2\mathrm{i}g(dx^j, dx^k)\omega^T(\partial_j)\xi_k = -2\mathrm{i}g(\omega^T, \xi)$.

EXAMPLE 2: Let $D = \gamma\nabla$ be given by a Dirac bundle (E, γ, ∇). We adopt all of the notations about ∇ used in the previous example. Then $\sigma_D^{(0)} = \mathrm{i}\gamma^j\xi_j$, $\sigma_D^{(1)} = \gamma^j b_j$ and, consequently,

$$\begin{aligned}
\mathrm{Sub}(D) &= \sigma_D^{(1)} + \frac{\mathrm{i}}{2}\cdot\frac{\partial^2\sigma_D^{(0)}}{\partial x^k\partial\xi_k} + \frac{\mathrm{i}}{2}\cdot\frac{\partial\sigma_D^{(0)}}{\partial\xi_k}\cdot\frac{\partial(\log\sqrt{G})}{\partial x^k}\\
&= \gamma^j b_j - \frac{1}{2}\cdot\frac{\partial\gamma^k}{\partial x^k} - \frac{1}{2}\cdot\gamma^k\cdot\Gamma_{kn}^n\\
&= \gamma^j b_j - \frac{1}{2}\cdot([\gamma^k, b_k] - \Gamma_{kn}^k\gamma^n) - \frac{1}{2}\cdot\gamma^k\cdot\Gamma_{kn}^n\\
&= \frac{\gamma^k b_k + b_k\gamma^k}{2},
\end{aligned}$$

where the third equality follows from (2.2). On each inner product space (T_xM, g_x), we introduce two bilinear maps J_x, K_x sending $X_x, Y_x \in T_xM$ respectively to $\gamma(X_x)\omega^T(Y_x)$ and $\omega^T(X_x)\gamma(Y_x)$. Then it is easy to see that

$$\mathrm{Sub}(D)(x,\xi) = \frac{\mathrm{Tr}(J_x) + \mathrm{Tr}(K_x)}{2},$$

which implies that $\mathrm{Sub}(D)(x,\xi)$ is actually independent of ξ.

EXAMPLE 3: Given two classical pseudo-differential operators A, B on smooth sections of E, it is easy to verify that (see also [40, (1.4)])

$$\mathrm{Sub}(AB) = \mathrm{Sub}(A)\cdot\sigma_B^{(0)} + \sigma_A^{(0)}\cdot\mathrm{Sub}(B) + \frac{1}{2\mathrm{i}}\{\sigma_A^{(0)}, \sigma_B^{(0)}\}, \tag{2.19}$$

where $\{\sigma_A^{(0)}, \sigma_B^{(0)}\}$ denotes the Poisson bracket between $\sigma_A^{(0)}$ and $\sigma_B^{(0)}$, that is,

$$\{\sigma_A^{(0)}, \sigma_B^{(0)}\} = \frac{\partial\sigma_A^{(0)}}{\partial\xi_k}\cdot\frac{\partial\sigma_B^{(0)}}{\partial x^k} - \frac{\partial\sigma_A^{(0)}}{\partial x^k}\cdot\frac{\partial\sigma_B^{(0)}}{\partial\xi_k}.$$

Given a non-negative self-adjoint Laplace type operator P and a $q \in \mathbb{R}$, it is well known [138] that P^q is a classical pseudo-differential operator of order $2q$. It is not hard to verify that (see also [40, (1.3)])

$$\mathrm{Sub}(P^q) = q\cdot(\sigma_P^{(0)})^{q-1}\cdot\mathrm{Sub}(P). \tag{2.20}$$

2.2.5 Wodzicki residues

Let M be a smooth closed manifold of dimension d. On the algebra $\Psi^\infty(M;E)$ of all classical pseudo-differential operators on $C^\infty(M;E)$, there exists a trace $\mathrm{res} : \Psi^\infty(M;E) \to \mathbb{C}$ called Wodzicki's residue or non-commutative residue. It is defined by

$$\mathrm{res}(A) = \int_M \mathrm{res}_x(A)dx,$$

where

$$\mathrm{res}_x(A)dx \triangleq \Big(\frac{1}{(2\pi)^d}\int_{|\xi|=1} \mathrm{Tr}(\sigma_{-d}(A)(x,\xi))dS(\xi)\Big)dx$$

is independent of the choice of local coordinates and thus is a global density on M, $\sigma_{-d}(A)(x,\xi)$ denotes the homogeneous part of degree $-d$ of the local full symbol of A, $dS(\xi)$ denotes the sphere measure on $|\xi| = 1$. To be clear, $|\xi| = 1$ is short for the set

$$\{(\xi_1,\ldots,\xi_d) \in \mathbb{R}^d : \xi_1^2 + \cdots + \xi_d^2 = 1\}$$

as there are no metric structures endowed with T_x^*M yet, and by trace we mean that res is a linear map satisfying

$$\mathrm{res}(AB) = \mathrm{res}(BA)$$

for all $A, B \in \Psi^\infty(M;E)$. If M is connected, any trace τ on $\Psi^\infty(M;E)$ is a multiple of res. Wodzicki's residue was introduced independently by Wodzicki [160] in 1984, and Guillemin [70] in 1985. In the case of the circle, the Wodzicki residue had been studied earlier by Manin [105] in 1978, and Adler [2] in 1979. Since its appearance, this concept has found many applications in both mathematics and mathematical physics.

The reader should distinguish the difference between the Wodzicki residue trace res and the standard operator trace tr. For example, if A is a classical pseudo-differential operator of order less than $-d$, then $\mathrm{res}(A) = 0$, but as A is trace class, we have

$$\mathrm{tr}(A) = \sum_{n=1}^{\infty} \langle Ae_n, e_n\rangle_{L^2(M;E)}$$

for an arbitrary orthonormal basis $\{e_n\}_{n=1}^\infty$ for $L^2(M;E)$. Note in general $\mathrm{tr}(A)$ needs not to be zero. The Kontsevich-Vishik trace [91] is an extension of the standard operator trace to some proper subset of $\Psi^\infty(M;E)$.

In the case that M admits a Riemannian metric g, any smooth density μ must be of the form $\mu = f\mu_g$ for some smooth function f on M. Thus for any $A \in \Psi^\infty(M;E)$, there exists a smooth function f_A on M such that $\mathrm{res}_x(A)dx = f_A\mu_g$. Then for any given $x_0 \in M$, we have

$$f_A(x_0) = \frac{1}{(2\pi)^d}\int_{|\xi|=1} \mathrm{Tr}(\sigma_{-d}(A)(x_0,\xi))dS(\xi),$$

where the local coordinates are chosen so that $\{\frac{\partial}{\partial x^i}\big|_{x_0}\}_{i=1}^d$ is an orthonormal basis for $(T_{x_0}M, g_{x_0})$. In particular, if A is of order $-d$, then in an invariant manner we also have

$$f_A(x_0) = \frac{1}{(2\pi)^d}\int_{S_{x_0}^*M} \mathrm{Tr}(\sigma_A),$$

where $S_{x_0}^*M$ denotes the unit cotangent sphere at x_0, σ_A denotes the principal symbol of A.

The Wodzicki residue is closely related to heat trace expansions. Suppose $A \in \Psi^\infty(M;E)$ is of order m and we are interested in calculating its Wodzicki residue by other means rather than its original definition. Assume further that M is a Riemannian manifold, over which E is a smooth complex hermitian vector bundle. Denote by $L^2(M;E)$ the Hilbert space of square integrable sections equipped with the natural inner product defined by the hermitian structure on the fibres and the metric measure on M. Let P be a non-negative self-adjoint Laplace type operator acting on smooth sections of E. For each $t > 0$, e^{-tP} defined by the functional calculus of self-adjoint operators is, a smoothing operator. This implies that Ae^{-tP} also is a smoothing operator for each $t > 0$ and, consequently, $\mathrm{tr}(Ae^{-tP})$ is well defined. One can establish the following widely used (though less precise) short-time asymptotic expansion (see §3.3)

$$\mathrm{tr}(Ae^{-tP}) \sim \sum_{k=0}^{\infty} \Big(\mathscr{B}_k(A,P) t^{\frac{k-d-m}{2}} + \mathscr{C}_k(A,P) t^k \log(t) + \mathscr{D}_k(A,P) t^k \Big) \quad (t \to 0^+). \tag{2.21}$$

Then the connecting formula is [70, 160] (see also [64, (0.2)], [96, (1.2)], [134, (1.16)])

$$\mathrm{res}(A) = -2\mathscr{C}_0(A,P), \tag{2.22}$$

which means in particular that $\mathscr{C}_0(A,P)$ is independent of the choice of P. Actually, plenty of the heat expansion coefficients are Wodzicki residues of certain operators (see Prop. 3.3.1).

In this thesis we will encounter lots of integration not only over a closed manifold but also over its (unit) cotangent bundle, so let us clearly state their precise definitions. Let (M,g) be a closed Riemannian manifold, and let μ_g be the associated Riemannian density. For any smooth function f on M, the integral of f over M is defined by (see (2.13) and (2.14))

$$\int_M f = \int_M f d\mu_g.$$

For any smooth function h on T^*M, we define

$$\int_{T^*M} h = \int_M \Big[\int_{T_x^*M} h \Big] d\mu_g(x).$$

Here the linear spaces T_x^*M have inner product structures g_x, so we can identify (T_x^*M, g_x) with the standard Euclidean space $\mathbb{R}^d$, and thus $\int_{T_x^*M} h$ can naturally be regarded as standard Lebesgue integrations. To be precise, letting $\{e_i\}_{i=1}^d$ be an orthonormal basis for T_x^*M, one can introduce a function $\widehat{h}$ on $\mathbb{R}^d$ such that

$$\widehat{h}(y_1, \ldots, y_d) = h(y_1 e_1 + \cdots + h_d e_d).$$

With this identification it is straightforward to set

$$\int_{T_x^*M} h = \int_{\mathbb{R}^d} \widehat{h}(y) dy.$$

The integration over the unit cotangent bundle can be defined in a similar way. To summarize, any integration over the (unit) cotangent bundle is always regarded as a repeated integral.

2.3 Fourier integral operators

In this part we do not heavily cite Hörmander's general theory of Fourier integral operators (FIOs), but focus on the local expressions of $e^{-\mathrm{i}t\sqrt{P}}$, where P is a non-negative self-adjoint Laplace type operator acting on smooth sections of a vector bundle. Let M be a closed smooth manifold of dimension d.

Assume first that $P : C^\infty(M) \to C^\infty(M)$ is a non-negative self-adjoint Laplace type operator. According to Seeley's construction of complex powers of P [138], $\sqrt{P}$ is a classical pseudo-differential operator of first order with nowhere vanishing principal symbol. Locally, $\sqrt{P}$ is of the form[2]

$$\sqrt{P} \sim \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \sum_{n=0}^{\infty} q_n(x,\xi) e^{\mathrm{i}(x-y)\cdot\xi} d\xi, \tag{2.23}$$

where each homogeneous symbol q_n is of order $1-n$. A breakthrough work by Hörmander [77] says that modulo smoothing operators $e^{-\mathrm{i}t\sqrt{P}}$ locally is of the form

$$e^{-\mathrm{i}t\sqrt{P}} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} a(t,x,y,\xi) e^{\mathrm{i}\theta(t,x,y,\xi)} d\xi \tag{2.24}$$

for sufficiently small times t, where the phase function θ is of the form

$$\theta = \psi(x,y,\xi) - t q_0(y,\xi). \tag{2.25}$$

Here $\psi = \psi(x,y,\xi)$ is a homogeneous symbol of first order, and the amplitude function $a = a(t,x,y,\xi)$ is a homogeneous symbol of order zero. To this end, by supposing that $a \sim \sum_{n=0}^{\infty} a_n$ and ψ are unknowns, where each a_n is a homogeneous symbol of order $-n$, we need to solve

$$\frac{d}{dt} e^{-\mathrm{i}t\sqrt{P}} = -\mathrm{i}\sqrt{P} e^{-\mathrm{i}t\sqrt{P}} \tag{2.26}$$

subject to the initial condition

$$\mathrm{Id} \sim \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \sum_{n=0}^{\infty} a_n(0,x,y,\xi) e^{\mathrm{i}\psi(x,y,\xi)} d\xi. \tag{2.27}$$

The left hand side of (2.26) is of the form

$$\frac{d}{dt} e^{-\mathrm{i}t\sqrt{P}} \sim \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \Big[-\mathrm{i} a_0 q_0(y,\xi) + \sum_{k=0}^{\infty} \big(-\mathrm{i} a_{k+1} q_0(y,\xi) + \frac{da_k}{dt} \big) \Big] e^{\mathrm{i}\theta(t,x,y,\xi)} d\xi. \tag{2.28}$$

The product rule [77] (see also [139, Thm. 18.2]) between the pseudo-differential operator $\sqrt{P}$ and the assumed Fourier integral operator $e^{-\mathrm{i}t\sqrt{P}}$ implies that the right-hand side of (2.26) is of the form

$$-\mathrm{i}\sqrt{P} e^{-\mathrm{i}t\sqrt{P}} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \Big[\sum_{\alpha} \sum_{j=0}^{\infty} \sum_{n=0}^{\infty} R_{\alpha,j,n}(t,x,y,\xi) \Big] e^{\mathrm{i}\theta(t,x,y,\xi)} d\xi, \tag{2.29}$$

[2] For simplicity we identify a continuous linear operator with its distributional kernel in this section. This causes no harm especially in the case that the operator, say for example $e^{-\mathrm{i}t\sqrt{P}}$, is bounded on $L^2(M)$. For details see §2.5.

where

$$R_{\alpha,j,n}(t,x,y,\xi) = -\mathrm{i}q_n^{(\alpha)}(x,\psi_x(x,y,\xi))\frac{D_z^\alpha(a_j(t,z,y,\xi)e^{\mathrm{i}\rho(z,x,y,\xi)})}{\alpha!}\Big|_{z=x}.$$

Here α is taken over all multiple indexes in $(\mathbb{N}\cup\{0\})^d$, $q_n^{(\alpha)}(x,\eta) = (\partial_\eta^\alpha q_n)(x,\eta)$,

$$\rho(z,x,y,\xi) = \psi(z,y,\xi) - \psi(x,y,\xi) - (z-x)\cdot\psi_x(x,y,\xi)$$

is a first order homogeneous symbol such that its zero and first order derivatives with respect to the z variable vanish at $z = x$. For simplicity, we introduce

$$T_{\alpha,j,n}(t,x,y,\xi) = -\mathrm{i}q_n^{(\alpha)}(x,\psi_x(x,y,\xi))\frac{(D_z^\alpha a_j)(t,z,y,\xi)}{\alpha!}\Big|_{z=x},$$

which is a homogeneous symbol of order $1-n-|\alpha|-j$. One can verify that 1) if $|\alpha|\le 1$, then $R_{\alpha,j,n} = T_{\alpha,j,n}$; and 2) if $|\alpha|\ge 2$, then $R_{\alpha,j,n}$ can be written as

$$R_{\alpha,j,n} = T_{\alpha,j,n} + \sum_k R_{\alpha,j,n,k}$$

where each $R_{\alpha,j,n,k}$ is a homogeneous symbol of order $-k$ between $1-n-|\alpha|-j+1$ and $1-n-|\alpha|-j+\frac{|\alpha|}{2}$. For any given $R_{\alpha,j,n,k}$,

$$-k \le 1-n-|\alpha|-j+\frac{|\alpha|}{2},$$

which implies that $j\le k$ as $|\alpha|\ge 2$. Note also for each non-negative integer k there are finitely many (α,j,n) such that $R_{\alpha,j,n,k}$ are of order $-k$.

Step 1: We study the first order terms of the amplitude function in (2.28) and (2.29) by solving the Eikonal equation

$$q_0(y,\xi) = q_0(x,\psi_x(x,y,\xi)) \tag{2.30}$$

for the unknown ψ subject to the initial condition $\psi_x(x,y,\xi)|_{y=x} = \xi$. This can be done by the theory of Hamilton-Jacobi equations. In particular, one can show that

$$\psi(x,y,\xi) = (x-y)\cdot\xi + O(|x-y|^2|\xi|). \tag{2.31}$$

Step 2: With ψ determined in the first step and with the property (2.31), one can recover the initial values $a_n(0,x,y,\xi)$ from the condition (2.27).

Step 3: For each non-negative integer k, we study the k-th order terms of the amplitude function in (2.28) and (2.29) by solving the k-th order transport equation

$$\frac{da_k}{dt} - \mathrm{i}a_{k+1}q_0(y,\xi) = \sum_{(-k)} T_{\alpha,j,n} + \sum_{(-k)} R_{\alpha,j,n,k},$$

where the notation $\sum\limits_{(-k)}$ means taking sum over all relevant homogeneous symbols of order $-k$. Obviously, $\sum\limits_{(-k)} R_{\alpha,j,n,k}$ is a finite sum not involved with $\{a_j\}_{j=k+1}^\infty$, so is

$$\mathrm{i}a_{k+1}q_0(y,\xi) + \sum_{(-k)} T_{\alpha,j,n}.$$

The initial condition for $a_k(0,x,y,\xi)$ has been determined in the second step. Therefore, one can successively solve the Cauchy problem for these equations for sufficiently small times t first for $k=0$, then for $k=1$, and so on.

The details of the above steps can be found in Hörmander's paper [77] and in [139, 146].

In general, let E be a vector bundle over M, and let P be a non-negative self-adjoint Laplace type operator acting on smooth sections of E. Similar to the trivial bundle case, one can show (e.g. [110]) that modulo smoothing operators $e^{-\mathrm{i}t\sqrt{P}}$ locally are of the form

$$e^{-\mathrm{i}t\sqrt{P}} = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} a(t,x,y,\xi)e^{\mathrm{i}\theta(t,x,y,\xi)}d\xi \tag{2.32}$$

for sufficiently small times t, where the scalar-valued phase function θ is the same as before, the amplitude function a is now a matrix-valued symbol of order zero. To be clear, as the principal symbol of $\sqrt{P}$ is proportional to the identity matrix, it can be written in the form $q_0(x,\xi)\mathrm{Id}$, where q_0 once again means a scalar-valued function.

2.4 Finite propagation speed

The d'Alembert formula

$$u(x,t) = \frac{1}{2}(f(x-t)+f(x+t)) + \frac{1}{2}\int_{x-t}^{x+t} h(s)ds \quad ((x,t)\in\mathbb{R}\times[0,\infty)) \tag{2.33}$$

provides the unique classical solution of the Cauchy problem for the one-dimensional wave equation

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \quad ((x,t)\in\mathbb{R}\times\mathbb{R}^+) \\ u(x,0) = f(x) \\ \frac{\partial u}{\partial t}(x,0) = h(x) \end{cases}$$

whenever the Cauchy data f,h are of a certain smoothness. This implies that the solution at a given point (x_0,t_0) depends only on the values of the Cauchy data in $[x_0-t_0, x_0+t_0]$. Similarly, the unique classical solution of the Cauchy problem for the d-dimensional wave equation

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} = \Delta u \quad ((x,t)\in\mathbb{R}^d\times\mathbb{R}^+) \\ u(x,0) = f(x) \\ \frac{\partial u}{\partial t}(x,0) = h(x) \end{cases}$$

at (x_0,t_0) depends similarly only on the values of the Cauchy data in the closed ball $\overline{B}(x_0,t_0)$. To be precise, if $d\geq 3$ is odd one has

$$\begin{aligned} u(x,t) = \frac{1}{1\cdot 3\cdots(d-2)|\mathbb{S}^{d-1}|}\Big[&\partial_t(t^{-1}\partial_t)^{(d-3)/2}\Big(t^{d-2}\int_{|y|=1} f(x+ty)d\sigma(y)\Big) \\ &+ (t^{-1}\partial_t)^{(d-3)/2}\Big(t^{d-2}\int_{|y|=1} h(x+ty)d\sigma(y)\Big)\Big], \end{aligned} \tag{2.34}$$

and if d is even one has

$$u(x,t) = \frac{2}{1\cdot 3\cdots(d-1)|\mathbb{S}^d|}\Big[\partial_t(t^{-1}\partial_t)^{(d-2)/2}\Big(t^{d-1}\int_{|y|\le 1}\frac{f(x+ty)}{\sqrt{1-|y|^2}}dy\Big) + (t^{-1}\partial_t)^{(d-2)/2}\Big(t^{d-1}\int_{|y|\le 1}\frac{h(x+ty)}{\sqrt{1-|y|^2}}dy\Big)\Big]. \tag{2.35}$$

Thus the space support of the solution expands at speed one, that is,

$$\mathrm{supp}(u(\cdot,t)) \subset \bigcup_{x\in \mathrm{supp}(f)\cup \mathrm{supp}(h)} \overline{B}(x,t). \tag{2.36}$$

Now let $U \subset \mathbb{R}^d$ be an open set. The following uniqueness proposition (e.g. [44, §7.2.4], [48, Thm. 5.3], [126, Lemma 2.3]) will play a crucial role in our study of the heat kernels in Chapter 5. According to Folland [48, p. 164], "This is a very strong result".

Proposition 2.4.1. *Suppose $u(x,t)$ is C^2 in $U\times[0,\infty)$ and that $\frac{\partial^2 u}{\partial t^2} = \Delta u$. Suppose $u(x,0) = \frac{\partial u}{\partial t}(x,0) = 0$ for all $x \in B(x_0,r_0)\subset U$. Then $u = 0$ in the backward light cone $|x-x_0| \le r_0 - t$.*

We briefly explain why the above proposition is so useful to our later study. First, it implies (2.36) for $U = \mathbb{R}^d$. Second, let Δ_U be an arbitrary non-negative self-adjoint extension of $-\Delta : C_c^\infty(U) \to C_c^\infty(U)$ in $L^2(U)$, and let $\phi \in C_c^\infty(U) \subset C_c^\infty(\mathbb{R}^d)$. Applying Proposition 2.4.1 to

$$u(x,t) = \cos(t\sqrt{\Delta_0})\phi\Big|_U - \cos(t\sqrt{\Delta_U})\phi$$

(see §5.2.2 for the proof of smoothness of $\cos(t\sqrt{\Delta_U})\phi$) implies that $\cos(t\sqrt{\Delta_0})\phi\big|_U$ agrees with $\cos(t\sqrt{\Delta_U})\phi$ on the region $U_{|t|} = \{z\in U : \mathrm{dist}(z,\partial U) > |t|\}$, where Δ_0 denotes the (unique) self-adjoint extension of $-\Delta : C_c^\infty(\mathbb{R}^d) \to C_c^\infty(\mathbb{R}^d)$ in $L^2(\mathbb{R}^d)$. But according to (2.33) – (2.35), $\cos(t\sqrt{\Delta_0})\phi$ is completely known in $\mathbb{R}^d$, so is $\cos(t\sqrt{\Delta_U})\phi$ in the region $U_{|t|}$. In other words, the operator kernel of $\cos(t\sqrt{\Delta_U})$ in $U_{|t|}\times U$ is completely known. This implies that the operator kernel of $\cos(t\sqrt{\Delta_U})$ at a given diagonal element $(x,x)\in U\times U$ is completely determined by that of $\cos(t\sqrt{\Delta_0})$ whenever $|t| < \rho(x)$, where $\rho(x)$ denotes the distance x to the boundary of U. This is quite an interesting property as it is independent of the choice of self-adjoint extensions.

For completeness we provide a proof of Proposition 2.4.1. Without loss of generality we can assume that u is real-valued and $x_0 = 0$. Define

$$E(t) = \int_{B(r_0-t)}\Big((\partial_t u)^2 + |\nabla_x u|^2\Big)dx \quad (0\le t < r_0),$$

which represents the energy of the wave in the region $B(r_0-t)$ at time t. Here $B(r)$ denotes the open ball centered at the origin in $\mathbb{R}^d$ with radius $r > 0$. We also let $S(r)$ denote the boundary of $B(r)$, and write σ for the surface measure on $S(r)$. Note

$$\frac{dE}{dt} = -\int_{S(r_0-t)}\Big((\partial_t u)^2 + |\nabla_x u|^2\Big)d\sigma + 2\int_{B(r_0-t)}\Big(\frac{\partial u}{\partial t}\frac{\partial^2 u}{\partial t^2} + \nabla_x u\cdot\nabla_x(\frac{\partial u}{\partial t})\Big)dx.$$

A use of $\frac{\partial^2 u}{\partial t^2} = \Delta_x u$ and application of Green's first identity (e.g. [48, (2.5)]) allow us to write the second integral in the form

$$2\int_{S(r_0-t)}\frac{\partial u}{\partial t}\frac{\partial u}{\partial \mathbf{n}}d\sigma,$$

where $\mathbf{n}$ denotes the unit outer normal vector on the sphere. Therefore, it follows from the Cauchy-Schwartz inequality that $\frac{dE}{dt} \leq 0$. But clearly $E \geq 0$, and $E(0) = 0$ since the Cauchy data vanish. Hence $E(t) = 0$ for all $0 \leq t < r_0$. Considering $u(x,0) = 0$ on $B(r_0)$, one gets $u = 0$ in the backward light cone $|x - x_0| \leq r_0 - t$. This finishes the proof of the proposition.

Generalizations of Proposition 2.4.1 to Schrödinger operators or manifold situations can be seen in [126, 140, 153, 154]. For example, suppose $u(x,t)$ is C^2 in $U \times [0,\infty)$ and that

$$\frac{\partial^2 u}{\partial t^2} = \Delta u + Vu$$

for some bounded function V on U. Suppose $u(x,0) = \frac{\partial u}{\partial t}(x,0) = 0$ for all $x \in B(x_0, r_0) \subset U$. We then still have $u = 0$ in the same backward light cone. To this end, it suffices to first study

$$E(t) = \int_{B(r_0-t)} \Big(u^2 + (\partial_t u)^2 + |\nabla_x u|^2\Big) dx \quad (0 \leq t < r_0)$$

in the same manner as above, then apply Gronwall's lemma appropriately.

2.5 Schwartz kernel theorem

Let $U \subset \mathbb{R}^d$ be an open set. The Schwartz kernel theorem (e.g. [79, Thm. 5.2.1]) says that every continuous linear map T from $C_c^\infty(U)$[3] to its dual space $\mathscr{D}'(U)$[4] is uniquely determined by an element $K_T \in \mathscr{D}'(U \times U)$ in the following way:

$$\langle T\phi, \psi\rangle = \langle K_T, \psi \otimes \phi\rangle \quad (\phi, \psi \in C_c^\infty(U)).$$

Here $\langle \cdot, \cdot \rangle$ denotes the dual between $C_c^\infty(U)$ and $\mathscr{D}'(U)$ or $C_c^\infty(U \times U)$ and $\mathscr{D}'(U \times U)$. One calls K_T the integral or operator kernel of T. If S is a bounded linear operator on $L^2(U)$, then it follows immediately from

$$|\langle S\phi, \psi\rangle_{L^2(U)}| \leq \|S\| \sqrt{\langle \phi, \phi\rangle_{L^2(U)}} \sqrt{\langle \psi, \psi\rangle_{L^2(U)}}$$

that the restriction T of S onto $C_c^\infty(U)$[5] is a continuous linear map from $C_c^\infty(U)$[6] to $\mathscr{D}'(U)$[7]. Since $C_c^\infty(U)$ is a dense subset of $L^2(U)$, we see that S is uniquely determined by T or its integral kernel K_T. For simplicity we do not distinguish S and T, and write K_S for K_T. In general, let $\mathbf{T}$ be a continuous linear map from $C_c^\infty(U; \mathbb{C}^N)$ to its dual space $\mathscr{D}'(U; \mathbb{C}^N)$, or be a bounded linear operator on $L^2(U; \mathbb{C}^N)$. For each fixed pair (i,j), $1 \leq i, j \leq N$, one can introduce a

[3] Here $C_c^\infty(U)$ is endowed with the following topology structure: a sequence of functions $\{\phi_n\}_{n=1}^\infty$ in $C_c^\infty(U)$ is said to converge to ϕ_0 in $C_c^\infty(U)$ if there exists a compact subset of U containing all of the supports of ϕ_n as subsets, and $\{\phi_n\}_{n=1}^\infty$ converges to ϕ in $C^k(U)$ for all $k \in \mathbb{N}$.

[4] An element of $\mathscr{D}'(U)$ is also called a distribution on U. The topology structure on $\mathscr{D}'(U)$ is endowed as follows: a sequence of distributions $\{Z_n\}_{n=1}^\infty$ on U is said to converge to Z_0 in $\mathscr{D}'(U)$ if $Z_n(\phi) \to Z_0(\phi)$ for all $\phi \in C_c^\infty(U)$.

[5] Here $C_c^\infty(U)$ is only regarded as a subset of $L^2(U)$.

[6] Here $C_c^\infty(U)$ is endowed with its own standard topology structure, not the one inherited from $L^2(U)$.

[7] This is due to the fact that $L^2(U)$ is continuously embedded in $\mathscr{D}'(U)$.

continuous linear map $\mathbf{T}_{ij}$ from $C_c^\infty(U)$ to $\mathscr{D}'(U)$ by defining

$$\langle \mathbf{T}_{ij}\phi, \psi\rangle = \langle \mathbf{T}\begin{pmatrix} 0 \\ \vdots \\ \phi \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \vdots \\ \psi \\ \vdots \\ 0 \end{pmatrix}\rangle,$$

where ϕ appears at the j-th position in $\begin{pmatrix} 0 \\ \vdots \\ \phi \\ \vdots \\ 0 \end{pmatrix}$, ψ appears at the i-th position in $\begin{pmatrix} 0 \\ \vdots \\ \psi \\ \vdots \\ 0 \end{pmatrix}$. We then have a matrix of integral kernels

$$K_{\mathbf{T}} = \begin{pmatrix} K_{\mathbf{T}_{11}} & \cdots & K_{\mathbf{T}_{1N}} \\ \vdots & \ddots & \vdots \\ K_{\mathbf{T}_{N1}} & \cdots & K_{\mathbf{T}_{NN}} \end{pmatrix},$$

which is called the integral or operator kernel of $\mathbf{T}$. Obviously, $\mathbf{T}$ is uniquely determined by its integral kernel because of linearity:

$$\langle \mathbf{T}\begin{pmatrix} \phi_1 \\ \vdots \\ \phi_N \end{pmatrix}, \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}\rangle = \sum_{i,j=1}^{N} \langle \mathbf{T}_{ij}\phi_j, \psi_i\rangle = \sum_{i,j=1}^{N} \langle K_{\mathbf{T}_{ij}}, \psi_i \otimes \phi_j\rangle.$$

We end this section with a few remarks.

First, let U_2 be another open set in a possibly different Euclidean space $\mathbb{R}^{d_2}$. The original Schwartz kernel theorem actually says that every continuous linear map T from $C_c^\infty(U)$ to $\mathscr{D}'(U_2)$ is uniquely determined by an element $K_T \in \mathscr{D}'(U_2 \times U)$ in the following way:

$$\langle T\phi, \psi\rangle = \langle K_T, \psi \otimes \phi\rangle \quad (\phi \in C_c^\infty(U), \psi \in C_c^\infty(U_2)).$$

Following the previous argument, one can define integral kernel for continuous linear maps from $C_c^\infty(U;\mathbb{C}^N)$ to $\mathscr{D}'(U_2;\mathbb{C}^{N_2})$ or bounded linear operators from $L^2(U;\mathbb{C}^N)$ to $L^2(U_2;\mathbb{C}^{N_2})$, where N_2 is an arbitrary positive integer.

Second, we should remind the reader that the Schwartz kernel theorem is a local statement. For example, given an operator acting on smooth sections of a vector bundle, one can induce locally-defined operators from one coordinate system to another, and define the corresponding integral kernels. This has been done many times in §2.2.2 and §2.2.4.

Finally, note that in various situations the integral kernels can be realized partially or globally as continuous or smooth (scalar or matrix-valued) functions. For example, the integral kernel of any pseudo-differential operator on U is smooth off the diagonal, and the Dirichlet heat kernel for U is smooth on $U \times U$ for any fixed time $t > 0$.

Chapter 3

Spectral counting functions

Let M be a closed smooth Riemannian manifold of dimension d and metric g. Let E be a smooth complex hermitian vector bundle over M. As usual we denote by $C^\infty(M;E)$ the space of smooth sections of E, and by $L^2(M;E)$ the Hilbert space of square integrable sections equipped with the natural inner product defined by the hermitian structure on the fibres and the metric measure μ_g on M.

We first recall some basic facts about operators of Laplace type. A second order partial differential operator $P : C^\infty(M;E) \to C^\infty(M;E)$ is said to be of Laplace type if its principal symbol σ_P is of the form $\sigma_P(\xi) = g_x(\xi,\xi)\mathrm{id}_{E_x}$ for all covectors $\xi \in T_x^*M$. In local coordinates this means that P is of the form

$$P = -g^{ij}(x)\partial_i\partial_j + a^k(x)\partial_k + b(x), \tag{3.1}$$

where a^k, b are smooth matrix-valued functions, and we have used Einstein's sum convention. Given a Laplace type operator P, it is known that there exist a unique connection ∇ on E and a unique bundle endomorphism $V \in C^\infty(M;\mathrm{End}(E))$ such that $P = \Delta^\nabla + V$. We assume that P is self-adjoint and non-negative. Thus there exists an orthonormal basis $\{\phi_j\}_{j=1}^\infty$ for $L^2(M;E)$ consisting of smooth eigensections such that $P\phi_j = \lambda_j^2\phi_j$, where λ_j are chosen to be non-negative and correspond to the eigenvalues of the operator $\sqrt{P}$.

Let A be a classical pseudo-differential operator of order $m \in \mathbb{R}$. The (microlocalized) spectral counting function $N_A(\lambda)$ of P is defined as

$$N_A(\lambda) = \sum_{\lambda_j<\lambda} \langle A\phi_j, \phi_j\rangle. \tag{3.2}$$

Let $\chi \in \mathscr{S}(\mathbb{R})$ be a Schwartz function such that the Fourier transform $\mathscr{F}\chi$ of χ is 1 near the origin and $\mathrm{supp}(\mathscr{F}\chi) \subset (-\delta,\delta)$, where δ is a positive constant smaller than half the radius of injectivity of M. It is well known (e.g. [40, 84, 85, 132, 133, 162] for various special cases) that

$$(\chi * N_A')(\lambda) = \sum_{j=1}^\infty \langle A\phi_j, \phi_j\rangle \chi(\lambda-\lambda_j) \sim \sum_{k=0}^\infty \mathscr{A}_k(A,P)\lambda^{d+m-k-1} \quad (\lambda\to\infty), \tag{3.3}$$

where the spectral counting coefficients $\mathscr{A}_k(A,P)$ do not depend on the choice of χ, and are locally computable in terms of the local full symbols of A and P. This can be derived from studying the Fourier integral operator representation of $Ae^{-\mathrm{i}t\sqrt{P}}$ via the stationary phase method.

Apart from the Fourier integral operator representation method, there exist several other ways to recover the mollified spectral counting coefficients $\mathscr{A}_k(A,P)$.

First, the (microlocalized) spectral zeta function $\zeta(s,A,P)$ is defined by

$$\zeta(s,A,P)=\sum_{\lambda_j>0}\frac{\langle A\phi_j,\phi_j\rangle}{\lambda_j^s}\quad(\mathrm{Re}(s)>d+m). \tag{3.4}$$

It is well known (e.g. [40, 162]) that $\zeta(s,A,P)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $s=d+m-k$ ($k=0,1,2,\ldots$) with residues $\mathscr{A}_k(A,P)$.

Second, the Mellin transform of

$$\mathrm{tr}(Ae^{-tP})-\sum_{\lambda_j=0}\langle A\phi_j,\phi_j\rangle\quad(t\in(0,\infty))$$

admits a meromorphic continuation $\zeta(2s,A,P)\Gamma(s)$ to $\mathbb{C}$ whose singularities can be completely determined from those of $\zeta(s,A,P)$ and $\Gamma(s)$. Here $\Gamma(s)$ denotes the classical Gamma function. After establishing a suitable vertical decay estimate for $\zeta(2s,A,P)\Gamma(s)$, one can deduce from the inverse Mellin transform theorem the following widely used heat expansion (e.g. [64, 67, 68, 101, 137])

$$\mathrm{tr}(Ae^{-tP})\sim\sum_{k=0}^{\infty}\left(\mathscr{B}_k(A,P)t^{\frac{k-d-m}{2}}+\mathscr{C}_k(A,P)t^k\log(t)+\mathscr{D}_k(A,P)t^k\right)\quad(t\to0^+). \tag{3.5}$$

The above notation system may bring confusion to the reader as it could happen that there are non-negative integers k such that $\frac{k-d-m}{2}$ are non-negative integers. In this case one can simply set $\mathscr{B}_k(A,P)=0$, thus (3.5) is well-defined. The relation between the mollified counting coefficients and some of the heat coefficients can be summarized as follows:

Case 1: If the order m of A is an integer, then

- $\mathscr{B}_k(A,P)=\frac{\Gamma(\frac{d+m-k}{2})}{2}\cdot\mathscr{A}_k(A,P)$ ($d+m-k$ is positive or negative but odd);
- $\mathscr{C}_k(A,P)=0$ ($d+m+2k<0$);
- $\mathscr{C}_k(A,P)=\frac{(-1)^{k+1}}{2\cdot k!}\cdot\mathscr{A}_{d+m+2k}(A,P)$ ($d+m+2k\geq0$).

Case 2: If the order m of A is not an integer, then for all non-negative integers k:

- $\mathscr{B}_k(A,P)=\frac{\Gamma(\frac{d+m-k}{2})}{2}\cdot\mathscr{A}_k(A,P)$;
- $\mathscr{C}_k(A,P)=0$.

Thus the heat expansion (3.5) contains all information about $\{\mathscr{A}_k(A,P)\}_{k=0}^{\infty}$.

In exactly the same way, the following resolvent trace expansion (e.g. [65, 67, 137])

$$\mathrm{tr}(A(1+tP)^{-\frac{N}{2}})\sim\sum_{k=0}^{\infty}\left(\mathscr{B}_k^{(N)}(A,P)t^{\frac{k-d-m}{2}}+\mathscr{C}_k^{(N)}(A,P)t^k\log(t)+\mathscr{D}_k^{(N)}(A,P)t^k\right)(t\to0^+) \tag{3.6}$$

also contains all information about $\{\mathscr{A}_k(A,P)\}_{k=0}^{\infty}$, where N is any complex number such that $\mathrm{Re}(N)>\max\{d+m,0\}$. Similar to the unambiguousness of (3.5), one can set $\mathscr{B}_k^{(N)}(A,P)=0$ whenever $\frac{k-d-m}{2}$ is a non-negative integer to guarantee (3.6) is well-defined.

To summarize, there exist at least four different ways, such as studying

- spectral counting functions,
- spectral zeta functions,
- heat expansions, and
- resolvent trace expansions,

to retrieve all the information about $\{\mathscr{A}_k(A,P)\}_{k=0}^{\infty}$. For example, using parametrix constructions in any of these methods results in the well-known leading term

$$\mathscr{A}_0(A,P) = \frac{1}{(2\pi)^d}\int_{T_1^*M} \mathrm{Tr}(\sigma_A). \tag{3.7}$$

In the second chapter we discussed the concepts of invariantly-defined principal and sub-principal symbols. In theory one can use parametrix constructions in any of these methods to express $\mathscr{A}_1(A,P)$ in terms of the principal and sub-principal symbols of both A and P.

The mollified spectral counting coefficients $\mathscr{A}_k(A,P)$ do not depend on the choice of χ, and are locally computable in terms of the local full symbols of A and P. But as we do not have invariantly-defined concepts of "sub-sub-principal symbol", "sub-sub-sub-principal symbol" and so on, it is not so convenient to regard $\mathscr{A}_k(A,P)$ ($k \geq 2$) from global viewpoint. In particular, the expressions of $\mathscr{A}_k(A,P)$ normally involve many summands of derivatives of the local full symbols of A and P, thus their geometric meanings are not easy to be retrieved.

In this chapter we will see that the Wodzicki residue can provide a clear interpretation of $\mathscr{A}_k(A,P)$ for all $k \geq 0$. Actually, there exist smooth functions $f_k(A,P)$ on M such that

$$\mathscr{A}_k(A,P) = \int_M f_k(A,P)d\mu_g \tag{3.8}$$

for all $k \geq 0$. In practice, one can extract microlocal information about P from $f_k(A,P)$ with A ranging all classical pseudo-differential operators or endomorphisms of the given bundle.

In the next chapter we will specialize in Dirac type operators. Let D be a self-adjoint Dirac type operator. There exists a discrete spectral resolution $\{\phi_j,\mu_j\}_{j=1}^{\infty}$ of D, where $\{\phi_j\}_{j=1}^{\infty}$ is an orthonormal basis for $L^2(M;E)$, and $D\phi_j = \mu_j\phi_j$ for each j. Obviously, ϕ_j will be eigensections of $P = P$ with eigenvalues μ_j^2. Therefore, using the notation from before $\lambda_j = |\mu_j|$. By setting

$$B^{\pm} = \frac{\mathrm{Sign}(D) \pm \mathrm{Id}_E}{2},$$

we see that $\mathscr{A}_k(B^{\pm},P)$ carry microlocal information about the positive (negative) spectrum of D. Later on we will extract this information from studying $f_k(FB^{\pm},P)$ with F ranging all smooth endomorphisms of E.

This chapter is arranged as follows. In Sections 3.1, 3.3 and 3.4 we provide proofs of (3.3), (3.5) and (3.6), respectively, and in Section 3.2 we determine the singularity structure of spectral zeta functions (3.4). The author should clearly state that he does not claim any originality over these four classical results. All of the other sections are devoted to providing explicit formulae for $\mathscr{A}_k(A,P)$. This will be performed by two methods: one is Wodzicki's residue in Section 3.5, the other is complex powers of elliptic operators in Section 3.7. In Section 3.8 we specialize in $\mathscr{A}_1(A,P)$. By the way, we study a case where A is a partial differential operator in Section 3.6.

3.1 FIO method

Formula (3.3) is essentially Proposition 2.1 in [40], Corollary 2.2 in [84], Theorem 2.2 in [133] and Proposition 1.1 in [162], except the authors either consider scalar operators or assume A is of order zero. Recall that $\chi \in \mathscr{S}(\mathbb{R})$ is chosen so that $\mathscr{F}\chi = 1$ near the origin and $\operatorname{supp}(\mathscr{F}\chi) \subset (-\delta, \delta)$, where δ is smaller than half the radius of injectivity of M. If t is sufficiently small, say $|t| < \delta_1 < \delta$, then locally the integral kernel $(Ae^{-\mathrm{i}t\sqrt{P}})(t,x,y)$ of the operator $Ae^{-\mathrm{i}tP^{1/2}}$ is well known to have the form

$$(Ae^{-\mathrm{i}t\sqrt{P}})(t,x,y) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} a(t,x,y,\xi)e^{\mathrm{i}\theta(t,x,y,\xi)}d\xi,$$

where a is a classical (matrix-valued) symbol of order m. This can be seen from (2.32) and the rule of product between a classical pseudo-differential operator and a Fourier integral operator. The scalar-valued phase function θ is of the form

$$\theta(t,x,y,\xi) = \psi(x,y,\xi) - tq_0(y,\xi),$$

where q_0 denotes the (scalar) principal symbol of $\sqrt{P}$,

$$\psi(x,y,\xi) = (x-y)\cdot\xi + O(|x-y|^2|\xi|).$$

For details see (2.25) and (2.31). It is also known that $\operatorname{tr}(Ae^{-\mathrm{i}t\sqrt{P}})$ is smooth in $(-\delta,\delta)\backslash\{0\}$, so we introduce a cut-off function $\varrho \in \mathscr{S}(\mathbb{R})$ satisfying $\varrho(t) = 1$ if $|t| < \frac{\delta_1}{2}$ and $\operatorname{supp}(\varrho) \subset (-\delta_1, \delta_1)$. Using integration by parts one gets

$$\begin{aligned}(\chi * N_A')(\lambda) =& \frac{1}{2\pi}\int_{\mathbb{R}}(\mathscr{F}\chi)(t)(\varrho(t)+1-\varrho(t))\operatorname{tr}(Ae^{-\mathrm{i}t\sqrt{P}})e^{\mathrm{i}\lambda t}dt\\ =& \frac{1}{(2\pi)^{d+1}}\int_M\int_{\mathbb{R}^d}\int_{\mathbb{R}}(\mathscr{F}\chi)(t)\varrho(t)\operatorname{Tr}(a(t,y,y,\xi))e^{-\mathrm{i}tq_0(y,\xi)}e^{\mathrm{i}\lambda t}dyd\xi dt\\ &+ o(\lambda^{-\infty}) \quad (\lambda\to\infty),\end{aligned}$$

where $o(\lambda^{-\infty})$ is short for $o(\lambda^{-h})$ for any positive integer h. Consider

$$I(y,\lambda) = \int_{\mathbb{R}^d}\int_{\mathbb{R}}(\mathscr{F}\chi)(t)\varrho(t)\operatorname{Tr}(a(t,y,y,\xi))e^{-\mathrm{i}tq_0(y,\xi)}e^{\mathrm{i}\lambda t}d\xi dt.$$

We here pass to polar coordinates by putting $\xi = \lambda r\omega$, $|\omega| = 1$, $d\xi = \lambda^d r^{d-1}drd\omega$. Then

$$I(y,\lambda) = \lambda^{d+m}\int_{\mathbb{S}^{d-1}}\Big[\int_{\mathbb{R}^+}\int_{\mathbb{R}}(\mathscr{F}\chi)(t)\varrho(t)\operatorname{Tr}(a(t,y,y,\omega))r^{d+m-1}e^{\mathrm{i}\lambda(t-trq_0(y,\omega))}drdt\Big]d\omega.$$

Here we apply the stationary phase method to the two-dimensional $drdt$ integral. The phase function is $\Phi(r,t) = t - trq_0(y,\omega)$, whose unique critical point close to $t = 0$ is given by

$$(r_0,t_0) = \Big(\frac{1}{q_0(y,\omega)}, 0\Big).$$

At this critical point the Hessian matrix Φ'' of the phase function satisfies $\det(\Phi'') = -q_0(y,\omega)^2 < 0$. Applying the stationary phase method (e.g. [62, Prop. 2.3], [149, p. 344]) yields a full asymptotic expansion for $I(y,\lambda)$ and proves (3.3) as a consequence. We should mention that to correctly apply the stationary phase method one needs to introduce a suitable cut-off function of the variable r. The details of this more careful treatment can be seen in [62, p.136].

3.2 Spectral zeta functions

3.2.1 Finite heat expansions

It is easy to show that

$$\langle T, \varphi_t \rangle = \langle \rho * T, \varphi_t \rangle + o(t^\infty)^1 \quad (t \to 0^+), \tag{3.9}$$

where T is a tempered distribution on $\mathbb{R}$, $\varphi \in \mathscr{S}(\mathbb{R})$, $\varphi_t(\lambda) = \varphi(t\lambda)$, and $\rho \in \mathscr{S}(\mathbb{R})$ is chosen so that $\mathscr{F}\rho = 1$ near the origin. Actually, this formula appears in equivalent forms in [40, 71, 162]. For completeness we provide a proof as follows. By definition we have

$$\langle T - \rho * T, \varphi_t \rangle = \langle \mathscr{F}T, (1 - \mathscr{F}\rho)\mathscr{F}^{-1}\varphi_t \rangle.$$

Fix a $\delta > 0$ such that $(\mathscr{F}\rho)(\xi) = 1$ for $|\xi| < \delta$. Then for any $|\xi| \geq \delta$, $N \in \mathbb{N}$, and any non-negative integer k,

$$\frac{d^k}{d\xi^k}(\mathscr{F}^{-1}\varphi_t) = \big(\frac{|\xi|}{t}\big)^N \Big(\frac{d^k}{d\xi^k}(\mathscr{F}^{-1}\varphi)\Big)(\frac{\xi}{t}) \cdot \frac{t^{N-k-1}}{|\xi|^N}.$$

This implies that there exists a positive constant C depending only on ρ, φ, N and k such that for all $\xi \in \mathbb{R}$ and $t > 0$,

$$\Big|\frac{d^k}{d\xi^k}\big[(1 - \mathscr{F}\rho)\mathscr{F}^{-1}\varphi_t\big]\Big| \leq \frac{C}{1 + |\xi|^N} \cdot t^{N-k-1}. \tag{3.10}$$

The structure of tempered distributions on $\mathbb{R}$ implies that there exist a non-negative integer k_0 and a slowly increasing continuous function h_0 on $\mathbb{R}$ such that $(\mathscr{F}T)(\xi) = \frac{d^k}{d\xi^k}h_0$. So we can set $k = k_0$ in (3.10) and let N be large enough to obtain (3.9).

As an immediate consequence of (3.9), one gets

$$\langle N'_A, (t\lambda)^h \varphi(t\lambda) \rangle = \langle \chi * N'_A, (t\lambda)^h \varphi(t\lambda) \rangle + o(t^\infty) \quad (t \to 0^+),$$

where $\varphi \in \mathscr{S}(\mathbb{R})$, and h is an arbitrary non-negative integer. Equivalently, we have

$$\langle N'_A, \lambda^h \varphi(t\lambda) \rangle = \langle \chi * N'_A, \lambda^h \varphi(t\lambda) \rangle + o(t^\infty) \quad (t \to 0^+). \tag{3.11}$$

Note the left hand side of (3.11) just is $\mathrm{tr}(AP^{\frac{h}{2}}\varphi(t\sqrt{P}))$. Now we claim the right hand side of (3.11) is of the following form

$$\sum_{k<d+m+h} \mathscr{A}_k(A, P) \cdot \int_0^\infty \lambda^{d+m+h-k-1}\varphi(\lambda)d\lambda \cdot t^{k-d-m-h} + o(t^{\lceil m \rceil - m - 1}). \tag{3.12}$$

To this end we first decompose

$$\begin{aligned}
\langle \chi * N'_A, \lambda^h \varphi(t\lambda) \rangle = &\int_{-\infty}^0 (\chi * N'_A)(\lambda) \cdot \lambda^h \varphi(t\lambda)d\lambda + \\
&\sum_{k<d+m+h} \int_0^\infty \mathscr{A}_k(A, P)\lambda^{d+m-k-1} \cdot \lambda^h \varphi(t\lambda)d\lambda + \\
&\int_0^\infty \big((\chi * N'_A)(\lambda) - \sum_{k<d+m+h} \mathscr{A}_k(A, P)\lambda^{d+m-k-1}\big) \cdot \lambda^h \varphi(t\lambda)d\lambda \\
&\triangleq \alpha_1(t) + \alpha_2(t) + \alpha_3(t).
\end{aligned}$$

[1] Here $o(t^\infty)$ means $o(t^h)$ for any positive integer h. Similarly, $o(t^{-\infty})$ means $o(t^{-h})$ for any positive integer h.

Since $\operatorname{supp}(N_A') \subset [0,\infty)$, it is easy to show that

$$(\chi * N_A')(\lambda) = o(|\lambda|^{-\infty}) \quad (\lambda \to -\infty). \tag{3.13}$$

To see this we let τ be a smooth function on $\mathbb{R}$ such that it vanishes on $(-\infty,-2]$ and equals one on $[-1,\infty)$, and let k_0 be a non-negative integer and h_0 be a slowly increasing continuous function on $\mathbb{R}$ such that $N_A' = \frac{d^{k_0}}{dy^k} h_0$. Then $N_A' = \tau(y)\frac{d^{k_0}}{dy^{k_0}} h_0$ and, consequently,

$$(\chi * N_A')(\lambda) = (-1)^{k_0} \int_{-2}^{\infty} h_0(y) \frac{d^{k_0}}{dy^{k_0}} \big(\tau(y)\chi(\lambda - y)\big) dy.$$

Hence to prove (3.13) it suffices to note that there exists a positive constant C_0 depending on τ, χ and large enough $N \in \mathbb{N}$ such that, for all $\lambda < -3 < -2 < y$,

$$\Big| \frac{d^{k_0}}{dy^{k_0}} \big(\tau(y)\chi(\lambda - y)\big) \Big| \le \frac{C_0}{|\lambda - y|^{2N}} \le \frac{C_0}{|y+3|^N} \cdot \frac{1}{|\lambda + 2|^N}.$$

It follows from (3.13) that $\alpha_1(t) = O(1)$ as $t \to 0^+$. Note also

$$\alpha_2(t) = \sum_{k<d+m+h} \mathscr{A}_k(A,P) \cdot \int_0^{\infty} \lambda^{d+m+h-k-1} \varphi(\lambda) d\lambda \cdot t^{k-d-m-h}.$$

For simplicity we introduce

$$f(\lambda) = \big((\chi * N_A')(\lambda) - \sum_{k<d+m+h} \mathscr{A}_k(A,P)\lambda^{d+m-k-1}\big) \cdot \lambda^h \quad (\lambda > 0)$$

and note $\alpha_3(t) = \int_0^\infty f(\lambda)\varphi(t\lambda)d\lambda$. To prove the claim we have two cases to consider.
Case 1: Suppose $d+m+h > 0$. Let $\widetilde{k}$ be the unique non-negative integer such that $\widetilde{k} < d+m+h \le \widetilde{k}+1$. Let $\beta \triangleq d+m+h-\widetilde{k}-1 \in (-1,0]$, which implies there exists a constant C_1 such that for all $\lambda \in (0,1)$, $|f(\lambda)| \le C_1\lambda^\beta$. According to (3.3), there exists another constant C_2 such that for all $\lambda \ge 1$, $|f(\lambda)| \le C_2\lambda^{\beta-1} \le C_2\lambda^{-1}$. So as $t \to 0^+$,

$$\begin{aligned}
|\alpha_3(t)| &\le C_1 \int_0^1 \lambda^\beta |\varphi(t\lambda)| d\lambda + C_2 \int_1^\infty \lambda^{-1}|\varphi(t\lambda)|d\lambda \\
&= C_1 \int_0^t \lambda^\beta |\varphi(\lambda)| d\lambda \cdot t^{-(\beta+1)} + C_2 \int_t^\infty \lambda^{-1}|\varphi(\lambda)|d\lambda \\
&= o(t^{-(\beta+1)}) + O(|\log(t)|) \\
&= o(t^{-(\beta+1)}).
\end{aligned}$$

Since $-(\beta+1) = \widetilde{k} - d - m - h = \lceil m \rceil - m - 1 < 0$, we are done in the first case.
Case 2: Suppose $d+m+h \le 0$. Obviously, there is a constant C_3 such that, for all $\lambda \in (0,1)$, $|f(\lambda)| \le C_3$. According to (3.3), $(\chi * N_A')(\lambda) = O(\lambda^{d+m-1})$ as $\lambda \to \infty$. Thus there is a constant C_4 such that, for all $\lambda \ge 1$, $|f(\lambda)| \le C_4\lambda^{-1}$. So as $t \to 0^+$,

$$\begin{aligned}
|\alpha_3(t)| &\le C_3 \int_0^1 |\varphi(t\lambda)| d\lambda + C_4 \int_1^\infty \lambda^{-1}|\varphi(t\lambda)|d\lambda \\
&= O(1) + O(|\log(t)|) \\
&= O(|\log(t)|).
\end{aligned}$$

But note $\lceil m \rceil - m - 1 < 0$, we are also done in the second case.

To summarize, we have shown

Proposition 3.2.1. *Suppose $\varphi \in \mathscr{S}(\mathbb{R})$. We have as $t \to 0^+$ that*

$$\mathrm{tr}(AP^{\frac{h}{2}}\varphi(t\sqrt{P})) = \sum_{k<d+m+h} \frac{\mathscr{A}_k(A,P)\int_0^\infty \lambda^{d+m+h-k-1}\varphi(\lambda)d\lambda}{t^{d+m+h-k}} + o(t^{\lceil m\rceil - m-1}).$$

3.2.2 Mellin transforms

The Mellin transform of a continuous function f on $(0,\infty)$ is the function $(Mf)(s)$ of the complex variable s, given by

$$(Mf)(s) = \int_0^\infty f(t)t^{s-1}dt$$

whenever the integral is well-defined. An open strip $\Pi(\beta_1,\beta_2) = \{s \in \mathbb{C} : \beta_1 < \mathrm{Re}(s) < \beta_2\}$ is called a basic strip of Mf if the integral is absolutely convergent in that strip. Given meromorphic functions u, v defined over an open subset Π of $\mathbb{C}$, we denote $u \asymp v$ $(s \in \Pi)$ to mean $u - v$ is analytic in Π. For example, assume f is a continuous function on $(0,\infty)$ satisfying $f(t) = o(t^{-\infty})$ as $t \to \infty$ and assume there exist real numbers $\omega_0 < \omega_1 < \cdots < \omega_N$ such that

$$f(t) = \sum_{k=0}^{N-1} a_k t^{\omega_k} + O(t^{\omega_N}) \quad (t \to 0^+). \tag{3.14}$$

Then one may easily check that $\Pi(-\omega_0,\infty)$ is a basic strip of Mf, and Mf admits a meromorphic continuation to $\Pi(-\omega_N,\infty)$ such that

$$(Mf)(s) \asymp \sum_{k=0}^{N-1} \frac{a_k}{s+\omega_k} \quad (s \in \Pi(-\omega_N,\infty)). \tag{3.15}$$

Actually, for any $s \in \Pi(\gamma_1,\gamma_2)$ with $-\omega_N < \gamma_1 < \gamma_2 < \infty$, one has

$$(Mf)(s) = \sum_{k=0}^{N-1} \frac{a_k}{s+\omega_k} + \int_0^1 \big(f(t) - \sum_{k=0}^{N-1} a_k t^{\omega_k}\big)t^{s-1}dt + \int_1^\infty f(t)t^{s-1}dt,$$

which immediately implies (3.15) as well as an upper bound estimate:

$$(Mf)(s) = O(1) \quad (s \in \Pi(\gamma_1,\gamma_2),\ |s| \to \infty). \tag{3.16}$$

Lemma 3.2.2 ([47])**.** *Let f be a continuous function over $(0,\infty)$. Assume there exist real numbers $\beta_1 < \beta_2 < \beta_3 < \beta_4$ such that*

- *$\Pi(\beta_3,\beta_4)$ is a basic strip of Mf,*
- *Mf admits a meromorphic continuation to $\Pi(\beta_1,\beta_4)$ with finite poles there,*
- *$Mf \asymp \sum_{(\omega,j)} \frac{C_{\omega,j}}{(s+\omega)^{j+1}}$ $(s \in \Pi(\beta_2,\beta_4))$,*
- *Mf is analytic on $\mathrm{Re}(s) = \beta_2$,*
- *$(Mf)(s) = O(|s|^{-2})$ $(s \in \Pi_{\beta_1,\beta_4}, |s| \to \infty)$.*

Then

$$f(t) = \sum_{(\omega,j)} C_{\omega,j}\Big(\frac{(-1)^j}{j!}t^\omega(\log t)^j\Big) + O(t^{-\beta_2}) \quad (t \to 0^+).$$

3.2.3 Spectral zeta functions

Let h be a positive integer such that $d+m+h>1$, and define

$$f_h(t)=\operatorname{tr}(AP^{\frac{h}{2}}e^{-tP})=\sum_{\lambda_j>0}\langle A\phi_j,\phi_j\rangle\lambda_j^h e^{-t\lambda_j^2}\quad(t>0).$$

Now we have two ways to study the Mellin transform of f_h. First, we list the eigenvalues $\{\lambda_j\}_{j=1}^{\infty}$ of $\sqrt{P}$ in non-decreasing order and thus by Weyl's law (e.g. [14]), $\lim_{j\to\infty}\lambda_j^d/j$ exists and is positive. It is easy to see (e.g. [25, 138]) that there exists a constant $C=C(A,P)$ such that $|\langle A\phi_j,\phi_j\rangle|\le C\lambda_j^m$ whenever $\lambda_j>0$. Consequently,

- f_h is smooth over $(0,\infty)$ with $f_h(t)=o(t^{-\infty})$ as $t\to\infty$;
- $\zeta(\cdot,A,P)$ is analytic in $\Pi(d+m,\infty)$;
- Mf_h has a basic strip $\Pi(\frac{d+m+h}{2},\infty)$ in which $(Mf_h)(s)=\zeta(2s-h,A,P)\Gamma(s)$.

Second, according to Proposition 3.2.1 f_h is easily seen to have the form (3.14):

$$f_h(t)=\sum_{k=0}^{N-1}\frac{\Gamma(\frac{d+m+h-k}{2})}{2}\cdot\mathscr{A}_k(A,P)\cdot t^{\frac{k-d-m-h}{2}}+O(t^{\omega_N})\quad(t\to0^+),$$

where $N=N_h=d+h+\lceil m\rceil-1\ge1$, $\omega_N=\frac{\lceil m\rceil-m-1}{2}<0$, $\omega_k=\omega_N-\frac{N-k}{2}=\frac{k-d-m-h}{2}$ $(k=0,1,\dots,N-1)$. So by (3.15), Mf_h, initially analytically defined in $\Pi(\frac{d+m+h}{2},\infty)$, admits a meromorphic continuation to $\Pi(-\omega_N,\infty)$ in which

$$(Mf_h)(s)\asymp\sum_{k=0}^{N-1}\frac{\Gamma(\frac{d+m+h-k}{2})}{2}\cdot\frac{\mathscr{A}_k(A,P)}{s-\frac{d+m+h-k}{2}}.$$

Considering in $\Pi(-\omega_N,\infty)$ the Gamma function Γ is analytic and has no zeros, it is easy to see that $\zeta(s,A,P)$, initially analytically defined in $\Pi(d+m,\infty)$, admits a meromorphic continuation to $\Pi(-2\omega_N-h,\infty)$ in which

$$\zeta(s,A,P)=\frac{(Mf_h)(\frac{s+h}{2})}{\Gamma(\frac{s+h}{2})}\asymp\sum_{k=0}^{N_h-1}\frac{\mathscr{A}_k(A,P)}{s-(d+m-k)}.\tag{3.17}$$

Letting $h\to\infty$ we get

Proposition 3.2.3. *$\zeta(s,A,P)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $s=d+m-k$ ($k=0,1,2,\dots$) with residues $\mathscr{A}_k(A,P)$.*

Remark 1. *Note that, if B is a smoothing operator on sections of E, then $\zeta(s,B,P)$ is an entire function on $\mathbb{C}$ and, consequently, $\mathscr{A}_k(A,P)=\mathscr{A}_k(A+B,P)$ for all k.*

Definition 3.2.4. *For any $q\in\mathbb{R}$, let $P^q:C^\infty(M;E)\to C^\infty(M;E)$ be the operator defined by the functional calculus of P if $q\ge0$ and by sending ϕ to $\sum_{\lambda_j>0}\lambda_j^{2q}\langle\phi,\phi_j\rangle\phi_j$ if $q<0$.*

According to a classical result by Seeley [138] (see also §3.7), P^q is a classical pseudo-differential operator of order $2q$ for any $q \in \mathbb{R}$.

Corollary 3.2.5. *For any real number q, $\mathscr{A}_k(A,P) = \mathscr{A}_k(AP^q,P)$ holds for all non-negative integers k.*

Proof. Note AP^q is a classical pseudo-differential operator of order $m+2q$. Thus $\zeta(s,AP^q,P)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $s = d+m+2q-k$ ($k=0,1,2,\ldots$) with residues $\mathscr{A}_k(AP^q,P)$. But noting that $\zeta(s,AP^q,P) = \zeta(s-2q,A,P)$, we must have $\mathscr{A}_k(AP^q,P) = \mathscr{A}_k(A,P)$. This finishes the proof of the corollary. □

3.3 Heat trace expansions

Define a smooth function f over $(0,\infty)$ by

$$f(t) = \sum_{\lambda_j>0} \langle A\phi_j,\phi_j\rangle e^{-t\lambda_j^2} = \mathrm{tr}(Ae^{-tP}) - \sum_{\lambda_j=0} \langle A\phi_j,\phi_j\rangle \quad (t>0).$$

Obviously, $\Pi(\max\{\frac{d+m}{2},0\},\infty)$ is a basic strip of Mf which admits a meromorphic continuation to $\mathbb{C}$ with $(Mf)(s) = \zeta(2s,A,P)\Gamma(s)$. Recall $\zeta(\cdot,A,P)$ is meromorphic on $\mathbb{C}$ whose only singularities are simple poles at $s = d+m-k$ ($k=0,1,2,\ldots$) with residues $\mathscr{A}_k(A,P)$, while Γ is meromorphic on $\mathbb{C}$ whose only singularities are simple poles at $s=-k$ ($k=0,1,2,\ldots$) with residues $\frac{(-1)^k}{k!}$. Hence to establish (3.5) via Lemma 3.2.2 it suffices to prove

$$(Mf)(s) = O(|s|^{-2}) \quad (s\in\Pi(-n,n),\ |s|\to\infty) \tag{3.18}$$

for all positive integers n. To this end we first assume $s\in\Pi(-n,n)$ ($n\in\mathbb{N}$), then let $h\geq n+2$ be a large enough integer so that one can use (3.17) to get

$$(Mf)(s) = \zeta(2s,A,P)\Gamma(s) = \frac{(Mf_{2h})(s+h)}{\Gamma(s+h)}\Gamma(s) = (Mf_{2h})(s+h)\prod_{i=0}^{h-1}\frac{1}{s+i}.$$

Thus by considering $s+h\in\Pi(2,n+h)$, (3.18) follows immediately from suitably applying (3.16) to uniformly bound $(Mf_{2h})(s+h)$ above for all $s\in\Pi(-n,n)$ with $|s|\to\infty$. This finishes the proof of (3.5). The precise relation between the mollified counting coefficients and some of the heat coefficients as mentioned in the introductory part is recorded as the following proposition whose details are omitted.

Proposition 3.3.1. *If the order m of A is an integer, then*

- $\mathscr{B}_k(A,P) = \frac{\Gamma(\frac{d+m-k}{2})}{2}\cdot\mathscr{A}_k(A,P)$ *($d+m-k$ is positive or negative but odd);*
- $\mathscr{C}_k(A,P) = 0$ *($d+m+2k<0$);*
- $\mathscr{C}_k(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot\mathscr{A}_{d+m+2k}(A,P)$ *($d+m+2k\geq 0$).*

If the order m of A is not an integer, then for all non-negative integers k:

- $\mathscr{B}_k(A,P) = \frac{\Gamma(\frac{d+m-k}{2})}{2}\cdot\mathscr{A}_k(A,P)$;
- $\mathscr{C}_k(A,P) = 0$.

3.4 Resolvent expansions

In this part we study the short time asymptotic expansion of the resolvent trace $(f^{(N)}(t) \triangleq)$ $\mathrm{tr}(A(1+tP)^{-N/2})$, where $N \in \mathbb{C}$ is such that $\mathrm{Re}(N) > \max\{d+m, 0\}$. Let $M^{(N)}$ denote the Mellin transform of

$$\mathrm{tr}(A(1+tP)^{-N/2}) - \sum_{\lambda_j=0} \langle A\phi_j, \phi_j\rangle \quad (t>0).$$

It is easy to verify that $M^{(N)}$ has a non-empty basic strip $\Pi(\max\{\frac{d+m}{2}, 0\}, \frac{\mathrm{Re}(N)}{2})$ in which $M^{(N)}(s) = \zeta(2s, A, P)B(s, \frac{N}{2} - s)$, where we recall the Beta function

$$B(\alpha,\beta) = \int_0^1 (1-t)^{\alpha-1}t^{\beta-1}dt = \int_0^\infty \frac{u^{\alpha-1}}{(1+u)^{\alpha+\beta}}du = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$$

is defined for $\mathrm{Re}(\alpha) > 0$ and $\mathrm{Re}(\beta) > 0$. Hence $M^{(N)}$ admits a meromorphic continuation to $\Pi(-\infty, \frac{\mathrm{Re}(N)}{2})$ in which

$$M^{(N)}(s) = \zeta(2s, A, P)\frac{\Gamma(s)\Gamma(\frac{N}{2}-s)}{\Gamma(\frac{N}{2})}. \tag{3.19}$$

For any real β in the strip $\Pi(\max\{\frac{d+m}{2}, 0\}, \frac{\mathrm{Re}(N)}{2})$ and any positive integer n, it is easy to see that

$$\sup_{s\in\Pi(-n,\beta)} \left|\Gamma(\frac{N}{2}-s)\right| \leq \max_{\frac{\mathrm{Re}(N)}{2}-\beta\leq t\leq\frac{\mathrm{Re}(N)}{2}+n} \Gamma(t) < \infty.$$

Consequently by (3.18),

$$M^{(N)}(s) = O(|s|^{-2}) \quad (s\in\Pi(-n,\beta), |s|\to\infty), \tag{3.20}$$

which immediately implies

$$f^{(N)}(t) \sim \sum_{k=0}^{\infty} \left(\mathscr{B}_k^{(N)}(A,P)t^{\frac{k-d-m}{2}} + \mathscr{C}_k^{(N)}(A,P)t^k\log(t) + \mathscr{D}_k^{(N)}(A,P)t^k\right) \quad (t\to 0^+) \tag{3.21}$$

via Lemma 3.2.2 as the singularities of $\zeta(\cdot, A, P)$ and Γ are known to be completely determined. The precise relation between the mollified counting coefficients and some of the resolvent trace coefficients is summarized in the following proposition:

Proposition 3.4.1. *If the order m of A is an integer, then*

- $\mathscr{B}_k^{(N)}(A,P) = \frac{\Gamma(\frac{d+m-k}{2})}{2}\cdot\frac{\Gamma(\frac{N+k-d-m}{2})}{\Gamma(\frac{N}{2})}\cdot\mathscr{A}_k(A,P)$ *($d+m-k$ is positive or negative but odd);*
- $\mathscr{C}_k^{(N)}(A,P) = 0$ *($d+m+2k<0$);*
- $\mathscr{C}_k^{(N)}(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot\frac{\Gamma(\frac{N}{2}+k)}{\Gamma(\frac{N}{2})}\cdot\mathscr{A}_{d+m+2k}(A,P)$ *($d+m+2k\geq 0$).*

If the order m of A is not an integer, then for all non-negative integers k:

- $\mathscr{B}_k^{(N)}(A,P) = \frac{\Gamma(\frac{d+m-k}{2})}{2}\cdot\frac{\Gamma(\frac{N+k-d-m}{2})}{\Gamma(\frac{N}{2})}\cdot\mathscr{A}_k(A,P)$*;*
- $\mathscr{C}_k^{(N)}(A,P) = 0$.

3.5 Wodzicki residues

Proposition 3.5.1. $\mathscr{A}_k(A,P) = \operatorname{res}(AP^{\frac{k-d-m}{2}})$.

Proof. Since $AP^{\frac{k-d-m}{2}}$ is of integer order $k-d$ and $d+(k-d)+2\cdot 0 = k \geq 0$, it follows first from Proposition 3.3.1 then from Proposition 3.2.5 that

$$-2\mathscr{C}_0(AP^{\frac{k-d-m}{2}},P) = \mathscr{A}_k(AP^{\frac{k-d-m}{2}},P) = \mathscr{A}_k(A,P).$$

But according to (2.22) we also have

$$-2\mathscr{C}_0(AP^{\frac{k-d-m}{2}},P) = \operatorname{res}(AP^{\frac{k-d-m}{2}}).$$

Combining the above two formulae yields the desired result. □

Proposition 3.5.2. $\mathscr{C}_k(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot \operatorname{res}(AP^k)$.

Proof. If A is of integer order $m \geq -d-2k$, then it follows first from Proposition 3.3.1 then from Proposition 3.5.1 that

$$\mathscr{C}_k(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot \mathscr{A}_{d+m+2k}(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot \operatorname{res}(AP^k).$$

If A is not of integer order or A is of integer order $m < -d-2k$, then it follows from definition that $\operatorname{res}(AP^k) = 0$ and from Proposition 3.3.1 that $\mathscr{C}_k(A,P) = 0$. This finishes the proof. □

We should remark that both propositions are known results. Proposition 3.5.1 can be found in [91, Prop. 4.2] and [137, P. 106]. Proposition 3.5.2 can be found in [53, Thm. 5.2].

Corollary 3.5.3. $\mathscr{C}_k^{(N)}(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot \frac{\Gamma(\frac{N}{2}+k)}{\Gamma(\frac{N}{2})}\cdot \operatorname{res}(AP^k)$.

Proof. If A is of integer order $m \geq -d-2k$, then it follows first from Proposition 3.4.1 then from Proposition 3.5.1 that

$$\mathscr{C}_k(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot \frac{\Gamma(\frac{N}{2}+k)}{\Gamma(\frac{N}{2})}\cdot \mathscr{A}_{d+m+2k}(A,P) = \frac{(-1)^{k+1}}{2\cdot k!}\cdot \frac{\Gamma(\frac{N}{2}+k)}{\Gamma(\frac{N}{2})}\cdot \operatorname{res}(AP^k).$$

If A is not of integer order or A is of integer order $m < -d-2k$, then it follows from definition that $\operatorname{res}(AP^k) = 0$ and from Proposition 3.4.1 that $\mathscr{C}_k(A,P) = 0$. This finishes the proof. □

Next we study the property $\mathscr{A}_k(A,P) = 0$ for certain operators $A \in \Psi(M;E)$. We denote by $\Psi^{\mathbb{Z}}_{\text{odd}}(M;E)$ the space of odd-class pseudo-differential operators and by $\Psi^{\mathbb{Z}}_{\text{even}}(M;E)$ the space of even-class pseudo-differential operators on sections of E, that is, $A \in \Psi^{\mathbb{Z}}_{\text{odd}}(M;E)$ if in local coordinates its symbol $\sum_{j\geq 0}\sigma_{m-j}(A)$ $(m\in\mathbb{Z})$ satisfies

$$\sigma_{m-j}(A)(x,-\xi) = (-1)^{m-j}\sigma_{m-j}(A)(x,\xi) \tag{3.22}$$

for all x,ξ and j, while $A \in \Psi^{\mathbb{Z}}_{\text{even}}(M;E)$ if in local coordinates

$$\sigma_{m-j}(A)(x,-\xi) = (-1)^{m-j+1}\sigma_{m-j}(A)(x,\xi) \tag{3.23}$$

for all x,ξ and j. For example, any partial differential operator is odd-class while $\sqrt{P}$ is even-class. An operator $A \in \Psi^{\mathbb{Z}}_{\text{odd}}(M;E)\cup\Psi^{\mathbb{Z}}_{\text{even}}(M;E)$ is said to be of regular parity class if its parity class agrees with that of d. It is easy to verify that $\operatorname{res}(A) = 0$ if A is of regular parity class.

Proposition 3.5.4. *Let $A \in \Psi^{\mathbb{Z}}_{\mathrm{odd}}(M;E) \cup \Psi^{\mathbb{Z}}_{\mathrm{even}}(M;E)$. If the parity class of A agrees with that of $k-m$, then $\mathscr{A}_k(A,P)=0$.*

Proof. We define a map τ by sending odd-class pseudo-differential operators to 0 and even-class ones to 1. Then (see [121, Prop. 1.11]) $\tau(AP^{\frac{k-d-m}{2}}) = \tau(A)+k-d-m \pmod 2$. Thus if the parity class of A agrees with that of $k-m$, or equivalently, the parity class of $\tau(AP^{\frac{k-d-m}{2}})$ does not agree with that of d, or further equivalently, the parity class of $AP^{\frac{k-d-m}{2}}$ agrees with that of d, then $AP^{\frac{k-d-m}{2}}$ is of regular parity class and, consequently by Proposition 3.5.1, $\mathscr{A}_k(A,P)=\mathrm{res}(AP^{\frac{k-d-m}{2}})=0$. □

Moreover, we explain how to calculate the local full symbol of AP^q for an arbitrary $q \in \mathbb{R}$. According to the product rule (2.12) for pseudo-differential operators, it suffices to do so for P^q. In the event that q is a non-negative integer, it is straightforward to apply (2.12). In the event that q is a negative integer, we apply (2.12) to $P^qP^{-q} \sim \mathrm{Id}_E$ to deduce the local full symbol of P^q. In the event that q is a half-integer, we apply (2.12) to $P^qP^q \sim P^{2q}$ to deduce the local full symbol of P^q by appealing to the fact that P^q is of scalar principal symbol. In the event that q is of the form $\frac{l}{2^n}$ for some $l \in \mathbb{Z}$ and $n \in \mathbb{N}$, we can do a similar job for P^q. Finally, we use the property ([138]) that the local full symbol of P^q at each fixed (x,ξ) is a continuous function of $q \in \mathbb{R}$ to reach the full generality.

We end this section with a remark. The heat expansion (3.5) can be written in a more rigorous way as

$$\mathrm{tr}(Ae^{-tP}) \sim \sum_{j\in\Lambda} \widetilde{\mathscr{B}}_j(A,P)t^{\frac{j-d-m}{2}} + \sum_{k=0}^{\infty}\big(\widetilde{\mathscr{C}}_k(A,P)t^k\log(t) + \widetilde{\mathscr{D}}_k(A,P)t^k\big), \tag{3.24}$$

where Λ means the set of non-negative integers j such that $\frac{j-d-m}{2}$ is not a non-negative integer. In this notation system $\widetilde{\mathscr{B}}_j(A,P)$, $\widetilde{\mathscr{C}}_k(A,P)$ and $\widetilde{\mathscr{D}}_k(A,P)$ are uniquely determined. According to Propositions 3.3.1, 3.5.1 and 3.5.2, $\widetilde{\mathscr{B}}_j(A,P)$ and $\widetilde{\mathscr{C}}_k(A,P)$ are certain Wodzicki residues. In most situations, $\widetilde{\mathscr{D}}_k(A,P)$ are not Wodzicki residues but operator traces. For the simplest example that A is smoothing operator, one can (regard A as of any real order and thus) deduce from (3.24) that

$$\mathrm{tr}(Ae^{-tP}) \sim \sum_{k=0}^{\infty} \widetilde{\mathscr{D}}_k(A,P)t^k.$$

In this situation it is so natural to expect $\mathrm{tr}(A)=\widetilde{\mathscr{D}}_0(A,P)$. Actually, if any of the following three cases happens, then $\widetilde{\mathscr{D}}_0(A,P)$ just is the Kontsevich-Vishik trace of A which is independent of the choice of P (e.g. [66, 91, 104]):

- $m<-d$;
- m is not an integer;
- A is of regular parity class.

Since the Kontsevich-Vishik trace agrees with the standard L^2-operator trace on trace class operators, the previous expectation is confirmed. Furthermore, if $A=Q$ is a partial differential operator and if d is even, then one can express $\widetilde{\mathscr{D}}_0(A,P)$ as the Wodzicki residue of a certain pseudo-differential operator with log-polyhomogeneous symbol (see [111, 117, 136] for details).

3.6 Heat kernel expansions

Let $Q : C^\infty(M;E) \to C^\infty(M;E)$ be a partial differential operator of order m. It is well known (e.g. [46, 56, 138]) that Qe^{-tP} is a smoothing operator with smooth kernel $K(t,x,y,Q,P)$ in the sense of

$$(Qe^{-tP}\phi)(x) = \int_M K(t,x,y,Q,P)\phi(y)d\mu_g(y), \tag{3.25}$$

where $K(t,x,y,Q,P)$ maps E_y to E_x, and the diagonal values of K admit a uniform small-time asymptotic expansion

$$K(t,x,x,Q,P) \sim \sum_{k=0}^{\infty} t^{\frac{k-d-m}{2}} \mathscr{H}_k(Q,P)(x) \quad (t \to 0^+), \tag{3.26}$$

where $\mathscr{H}_k(Q,P) \in C^\infty(M;\mathrm{End}(E))$ vanishes if $k+m$ is odd. How to express $\mathscr{H}_k(\mathrm{Id}_E,P)$, say for example $k \leq 10$, is a well-studied topic in the theory of heat trace expansions [57, 58]. In the following we explain how to extract $\mathscr{H}_k(Q,P)$ from the viewpoint of Wodzicki's residue. To the best of the author's knowledge, it seems that no explicit formula for $\mathscr{H}_k(D,D^2)$ with k odd is stated in the literature. Here D is a self-adjoint Dirac type operator on smooth sections of E.

It follows from (3.26) that

$$\mathrm{tr}(Qe^{-tP}) \sim \sum_{k=0}^{\infty} t^{\frac{k-d-m}{2}} \int_M \mathrm{Tr}_E(\mathscr{H}_k(Q,P))d\mu_g \quad (t \to 0^+),$$

which comparing with (3.5) and appealing to Propositions 3.3.1, 3.5.1 yields

$$\int_M \mathrm{Tr}_E(\mathscr{H}_k(Q,P))d\mu_g = \frac{\Gamma(\frac{d+m-k}{2})}{2} \cdot \mathrm{res}(QP^{\frac{k-d-m}{2}})$$

for any k such that $\frac{k-d-m}{2}$ is not a non-negative integer. Let F denote a smooth endomorphism of E. Obviously, $\mathscr{H}_k(FQ,P) = F\mathscr{H}_k(Q,P)$ for any $k \geq 0$. So we can get

$$\int_M \mathrm{Tr}_E(F\mathscr{H}_k(Q,P))d\mu_g = \frac{\Gamma(\frac{d+m-k}{2})}{2} \cdot \mathrm{res}(FQP^{\frac{k-d-m}{2}}) \tag{3.27}$$

for any k such that $\frac{k-d-m}{2}$ is not a non-negative integer. Note

$$\begin{aligned}\mathrm{res}_x(FQP^{\frac{k-d-m}{2}})dx &= \Big(\frac{1}{(2\pi)^d}\int_{|\xi|=1} \mathrm{Tr}(\sigma_{-d}(FQP^{\frac{k-d-m}{2}})(x,\xi))dS(\xi)\Big)dx \\ &= \Big(\mathrm{Tr}\Big[F\Big(\frac{1}{(2\pi)^d}\int_{|\xi|=1} \sigma_{-d}(QP^{\frac{k-d-m}{2}})(x,\xi)dS(\xi)\Big)\Big]\Big)dx.\end{aligned} \tag{3.28}$$

Comparing (3.27) with (3.28) yields the following

Theorem 3.6.1. *Fix a local coordinate system around $x_0 \in M$ such that the tangent vectors at x_0 form an orthonormal basis for $(T_{x_0}M, g_{x_0})$. Suppose $\frac{k-d-m}{2}$ is not a non-negative integer. Then*

$$\mathscr{H}_k(Q,P)(x_0) = \frac{\Gamma(\frac{d+m-k}{2})}{2\cdot(2\pi)^d} \cdot \int_{|\xi|=1} \sigma_{-d}(QP^{\frac{k-d-m}{2}})(x_0,\xi)dS(\xi).$$

As an immediate consequence, all of the endomorphisms $\{\mathscr{H}_k(Q,P)\}_{k=0}^\infty$ can be determined by the above method if the dimension of M is odd. The reason is that if $\frac{k-d-m}{2}$ is a non-negative integer, then $k+m$ is odd and thus $\mathscr{H}_k(Q,P) = 0$.

3.7 Seeley's method

Let $k \geq 0$ be a fixed integer. By Corollary 3.2.5, $\mathscr{A}_k(A,P) = \mathscr{A}_k(AP^q,P)$ for any positive integer q. Thus to study $\mathscr{A}_k(A,P)$ one can assume the order m of A is bigger than $k-d$, otherwise we study $\mathscr{A}_k(AP^q,P)$ for some large enough integer q. Actually, as q is a non-negative integer, the local full symbol of AP^q is easily to be determined by those of A and P. So from now on we assume $m > k-d$ or equivalently $k < d+m$. Our analysis below will be purely formal since the questions of convergence have already been dealt with by Seeley in [138].

Let P_0 denote the orthogonal projection onto the finite-dimensional null space of the non-negative self-adjoint Laplacian P. Note the meromorphic continuation of

$$\mathrm{tr}(A(P+P_0)^{-s/2}) \quad (\mathrm{Re}(s) > d+m > k \geq 0)$$

to $\mathbb{C}$ denoted by $Z(s)$ differs from the spectral zeta function $\zeta(s,A,P)$ only by a constant-valued function. Thus $Z(s)$ also has a simple pole at $s = d+m-k$ with the same residue $\mathscr{A}_k(A,P)$. For simplicity we denote $P+P_0$ by P, which is a positive self-adjoint classical pseudo-differential operator of second order.

Let $\varrho = \varrho(R)$ be the contour in the complex plane obtained by joining two lines parallel to the negative real axis by a counter-clockwise half circle around the origin whose radius R is less than the least eigenvalue of P. It is well known [139] that

$$P^{-s} = \frac{1}{2\pi i}\int_{\varrho} \lambda^{-s}(P-\lambda)^{-1}d\lambda \quad (\mathrm{Re}(s) > 0). \tag{3.29}$$

Seeley ([138]) showed that P^{-s} $(\mathrm{Re}(s) > 0)$ are classical pseudo-differential operators of order $-2s$ whose full symbols can be determined as follows:

For any $x_0 \in M$, let $x = (x^1,\ldots,x^d)$ be a system of local coordinates centered at x_0, and let $e = (e_1,\ldots,e_r)$ be a local frame for E near x_0. Using this local system, the full symbol of P is easily seen to be asymptotically equivalent to

$$\begin{aligned}\sigma_P^{Full}(x,\xi) &\sim g^{ij}(x)\xi_i\xi_j + \mathrm{i}a^k(x)\xi_k + b(x) \\ &\triangleq p_0(x,\xi) + p_1(x,\xi) + p_2(x,\xi),\end{aligned} \tag{3.30}$$

where we remind that P actually denotes $P+P_0$ with the original P locally being of the form (3.1). Seeley's idea is to first regard $(P-\lambda)^{-1}$ as a λ-dependent pseudo-differential operator with its full symbol being asymptotically equivalent to some $\sum_{n=0}^{\infty} b_n(x,\xi;\lambda)$, then study (3.29) via $\sum_{n=0}^{\infty} b_n$ to approximate the full symbols of P^{-s}. Following this plan, one can first recursively define for $|\xi| \geq 1$ and $\lambda \in \varrho(R)$ with R being sufficiently small that

$$b_0(x,\xi;\lambda) = (g^{ij}(x)\xi_i\xi_j - \lambda)^{-1}, \tag{3.31}$$

$$b_n(x,\xi;\lambda) = (-b_0)\cdot\Big(\sum_{\substack{i<n \\ i+j+|\alpha|=n}} \frac{(\partial_\xi^\alpha b_i)(D_x^\alpha p_j)}{\alpha!}\Big) \quad (n \geq 1), \tag{3.32}$$

then introduce a sequence of pseudo-differential operators with corresponding full symbols

$$e_n(x,\xi;s) = \frac{1}{2\pi i}\int_{\varrho} \lambda^{-s} b_n(x,\xi;\lambda)d\lambda \quad (n \geq 0) \tag{3.33}$$

of homogeneous degrees $-2s-n$. Actually, for all $|\xi|\geq 1$ and $t\geq 1$, one can deduce from the simple fact $b_n(x,t\xi;t^2\tau)=t^{-2-n}b_n(x,\xi;\tau)$ ($\tau\in\varrho(\frac{R}{t^2})$) that

$$\begin{aligned}e_n(x,t\xi;s)&=\frac{1}{2\pi i}\int_{\varrho}\lambda^{-s}b_n(x,t\xi;\lambda)d\lambda\\&=\frac{1}{2\pi i}\int_{\varrho(\frac{R}{t^2})}(t^2\tau)^{-s}b_n(x,t\xi;t^2\tau)d(t^2\tau)\\&=t^{-2s-n}e_n(x,\xi;s),\end{aligned}$$

where we recall $\varrho(\frac{R}{t^2})$ denotes the $\frac{1}{t^2}$–contraction of ϱ. It was shown in [138] by Seeley that P^{-s} $(\mathrm{Re}(s)>0)$ are classical pseudo-differential operators of order $-2s$ whose full symbols are asymptotically equivalent to $\sum_{n=0}^{\infty}e_n(x,\xi;s)$.

Recall that A is a classical pseudo-differential operator or order $m>k-d$. Thus $AP^{-s/2}$ $(\mathrm{Re}(s)>0)$ are classical pseudo-differential operators of order $m-s$ whose full symbols are asymptotically equivalent to

$$\sum_{\alpha}\sum_{j}\sum_{n}\frac{1}{\alpha!}\cdot(\partial_{\xi}^{\alpha}\sigma_A^{(j)})(x,\xi)\cdot(D_x^{\alpha}e_n)(x,\xi;\frac{s}{2})=\sum_{q=0}^{\infty}\mathbf{I}_q(x,\xi;s),\tag{3.34}$$

where the full symbol of A is asymptotically equivalent to a sum of homogeneous symbols $\sigma_A^{(j)}$ $(j=0,1,2,\ldots)$ of degrees $m-j$, and

$$\mathbf{I}_q(x,\xi;s)\triangleq\sum_{|\alpha|+j+n=q}\frac{1}{\alpha!}\cdot(\partial_{\xi}^{\alpha}\sigma_A^{(j)})(x,\xi)\cdot(D_x^{\alpha}e_n)(x,\xi;\frac{s}{2})$$

are homogeneous symbols of degrees $m-s-q$. For each non-negative integer q, the meromorphic continuation of

$$\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\mathrm{Tr}(\mathbf{I}_q(x,\xi;s))d\xi$$

to the right half plane $\Pi(0,\infty)$ differs from the following meromorphic function

$$\frac{1}{(2\pi)^d}\int_{\mathbb{S}^{d-1}}\mathrm{Tr}(\mathbf{I}_q(x,\omega;s))d\omega\cdot\frac{1}{s-(d+m-q)}\tag{3.35}$$

by an analytic function. On the other hand, if $\mathrm{Re}(s)>d+m$, then $AP^{-s/2}$ is trace class whose trace satisfies

$$Z(s)=\int_M\mathrm{Tr}_{E_x}(K(x,x;s))d\mu_g(x)\quad(\mathrm{Re}(s)>d+m),\tag{3.36}$$

where we denote by $K(x,y;s)$ the continuous Schwartz kernel of $AP^{-s/2}$, that is,

$$(AP^{-s/2}u)(x)=\int_M K(x,y;s)u(y)d\mu_g(y),$$

where $K(x,y;s)$ maps E_y to E_x. Thus to study the meromorphic continuation of $Z(s)$, it suffices to study that of $\mathrm{Tr}_{E_x}(K(x,x;s))$ at each fixed $x\in M$. By considering (3.34), (3.35) as well as the metric measure μ_g in (3.36), it is easy to modify the argument in [138] to determine $\mathscr{A}_k(A,P)$ $(k<d+m)$ as follows (the details of the proof are left to the interested reader):

Proposition 3.7.1. *Suppose $k < d + m$. Then*

$$\mathscr{A}_k(A, P) = \int_M \mathscr{A}_k(A, P)(x) d\mu_g(x),$$

where in a local coordinate system $(x^1, \ldots, x^d)$ centered at any prescribed $x_0 \in M$ with $\det(g_{ij}(x_0)) = 1$,

$$\mathscr{A}_k(A, P)(x_0) = \sum_{|\alpha|+j+n=k} \frac{1}{(2\pi)^d \alpha!} \int_{\mathbb{S}^{d-1}} \mathrm{Tr}((\partial_\xi^\alpha \sigma_A^{(j)})(x_0, \omega)(D_x^\alpha e_n)(x_0, \omega; \frac{d+m-k}{2})).$$

Finally, we collect a few formulae for $e_n(x, \xi; s)$ for later use. Suppose $\mathrm{Re}(s) > 0$, $|\xi| \geq 1$, and $\lambda \in \varrho(R)$ with R being sufficiently small. Denote $\|\xi\| = (g^{ij}(x)\xi_i\xi_j)^{1/2}$ for simplicity. First, it is easy to verify that (we repeat b_0 here for completeness)

$$b_0(x, \xi, \lambda) = (\|\xi\|^2 - \lambda)^{-1}, \tag{3.37}$$

$$b_1(x, \xi, \lambda) = \frac{-\mathrm{i}a^k(x)\xi_k}{(\|\xi\|^2 - \lambda)^2} + \frac{2g^{kn}(x)\xi_n(D_{x_k}g^{ij})(x)\xi_i\xi_j}{(\|\xi\|^2 - \lambda)^3}. \tag{3.38}$$

By considering $\mathrm{Re}(s) > 0$, it is easy to use Cauchy's integral theorem to show

$$e_n(x, \xi; s) = \frac{1}{2\pi i} \int_{\varrho(x,\xi)} \lambda^{-s} b_n(x, \xi; \lambda) d\lambda \quad (n \geq 0), \tag{3.39}$$

where $\varrho(x, \xi)$ denotes any clockwise circle centered at $\|\xi\|^2$ in the right half plane $\Pi(0, \infty)$. Substituting (3.37) and (3.38) respectively into (3.39) yields for $|\xi| \geq 1$ that

$$e_0(x, \xi; s) = \|\xi\|^{-2s}, \tag{3.40}$$

$$\begin{aligned} e_1(x, \xi; s) =& (-\mathrm{i}a^k(x)\xi_k) \cdot s \cdot \|\xi\|^{-2s-2} + \\ & (g^{kn}(x)\xi_n(D_{x_k}g^{ij})(x)\xi_i\xi_j) \cdot s(s+1) \cdot \|\xi\|^{-2s-4}. \end{aligned} \tag{3.41}$$

If we assume the local coordinate system centered at a fixed point $x_0 \in M$ is a Riemannian normal one, then the above formulae at x_0 can be greatly simplified. For example, for $|\xi| \geq 1$ one easily has

$$e_0(x_0, \xi; s) = |\xi|^{-2s}, \tag{3.42}$$

$$(D_{x_j} e_0)(x_0, \xi; s) = 0 \quad (j = 1, 2, \ldots, d), \tag{3.43}$$

$$e_1(x_0, \xi; s) = (-\mathrm{i}a^k(x)\xi_k) \cdot s \cdot |\xi|^{-2s-2}. \tag{3.44}$$

As an application, it follows from (3.42) and Proposition 3.7.1 that if $m > -d$ then

$$\mathscr{A}_0(A, P) = \frac{1}{(2\pi)^d} \int_{T_1^*M} \mathrm{Tr}(\sigma_A), \tag{3.45}$$

where we recall that T_1^*M denotes the unit cotangent bundle of M, σ_A denotes the principal symbol of A. By considering the fact $\mathscr{A}_0(A, P) = \mathscr{A}_0(AP^q, P)$ for any non-negative integer q, one can drop the assumption $m > -d$ in (3.45) to get (3.7).

There exist other methods to determine the coefficients $\mathscr{A}_k(A, P)$ except Propositions 3.5.1 and 3.7.1. For example, one can follow the analysis in §3.1 more carefully (see also [40]) or adapt the heat trace argument in [54] to do so.

3.8 Leading coefficients

In this section, we provide a formula for $\mathscr{A}_1(A,P)$ in terms of the principal and sub-principal symbols of both A and P. This brings a clear geometric interpretation of $\mathscr{A}_1(A,P)$, and could help characterize a certain class of operators for which the second coefficient vanishes. A key ingredient (e.g. [45, 144]) is that, if f is a smooth homogeneous function of degree $1-d$ on $\mathbb{R}^d\backslash\{0\}$, then $\int_{|\xi|=1}\frac{\partial f}{\partial \xi_k}dS(\xi)=0$ for each k. For example, if $T: C^\infty(M;E)\to C^\infty(M;E)$ is a classical pseudo-differential operator of order $1-d$, then it is easy to see that

$$\int_{|\xi|=1}\mathrm{Tr}(\sigma_T^{(1)}(x,\xi))dS(\xi)=\int_{|\xi|=1}\mathrm{Tr}(\mathrm{Sub}(T)(x,\xi))dS(\xi).$$

Consequently, the global density $\mathrm{res}_x(T)dx$ is of the form

$$\Big(\frac{1}{(2\pi)^d}\int_{|\xi|=1}\mathrm{Tr}(\mathrm{Sub}(T)(x,\xi))dS(\xi)\Big)dx,$$

which is independent of the choice of local coordinates of M and local frames for E. Thus if T is a classical pseudo-differential operator of order $1-d$, then

$$\mathrm{res}(T)=\frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}(\mathrm{Sub}(T)), \tag{3.46}$$

which is simply short for

$$\int_M\Big(\frac{1}{(2\pi)^d}\int_{|\xi|=1}\mathrm{Tr}(\mathrm{Sub}(T)(x,\xi))dS(\xi)\Big)dx.$$

Lemma 3.8.1. *Let T_1,T_2 be classical pseudo-differential operators on smooth sections of E such that the sum of the order of T_1 and T_2 is $1-d$. Then*

$$\mathrm{res}(T_1T_2)=\frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}(\mathrm{Sub}(T_1)\cdot\sigma_{T_2}^{(0)}+\sigma_{T_1}^{(0)}\cdot\mathrm{Sub}(T_2)).$$

Proof. Since $\mathrm{res}(T_1T_2)=\mathrm{res}(T_2T_1)$, it thus follows from (3.46) that

$$\mathrm{res}(T_1T_2)=\frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}\big(\frac{\mathrm{Sub}(T_1T_2)+\mathrm{Sub}(T_2T_1)}{2}\big),$$

which proves the lemma from (2.19) as $\mathrm{Tr}(\{\sigma_{T_1}^{(0)},\sigma_{T_2}^{(0)}\}+\{\sigma_{T_2}^{(0)},\sigma_{T_1}^{(0)}\})=0$. We are done. □

According to Proposition 3.5.1 and Lemma 3.8.1, one gets

$$\mathscr{A}_1(A,P)=\frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}\big(\mathrm{Sub}(A)\cdot\sigma^{(0)}_{P^{\frac{1-d-m}{2}}}+\sigma_A^{(0)}\cdot\mathrm{Sub}(P^{\frac{1-d-m}{2}})\big). \tag{3.47}$$

According to (2.20), we have

$$\mathrm{Sub}(P^q)=q\cdot(\sigma_P^{(0)})^{q-1}\cdot\mathrm{Sub}(P) \tag{3.48}$$

for any $q\in\mathbb{R}$. Therefore, by combining (3.47) – (3.48) and by considering $\sigma_{P^q}^{(0)}=(\sigma_P^{(0)})^q$, we get

Theorem 3.8.2.

$$\mathscr{A}_1(A,P)=\frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}\big(\mathrm{Sub}(A)+\frac{1-d-m}{2}\cdot\sigma_A^{(0)}\cdot\mathrm{Sub}(P)\big).$$

Chapter 4

Dirac type operators

We follow all of the assumptions and notations about M (closed smooth Riemannian manifold of dimension d and metric g), E (hermitian vector bundle over M), A (classical pseudo-differential operator of order m), P (self-adjoint non-negative Laplacian with spectral resolution $\{\phi_j, \lambda_j^2\}_{j=1}^{\infty}$), χ ($\mathscr{F}\chi$ is of sufficiently small support and equals one near the origin), and Q (partial differential operator of order m) used in the previous chapter.

In this chapter we will focus on $P = D^2$, where D is a self-adjoint Dirac type operator acting on smooth sections of E. There exists a discrete spectral resolution $\{\phi_j, \mu_j\}_{j=1}^{\infty}$ of D, where $\{\phi_j\}_{j=1}^{\infty}$ is an orthonormal basis for $L^2(M;E)$, and $D\phi_j = \mu_j\phi_j$ for each j. Obviously, ϕ_j will be eigensections of $P = D^2$ with eigenvalues μ_j^2. Therefore, using the notation from before $\lambda_j = |\mu_j|$. The microlocalized spectral counting function $N_A(\mu)$ of D is defined as

$$N_A(\mu) = \begin{cases} \sum_{0\le\mu_j<\mu}\langle A\phi_j, \phi_j\rangle & \text{if } \mu > 0, \\ \sum_{\mu\le\mu_j<0}\langle A\phi_j, \phi_j\rangle & \text{if } \mu \le 0. \end{cases}$$

Thus, $N_A(\mu)$ is a piecewise constant function on $\mathbb{R}$ such that

$$N_A'(\mu) = \sum_{j=1}^{\infty}\langle A\phi_j, \phi_j\rangle\delta_{\mu_j},$$

where δ_{μ_j} denotes the delta function on $\mathbb{R}$ centered at μ_j. Similar to (3.3) in the previous chapter, one can show that

$$(\chi * N_A')(\mu) = \sum_{j=1}^{\infty}\langle A\phi_j, \phi_j\rangle\chi(\mu-\mu_j) \sim \sum_{k=0}^{\infty}\mathscr{A}_k(A,D)\mu^{d+m-k-1} \quad (\mu\to\infty). \tag{4.1}$$

The corresponding expansion for $\mu \to -\infty$ can be easily obtained by replacing D with $-D$:

$$(\chi * N_A')(\mu) \sim \sum_{k=0}^{\infty}\mathscr{A}_k(A,-D)|\mu|^{d+m-k-1} \quad (\mu\to-\infty). \tag{4.2}$$

Therefore, the function $\chi * N_A'$ contains all information about $\{\mathscr{A}_k(A,\pm D)\}_{k=0}^{\infty}$.

Recall that D can always be written as $D = \gamma\nabla + \psi$, where (E,γ,∇) is some Dirac bundle with its Clifford module structure γ uniquely determined by the principal symbol of D, ψ is the potential of D associated with the Dirac bundle (E,γ,∇). In case $\psi = 0$ then P is called the generalized Dirac operator associated with the Dirac bundle (E,γ,∇).

The first purpose of this chapter is to explicitly determine $\mathscr{A}_k(A, D)$. In particular, for any bundle endomorphism F of E, we can express $\mathscr{A}_1(F, D)$ in terms of geometric quantities such as $g, \gamma, \nabla, \psi, F$. To compare, Sandoval [133] obtained an explicit expression of $\mathscr{A}_1(\mathrm{Id}_E, D)$, while Branson and Gilkey [22] can also do so for $\mathscr{A}_1(F, D)$ whenever F is of the form $f\mathrm{Id}_E$, where f is a smooth function on M. In the case of more general first order systems with $F = \mathrm{Id}_E$ a formula was also recently obtained by Chervova, Downes and Vassiliev [30].

The second purpose of this chapter is to show that $\mathscr{H}_1(D, D^2) = 0$ (see §3.6) if and only if D is a generalized Dirac operator. Here D can mean any Dirac type operator on smooth sections of E without the self-adjointness assumption. In the case of dimension three and rank two, a spectral theoretic characterization of the so-called massless Dirac operator was recently obtained by Chervova, Downes and Vassiliev [31].

4.1 Spectral counting coefficients

We first give a proof of (4.1). To this end we introduce a classical pseudo-differential operator B of order m by defining

$$B = A\frac{\mathrm{Sign}(D) + \mathrm{Id}_E}{2}.$$

Since $\mathrm{supp}(N'_A - N'_B) \subset (-\infty, 0]$, we get (see also the proof of (3.13))

$$(\chi * N'_A)(\mu) - (\chi * N'_B)(\mu) = o(\mu^{-\infty}) \quad (\mu \to \infty).$$

By appealing to (3.3) with A, P, λ, λ_j replaced respectively by $B, D^2, \mu, |\mu_j|$, we obtain as $\mu \to \infty$ that

$$\begin{aligned}(\chi * N'_B)(\mu) &= \sum_{j=1}^{\infty} \langle B\phi_j, \phi_j\rangle \chi(\mu - \mu_j) \\ &= \sum_{j=1}^{\infty} \langle B\phi_j, \phi_j\rangle \chi(\mu - |\mu_j|) \\ &\sim \sum_{k=0}^{\infty} \mathscr{A}_k(B, D^2)\mu^{d+m-k-1},\end{aligned}$$

which proves (4.1) as well as

$$\mathscr{A}_k(A, D) = \mathscr{A}_k(A\frac{\mathrm{Sign}(D) + \mathrm{Id}_E}{2}, D^2) \tag{4.3}$$

for all non-negative integers k.

Theorem 4.1.1. $\mathscr{A}_k(A, D) = \mathrm{res}(A\frac{|D|+D}{2}|D|^{k-d-m-1})$.

Here $|D|^{k-d-m-1}$ is understood as $P^{\frac{k-d-m-1}{2}}$ with $P = D^2$ (see Defn. 3.2.4). To give a proof of Theorem 4.1.1, it suffices to deduce from (4.3) and Proposition 3.5.1 that

$$\mathscr{A}_k(A, D) = \mathrm{res}(A\frac{\mathrm{Sign}(D) + \mathrm{Id}_E}{2}|D|^{k-d-m}) = \mathrm{res}(A\frac{D + |D|}{2}|D|^{k-d-m-1}).$$

As an immediate consequence, we get

Corollary 4.1.2. $\mathscr{A}_k(A, -D) = \mathrm{res}(A\frac{|D|-D}{2}|D|^{k-d-m-1})$.

Suppose D is of the form $\gamma\nabla + \psi$ for some Dirac bundle (E, γ, ∇). Define $\widehat{\psi} = \gamma(e_i)\psi\gamma(e_i)$, where $\{e_i\}_{i=1}^d$ is an arbitrary local orthonormal frame in T^*M. Obviously, $\widehat{\psi} \in C^\infty(M; \mathrm{End}(E))$ is independent of the choice of local orthonormal frames.

Theorem 4.1.3. *Let D be a self-adjoint Dirac type operator of potential ψ associated with the Dirac bundle (E, γ, ∇) and let F be a smooth bundle endomorphism of E. Then*

$$\mathscr{A}_1(F, D) = \frac{1}{(4\pi)^{d/2} \cdot \Gamma(\frac{d}{2})} \int_M \mathrm{Tr}\Big(F \cdot \frac{\widehat{\psi} - (d-2)\psi}{2}\Big). \tag{4.4}$$

Proof. It follows from Theorem 3.8.2 that $\mathscr{A}_1(F, D^2) = 0$. So according to (4.3) and Corollary 3.2.5, we get $\mathscr{A}_1(F, D) = \frac{\mathscr{A}_1(FD, D^2)}{2}$. By Proposition 3.5.1, we also have

$$\mathscr{A}_1(FD, D^2) = \mathrm{res}(FD|D|^{-d}) = \mathrm{res}(F|D|^{-d}D) = \mathrm{res}(DF|D|^{-d}) = \mathscr{A}_1(DF, D^2).$$

Consequently,

$$\mathscr{A}_1(F, D) = \frac{\mathscr{A}_1(FD, D^2) + \mathscr{A}_1(DF, D^2)}{4},$$

and by Theorem 3.8.2 we get

$$\mathscr{A}_1(F, D) = \frac{1}{(2\pi)^d} \int_{T_1^*M} \mathrm{Tr}\Big(F \cdot \Big[\frac{\mathrm{Sub}(D)}{2} - \frac{d}{2} \cdot \frac{\sigma_D^{(0)} \cdot \mathrm{Sub}(D^2) + \mathrm{Sub}(D^2) \cdot \sigma_D^{(0)}}{4}\Big]\Big). \tag{4.5}$$

In local coordinates around a fixed point $x_0 \in M$, we assume $\nabla_{\partial_j} = \partial_j + b_j$, where b_j are smooth matrix-valued functions. Then $\sigma_D^{(0)}(x_0, \xi) = \mathrm{i}\gamma^j(x_0)\xi_j$, $\sigma_D^{(1)}(x_0, \xi) = \gamma^j(x_0)b_j(x_0) + \psi(x_0)$. The compatibility condition (2.2) implies $\frac{\partial \gamma^k}{\partial x^j} = [\gamma^k, b_j] - \Gamma_{jn}^k \gamma^n$, where Γ_{jn}^k are the standard Christoffel symbols. We further assume the local coordinate system is a Riemannian normal one centered at x_0. This implies $\big(\frac{\partial \gamma^k}{\partial x^j}\big)(x_0) = [\gamma^k(x_0), b_j(x_0)]$, and, consequently, by the definition of the sub-principal symbol of D we get

$$\mathrm{Sub}(D)(x_0, \xi) = \gamma^j(x_0)b_j(x_0) + \psi(x_0) - \frac{1}{2}\big(\frac{\partial \gamma^k}{\partial x^k}\big)(x_0) = \big(\frac{\gamma^j b_j + b_j \gamma^j}{2} + \psi\big)(x_0).$$

Similarly, one can show that $\sigma_{D^2}^{(0)}(x_0, \xi) = |\xi|^2$, $\sigma_{D^2}^{(1)}(x_0, \xi) = \mathrm{i}(\gamma^k\psi + \psi\gamma^k - 2b_k)(x_0)\xi_k$, and

$$\mathrm{Sub}(D^2)(x_0, \xi) = \mathrm{i}(\gamma^k\psi + \psi\gamma^k - 2b_k)(x_0)\xi_k.$$

Consequently,

$$(\sigma_D^{(0)} \cdot \mathrm{Sub}(D^2))(x_0, \xi) = -(\gamma^j\gamma^k\psi + \gamma^j\psi\gamma^k - 2\gamma^j b_k)(x_0)\xi_j\xi_k,$$
$$(\mathrm{Sub}(D^2) \cdot \sigma_D^{(0)})(x_0, \xi) = -(\gamma^k\psi\gamma^j + \psi\gamma^k\gamma^j - 2b_k\gamma^j)(x_0)\xi_k\xi_j.$$

Based on the relevant formulae obtained previously, we can get

$$\int_{|\xi|=1} \mathrm{Tr}(F \cdot \mathrm{Sub}(D))(x_0, \xi)dS(\xi) = \mathrm{Tr}\big(F\frac{\gamma^j b_j + b_j\gamma^j}{2} + F\psi\big)(x_0) \cdot \mathrm{Vol}(\mathbb{S}^{d-1}),$$

$$\int_{|\xi|=1} \mathrm{Tr}(F \cdot \sigma_D^{(0)} \cdot \mathrm{Sub}(D^2))(x_0, \xi)dS(\xi) = \mathrm{Tr}\big(F\psi - \frac{F\widehat{\psi}}{d} + 2\frac{F\gamma^j b_j}{d}\big)(x_0) \cdot \mathrm{Vol}(\mathbb{S}^{d-1}),$$

$$\int_{|\xi|=1} \mathrm{Tr}(F \cdot \mathrm{Sub}(D^2) \cdot \sigma_D^{(0)})(x_0, \xi)dS(\xi) = \mathrm{Tr}\big(F\psi - \frac{F\widehat{\psi}}{d} + 2\frac{Fb_j\gamma^j}{d}\big)(x_0) \cdot \mathrm{Vol}(\mathbb{S}^{d-1}).$$

Theorem 4.1.3 follows from these formulae as well as from the fact $\mathrm{Vol}(\mathbb{S}^{d-1}) = \frac{2\pi^{d/2}}{\Gamma(d/2)}$. □

Recall that (see §3.6) De^{-tD^2} is a smoothing operator with smooth kernel $K(t,x,y,D,D^2)$ in the sense of

$$(De^{-tD^2}\phi)(x) = \int_M K(t,x,y,Q,P)\phi(y)d\mu_g(y), \tag{4.6}$$

where $K(t,x,y,D,D^2)$ maps E_y to E_x, and the diagonal values of K admit a uniform small-time asymptotic expansion

$$K(t,x,x,D,D^2) \sim \sum_{k=0}^{\infty} t^{\frac{k-d-1}{2}} \mathscr{H}_k(D,D^2)(x) \quad (t \to 0^+), \tag{4.7}$$

where $\mathscr{H}_k(D,D^2) \in C^\infty(M;\mathrm{End}(E))$ vanishes if k is even.

Corollary 4.1.4. *Let D be a self-adjoint Dirac type operator of potential ψ associated with the Dirac bundle (E,γ,∇). Then $\mathscr{H}_1(D,D^2) = \frac{1}{(4\pi)^{d/2}} \cdot \frac{\widehat{\psi}-(d-2)\psi}{2}$.*

Proof. The proof of Theorem 4.1.3 also gives that

$$\mathscr{A}_1(FD,D^2) = \frac{1}{(4\pi)^{d/2}\cdot\Gamma(\frac{d}{2})}\int_M \mathrm{Tr}\Big(F\cdot\big(\widehat{\psi}-(d-2)\psi\big)\Big). \tag{4.8}$$

On the other hand, it is easy to see that

$$\mathscr{B}_1(FD,D^2) = \int_M \mathrm{Tr}\big(F\mathscr{H}_1(D,D^2)\big).$$

According to Proposition 3.3.1, we get $\mathscr{B}_1(FD,D^2) = \frac{\Gamma(\frac{d}{2})}{2}\cdot\mathscr{A}_1(FD,D^2)$. Consequently,

$$\int_M \mathrm{Tr}\big(F\mathscr{H}_1(D,D^2)\big) = \frac{1}{(4\pi)^{d/2}}\int_M \mathrm{Tr}\Big(F\cdot\frac{\widehat{\psi}-(d-2)\psi}{2}\Big),$$

which proves the corollary as F can be any smooth endomorphism of E. We are done. □

The asymmetry of the spectrum about the origin can be examined by studying (see also [133])

$$\omega_k(D) \doteq \frac{\mathscr{A}_k(\mathrm{Id}_E,D)-\mathscr{A}_k(\mathrm{Id}_E,-D)}{2} \tag{4.9}$$

for all non-negative integers k. It follows from Theorem 4.1.1 and Corollary 4.1.2 that

$$\omega_k(D) = \mathrm{res}(D|D|^{k-d-1}). \tag{4.10}$$

On the other hand, it follows from (4.3) that $\omega_k(D) = \mathscr{A}_k(D|D|^{-1},D^2)$, which yields

$$\omega_k(D) = \mathscr{A}_k(D,D^2) \tag{4.11}$$

from Corollary 3.2.5. By definition we have

$$\omega_0(D) = \frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}(\sigma_{D|D|^{-d-1}}) = \frac{1}{(2\pi)^d}\int_{T_1^*M}\mathrm{Tr}(\sigma_D) = 0, \tag{4.12}$$

which implies that the positive and negative parts of the spectrum are symmetric with respect to the origin. According to (4.8) and (4.11), we have

$$\omega_1(D) = \frac{1}{(4\pi)^{d/2}\cdot\Gamma(\frac{d}{2})}\int_M \mathrm{Tr}\big(\widehat{\psi}-(d-2)\psi\big). \tag{4.13}$$

In particular, if D is a generalized Dirac operator, then $\omega_1(D) = 0$ (see also [22]).

Similar to the (microlocalized) spectral zeta function (3.4), we introduce the (microlocalized) spectral eta function (e.g. [22, 59]) by defining

$$\eta(s, A, D) = \sum_{\mu_j \neq 0} \frac{\langle A\phi_j, \phi_j \rangle}{|\mu_j|^s} \cdot \mathrm{Sign}(\mu_j) \quad (\mathrm{Re}(s) > d + m). \tag{4.14}$$

But it is easy to see that

$$\eta(s, A, D) = \zeta(s, A \cdot \mathrm{Sign}(D), D^2). \tag{4.15}$$

So according to Propositions 3.2.3, 3.5.1, we get

Proposition 4.1.5. *$\eta(s, A, D)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $s = d + m - k$ ($k = 0, 1, 2, \ldots$) with residues $\mathrm{res}(AD|D|^{k-d-m-1})$.*

In the event that A is the identity operator, we see from (4.10) that $\eta(s, D) = \eta(s, \mathrm{Id}, D)$ admits a meromorphic continuation to $\mathbb{C}$ whose only singularities are simple poles at $s = d - k$ ($k = 0, 1, 2, \ldots$) with residues $\omega_k(D) = \mathrm{res}(D|D|^{k-d-1})$. This means in particular that the spectral eta function carries all information of the asymmetry of the spectrum about the origin. For example, we know that D is odd-class, $|D|$ is even-class and, consequently (see also [121, Prop. 1.11]), both $|D|^{-1}$ and $D|D|^{-1}$ are even-class. Thus $\mathrm{res}(D|D|^{-1}) = 0$ if d is even. Equivalently, the spectral eta function (4.14) is regular at the origin if the dimension of M is even. We remark that this is a known result by P. Gilkey [55].

4.2 Second coefficient

It is well known that (4.6) and (4.7) hold for an arbitrary Dirac type operator $D = \gamma\widetilde{\nabla} + \psi$ acting on smooth sections of E without any self-adjointness assumption. In the event that D is indeed self-adjoint we have shown in Corollary 4.1.4 that $\mathscr{H}_1(D, D^2) = \frac{1}{(4\pi)^{d/2}} \cdot \frac{\widehat{\psi} - (d-2)\psi}{2}$. The purpose of this section is to show this formula still holds in general.

Theorem 4.2.1. *Let D be a Dirac type operator of potential ψ associated with the Dirac bundle $(E, \gamma, \widetilde{\nabla})$. Then $\mathscr{H}_1(D, D^2) = \frac{1}{(4\pi)^{d/2}} \cdot \frac{\widehat{\psi} - (d-2)\psi}{2}$.*

We first explain how to prove this theorem. Let $\epsilon > 0$ be a parameter and let F be a smooth endomorphism of E. Consider the Dirac type operator D_ϵ of potential $\psi_\epsilon = \psi - \epsilon F$ associated with the Dirac bundle $(E, \gamma, \widetilde{\nabla})$. The Bochner-Weitzenböck technique permits us to find a unique connection ∇_ϵ on E and a unique $V_\epsilon \in C^\infty(M; \mathrm{End}(E))$ such that

$$(D - \epsilon F)^2 = \Delta^{\nabla_\epsilon} + V_\epsilon.$$

But it is known (e.g. [22, Lemma 2.1], [57, Thm. 3.3.1]) that

$$\int_M \mathrm{Tr}(F\mathscr{H}_1(D, D^2)) = \frac{-1}{2 \cdot (4\pi)^{d/2}} \cdot \frac{d}{d\epsilon}\Big|_{\epsilon=0} \int_M \mathrm{Tr}(V_\epsilon). \tag{4.16}$$

As we have done a few times in this thesis, we will recover $\mathscr{H}_1(D, D^2)$ by studying the right-hand side of (4.16) with F ranging all smooth endomorphisms of E. To compare, Branson and Gilkey [22] only considered scalar variations as they thought "otherwise the formulas become more complicated".

Proof of Theorem 4.2.1. Let $L_\epsilon : TM \to \mathrm{End}(E)$ denote the map defined by

$$L_\epsilon(X) = \frac{\gamma(X)\psi_\epsilon + \psi_\epsilon\gamma(X)}{2}.$$

According to Proposition 2.1.1 we have locally that (see (2.4) in §2.1.5 for the meaning of $\overline{\nabla}$)

$$V_\epsilon = \frac{1}{2}\gamma^i\gamma^j R^{\widetilde{\nabla}}_{ij} + \frac{1}{2}[\gamma^i, \overline{\nabla}_i\psi_\epsilon] + (L_\epsilon)^i(L_\epsilon)_i + \psi_\epsilon^2.$$

Thus

$$\frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathrm{Tr}(V_\epsilon) = \mathrm{Tr}\big((L_{-F})^i(L_\psi)_i + (L_\psi)^i(L_{-F})_i\big) - 2\mathrm{Tr}(F\psi),$$

which gives

$$\frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathrm{Tr}(V_\epsilon) = \mathrm{Tr}\big(F((d-2)\psi - \widehat{\psi})\big)$$

from the facts $\gamma^i\gamma_i = -d$ and $\widehat{\psi} = \gamma^i\psi\gamma_i = \gamma_i\psi\gamma^i$. Now (4.16) reads

$$\int_M \mathrm{Tr}(F\mathscr{H}_1(D, D^2)) = \frac{1}{(4\pi)^{d/2}} \cdot \int_M \mathrm{Tr}\big(F\frac{\widehat{\psi} - (d-2)\psi}{2}\big),$$

which suffices to prove the theorem as F can be any smooth endomorphism of E. □

4.3 Characterization

Theorem 4.3.1. *Let D be a Dirac type operator. Then $\mathscr{H}_1(D, D^2) = 0$ if and only if D is a generalized Dirac operator.*

We first explain how to prove this theorem. Let D be a Dirac type operator of potential ψ associated with the Dirac bundle (E, γ, ∇). According to Theorem 4.2.1, $\mathscr{H}_1(D, D^2) = 0$ if and only if $\widehat{\psi} = (d-2)\psi$. Thus to prove Theorem 4.3.1 it suffices to show that, if $\widehat{\psi} = (d-2)\psi$, then there exists a connection $\widetilde{\nabla}$ on E compatible with γ such that $D = \gamma\widetilde{\nabla}$. Note any connection on E is of the form $\nabla_L = \nabla + L$, where

$$L : C^\infty(M; TM) \to C^\infty(M; \mathrm{End}(E))$$

is a $C^\infty(M)$-linear map. It is easy to check that ∇_L is compatible with γ if and only if $L(X)$ commutes with $\gamma(Y)$ for all $X, Y \in C^\infty(M; TM)$. Suppose we do have such a map L satisfying $D = \gamma\nabla_L$. Letting $\{e_k\}_{k=1}^d$ be a local orthonormal frame in TM, we have $D = \gamma\nabla + \gamma(e_k)L(e_k)$, which means $\psi = \gamma(e_k)L(e_k)$. Consequently, for any fixed $i \in \{1, \ldots, d\}$,

$$\frac{\gamma(e_i)\psi + \psi\gamma(e_i)}{2} = L(e_k)\frac{\gamma(e_i)\gamma(e_k) + \gamma(e_k)\gamma(e_i)}{2} = -L(e_i).$$

This implies that globally L is uniquely of the following form

$$L(X) = -\frac{\gamma(X)\psi + \psi\gamma(X)}{2} \tag{4.17}$$

for any $X \in C^\infty(M; TM)$. Thus to prove Theorem 4.3.1, assuming $\widehat{\psi} = (d-2)\psi$ and defining $\widetilde{\nabla} = \nabla + L$ with L given by (4.17), we need only to show that

- 1) $D = \gamma\widetilde{\nabla}$;
- 2) $\widetilde{\nabla}$ is compatible with γ.

The first property can be verified in the following way. Let $\{e_k\}_{k=1}^d$ be a local orthonormal frame in TM, then

$$\gamma(e_k)L(e_k) = -\gamma(e_k)\frac{\gamma(e_k)\psi + \psi\gamma(e_k)}{2} = \frac{d\psi - \widehat{\psi}}{2} = \psi,$$

which gives

$$D = \gamma\nabla + \psi = \gamma\nabla + \gamma(e_k)L(e_k) = \gamma\widetilde{\nabla}.$$

To prove the second property we need to show that $L(X)$ commutes with $\gamma(Y)$ for all $X, Y \in C^\infty(M; TM)$. But considering L and γ are $C^\infty(M)$-linear maps, it suffices to prove that $L_x(X_x)$ commutes with $\gamma_x(Y_x)$ for all $X_x, Y_x \in T_xM$ at each $x \in M$. This is guaranteed by the next proposition and a proof of Theorem 4.3.1 is obtained.

Proposition 4.3.2. *Let (W, γ) be a complex $\mathrm{Cl}(\mathbb{R}^d)$-module. Let $\psi \in \mathrm{End}(W)$ be such that $\widehat{\psi} = (d-2)\psi$, and let $L : \mathbb{R}^d \to \mathrm{End}(W)$ be the linear map defined by*

$$L(X) = -\frac{\gamma(X)\psi + \psi\gamma(X)}{2} \quad (X \in \mathbb{R}^d).$$

Then $L(X)$ commutes with $\gamma(Y)$ for all $X, Y \in \mathbb{R}^d$.

Ahead of giving the details of the proof of Proposition 4.3.2, we collect some basic facts about the Clifford modules (e.g. [49, 52, 94, 135]). Let $\mathrm{Cl}(\mathbb{R}^d)$ be the complex Clifford algebra generated by $(\mathbb{R}^d, \langle\cdot,\cdot\rangle)$ subject to the commutation relation

$$X * Y + Y * X = -2\langle X, Y\rangle,$$

where $X, Y \in \mathbb{R}^d$, $\langle\cdot,\cdot\rangle$ denotes the standard Euclidean metric on $\mathbb{R}^d$, and $*$ denotes the Clifford algebra operation. Any complex $\mathrm{Cl}(\mathbb{R}^d)$-module W with structure γ (unital algebra morphism from $\mathrm{Cl}(\mathbb{R}^d)$ to $\mathrm{End}(W)$) studied in this thesis is always assumed to be of dimension in $\mathbb{N}$. A complex $\mathrm{Cl}(\mathbb{R}^d)$-module (W, γ) is said to be *irreducible* if for any decomposition $W = W_1 \oplus W_2$ into subspaces invariant under γ one has $W_1 = W$ or $W_2 = W$. It is known that a complex $\mathrm{Cl}(\mathbb{R}^d)$-module is irreducible if and only if it is of complex dimension $2^{\lfloor \frac{d}{2} \rfloor}$. Two complex $\mathrm{Cl}(\mathbb{R}^d)$-modules (W_1, γ) and $(W_2, \widetilde{\gamma})$ are said to be *equivalent* if there exists an invertible element $\kappa \in \mathrm{Hom}(W_1, W_2)$ such that $\widetilde{\gamma} = \kappa^*\gamma$, where κ^* is defined by sending $\varrho \in \mathrm{End}(W_1)$ to $\kappa\varrho\kappa^{-1} \in \mathrm{End}(W_2)$. Up to isomorphism there are exactly $\frac{3-(-1)^d}{2}$ inequivalent irreducible complex $\mathrm{Cl}(\mathbb{R}^d)$-modules. It is also known that any complex $\mathrm{Cl}(\mathbb{R}^d)$-module is a sum of irreducible ones.

Let (W, γ) be a complex $\mathrm{Cl}(\mathbb{R}^d)$-module and define

$$\widehat{\psi} = \sum_{k=1}^{d} \gamma(e_k)\psi\gamma(e_k)$$

for any $\psi \in \mathrm{End}(W)$, where $\{e_k\}_{k=1}^d$ is an arbitrary orthonormal basis for $(\mathbb{R}^d, \langle\cdot,\cdot\rangle)$. Let

$$\mathrm{End}_k(W) := \mathrm{Span}_{\mathbb{C}}\big\{\gamma(e_{i_1})\gamma(e_{i_2})\cdots\gamma(e_{i_k}) : 1 \le i_1 < i_2 < \cdots < i_k \le d\big\},$$

for $k > 0$ and let $\mathrm{End}_0(W)$ be the complex span of the identity map. A simple computation[1] using the Clifford algebra relations shows that $\mathrm{End}_k(W)$ is an eigenspace for the map $\psi \mapsto \widehat{\psi}$ with eigenvalue $(-1)^k(2k-d)$. It is clear that Clifford multiplication by the volume element $\Theta_d = \gamma(e_1)\gamma(e_2)\cdots\gamma(e_d)$ defines the linear map $\psi \mapsto \Theta_d * \psi$ from $\mathrm{End}_k(W)$ to $\mathrm{End}_{d-k}(W)$. If the module is irreducible the subspaces $\mathrm{End}_k(W)$ generate $\mathrm{End}(W)$ and therefore this gives a decomposition into eigenspaces. Hence, in the irreducible case we have

$$\mathrm{End}(W) = \bigoplus_{k=0}^{d} \mathrm{End}_k(W) \quad \text{if } d \text{ is even,} \tag{4.18}$$

$$\mathrm{End}(W) = \bigoplus_{k=0}^{\frac{d-1}{2}} \mathrm{End}_k(W) \quad \text{if } d \text{ is odd.} \tag{4.19}$$

In the latter case we have used $\mathrm{End}_{d-k}(W) = \mathrm{End}_k(W)$. This can be seen directly because Clifford multiplication by the volume element commutes with the Clifford action, and therefore, by Schur's lemma, the volume element Θ_d must be a multiple of the identity. As an immediate consequence of this discussion we get the following proposition.

Proposition 4.3.3. *If (W,γ) is irreducible, then the $d-2$ eigenspace of the map $\psi \mapsto \widehat{\psi}$ equals $\mathrm{End}_1(W) = \mathrm{Span}_{\mathbb{C}}\gamma(\mathbb{R}^d)$. If furthermore d is odd, then $2-d$ is not an eigenvalue of the map $\psi \mapsto \widehat{\psi}$.*

Proof of Proposition 4.3.2. Let (W,γ) denote an arbitrary (finite-dimensional) complex $\mathrm{Cl}(\mathbb{R}^d)$-module and let $(W_0,\gamma^{(0)})$ be an irreducible complex $\mathrm{Cl}(\mathbb{R}^d)$-module. It is easy to see that up to isomorphism $(W_0,\gamma^{(0)})$ can represent all irreducible complex $\mathrm{Cl}(\mathbb{R}^d)$-modules if d is even, and so for $(W_0,\pm\gamma^{(0)})$ if d is odd. We then have two cases to consider.

Case 1: Suppose d is even. In this case there exists a (finite-dimensional) complex vector space V such that (W,γ) is equivalent to $(W_0\otimes V,\widetilde{\gamma})$, where the Clifford structure $\widetilde{\gamma}$ on $W_0\otimes V$ is applied only to the first tensor factor W_0. To be precise,

$$\widetilde{\gamma}(Y) = \gamma^{(0)}(Y)\otimes \mathrm{Id}_V$$

for any $Y \in \mathbb{R}^d$. Without loss of generality we can assume that $(W,\gamma) = (W_0\otimes V,\widetilde{\gamma})$, since the general cases can be dealt with simply by studying isomorphism between Clifford modules. Then as an application of Proposition 4.3.3, we claim that the $d-2$ eigenspace of the map $\psi \mapsto \widehat{\psi}$ equals $\gamma^{(0)}(\mathbb{R}^d)\otimes \mathrm{End}(V)$. To prove this claim, it suffices to first fix a linear basis $\{K_i\}$ for $\mathrm{End}(V)$, then express ψ with $\widehat{\psi} = (d-2)\psi$ uniquely as $\psi_i^{(0)}\otimes K_i$ where $\psi_i^{(0)} \in \mathrm{End}(W_0)$, note

$$\widehat{\psi_i^{(0)}}\otimes K_i = \widehat{\psi} = (d-2)\psi = (d-2)\psi_i^{(0)}\otimes K_i,$$

and finally apply Proposition 4.3.3 appropriately. This claim immediately implies that

$$L(\mathbb{R}^d) = \{\mathrm{Id}_{W_0}\}\otimes \mathrm{End}(V),$$

which obviously commutes with $\gamma(\mathbb{R}^d) = \gamma^{(0)}(\mathbb{R}^d)\otimes\{\mathrm{Id}_V\}$.

[1] It suffices to study $\gamma(e_1)\gamma(e_2)\cdots\gamma(e_k) \in \mathrm{End}_k(W)$.

Case 2: Suppose d is odd. In this case there exist (finite-dimensional) complex vector spaces V_1, V_2 such that (W, γ) is equivalent to $((W_0 \otimes V_1) \oplus (W_0 \otimes V_2), \widetilde{\gamma})$, where the Clifford structure $\widetilde{\gamma}$ on $(W_0 \otimes V_1) \oplus (W_0 \otimes V_2)$ applied only to W_0 is defined by

$$\widetilde{\gamma}(Y) = \big(\gamma^{(0)}(Y) \otimes \mathrm{Id}_{V_1}\big) \bigoplus \big(- \gamma^{(0)}(Y) \otimes \mathrm{Id}_{V_2}\big)$$

for any $Y \in \mathbb{R}^d$. Similar to the discussion in the previous case, we assume without loss of generality that $(W, \gamma) = ((W_0 \otimes V_1) \oplus (W_0 \otimes V_2), \widetilde{\gamma})$. Then as an application of Proposition 4.3.3, we claim that the $d-2$ eigenspace of the map $\psi \mapsto \widehat{\psi}$ equals $(\gamma^{(0)}(\mathbb{R}^d) \otimes \mathrm{End}(V_1)) \oplus (\gamma^{(0)}(\mathbb{R}^d) \otimes \mathrm{End}(V_2))$. To prove this claim, we first choose a linear basis $\{K_i^{\alpha\beta}\}$ for each $\mathrm{Hom}(V_\alpha, V_\beta)$, then express ψ with $\widehat{\psi} = (d-2)\psi$ uniquely as

$$\big(\psi_i^{(11)} \otimes K_i^{(11)}\big) \bigoplus \big(\psi_j^{(22)} \otimes K_j^{(22)}\big) + \big(\psi_i^{(12)} \otimes K_i^{(12)}\big) \bigoplus \big(\psi_j^{(21)} \otimes K_j^{(21)}\big),$$

where $\psi_i^{(\alpha\beta)} \in \mathrm{End}(W_0)$. Here to be clear, $W = (W_0 \otimes V_1) \oplus (W_0 \otimes V_2)$ is naturally identified with $(W_0 \otimes V_2) \oplus (W_0 \otimes V_1)$ by interchanging the positions, thus any element in W mapped via the second summand is indeed contained in W. Following this convention, it is straightforward to check that

$$\widehat{\psi} = \big(\widehat{\psi_i^{(11)}} \otimes K_i^{(11)}\big) \bigoplus \big(\widehat{\psi_j^{(22)}} \otimes K_j^{(22)}\big) + \big(- \widehat{\psi_i^{(12)}} \otimes K_i^{(12)}\big) \bigoplus \big(- \widehat{\psi_j^{(21)}} \otimes K_j^{(21)}\big).$$

Thus the claim is an immediate consequence of Proposition 4.3.3. This claim implies that

$$L(\mathbb{R}^d) = \big(\{\mathrm{Id}_{W_0}\} \otimes \mathrm{End}(V_1)\big) \bigoplus \big(\{\mathrm{Id}_{W_0}\} \otimes \mathrm{End}(V_2)\big),$$

which commutes with $\widetilde{\gamma}(Y)$ for any $Y \in \mathbb{R}^d$. This finishes the proof of Proposition 4.3.2. $\square$

Chapter 5

Heat kernel estimates

In the previous two chapters we studied various spectral invariants for Laplace and Dirac type operators acting on smooth sections of vector bundles over closed Riemannian manifolds. In the following two chapters we will study vector-valued and scalar-valued Laplace operators on bounded Euclidean domains. Given that in the new background many relevant quantitative estimates are available, we will establish various uniform bounds rather than well-studied asymptotic limits in the previous setting of closed manifolds. Contrary to closed eigenvalue problems, there are plenty of non-negative self-adjoint extensions of the standard Laplace operator on bounded Euclidean domains. An important feature of Chapter 5 is to provide a unified approach to the heat kernel of these operators regardless of the choice of self-adjoint extensions. The reader may feel later that there are no obvious connections between Chapters 5 and 6 except estimate (5.7), which is (6.13) in two dimensions. Actually, we were not aware of the precise form of this estimate for a long time, but were still able to recover an optimal estimate (Theorem 5.5.1) by appealing to the finite propagation speed for wave equations. Our plan was to apply our own estimate to Chapter 6, so the coherence between both chapters does exist. But unfortunately, Theorem 5.5.1 is weaker than (5.7) in two dimensions. This is the reason why we will develop Chapters 5 and 6 quite independently.

Let $U_0 \subset \mathbb{R}^d$ be a bounded domain of smooth boundary. Let $\{\lambda_n^{(+)}\}_{n=1}^\infty$ ($\{\lambda_n^{(-)}\}_{n=1}^\infty$) denote the eigenvalues, listed in non-decreasing order, of the Dirichlet (Neumann) Laplacian $\Delta_{U_0}^{(+)}$ ($\Delta_{U_0}^{(-)}$) on $L^2(U_0)$. The classical Weyl law states that

$$\lim_{n\to\infty} \frac{(\lambda_n^{(\pm)})^{d/2}}{n} = \frac{(4\pi)^{d/2}\Gamma(\frac{d}{2}+1)}{|U_0|},$$

which means in particular that one can hear the volume of U_0 from either its Dirichlet or Neumann spectrum. It is well known (e.g. [23]) that

$$\sum_{n=1}^\infty e^{-\lambda_n^{(\pm)}t} = (4\pi t)^{-d/2}\Big(|U_0| \mp \frac{\sqrt{\pi t}}{2}|\partial U_0| + o(t^{1/2})\Big) \quad (t \to 0^+),$$

which implies that the surface area of the boundary ∂U_0 can also be heard from either its Dirichlet or Neumann spectrum. There are plenty of works adapting the techniques of one problem to the study of the other, and thus yielding many similar estimates for both problems.

An important feature is many twin inequalities for both problems hold in opposite directions. To name just one example, the long-standing Polya conjecture claims that

$$\frac{(\lambda_{n+1}^{(-)})^{d/2}}{n} \leq \frac{(4\pi)^{d/2}\Gamma(\frac{d}{2}+1)}{|U_0|} \leq \frac{(\lambda_n^{(+)})^{d/2}}{n} \quad (n \in \mathbb{N}).$$

A notable distinction between both problems is that the Dirichlet heat kernel has full domain monotonicity, while that of Neumann has only partial. The fundamental solution $K_{U_0}^{(+)}(t)$ $(t > 0)$ of the heat equation with Dirichlet boundary conditions can be constructed via spectral calculus as $K_{U_0}^{(+)}(t) = \exp(-t\Delta_{U_0}^{(+)})$. The integral kernel $K_{U_0}^{(+)}(x, y; t)$ of $K_{U_0}^{(+)}(t)$ defined by

$$(K_{U_0}^{(+)} f)(x) = \int_{U_0} K_{U_0}^{(+)}(x, y; t) f(y) dy$$

is a positive smooth function on $U_0 \times U_0 \times \mathbb{R}^+$. It describes the propagation of heat from the point x to the point y in time t. The full domain monotonicity of the Dirichlet heat kernel claims for any two bounded domains $U_0 \subset U_1$ of smooth boundary that

$$K_{U_0}^{(+)}(x, y; t) \leq K_{U_1}^{(+)}(x, y; t) \quad ((x, y, t) \in U_0 \times U_0 \times \mathbb{R}^+). \tag{5.1}$$

This follows from the maximum principle for elliptic equations (e.g. [36]) or the probabilistic interpretation of the Dirichlet heat kernel (e.g. [123, 127, 143]). In contrast to Dirichlet boundary problems, there is no general domain monotonicity principle [8] claiming for any two bounded domains $U_0 \subset U_1$ of smooth boundary that

$$K_{U_1}^{(-)}(x, y; t) \leq K_{U_0}^{(-)}(x, y; t) \quad ((x, y, t) \in U_0 \times U_0 \times \mathbb{R}^+), \tag{5.2}$$

where $K_{U_i}^{(-)}(x, y; t)$ denotes the integral kernel of the fundamental solution of the heat equation with Neumann boundary conditions on ∂U_i. The partial domain monotonicity of the Neumann heat kernel means in this thesis exactly a result by Kendall [89] (see also [115]; if U_0 is convex then see [26]) stating

$$K_{U_0}^{(-)}(x, x; t) \leq K_{B_x}^{(-)}(x, x; t) \quad ((x, t) \in U_0 \times \mathbb{R}^+), \tag{5.3}$$

where $B_x \subset U_0$ denotes the largest open ball centred at x. The full domain monotonicity of the Dirichlet heat kernel has proven to be an extremely fundamental property, but the partial one of the Neumann heat kernel has no exciting applications yet. For example, suppose an open manifold is the union of an increasing sequence of open subsets, then the Dirichlet heat kernel for the open manifold is the pointwise limit of the counterparts of sequence of subsets [36].

Without the full domain monotonicity some results about the Dirichlet boundary problems have not found corresponding Neumann counterparts yet. For example, many known estimates about the Neumann heat kernel (e.g. [26, 35, 72, 81, 89, 92, 115]) need to impose certain geometric assumptions on boundaries.

Let us return to Dirichlet boundary problems once again. On physical grounds one expects that for small times the Dirichlet heat kernel is dominated by local contributions that do not involve the boundary of U_0. This is essentially the principle of not feeling the boundary by

Kac [87]. The precise information of the small-time Dirichlet heat kernel should also count the contributions that involve the boundary of U_0. In practice this part needs to be analysed independently.

In this chapter we will show that the heat kernels for vector-valued non-negative Laplacians can be always treated in the above manner. In particular, we can study the Neumann heat kernels without imposing geometric assumptions on boundaries as mentioned earlier except smoothness. Actually, we will prove that Kac's principle of not feeling the boundary can be obtained for any self-adjoint extension of the Laplace operator acting on vector-valued functions on a Euclidean domain. They can be derived from a combination of finite propagation speed estimates and explicit Fourier Tauberian theorems that were found by Safarov in [130]. The idea of using finite propagation speed estimates in this context is not new and is already present in the classical paper [28]. It has since been used by many authors to derive heat kernel bounds on manifolds (e.g. [16, 33, 37, 103, 118, 141]). The implied constants are independent of the boundary conditions.

Explicit estimates like these are important in spectral geometry. For example the meromorphic extension of the local spectral zeta function is usually based on the expansion of the heat kernel [56]. The above estimates directly lead to bounds on the local spectral zeta functions or other spectral invariants [42]. A particular example of such a local spectral function is the Casimir energy density that plays a distinguished role in physics. For these applications it is important to allow for boundary conditions other than Dirichlet. For example Casimir interaction between two conducting obstacles is described by the Casimir energy density of the photon field. This is obtained from the Laplace operator acting on one forms with electromagnetic boundary conditions. We would like to refer the reader to [20] for further details and references on Casimir energy density computations.

This chapter is arranged as follows. In Section 5.1 we give details of Kac's original principle of not feeling the boundary. In Section 5.2 we study smoothness and the finite propagation speed of solutions of wave equations. In Section 5.3 we establish Kac's principle in terms of integral kernel bounds for higher order inverses of the given Laplacian. In Section 5.4 we apply Safarov's Fourier Tauberian theorems to study higher order inverses of the given Laplacian, while in Section 5.5 (5.6) we use the full (partial) domain monotonicity of the Dirichlet (Neumann) heat kernel to do so.

5.1 Kac's principle

Let $U \subset \mathbb{R}^d$ be an arbitrary open set, and let $K_U^{(+)}(x, y; t)$ be the integral kernel of $\exp(-t\Delta_U^{(+)})$. In the previous introductory part we assumed that $U = U_0$ is of smooth boundary. According to the full domain monotonicity of the Dirichlet heat kernel, we see that $K_U^{(+)}(x, y; t)$ is well-defined without any boundedness or smoothness assumptions on U.

Kac's original principle of not feeling the boundary [87] (see also [88]) is as simple as follows: take a point x in U and let $C_x \subset U$ denote the largest open cube centred at x, then this principle basically is

$$K_{C_x}^{(+)}(x, x; t) \leq K_U^{(+)}(x, x; t) \leq K_{\mathbb{R}^d}^{(+)}(x, x; t) \quad (t > 0). \tag{5.4}$$

The reason for picking up a cube is all of the eigenvalues and eigenfunctions of any Dirichlet Laplacians on cubes can be explicitly determined. One can then use the Poisson summation formula to get very precise short time asymptotic expansions for $K^{(+)}_{C_x}(x,x;t)$, and find they are close to

$$K^{(+)}_{\mathbb{R}^d}(x,x;t) = \frac{1}{(4\pi t)^{d/2}}.$$

Consequently, $K^{(+)}_U(x,x;t)$ is forced to be close to $(4\pi t)^{-d/2}$ for small times t by (5.4). A detailed analysis of (5.4) [9] leads to

$$\Big|K^{(+)}_U(x,x;t) - \frac{1}{(4\pi t)^{d/2}}\Big| \le \frac{2d}{(4\pi t)^{d/2}} \exp(-\frac{\rho(x)^2}{dt}), \tag{5.5}$$

where $\rho(x)$ denotes the distance of x to ∂U. This estimate has been widely used in the study of short time asymptotic expansions of the Dirichlet heat trace. For example, Kac [88] explicitly determined β_1 in

$$\sum_{n=1}^{\infty} e^{-\lambda_n^{(+)}t} = \frac{1}{4\pi t}\Big(|U| - \frac{\sqrt{\pi t}}{2}|\partial U| + \beta_1 + O(e^{-\beta_2/t})\Big) \quad (t \to 0^+),$$

provided $U \subset \mathbb{R}^2$ is a convex polygon without acute or right angles, while M. van den Berg and S. Srisatkunarahaj [12] can do so for both β_1 and β_2 whenever $U \subset \mathbb{R}^2$ is an arbitrary polygon.

According to probabilistic interpretation of the Dirichlet heat kernel, one can expect that

$$K^{(+)}_{B_x}(x,x;t) \le K^{(+)}_U(x,x;t) \le K^{(+)}_{\mathbb{R}^d}(x,x;t) \quad (t > 0) \tag{5.6}$$

may yield better estimates than (5.5), where $B_x \subset U$ denotes the largest open ball centred at x. But it is difficult to adopt the previous method to improve (5.5) because it is hard to get precise values of normalised eigenfunctions at the centre x. Even so, M. van den Berg [10] used dimension induction on Brownian motions to improve (5.5) to

$$\Big|K^{(+)}_U(x,x;t) - \frac{1}{(4\pi t)^{d/2}}\Big| \le \frac{1}{(4\pi t)^{d/2}} \exp(-\frac{\rho(x)^2}{t}) \sum_{j=1}^{d} \frac{2^j}{(j-1)!}(\frac{\rho(x)^2}{t})^{j-1}. \tag{5.7}$$

The exponential factor is sharp as it is known (e.g. [10, 82]) that

$$\lim_{t\to 0^+} t \log\Big(1 - \frac{K^{(+)}_U(x,x;t)}{K^{(+)}_{\mathbb{R}^d}(x,x;t)}\Big) = -\rho^2(x).$$

These estimates show that as t goes to 0 the error in approximating the heat kernel by $(4\pi t)^{-d/2}$ is exponentially small with decay rate determined by the distance to the boundary.

5.2 Finite propagation speed

5.2.1 Functional calculus

Consider in the Hilbert space H an arbitrary self-adjoint operator A. By the spectral theorem one can write $A = \int_{\mathbb{R}} \lambda d\Pi(\lambda)$, where $\Pi(\lambda)$ ($\lambda \in \mathbb{R}$) denotes the spectral projection of A onto

$(-\infty, \lambda]$. For any element φ in H, $d\langle\varphi, \Pi(\lambda)\varphi\rangle$ is a finite Borel measure on $\mathbb{R}$. Let f, f_1, f_2 denote real-valued Borel functions. It is known that φ lies in the domain of $f(A)$ if and only if

$$\int_{\mathbb{R}} f(\lambda)^2 d\langle\varphi, \Pi(\lambda)\varphi\rangle < \infty.$$

Suppose this is the case then

$$\langle f(A)\varphi, \varphi\rangle_H = \int_{\mathbb{R}} f(\lambda) d\langle\varphi, \Pi(\lambda)\varphi\rangle. \tag{5.8}$$

It is also known that

$$\mathrm{Dom}(f_1(A)f_2(A)) = \mathrm{Dom}(f_2(A)) \cap \mathrm{Dom}((f_1f_2)(A)) \tag{5.9}$$

and $(f_1f_2)(A)$ is an extension of $f_1(A)f_2(A)$. All these basic facts can be found in [32, 125]. Now let ϕ, ψ be two arbitrary elements in $\cap_{k=1}^{\infty}\mathrm{Dom}(A^k)$. By polarization one has for each $s \in \mathbb{R}$,

$$\langle\cos(s\sqrt{|A|})\phi, \psi\rangle_H = \int_{\mathbb{R}} \cos(s\sqrt{|\lambda|}) \frac{d\langle\phi+\psi, \Pi(\lambda)(\phi+\psi)\rangle - d\langle\phi, \Pi(\lambda)\phi\rangle - d\langle\psi, \Pi(\lambda)\psi\rangle}{2}.$$

Obviously, $(1+\lambda^{2k})d\langle h, \Pi(\lambda)h\rangle$ is a finite Borel measure on $\mathbb{R}$ for any $k \in \mathbb{N}$, $h \in \cap_{k=1}^{\infty}\mathrm{Dom}(A^k)$. This implies that $\langle\cos(s\sqrt{|A|})\phi, \psi\rangle_H$ is a smooth function of $s \in \mathbb{R}$ and its rigorous derivatives can be obtained formally.

5.2.2 Finite propagation speed

In order to make use of Proposition 2.4.1, we need study smoothness of the solution of the wave equation subject to general non-negative boundary conditions. We begin with the scalar case.

Consider in the Hilbert space $L^2(U)$ an arbitrary non-negative self-adjoint extension Δ_U of $-\Delta : C_c^\infty(U) \to C_c^\infty(U)$. When $U = \mathbb{R}^d$ the counterpart for Δ_U is denoted by Δ_0. Let ϕ denote an element of $C_c^\infty(U)$. We claim that $(\cos(s\sqrt{\Delta_U})\phi)(x)$ is smooth in $U \times \mathbb{R}$ and

$$\frac{\partial^2}{\partial s^2}\cos(s\sqrt{\Delta_U})\phi = \Delta\cos(s\sqrt{\Delta_U})\phi. \tag{5.10}$$

This implies that $u(x,t) = \cos(t\sqrt{\Delta_U})\phi$ solves the wave equation $\frac{\partial^2 u}{\partial t^2} = \Delta u$. The proof is as follows. First, let $s \in \mathbb{R}$ be fixed and suppose $k \in \mathbb{N}$. Note $\cos(s\sqrt{\Delta_U})\phi$ lies in the domain of $(\Delta_U)^k$ because (see (5.9) in §5.2.1)

$$(\Delta_U)^k\cos(s\sqrt{\Delta_U})\phi = \cos(s\sqrt{\Delta_U})(\Delta_U)^k\phi = \cos(s\sqrt{\Delta_U})(-\Delta)^k\phi.$$

Let $\psi \in C_c^\infty(U)$ be an arbitrary test function. Note

$$\begin{aligned}\langle(\Delta_U)^k\cos(s\sqrt{\Delta_U})\phi, \psi\rangle_{L^2(U)} &= \langle\cos(s\sqrt{\Delta_U})\phi, (\Delta_U)^k\psi\rangle_{L^2(U)} \\ &= \langle\cos(s\sqrt{\Delta_U})\phi, (-\Delta)^k\psi\rangle_{L^2(U)}.\end{aligned}$$

This implies that the weak derivative of $\cos(s\sqrt{\Delta_U})\phi$ under $(-\Delta)^k$ is just $(\Delta_U)^k\cos(s\sqrt{\Delta_U})\phi$, which is an $L^2(U)$ function. Thus it follows from the elliptic regularity theorem by letting k be large enough (e.g. [44, 48]) that $\cos(s\sqrt{\Delta_U})\phi$ is smooth in U. By the way, we have obtained

$$(\Delta_U)^k\cos(s\sqrt{\Delta_U})\phi = (-\Delta)^k\cos(s\sqrt{\Delta_U})\phi = \cos(s\sqrt{\Delta_U})(-\Delta)^k\phi. \tag{5.11}$$

To finish the proof of the claim we also need to show that $\cos(s\sqrt{\Delta_U})\phi$ is smooth with respect to the time variable s. Note $\|\cos(s\sqrt{|\lambda|})\|_{L^\infty(\mathbb{R}\times\mathbb{R})} \leq 1$ and $\cos(s\sqrt{|\lambda|})$ is a continuous function of $s \in \mathbb{R}$ for each fixed $\lambda \in \mathbb{R}$. By the functional calculus of self-adjoint operators (see [125, Thm. VIII.5 (d)]), $\cos(s\sqrt{\Delta_U})\phi$ is an $L^2(U)$-valued continuous function of $s \in \mathbb{R}$. By appealing to Taylor's theorem with integral remainder, we can rewrite $\langle\cos(s\sqrt{\Delta_U})\phi,\psi\rangle_{L^2(U)}$ as (see §5.2.1)

$$\begin{aligned}\langle\cos(s\sqrt{\Delta_U})\phi,\psi\rangle_{L^2(U)} &= \langle\phi,\psi\rangle_{L^2(U)} + \int_0^s (s-z)\langle\cos(z\sqrt{\Delta_U})\Delta\phi,\psi\rangle_{L^2(U)}dz \\ &= \langle\phi + \int_0^s (s-z)\cos(z\sqrt{\Delta_U})\Delta\phi dz,\psi\rangle_{L^2(U)},\end{aligned}$$

which implies that

$$\cos(s\sqrt{\Delta_U})\phi = \phi + \int_0^s (s-z)\cos(z\sqrt{\Delta_U})\Delta\phi dz. \tag{5.12}$$

Self-repeating the above formula implies that $\cos(s\sqrt{\Delta_U})\phi$ is also of the following form

$$\sum_{k=0}^N \frac{s^{2k}\Delta^k\phi}{(2k)!} + \int_0^s\int_0^{z_0}\cdots\int_0^{z_{N-1}}(s-z_0)(z_0-z_1)\cdots(z_{N-1}-z_N)\cos(z_N\sqrt{\Delta_U})\Delta^{N+1}\phi dz_N\cdots dz_1dz_0.$$

Define $Z(x,s) = (\cos(s\sqrt{\Delta_U})\phi)(x)$, which is square integrable on $U\times[a,b]$ for any bounded intervals $[a,b]$. This implies for almost every $x \in U$ that $Z(x,\cdot)$ is locally (square) integrable on $\mathbb{R}$. Thus according to the last formula on the previous page, for almost every $x \in U$ we have that $Z(x,\cdot)$ is smooth on $\mathbb{R}$. But this is not enough to prove the claim and we need turn to the elliptic regularity theorem once again. Letting $\kappa \in C_c^\infty(U\times\mathbb{R})$ be an arbitrary element, define

$$\langle Z,\kappa\rangle = \int_{\mathbb{R}}\langle\cos(s\sqrt{\Delta_U})\phi,\kappa(\cdot,s)\rangle_{L^2(U)}ds.$$

Let $k \in \mathbb{N}$. According to (5.11) it is easy to show that the weak derivative of Z under $(-\Delta)^k = (-\Delta_x)^k$ is just $(\cos(s\sqrt{\Delta_U})(-\Delta)^k\phi)(x)$, which is an $L^2_{\text{loc}}(U\times\mathbb{R})$ function. According to (5.12), it is easy to show that the weak derivative of Z under $-\frac{d^2}{ds^2}$ is $(\cos(s\sqrt{\Delta_U})(\Delta\phi)(x)$ because we have shown that $Z(x,\cdot)$ is smooth on $\mathbb{R}$ for almost every $x \in U$. Self-repeating this fact implies that the weak derivative of Z under $(-\frac{d^2}{ds^2})^k$ is $(\cos(s\sqrt{\Delta_U})(\Delta^k\phi)(x)$, which is an $L^2_{\text{loc}}(U\times\mathbb{R})$ function. Consequently, the weak derivative of Z under the elliptic operator $(-\Delta_x)^k + (-\frac{d^2}{ds^2})^k$ is an $L^2_{\text{loc}}(U\times\mathbb{R})$ function. It then follows on from the elliptic regularity theorem by letting k be large enough that Z is a smooth function on $U\times\mathbb{R}$. Finally, (5.10) follows straight on from (5.12). This finishes the proof of the claim.

Proposition 5.2.1. *Let $\phi \in C_c^\infty(U)$ be such that the s-neighborhood of its support is a compact subset of U for some $s \geq 0$. Then $\cos(s\sqrt{\Delta_0})\phi$ is compactly supported in U and completely agrees with $\cos(s\sqrt{\Delta_U})\phi$ in U.*

Proof. According to the finite propagation speed (2.36), $\cos(s\sqrt{\Delta_0})\phi$ is compactly supported in U. To prove the second assertion we need only to show for any $\psi \in C_c^\infty(U)$ that

$$\langle \psi, \cos(s\sqrt{\Delta_U})\phi\rangle_{L^2(U)} = \langle \psi, \cos(s\sqrt{\Delta_0})\phi\rangle_{L^2(\mathbb{R}^d)},$$

which is equivalent to

$$\int_U \Big[\cos(s\sqrt{\Delta_U})\psi - \cos(s\sqrt{\Delta_0})\psi\Big](x)\cdot\overline{\phi(x)}dx = 0.$$

Note $u(x,t) = \cos(t\sqrt{\Delta_U})\psi - \cos(t\sqrt{\Delta_0})\psi$ solves the wave equation with $u(x,0) = \frac{\partial u}{\partial t}(x,0) = 0$. It thus follows from Proposition 2.4.1 that $u(\cdot, s)$ vanishes on

$$U_s = \{y \in U : \mathrm{dist}(y, \partial U) > s\}.$$

The assumption of the proposition actually means that the support of ϕ is contained in U_s. Hence the proof of the proposition is achieved. □

In general, let $N \in \mathbb{N}$ and consider in the Hilbert space $L^2(U;\mathbb{C}^N)$ an arbitrary non-negative self-adjoint extension, denoted by Δ_U, of $-\Delta : C_c^\infty(U;\mathbb{C}^N) \to C_c^\infty(U;\mathbb{C}^N)$ acting component-wise. When $U = \mathbb{R}^d$ the counterpart for Δ_U is also denoted by Δ_0.

Proposition 5.2.2. *Let $\phi \in C_c^\infty(U;\mathbb{C}^N)$ be such that the s-neighborhood of its support is a compact subset of U for some $s \geq 0$. Then $\cos(s\sqrt{\Delta_0})\phi$ is compactly supported in U and completely agrees with $\cos(s\sqrt{\Delta_U})\phi$ in U.*

To prove this proposition it suffices to follow the proof of the previous proposition by applying Proposition 2.4.1 component-wise. We omit the details.

5.3 Heat kernel bounds (I)

Let us assume that, as before, U is an open set in $\mathbb{R}^d$, $\rho(x)$ denotes the distance from $x \in U$ to ∂U, N is a positive integer, and Δ_U is an arbitrary non-negative self-adjoint extension of the (negative) Laplacian $-\Delta : C_c^\infty(U;\mathbb{C}^N) \to C_c^\infty(U;\mathbb{C}^N)$ acting component-wise on the Hilbert space $L^2(U;\mathbb{C}^N)$. The heat kernel for Δ_U, denoted by (see §2.5)

$$\mathbf{K}_U(x,y;t) = \begin{pmatrix} K_U^{(11)}(x,y;t) & \cdots & K_U^{(1N)}(x,y;t) \\ \vdots & \ddots & \vdots \\ K_U^{(N1)}(x,y;t) & \cdots & K_U^{(NN)}(x,y;t) \end{pmatrix},$$

means the integral kernel of $e^{-t\Delta_U}$ ($t > 0$), which is defined by the functional calculus of self-adjoint operators. When $U = \mathbb{R}^d$ the counterpart for Δ_U and $\mathbf{K}_U(x,y;t)$ is denoted respectively by Δ_0 and $\mathbf{K}_0(x,y;t)$. Of course,

$$\mathbf{K}_0(x,y;t) = (4\pi t)^{-d/2}\exp(-\frac{|x-y|^2}{4t})\mathrm{Id}_N. \tag{5.13}$$

Any matrix of size $N \times N$ can naturally be regarded as a linear operator on the Hilbert space $\mathbb{C}^N$, so we let $\|\cdot\|$ denote its operator norm. Let $m \in \mathbb{N}$ with $m > \frac{d}{2}$. Let V denote either U or 0. Let $\mathbf{G}_V^{(m)}$ denote the integral kernel of the operator $(1+\Delta_V)^{-m}$. In later sections in case $N = 1$ we also write $G_V^{(m)}$ for $\mathbf{G}_V^{(m)}$. It is known that

$$\mathbf{G}_0^{(m)}(x,x) = \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!}\mathrm{Id}_N. \tag{5.14}$$

For any $R > 0$ define

$$J_m(R;t) = \inf_{\psi \in A_R} J_m(\psi;t) \quad (R > 0), \tag{5.15}$$

where A_R is the set of real-valued functions ψ in $C^{2m}(\mathbb{R})$ such that $\mathrm{Supp}(1-\psi) \subset (-R,R)$, and

$$J_m(\psi;t) = \int_{\mathbb{R}} \left|(1-\frac{d^2}{ds^2})^m \left(\psi(s)e^{-\frac{s^2}{4t}}\right)\right| ds. \tag{5.16}$$

Theorem 5.3.1. *The following pointwise estimate holds for the heat kernel:*

$$\begin{aligned}&\|\mathbf{K}_U(x,y;t) - \mathbf{K}_0(x,y;t)\| \\ &\quad \le \Big(\big(\|\mathbf{G}_U^{(m)}(x,x)\|\|\mathbf{G}_U^{(m)}(y,y)\|\big)^{\frac{1}{2}} + \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!}\Big)\frac{J_m(\rho(x)+\rho(y);t)}{2\sqrt{\pi t}}.\end{aligned}$$

Proof. Let $x, y \in U$, $v, w \in \mathbb{C}^N$, and let $\psi \in A_R$ where $R = \rho(x) + \rho(y)$. Denote $\delta_x^{(v)} = \delta_x \otimes v$, where δ_x is the Dirac delta function at x. Here

$$\delta_x \otimes v = \begin{pmatrix} v_1\delta_x \\ \vdots \\ v_N\delta_x \end{pmatrix} \quad \text{where} \quad v = \begin{pmatrix} v_1 \\ \vdots \\ v_N \end{pmatrix}.$$

Strictly speaking, $\delta_x \otimes v$ is not in the domain of the self-adjoint operators $e^{-t\Delta_V}$ and $\cos(s\sqrt{\Delta_V})$. So to be clear, we actually let $\delta_x^{(v)}$ be short for a $C_c^\infty(U;\mathbb{C}^N)$ approximation of $\delta_x \otimes v$ in the distributional sense. For example, one can either regard $\delta_x^{(v)}$ as an element in $C_c^\infty(U;\mathbb{C}^N)$ with sufficiently small support that is sufficiently close to $\delta_x \otimes v$, or treat any formula related to $\delta_x^{(v)}$ just as its limit. In this manner letting ϕ_1 (ϕ_2) be a $C_c^\infty(U)$ function with integral one and support contained in a small neighborhood of x (y), then $\delta_x \otimes v$ ($\delta_y \otimes w$) needs to be replaced by

$$\phi_1 \otimes v = \begin{pmatrix} v_1\phi_1 \\ \vdots \\ v_N\phi_1 \end{pmatrix} \quad \left(\phi_2 \otimes w = \begin{pmatrix} w_1\phi_2 \\ \vdots \\ w_N\phi_2 \end{pmatrix}\right),$$

which is a $C_c^\infty(U;\mathbb{C}^N)$ function. If the reader prefers the notations $\phi_1 \otimes v$, $\phi_2 \otimes w$, then it suffices to follow our argument below and finally take a suitable limit. It is well known (e.g. [154]) that

$$e^{-t\Delta_V} = \frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}} \cos(s\sqrt{\Delta_V})e^{-\frac{s^2}{4t}}ds,$$

which implies (see the next page for details) that

$$e^{-t\Delta_V} = \frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}} \cos(s\sqrt{\Delta_V})(1-\psi(s))e^{-\frac{s^2}{4t}}ds + \frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}}(1+\Delta_V)^{-m}\cos(s\sqrt{\Delta_V})(1-\frac{d^2}{ds^2})^m(\psi(s)e^{-\frac{s^2}{4t}})ds. \tag{5.17}$$

According to Proposition 5.2.2 we see that if $|s_1| < \rho(x)$ ($|s_2| < \rho(y)$) then $\cos(s_1\sqrt{\Delta_0})\delta_x^{(v)}$ ($\cos(s_2\sqrt{\Delta_0})\delta_y^{(w)}$) has compact support in U and agrees with $\cos(s_1\sqrt{\Delta_U})\delta_x^{(v)}$ ($\cos(s_2\sqrt{\Delta_U})\delta_y^{(w)}$). Note any $s \in \mathbb{R}$ with $|s| < \rho(x)+\rho(y)$ can be written as $s = s_1 + s_2$ with $|s_1| < \rho(x)$, $|s_2| < \rho(y)$, $s_1 s_2 \geq 0$. With this decomposition available and by considering

$$\cos(s\sqrt{\Delta_V}) = 2\cos(s_1\sqrt{\Delta_V})\cos(s_2\sqrt{\Delta_V}) - \cos((s_1-s_2)\sqrt{\Delta_V})\cos(0\sqrt{\Delta_V})$$

as well as $|s_1 - s_2| < \max\{\rho(x),\rho(y)\}$, $0 < \min\{\rho(x),\rho(y)\}$, one obtains

$$\langle \delta_x^{(v)}, \cos(s\sqrt{\Delta_U})\delta_y^{(w)}\rangle - \langle \delta_x^{(v)}, \cos(s\sqrt{\Delta_0})\delta_y^{(w)}\rangle = 0 \tag{5.18}$$

for any $s \in \mathbb{R}$ with $|s| < \rho(x)+\rho(y)$. As $\mathrm{supp}(1-\psi) \subset (-\rho(x)-\rho(y), \rho(x)+\rho(y))$, we get

$$(1-\psi(s))\langle \delta_x^{(v)}, \cos(s\sqrt{\Delta_U})\delta_y^{(w)}\rangle - (1-\psi(s))\langle \delta_x^{(v)}, \cos(s\sqrt{\Delta_0})\delta_y^{(w)}\rangle = 0 \tag{5.19}$$

for any $s \in \mathbb{R}$. On the other hand, note

$$\langle \delta_x^{(v)}, (1+\Delta_V)^{-m}\cos(s\sqrt{\Delta_V})\delta_y^{(w)}\rangle = \langle (1+\Delta_V)^{-\frac{m}{2}}\delta_x^{(v)}, \cos(s\sqrt{\Delta_V})(1+\Delta_V)^{-\frac{m}{2}}\delta_y^{(w)}\rangle,$$

and by applying the Cauchy-Schwarz inequality several times we get

$$\begin{aligned} |\langle \delta_x^{(v)}, (1+\Delta_V)^{-m}\cos(s\sqrt{\Delta_V})\delta_y^{(w)}\rangle| &= |\langle (1+\Delta_V)^{-\frac{m}{2}}\delta_x^{(v)}, \cos(s\sqrt{\Delta_V})(1+\Delta_V)^{-\frac{m}{2}}\delta_y^{(w)}\rangle| \\ &\leq |(1+\Delta_V)^{-\frac{m}{2}}\delta_x^{(v)}||(1+\Delta_V)^{-\frac{m}{2}}\delta_y^{(w)}| \\ &\leq |v||w|\big(\|\mathbf{G}_V^{(m)}(x,x)\|\|\mathbf{G}_V^{(m)}(y,y)\|\big)^{1/2} \end{aligned} \tag{5.20}$$

for any $s \in \mathbb{R}$. Combining (5.19), (5.20), (5.14) with (5.17) suffices to conclude the proof. □

The prototype of (5.17) appeared in [16] and we explain why it is a correct fact. Since both sides of (5.17) are bounded operators, it suffices to show that

$$\langle e^{-t\Delta_V}\varphi_1, \varphi_2\rangle = \frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}}\langle \cos(s\sqrt{\Delta_V})\varphi_1, \varphi_2\rangle(1-\psi(s))e^{-\frac{s^2}{4t}}ds + \frac{1}{2\sqrt{\pi t}}\int_{\mathbb{R}}\langle (1+\Delta_V)^{-m}\cos(s\sqrt{\Delta_V})\varphi_1, \varphi_2\rangle(1-\frac{d^2}{ds^2})^m(\psi(s)e^{-\frac{s^2}{4t}})ds$$

for any $\varphi_1, \varphi_2 \in C_c^\infty(U;\mathbb{C}^N)$. According to the discussion in §5.2.1, one can apply integration by parts to the right-hand side of the above equality, and thus obtain (5.17).

This rest of this section is devoted to bounding $J_m(R;t)$ with $R = \rho(x)+\rho(y)$, while the next section is devoted to bounding $\|\mathbf{G}_U^{(m)}(x,x)\|$. In general we suppose $R > 0$ is arbitrary. The Hermite polynomials

$$H_n(s) = (-1)^n e^{s^2}\frac{d^n}{ds^n}e^{-s^2} \quad (n = 0,1,2,\ldots)$$

can be written as

$$H_n(s) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^k n!}{k!(n-2k)!}(2s)^{n-2k},$$

from which it is easy to deduce that

$$\frac{d^n}{ds^n}(e^{-\frac{s^2}{4t}}) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-\frac{1}{2})^n(-1)^k n!}{k!(n-2k)!} t^{k-n} s^{n-2k} e^{-\frac{s^2}{4t}} \quad (n = 0, 1, 2, \ldots).$$

Consequently, by Leibniz's rule one gets for any non-negative integer $n \leq 2m$ that

$$\frac{d^n}{ds^n}\left(\psi(s)e^{-\frac{s^2}{4t}}\right) = \sum_{j=0}^{n} \sum_{k=0}^{\lfloor \frac{j}{2} \rfloor} \binom{n}{j} \psi^{(n-j)} \frac{(-\frac{1}{2})^j(-1)^k j!}{k!(j-2k)!} t^{k-j} s^{j-2k} e^{-\frac{s^2}{4t}}.$$

To optimize the choice of cutoff functions, we first let ψ_0 denote a fixed real-valued function in $C^{2m}(\mathbb{R})$ such that $\psi_0(s) = 0$ for $s \leq 0$, and $\psi_0(s) = 1$ for $s \geq 1$. Later on we will give concrete examples of ψ_0 and thus

$$M_j(\psi_0) = \max_{0 \leq s \leq 1} \left| \frac{d^j \psi_0}{ds^j}(s) \right| \quad (j = 0, 1, \ldots, 2m)$$

can be explicitly determined. Then for any $0 < \epsilon_1 < \epsilon_2 < R$, define

$$\psi_{\epsilon_1, \epsilon_2}(s) = \psi_0\left(\frac{|s| - \epsilon_1}{\epsilon_2 - \epsilon_1}\right),$$

which is an even function in $C^{2m}(\mathbb{R})$ with $\mathrm{Supp}(1 - \psi_{\epsilon_1,\epsilon_2}) \subset (-R, R)$. We let the parameters ϵ_1, ϵ_2 (depending on both R and t) behave in the following way:

- $\epsilon_2 \to R$;
- $\epsilon_2 - \epsilon_1 \equiv \frac{2t}{R}$.

With the help of Lemma 5.3.3, it is not hard to show that, if $0 < t \leq \frac{R^2}{8}$, then

$$\lim_{\epsilon_2 \to R} \int_{\mathbb{R}} \left| \frac{d^n}{ds^n}(\psi_{\epsilon_1,\epsilon_2}(s)e^{-\frac{s^2}{4t}}) \right| ds \leq Z(n, \psi_0, R; t)e^{-\frac{R^2}{4t}} \quad (n \leq 2m), \tag{5.21}$$

where $Z(n, \psi_0, R; t)$ is short for the rational function

$$\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!\lceil \frac{n-2k-1}{2} \rceil! M_0(\psi_0) e^2 R^{n-2k-1}}{2^{2n-2k-1} k!(n-2k)!} t^{1+k-n} + \sum_{j=0}^{n-1} \sum_{k=0}^{\lfloor \frac{j}{2} \rfloor} \frac{n! M_{n-j}(\psi_0) e R^{n-2k-1}}{2^{n-2} k!(j-2k)!(n-j)!} t^{1+k-n}.$$

In general, it follows directly from Leibniz's rule and (5.21) that

Proposition 5.3.2. *Suppose* $0 < t \leq \frac{R^2}{8}$. *Then*

$$J_m(R; t) \leq \sum_{n=0}^{m} \binom{m}{n} Z(2n, \psi_0, R; t)e^{-\frac{R^2}{4t}}.$$

Lemma 5.3.3. *If β is a non-negative integer and if $\rho \geq 2\sqrt{t}$, then*

$$\int_\rho^\infty s^\beta e^{-\frac{s^2}{4t}} ds \leq \left\lceil \frac{\beta-1}{2} \right\rceil ! 2e\rho^{\beta-1} t e^{-\frac{\rho^2}{4t}}.$$

Proof. Note first

$$\int_\rho^\infty s^\beta e^{-\frac{s^2}{4t}} ds = 2^\beta t^{\frac{\beta+1}{2}} \Gamma(\frac{\beta+1}{2}, \frac{\rho^2}{4t}),$$

where $\Gamma(\cdot,\cdot)$ is the upper incomplete Gamma function. If $\frac{\beta+1}{2}$ is a positive integer, then it is known that $\Gamma(\frac{\beta+1}{2}, r) = (\frac{\beta-1}{2})!\, e^{-r} \sum_{k=0}^{\frac{\beta-1}{2}} \frac{r^k}{k!}$ for all $r > 0$. This partially proves the lemma simply by considering $\frac{\rho^2}{4t} \geq 1$. If $\frac{\beta+1}{2}$ is a positive half-integer, then we can use $\Gamma(\frac{\beta+1}{2}, r) \leq \frac{1}{\sqrt{r}} \Gamma(\frac{\beta+2}{2}, r)$ and the previous explicit formula for $\Gamma(\frac{\beta+2}{2}, r)$ to prove the remaining part of the lemma. This finishes the proof. □

Although there are many test functions for ψ_0, we use an interpolating polynomial because $M_j(\psi_0)$ can be determined rather easily. For any $n \in \mathbb{N}$, there exists a unique polynomial P_n of degree $\leq 2n+1$ such that $P_n(0) = 0$, $P_n(1) = 1$, and

$$\frac{d^i}{ds^i} P_n \Big|_{s=0} = \frac{d^i}{ds^i} P_n \Big|_{s=1} = 0 \quad (1 \leq i \leq n).$$

We then define a function $\widetilde{P}_n$ on $\mathbb{R}$ such that it agrees with P_n on $[0,1]$, equals 0 on $(-\infty, 0)$, and equals 1 on $(1, \infty)$. It is easy to check that $\widetilde{P}_n \in C^n(\mathbb{R})$. This means in particular that one can set $\psi_0 = \widetilde{P}_{2m}$. A few examples of P_n are listed below:

$$\begin{aligned}
P_1(s) &= 3s^2 - 2s^3, \\
P_2(s) &= 10s^3 - 15s^4 + 6s^5, \\
P_3(s) &= 35s^4 - 84s^5 + 70s^6 - 20s^7, \\
P_4(s) &= 126s^5 - 420s^6 + 540s^7 - 315s^8 + 70s^9.
\end{aligned}$$

5.4 Heat kernel bounds (II)

Let $m \in \mathbb{N}$ with $m > \frac{d}{2}$. In this section we establish a universal upper bound for $\|\mathbf{G}_U^{(m)}(x,x)\|$ only in terms of $\rho(x)$. Let ω_d denote the volume of the unit ball in $\mathbb{R}^d$, $B(\cdot,\cdot)$ the Beta function, $\rho(x,y) = \min(\rho(x), \rho(y))$ and $\gamma_d = \lceil \frac{d+1}{2} \rceil$. Define a series of constants as follows:

$$\begin{aligned}
C_d^{(1)} &= \omega_d (2\pi)^{-d}, \\
C_d^{(2)} &= d C_d^{(1)} (2\pi^{-1} (C_d^{(3)})^2 + C_d^{(3)}), \\
C_d^{(3)} &= 2\gamma_d 3^{\frac{1}{2\gamma_d}}, \\
C_d^{(4)} &= C_d^{(1)} + \frac{d-1}{d} 2^{d-2} C_d^{(2)}, \\
C_d^{(5)} &= 2^{d-2} C_d^{(2)} ((C_d^{(3)})^{d-1} + \frac{1}{d}), \\
C_d^{(6)} &= m C_d^{(4)} B(1 + \frac{d}{2}, m - \frac{d}{2}).
\end{aligned}$$

Theorem 5.4.1. *As (non-negative) self-adjoint matrices we have*

$$\mathbf{G}_U^{(m)}(x,x) \le \big(C_d^{(5)}\rho(x)^{-d} + C_d^{(6)}\big)\mathrm{Id}_N.$$

Corollary 5.4.2. *The following pointwise estimate holds for the heat kernel:*

$$\|\mathbf{K}_U(x,y;t) - \mathbf{K}_0(x,y;t)\| \le \big(C_d^{(5)}\rho(x,y)^{-d} + C_d^{(6)} + \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!}\big) \cdot \frac{J_m(\rho(x)+\rho(y);t)}{2\sqrt{\pi t}}.$$

Theorem 5.4.3. *There exist constants C_1, C_2 depending only on d such that if $t \le \frac{(\rho(x)+\rho(y))^2}{8}$ then*

$$\|\mathbf{K}_U(x,y;t) - \mathbf{K}_0(x,y;t)\| \le \big(C_1\rho(x,y)^{-d} + C_2\big) \cdot \frac{\exp\left(-\frac{(\rho(x)+\rho(y))^2}{4t}\right)}{t^{2\lceil\frac{d+1}{2}\rceil-\frac{1}{2}}}.$$

It follows on from Theorem 5.4.1 that $\|\mathbf{G}_U^{(m)}(x,x)\| \le C_d^{(5)}\rho(x)^{-d} + C_d^{(6)}$. Thus Corollary 5.4.2 is an immediate consequence of Theorem 5.3.1. Theorem 5.4.3 is the main result of this chapter. It follows from Proposition 5.3.2 and Corollary 5.4.2. Obviously, the constants C_1, C_2 in Theorem 5.4.3 can be explicitly given. In the rest of this section, we provide a proof of Theorem 5.4.1.

Proof of Theorem 5.4.1. According to the spectral theorem one has $\Delta_U = \int_0^\infty \lambda\, d\Pi(\lambda)$, where $\Pi(\lambda)$ ($\lambda \ge 0$) denotes the spectral projection of Δ_U onto the interval $[0,\lambda]$. The so-called spectral function $\mathbf{e}(x,y;\lambda)$, defined to be the integral kernel of $\Pi(\lambda)$, is smooth in $U \times U$ for each fixed λ.

If $N = 1$ we also write $e(x,y;\lambda)$ for $\mathbf{e}(x,y;\lambda)$. Safarov [130, Cor. 3.1] proved for every $x \in U$ and all $\lambda > 0$ that

$$e(x,x;\lambda) \le C_d^{(1)}\lambda^{d/2} + \frac{C_d^{(2)}}{\rho(x)}\Big(\lambda^{1/2} + \frac{C_d^{(3)}}{\rho(x)}\Big)^{d-1}. \tag{5.22}$$

We should mention that Safarov originally established (5.22) by understanding $e(x,x;\lambda)$ as the integral kernel of $\frac{\Pi(\lambda-0)+\Pi(\lambda+0)}{2}$. As the right-hand side of (5.22) is a continuous function of $\lambda > 0$, we see that (5.22) also holds for our choice of the spectral function. The key points (see explanations at the end of this section) for proving (5.22) are the facts (see [130, Lemma 2.7, Cor. 3.1]) that $\chi_+(\lambda)e(x,x;\lambda^2)$ is a non-decreasing function of λ on $\mathbb{R}$, and the cosine Fourier transform of

$$(C_d^{(1)})^{-1} \cdot \frac{d}{d\lambda}\big(\chi_+(\lambda)e(x,x;\lambda^2)\big)$$

coincides on the interval $(-\rho(x),\rho(x))$ with the cosine Fourier transform of $d\lambda_+^{d-1}$. Here χ_+ is the characteristic function of the positive axis. The latter property can be seen from the finite propagation speed for wave equations.

In the vector-valued situation, we claim as (non-negative) self-adjoint matrices,

$$\mathbf{e}(x,x;\lambda) \le \Big(C_d^{(1)}\lambda^{d/2} + \frac{C_d^{(2)}}{\rho(x)}\Big(\lambda^{1/2} + \frac{C_d^{(3)}}{\rho(x)}\Big)^{d-1}\Big)\mathrm{Id}_N \tag{5.23}$$

for every $x \in U$ and all $\lambda > 0$. To this end we see once again from the finite propagation speed for wave equations that, for each fixed unit vector $v \in \mathbb{C}^N$, the cosine Fourier transform of

$$(C_d^{(1)})^{-1} \cdot \frac{d}{d\lambda}\big(\chi_+(\lambda)\langle \delta_x^{(v)}, \Pi(\lambda^2)\delta_x^{(v)}\rangle\big)$$

coincides on the interval $(-\rho(x), \rho(x))$ with the cosine Fourier transform of $d\lambda_+^{d-1}$. On the other hand, $\chi_+(\lambda)\langle \delta_x^{(v)}, \Pi(\lambda^2)\delta_x^{(v)}\rangle$ is a non-decreasing function of λ on $\mathbb{R}$. So similar to (5.22) we have

$$\langle \delta_x^{(v)}, \Pi(\lambda)\delta_x^{(v)}\rangle \le C_d^{(1)}\lambda^{d/2} + \frac{C_d^{(2)}}{\rho(x)}\Big(\lambda^{1/2} + \frac{C_d^{(3)}}{\rho(x)}\Big)^{d-1} \quad (x \in U, \lambda > 0), \tag{5.24}$$

which proves (5.23). For simplicity, applying Hölder's and Young's inequalities to the right-hand side of (5.23) gives for every $x \in U$ and all $\lambda > 0$ that

$$\mathbf{e}(x, x; \lambda) \le (C_d^{(4)}\lambda^{d/2} + C_d^{(5)}\rho(x)^{-d})\mathrm{Id}_N. \tag{5.25}$$

According to the functional calculus of self-adjoint operators, we have

$$(1 + \Delta_U)^{-m} = \int_0^\infty \frac{1}{(1+\lambda)^m} d\Pi(\lambda).$$

Considering $m > \frac{d}{2}$, (5.25), $\mathbf{e}(x, x; 0) \ge 0$, and the following equivalent representation of the classical Beta function

$$B(\alpha, \beta) = \int_0^\infty \frac{\lambda^{\alpha-1}}{(1+\lambda)^{\alpha+\beta}} d\lambda \quad (\mathrm{Re}(\alpha) > 0,\ \mathrm{Re}(\beta) > 0),$$

one can use integration by parts to get (see §5.5 for details)

$$\begin{aligned} \mathbf{G}_U^{(m)}(x, x) &= \int_0^\infty \frac{1}{(1+\lambda)^m} d\mathbf{e}(x, x; \lambda) \\ &= m\int_0^\infty \frac{\mathbf{e}(x, x; \lambda)}{(1+\lambda)^{m+1}} d\lambda - \mathbf{e}(x, x; 0) \\ &\le \Big(m\int_0^\infty \frac{C_d^{(4)}\lambda^{d/2} + C_d^{(5)}\rho(x)^{-d}}{(1+\lambda)^{m+1}} d\lambda\Big)\mathrm{Id}_N \\ &= \big(C_d^{(6)} + C_d^{(5)}\rho(x)^{-d}\big)\mathrm{Id}_N. \end{aligned} \tag{5.26}$$

This finishes the proof of Theorem 5.4.1. □

We finish this section with some explanations on Safarov's proof of (5.22). Actually Safarov first established general Fourier Tauberian theorems, then studied as applications the growth of spectral functions. With regard to the general theorems, we refer the reader to [130] for the detailed proofs, and to [131] for some nice interpretations. From now on we focus on the spectral functions, and write e_{Δ_U} for e to clearly emphasize the dependence on Δ_U. Obviously (e.g. [150, (3.2)]),

$$e_{\Delta_0}(x, x; \lambda) = C_d^{(1)}\lambda^{d/2} \quad (\lambda > 0).$$

So the natural questions for general Δ_U are 1) where does the contribution of the term

$$\frac{C_d^{(2)}}{\rho(x)}\Big(\lambda^{1/2}+\frac{C_d^{(3)}}{\rho(x)}\Big)^{d-1}$$

on the right-hand side of (5.22) come from, and 2) why does it depend on the distance $\rho(x)$ of x to the boundary of U. To answer both questions we assume for simplicity that U is a bounded domain, and Δ_U has a discrete spectral resolution $\{\lambda_j,\phi_j\}_{j=1}^{\infty}$, where the eigenfunctions ϕ_j are chosen to be real-valued. Then

$$e_{\Delta_U}(x,y;\lambda)=\sum_{\lambda_j\le\lambda}\phi_j(x)\phi_j(y)$$

and, consequently,

$$\frac{\partial}{\partial\lambda}e_{\Delta_U}(x,y;\lambda^2)=\sum_{j=1}^{\infty}2\lambda\delta_{\lambda_j}(\lambda^2)\phi_j(x)\phi_j(y).$$

It is well known that the asymptotic behaviour of a sufficiently nice function $f(\lambda)$ for large λ is determined by singularities of its Fourier transform. So we study

$$\mathscr{F}(\frac{\partial}{\partial\lambda}e_{\Delta_U}(x,y;\lambda^2))(t)=\int_{\mathbb{R}}e^{-\mathrm{i}\lambda t}\frac{\partial}{\partial\lambda}e_{\Delta_U}(x,y;\lambda^2)d\lambda=-4\mathrm{i}\sum_{j=1}^{\infty}\sqrt{\lambda_j}\sin(t\sqrt{\lambda_j})\phi_j(x)\phi_j(y),$$

which is precisely the time derivative of the fundamental solution $u_{\Delta_U}(x,y;t)$ of the following wave equation

$$\begin{cases}\frac{\partial^2u}{\partial t^2}=\Delta u,\\ u|_{t=0}=4\delta(x-y),\\ \frac{\partial u}{\partial t}\Big|_{t=0}=0,\end{cases}$$

with an appropriate boundary condition given by Δ_U. If we could well describe singularities of $u_{\Delta_U}(x,y;t)$, then, taking the inverse Fourier transform, we would obtain an asymptotic formula for $\frac{\partial}{\partial\lambda}e_{\Delta_U}(x,y;\lambda^2)$, which yields a natural asymptotic formula for $e_{\Delta_U}(x,y;\lambda)$. According to finite propagation speed estimates (Propositions 5.2.1 and 5.2.2), $u_{\Delta_U}(x,x;t)$ completely agrees with $u_{\Delta_0}(x,x;t)$ whenever $|t|<\rho(x)$. So in principle we have already answered the second question, and it remains only to deal with $u_{\Delta_U}(x,x;t)$, $u_{\Delta_0}(x,x;t)$ both for $|t|>\rho(x)$. But this is the central part of the analysis in [130], to which the reader can refer for the details of the deduction of the explicit constants. By the way, one may feel that the above strategy is very similar to the proof of Theorem 5.3.1, and it should not be a coincidence at all.

5.5 Dirichlet boundary conditions

Let $m\in\mathbb{N}$ with $m>\frac{d}{2}$. In this section we give a replacement of Theorem 5.4.1 for $G_U^{(m)}(x,x)$ where $G_U^{(m)}$ is interpreted in accordance with the choice that Δ_U denotes the Dirichlet Laplacian on an open set $U\subset\mathbb{R}^d$. Note first (e.g. [21, (3.33)], [34, §3.4])

$$G_U^{(m)}(x,x)=\frac{1}{(m-1)!}\int_0^{\infty}t^{m-1}e^{-t}K_U^{(+)}(x,x;t)dt, \tag{5.27}$$

which combined with the full domain monotonicity of the Dirichlet heat kernel (5.4) yields

$$G_U^{(m)}(x,x) \le G_{\mathbb{R}^d}^{(m)}(x,x) \quad (x \in U). \tag{5.28}$$

But it is well known (see (5.14)) that

$$G_{\mathbb{R}^d}^{(m)} = \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!}.$$

So we get

$$G_U^{(m)}(x,x) \le \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!} \quad (x \in U), \tag{5.29}$$

which yields from Theorem 5.3.1 that

Theorem 5.5.1. *The following pointwise estimate holds for the Dirichlet heat kernel:*

$$|K_U^{(+)}(x,y;t) - (4\pi t)^{-d/2}\exp(-\frac{|x-y|^2}{4t})| \le \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!} \cdot \frac{J_m(\rho(x)+\rho(y);t)}{\sqrt{\pi t}}.$$

We should mention that the prototype of Theorem 5.3.1 first appeared in [16] by Bironneau for two-dimensional Dirichlet boundary problems. But unfortunately, both Theorem 7.5 in [16] and Theorem 5.5.1 for $d = 2$ are weaker than M. van den Berg's (5.7) for the short-time diagonal element of the Dirichlet heat kernel. Even so, one can check that Theorem 5.5.1 is a slight improvement of (5.7) if $d \ge 5$.

For completeness, we provide a short proof of (5.27). According to the functional calculus of self-adjoint operators, one gets

$$(1+\Delta_U^{(+)})^{-m} = \frac{1}{(m-1)!}\int_0^\infty t^{m-1}e^{-t}e^{-t\Delta_U^{(+)}}dt,$$

and consequently

$$\langle (1+\Delta_U^{(+)})^{-m}\phi,\psi\rangle = \frac{1}{(m-1)!}\int_0^\infty t^{m-1}e^{-t}\langle e^{-t\Delta_U^{(+)}}\phi,\psi\rangle dt$$

for any $\phi,\psi \in C_c^\infty(U)$. Letting $\{\phi_n\}_{n=1}^\infty$ be an approximation of identity at $x \in U$, that is, each ϕ_n is a non-negative $C_c^\infty(U)$ function with integral one and support contained in $B(x,1/n)$, we get

$$\langle (1+\Delta_U^{(+)})^{-m}\phi_n,\phi_n\rangle = \frac{1}{(m-1)!}\int_0^\infty t^{m-1}e^{-t}\langle e^{-t\Delta_U^{(+)}}\phi_n,\phi_n\rangle dt. \tag{5.30}$$

Note also

$$0 \le \langle e^{-t\Delta_U^{(+)}}\phi_n,\phi_n\rangle = \int_U\int_U K_U^{(+)}(y,z;t)\phi_n(y)\phi_n(z)dydz \le \frac{1}{(4\pi t)^{d/2}}, \tag{5.31}$$

and $t^{m-\frac{d}{2}-1}e^{-t}$ is a non-negative integrable function on $(0,\infty)$. Thus one can use Lebesgue's dominated convergence theorem to deduce (5.27) from (5.30).

In essentially the same way, we can use Lebesgue's dominated convergence theorem to give a rigorous proof of (5.26). Here (5.24) or (5.25) plays the role of $K_U^{(+)}(y,z;t) \le (4\pi t)^{-d/2}$. We

need be slightly careful as the right-hand side of (5.25) depends on the distance of x to the boundary of U. But this is not a big problem as any sequence of functions of approximation of identity at $x \in U$ will eventually be supported in $B(x, \frac{\rho(x)}{2})$, which means in particular that the dominating function can be chosen depending only on $\frac{\rho(x)}{2}$. For example, let ϕ be an arbitrary non-negative function in $C_c^\infty(U)$ with integral one and support contained in $B(x, \frac{\rho(x)}{2})$. We then have

$$\langle \begin{pmatrix} \phi \\ \vdots \\ \phi \end{pmatrix}, \Pi(\lambda) \begin{pmatrix} \phi \\ \vdots \\ \phi \end{pmatrix} \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} e_{ij}(x_{ij}, y_{ij}; \lambda)$$

for some $x_{ij}, y_{ij} \in B(x, \frac{\rho(x)}{2})$, where $\mathbf{e} = (e_{ij})$. Similar to the proof of (5.20) one can deduce from (5.24) or (5.25) that

$$|e_{ij}(x_{ij}, y_{ij}; \lambda)| \leq \sqrt{e_{ii}(x_{ij}, x_{ij}; \lambda) e_{ij}(y_{ij}, y_{ij}; \lambda)} \leq C_d^{(4)} \lambda^{d/2} + C_d^{(5)} (\frac{\rho(x)}{2})^{-d}.$$

This implies that

$$0 \leq \langle \begin{pmatrix} \phi \\ \vdots \\ \phi \end{pmatrix}, \Pi(\lambda) \begin{pmatrix} \phi \\ \vdots \\ \phi \end{pmatrix} \rangle \leq N^2 \Big(C_d^{(4)} \lambda^{d/2} + C_d^{(5)} (\frac{\rho(x)}{2})^{-d} \Big), \tag{5.32}$$

which plays the role of (5.31) during the application of Lebesgue's theorem.

5.6 Neumann boundary conditions

Recall $K_U^{(-)}(x, y; t)$ denotes the Neumann heat kernel for a smooth bounded open set $U \subset \mathbb{R}^d$. As an application of Theorem 5.4.3 (or Proposition 5.3.2 and Theorem 5.6.2 with $m = \lceil \frac{d+1}{2} \rceil$), there exists a positive function h on U such that if $0 < t \leq \frac{\rho(x)^2}{2}$ then

$$K_U^{(-)}(x, x; t) \leq (4\pi t)^{-d/2} + h(x) \cdot t^{-\alpha} \cdot \exp(-\frac{\rho(x)^2}{t}), \tag{5.33}$$

where $\alpha = 2\lceil \frac{d+1}{2} \rceil - \frac{1}{2}$. This answers a question raised by Lacey [92] who conjectured that for the class of smooth bounded strictly star-shaped domains (5.33) holds for some $\alpha > \frac{d}{2}$ as long as time t is sufficiently small. Lacey also asked to extend the main result in [92] to unbounded domains, domains with non-smooth boundary, or more general boundary conditions. Because of Theorem 5.4.3 this is indeed doable for the diagonal element of the Neumann heat kernel.

In the following we will give a replacement of Theorem 5.4.1 for $G_U^{(m)}(x, x)$ without using Safarov's estimates. Here $G_U^{(m)}$ is interpreted in accordance with the choice that Δ_U denotes the Neumann Laplacian on U. This can be done by mainly appealing to the partial domain monotonicity of the Neumann heat kernel (see (5.3)). Let $\Delta_d^{(-)}$ ($\mathbb{U}_d(x, y; t)$) be short for the Neumann Laplacian (heat kernel) on (for) the d-dimensional unit open ball.

Theorem 5.6.1. *The following pointwise estimate holds:*

$$G_U^{(m)}(x, x) \leq \frac{\rho(x)^{2m-d}}{(m-1)! \omega_d} \cdot \int_0^1 t^{m-1} \mathrm{Tr}(e^{-t\Delta_d^{(-)}}) dt + \frac{\mathrm{Tr}(e^{-\Delta_d^{(-)}})}{\omega_d \rho(x)^d}.$$

Proof. Similar to (5.27) one can show that (see the end of this section for details)

$$G_U^{(m)}(x,x) = \frac{1}{(m-1)!}\int_0^\infty t^{m-1}e^{-t}K_U^{(-)}(x,x;t)dt. \tag{5.34}$$

This combined with the partial domain monotonicity of the Neumann heat kernel (5.3) yields

$$G_U^{(m)}(x,x) \le G_{B_x}^{(m)}(x,x) \quad (x \in U). \tag{5.35}$$

The Pascu-Gageonea resolution [116] of the Laugesen-Morpurgo conjecture [93] says that

$$\mathbb{U}_d(x,x;t) < \mathbb{U}_d(y,y;t) \tag{5.36}$$

holds for all $t > 0$ and all x, y in the d-dimensional unit ball with $|x| < |y|$. This result implies that

$$\mathbb{U}_d(0,0;t) < \frac{\mathrm{Tr}(e^{-t\Delta_d^{(-)}})}{\omega_d}. \tag{5.37}$$

Now let $x \in U$ be fixed. It is straightforward to verify that

$$K_{B_x}^{(-)}(x,x;t) = \frac{\mathbb{U}_d\big(0,0;\dfrac{t}{\rho(x)^2}\big)}{\rho(x)^d}. \tag{5.38}$$

Hence by considering (5.35), (5.34) with U replaced by B_x, (5.38) and (5.37), we get

$$\begin{aligned}
G_U^{(m)}(x,x) &\le \frac{1}{(m-1)!}\cdot\int_0^\infty t^{m-1}e^{-t}\frac{\mathrm{Tr}(e^{-\frac{t}{\rho(x)^2}\Delta_d^{(-)}})}{\omega_d\rho(x)^d}dt \\
&= \frac{\rho(x)^{2m-d}}{(m-1)!\omega_d}\cdot\int_0^\infty t^{m-1}e^{-t\rho(x)^2}\mathrm{Tr}(e^{-t\Delta_d^{(-)}})dt \\
&\le \frac{\rho(x)^{2m-d}}{(m-1)!\omega_d}\cdot\Big(\int_0^1 t^{m-1}\mathrm{Tr}(e^{-t\Delta_d^{(-)}})dt + \mathrm{Tr}(e^{-\Delta_d^{(-)}})\int_0^\infty t^{m-1}e^{-t\rho(x)^2}dt\Big) \\
&= \frac{\rho(x)^{2m-d}}{(m-1)!\omega_d}\cdot\int_0^1 t^{m-1}\mathrm{Tr}(e^{-t\Delta_d^{(-)}})dt + \frac{\mathrm{Tr}(e^{-\Delta_d^{(-)}})}{\omega_d\rho(x)^d},
\end{aligned}$$

where in the last inequality we have used the fact $\mathrm{Tr}(e^{-t\Delta_d^{(-)}}) \le \mathrm{Tr}(e^{-\Delta_d^{(-)}})$ for all $t \ge 1$. This finishes the proof of the theorem. □

Theorem 5.6.2. *Let $U \subset \mathbb{R}^d$ be a smooth bounded open set and let $m \in \mathbb{N}$ be such that $m > \frac{d}{2}$. For any $t > 0$ and any x, y in U one has*

$$\big|K_U^{(-)}(x,y;t) - (4\pi t)^{-d/2}\exp(-\frac{|x-y|^2}{4t})\big| \le N_d(x,y)\cdot\frac{J_m(\rho(x)+\rho(y);t)}{2\sqrt{\pi t}},$$

where

$$\begin{aligned}
N_d(x,y) = &\frac{\displaystyle\int_0^1 t^{m-1}\mathrm{Tr}(e^{-t\Delta_d^{(-)}})dt}{(m-1)!\omega_d}\cdot(\max\{\rho(x),\rho(y)\})^{2m-d} + \frac{\Gamma(m-\frac{d}{2})}{(4\pi)^{\frac{d}{2}}(m-1)!} + \\
&\frac{\mathrm{Tr}(e^{-\Delta_d^{(-)}})}{\omega_d}\cdot(\min\{\rho(x),\rho(y)\})^{-d}.
\end{aligned}$$

This is an application of Theorems 5.3.1 and 5.6.1.

For completeness, we provide a proof of (5.34). In the case of Dirichlet boundary problems, the key point of using Lebesgue's dominated convergence theorem to prove (5.27) is the following upper bound

$$K_U^{(+)}(y,z;t) \leq \frac{1}{(4\pi t)^{d/2}} \tag{5.39}$$

for all $t > 0$ and all y, z close enough to any prescribed $x \in U$. In the case of Neumann boundary problems, we first recall Kendall's intermediate ball theorem [89], which says that if B is a ball of center y contained in U then

$$K_U^{(-)}(y,z;t) \leq K_B^{(-)}(y,z;t) \tag{5.40}$$

for all $t > 0$ and $z \in B$. Suppose $y, z \in B(x, \frac{\rho(x)}{8})$. Obviously, $z \in B(y, \frac{\rho(x)}{4}) \subset B(y, \frac{\rho(x)}{2}) \subset U$. Applying first (5.40) with $B = B(y, \frac{\rho(x)}{2})$ then the Pascu-Gageonea resolution of the Laugesen-Morpurgo conjecture (see (5.36)) gives

$$\begin{aligned}
K_U^{(-)}(y,z;t) &\leq K_B^{(-)}(y,z;t) \quad (\text{Kendall}) \\
&\leq \big(K_B^{(-)}(y,y;t)K_B^{(-)}(z,z;t)\big)^{1/2} \\
&\leq K_B^{(-)}(z,z;t) \quad (\text{Pascu} - \text{Gageonea}) \\
&\leq \frac{\mathrm{tr}(e^{-t\Delta_B^{(-)}})}{|B(y,\frac{\rho(x)}{2})\backslash B(y,\frac{\rho(x)}{4})|} \quad (\text{Pascu} - \text{Gageonea}) \\
&= \frac{\mathrm{tr}(e^{-\frac{4t}{\rho(x)^2}\Delta_d^{(-)}})}{((\frac{\rho(x)}{2})^d - (\frac{\rho(x)}{4})^d)\omega_d},
\end{aligned}$$

which plays the role of (5.39) in the application of Lebesgue's dominated convergence theorem as follows. Letting $\{\phi_n\}_{n=1}^\infty$ be an approximation of identity at $x \in U$ such that each ϕ_n is a non-negative $C_c^\infty(U)$ function with integral one and support contained in $B(x, \min\{\frac{1}{n}, \frac{\rho(x)}{2}\})$, we get

$$\langle (1+\Delta_U^{(-)})^{-m}\phi_n, \phi_n\rangle = \frac{1}{(m-1)!}\int_0^\infty t^{m-1}e^{-t}\langle e^{-t\Delta_U^{(-)}}\phi_n, \phi_n\rangle dt. \tag{5.41}$$

Note also

$$0 \leq \langle e^{-t\Delta_U^{(-)}}\phi_n, \phi_n\rangle = \int_U\int_U K_U^{(-)}(y,z;t)\phi_n(y)\phi_n(z)dydz \leq \frac{\mathrm{tr}(e^{-\frac{4t}{\rho(x)^2}\Delta_d^{(-)}})}{((\frac{\rho(x)}{2})^d - (\frac{\rho(x)}{4})^d)\omega_d}, \tag{5.42}$$

and

$$t^{m-1}e^{-t}\mathrm{tr}(e^{-\frac{4t}{\rho(x)^2}\Delta_d^{(-)}})$$

is a non-negative integrable function on $(0,\infty)$ (e.g. [23]). Thus one can use Lebesgue's dominated convergence theorem to deduce (5.34) from (5.41). We are done.

Chapter 6

Spectral zeta functions

Let U be a bounded open subset of $\mathbb{R}^2$. The spectrum of the Dirichlet Laplacian Δ_U on U consists of a sequence of non-decreasing positive eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$. Weyl's law in two dimensions states that

$$\lim_{n\to\infty} \frac{\lambda_n}{n} = \frac{4\pi}{|U|},$$

where $|U|$ denotes the Lebesgue measure of U. This implies that the spectral zeta function of Δ_U, defined by

$$\zeta_U(s) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s},$$

is analytic on $\mathrm{Re}(s) > 1$. Throughout the chapter we assume that the Dirichlet heat trace for U is of the following small-time asymptotic expansion:

$$\mathrm{tr}(e^{-t\Delta_U}) \sim \sum_{k=0}^{\infty} a_k(U) t^{\frac{k-2}{2}} \quad (t \to 0^+). \tag{6.1}$$

To be clear, the asymptotical notation $\sim$ means that, for any non-negative integer L and any $\epsilon > 0$, there exists a constant C such that

$$\left| \mathrm{tr}(e^{-t\Delta_U}) - \sum_{k=0}^{L} a_k(U) t^{\frac{k-2}{2}} \right| \leq C t^{\frac{L-1}{2}} \quad (0 < t < \epsilon). \tag{6.2}$$

For example, bounded domains with smooth [145] or polygonal [6, 12, 88] boundary have this property. Later on we will see that the spectral zeta function of Δ_U admits a meromorphic continuation to the complex plane $\mathbb{C}$ whose singularities are only simple poles at $\frac{2-k}{2}$ $(k \geq 0)$. The corresponding residues at these simple poles are denoted by $r_k(U)$.

The purpose of this chapter is to make an attempt at calculating some specific values of two-dimensional Dirichlet spectral zeta functions with high precision, depending on in general how precisely the first several hundred or one thousand Dirichlet eigenvalues can be numerically given by other means. In particular, we are interested in approximating

$$\exp\Big(- \frac{d\zeta_U}{ds}\Big|_{s=0} \Big),$$

which is known as the spectral determinant of U, and

$$\frac{1}{2}\Big(\zeta_U(s) - \frac{r_3(U)}{s+\frac{1}{2}}\Big)\Big|_{s=-\frac{1}{2}},$$

which is called the Casimir energy (or vacuum energy) of U in physics [1, 20, 42, 43].

To the best of our knowledge, there are explicit formulae for the spectral determinant only in the event that U is a disk, annulus [159], triangle, rectangle, or regular polygon [4]. Any of these planar regions is determined by no more than three parameters, and in higher dimensions there exist many generalization works [18, 19, 43, 148]. Similarly, explicit formulae for the Casimir energy are known only for certain triangles and all rectangles (see [1] and references therein).

A technical difficulty that allows us to study squares only as examples in this chapter is there are no rigorous completeness tests for sequences of computed eigenvalues generated by computer programs. As an application of Theorem 6.3.2 in this chapter, this issue has been solved effectively in [17], to which we refer the reader for more numerical examples.

6.1 An algorithm

It is well known that

$$\zeta_U(s) = \frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\mathrm{tr}(e^{-t\Delta_U})dt \quad (\mathrm{Re}(s) > 1).$$

For any fixed $s_0 \in \mathbb{C}$, let $L = L_{s_0}$ be an arbitrary non-negative integer such that

$$\mathrm{Re}(s_0) + \frac{L-1}{2} > 0.$$

Note for any $\mathrm{Re}(s) > 1$ and $\epsilon > 0$ that

$$\begin{aligned}\zeta_U(s) - \sum_{k=0}^{L}\frac{a_k(U)\epsilon^{s+\frac{k-2}{2}}}{\Gamma(s)(s+\frac{k-2}{2})} =& \frac{1}{\Gamma(s)}\int_0^\epsilon t^{s-1}\Big(\mathrm{tr}(e^{-t\Delta_U}) - \sum_{k=0}^{L}a_k(U)t^{\frac{k-2}{2}}\Big)dt + \\ & \sum_{n=1}^{\infty}\frac{1}{\Gamma(s)}\int_\epsilon^\infty t^{s-1}e^{-t\lambda_n}dt. \end{aligned} \tag{6.3}$$

Obviously, the right-hand side is analytic on the half-plane $\mathrm{Re}(s) > \frac{1-L}{2}$ because there exists a constant C_ϵ depending only on ϵ such that

$$\Big|\mathrm{tr}(e^{-t\Delta_U}) - \sum_{k=0}^{L}a_k(U)t^{\frac{k-2}{2}}\Big| \le C_\epsilon t^{\frac{L-1}{2}} \quad (0 < t < \epsilon). \tag{6.4}$$

Hence the unique meromorphic continuation of ζ_U to the half-plane $\mathrm{Re}(s) > \frac{1-L}{2}$ still satisfies (6.3). This implies that s_0 is a regular point or at most a simple pole of ζ_U. Around s_0 one can easily show for all non-negative integers j that

$$\begin{aligned}\frac{d^j}{ds^j}\Big(\zeta_U(s) - \sum_{k=0}^{L}\frac{a_k(U)\epsilon^{s+\frac{k-2}{2}}}{\Gamma(s)(s+\frac{k-2}{2})}\Big) =& \int_0^\epsilon \frac{d^j}{ds^j}\Big(\frac{t^{s-1}}{\Gamma(s)}\Big)\Big(\mathrm{tr}(e^{-t\Delta_U}) - \sum_{k=0}^{L}a_k(U)t^{\frac{k-2}{2}}\Big)dt + \\ & \sum_{n=1}^{\infty}\int_\epsilon^\infty \frac{d^j}{ds^j}\Big(\frac{t^{s-1}}{\Gamma(s)}\Big)e^{-t\lambda_n}dt. \end{aligned} \tag{6.5}$$

Formulae (6.3) and (6.5) in this and much general context are known to many authors (e.g. [4, 16, 38, 69, 114, 147, 151, 152]). A typical example is to study the spectral determinant of U in this manner (e.g. [16, 147, 151, 152]). Also, note around $s_0 = -\frac{1}{2}$ that

$$\zeta_U(s) - \frac{a_3(U)\epsilon^{s+\frac{1}{2}}}{\Gamma(s)(s+\frac{1}{2})} = \sum_{\substack{k=0\\k\neq 3}}^{L} \frac{a_k(U)\epsilon^{s+\frac{k-2}{2}}}{\Gamma(s)(s+\frac{k-2}{2})} + \sum_{n=1}^{\infty} \frac{1}{\Gamma(s)} \int_{\epsilon}^{\infty} t^{s-1} e^{-t\lambda_n} dt + \frac{1}{\Gamma(s)} \int_0^{\epsilon} t^{s-1} \Big(\mathrm{tr}(e^{-t\Delta_U}) - \sum_{k=0}^{L} a_k(U) t^{\frac{k-2}{2}} \Big) dt, \tag{6.6}$$

whose precise value at $s_0 = -\frac{1}{2}$ essentially (but in general not precisely, see the tiny difference between Corollaries 6.2.4 and 6.2.5) is the Casimir energy of U.

Based on (6.3) and (6.5) we explain in general how to extract numerical information about the spectral zeta function at a given point. We should mention that the following method is essentially a known strategy, which was first discovered by Strohmaier and Uski [152] as they studied similar problems for hyperbolic surfaces.

1) Following Kac's principle of not feeling the boundary, the coefficients $a_k(U)$ $(k \geq 1)$ are determined by the geometry of the boundary of U. In the case of smooth boundaries there exist explicit formulae for the first few leading coefficients (see [158] for a summary of results), and in the case of polygonal boundaries all of the coefficients are explicitly known [12].

2) Obviously, explicit upper bounds for C_ϵ are needed. One way out is to carefully trace back the details of the proof of (6.4) in the literature. Alternatively, note that C_ϵ should not be far away from $|a_{L+1}(U)|$ provided ϵ is very small. Thus the precise value of $a_{L+1}(U)$ is of practical importance. In particular, in the case of polygonal boundaries M. van den Berg and S. Srisatkunarajah's [12] exponentially decayed upper bounds for the left-hand side of (6.4) will be substantially improved in this chapter.

3) A high precision approximate value of λ_n could yield an approximate value of

$$\int_{\epsilon}^{\infty} \frac{d^j}{ds^j} \Big(\frac{t^{s-1}}{\Gamma(s)} \Big) e^{-t\lambda_n} dt \tag{6.7}$$

with high precision. Note that the MPSpack program, developed systematically by A. Barnett and T. Betcke [7], can provide approximate value of the first several hundred or one thousand Dirichlet eigenvalues with high precision for certain planar domains. On the other hand, for large eigenvalues one can use Weyl's law to well control λ_n and the related formula (6.7).

We should mention that Bironneau [16] obtained lots of numerical estimates on the spectral determinant and Casimir energy for various polygons in Chapter 8 of his doctoral dissertation. For example, he obtained many approximate values in Sections 8.1 – 8.6, and even proposed a conjecture about the extremal properties of the spectral determinant of polygonal regions in Section 8.7 of the dissertation. However, the error estimates stated in Sections 8.1 – 8.6 of [16] are unlikely to be true because the statement of the basic tool Theorem 7.7 therein is not true (see §6.3.1 for details).

6.2 Error estimates

For simplicity let $Z(t)$ denote the partition function $\mathrm{tr}(e^{-t\Delta_U})$, and let $Z_L(t)$ ($L \geq 0$) be short for $\sum_{k=0}^{L} a_k(U) t^{\frac{k-2}{2}}$.

Theorem 6.2.1. *Suppose $\lambda_N \epsilon \geq 2$. Then on the half-plane $\mathrm{Re}(s) > \frac{1-L}{2}$ we have*

$$\left| \frac{d^j}{ds^j}\Big(\zeta_U(s) - \sum_{k=0}^{L} \frac{a_k(U)\epsilon^{s+\frac{k-2}{2}}}{\Gamma(s)(s+\frac{k-2}{2})}\Big) - \sum_{n=1}^{N} \int_{\epsilon}^{\infty} \frac{d^j}{ds^j}\big(\frac{t^{s-1}}{\Gamma(s)}\big) e^{-t\lambda_n} dt \right| \leq$$
$$\int_0^{\epsilon} \Big| \frac{d^j}{ds^j}\big(\frac{t^{s-1}}{\Gamma(s)}\big)\Big| \Big| Z(t) - Z_L(t) \Big| dt + \frac{|U|^2 \lambda_N^2}{4\pi^2 N} \int_{\epsilon}^{\infty} \Big| \frac{d^j}{ds^j}\big(\frac{t^{s-1}}{\Gamma(s)}\big)\Big| e^{-t\lambda_N} dt.$$

Proof. Considering $\lambda_N \epsilon \geq 2$ and $z^2 e^{-z}$ is decreasing on the interval $z \geq 2$, we get

$$(\lambda_n t)^2 e^{-t\lambda_n} \leq (\lambda_N t)^2 e^{-t\lambda_N}$$

for any $n > N$ and $t \geq \epsilon$. The classical Li-Yau inequality [100] says that $\lambda_n \geq \frac{2\pi n}{|U|}$ for any $n \in \mathbb{N}$. Hence for any $t \geq \epsilon$,

$$\sum_{n>N} e^{-t\lambda_n} \leq \sum_{n>N} \frac{|U|^2 \lambda_N^2}{4\pi^2 n^2} e^{-t\lambda_N} \leq \frac{|U|^2 \lambda_N^2}{4\pi^2 N} e^{-t\lambda_N},$$

which suffices to conclude the proof by (6.5). □

Recall

$$\frac{d\Gamma}{ds}\Big|_{s=1} = -\gamma,$$

where $\gamma = 0.57721566490153286060\cdots$ is the Euler-Mascheroni constant. Note

$$\int_{\epsilon}^{\infty} t^{-1} e^{-t\lambda_N} dt = \int_{\lambda_N \epsilon}^{\infty} t^{-1} e^{-t} dt \leq \frac{1}{\lambda_N \epsilon} e^{-\lambda_N \epsilon}.$$

Thus applying Theorem 6.2.1 with $j = 1$ at the origin yields

Corollary 6.2.2. *Let $L \geq 2$ and suppose $\lambda_N \epsilon \geq 2$. Then*

$$\left| \frac{d\zeta_U}{ds}\Big|_{s=0} - a_2(U)(\gamma + \log\epsilon) - \sum_{\substack{k=0 \\ k\neq 2}}^{L} \frac{a_k(U)}{\frac{k-2}{2}} \epsilon^{\frac{k-2}{2}} - \sum_{n=1}^{N} \int_{\lambda_n \epsilon}^{\infty} t^{-1} e^{-t} dt \right| \leq$$
$$\int_0^{\epsilon} \Big| \frac{Z(t) - Z_L(t)}{t} \Big| dt + \frac{|U|^2 \lambda_N}{4\pi^2 N \epsilon} e^{-\lambda_N \epsilon}.$$

In the event that U is a polygon $a_k(U) = 0$ for all $k \geq 3$. So we get

Corollary 6.2.3. *Let U be a polygon and suppose $\lambda_N \epsilon \geq 2$. Then*

$$\left| \frac{d\zeta_U}{ds}\Big|_{s=0} + \frac{a_0(U)}{\epsilon} + \frac{2a_1(U)}{\sqrt{\epsilon}} - a_2(U)(\gamma + \log\epsilon) - \sum_{n=1}^{N} \int_{\lambda_n \epsilon}^{\infty} t^{-1} e^{-t} dt \right| \leq$$
$$\int_0^{\epsilon} \Big| \frac{Z(t) - Z_2(t)}{t} \Big| dt + \frac{|U|^2 \lambda_N}{4\pi^2 N \epsilon} e^{-\lambda_N \epsilon}.$$

Similarly,

$$\int_\epsilon^\infty t^{-3/2}e^{-t\lambda_N}dt = \sqrt{\lambda_N}\int_{\lambda_N\epsilon}^\infty t^{-3/2}e^{-t}dt \le \frac{1}{\lambda_N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.$$

Thus applying Theorem 6.2.1 with $j=0$ at $s=-\frac{1}{2}$ yields

Corollary 6.2.4. *Let $L\ge 3$ and suppose $\lambda_N\epsilon\ge 2$. Then*

$$\left|\Big(\zeta_U(s)-\frac{a_3(U)\epsilon^{s+\frac{1}{2}}}{\Gamma(s)(s+\frac{1}{2})}\Big)\Big|_{s=-\frac{1}{2}} - \sum_{\substack{k=0\\k\neq 3}}^{L}\frac{a_k(U)}{(3-k)\sqrt{\pi}}\epsilon^{\frac{k-3}{2}} + \sum_{n=1}^{N}\frac{1}{2\sqrt{\pi}}\int_\epsilon^\infty t^{-3/2}e^{-t\lambda_n}dt\right| \le$$
$$\frac{1}{2\sqrt{\pi}}\int_0^\epsilon\Big|\frac{Z(t)-Z_L(t)}{t^{3/2}}\Big|dt + \frac{|U|^2\lambda_N}{8\pi^{5/2}N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.$$

Recall[1]

$$\frac{d\Gamma}{ds}\Big|_{s=\frac{1}{2}} = -(\gamma+\log 4)\sqrt{\pi},$$

which gives

$$\frac{d\Gamma}{ds}\Big|_{s=-\frac{1}{2}} = (2\gamma+2\log 4-4)\sqrt{\pi}.$$

Thus around $s=-\frac{1}{2}$ we have the following first order Taylor expansion

$$\frac{\epsilon^{s+\frac{1}{2}}}{\Gamma(s)} = -\frac{1}{2\sqrt{\pi}} + \Big(\frac{2-\gamma-\log 4-\log\epsilon}{2\sqrt{\pi}}\Big)(s+\frac{1}{2}) + \cdots.$$

Corollary 6.2.5. *Let $L\ge 3$ and suppose $\lambda_N\epsilon\ge 2$. Then*

$$\left|\Big(\zeta_U(s)+\frac{a_3(U)}{2\sqrt{\pi}(s+\frac{1}{2})}\Big)\Big|_{s=-\frac{1}{2}} - a_3(U)\Big(\frac{2-\gamma-\log 4-\log\epsilon}{2\sqrt{\pi}}\Big) - \sum_{\substack{k=0\\k\neq 3}}^{L}\frac{a_k(U)}{(3-k)\sqrt{\pi}}\epsilon^{\frac{k-3}{2}}\right.$$
$$\left. + \sum_{n=1}^{N}\frac{1}{2\sqrt{\pi}}\int_\epsilon^\infty t^{-3/2}e^{-t\lambda_n}dt\right| \le \frac{1}{2\sqrt{\pi}}\int_0^\epsilon\Big|\frac{Z(t)-Z_L(t)}{t^{3/2}}\Big|dt + \frac{|U|^2\lambda_N}{8\pi^{5/2}N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.$$

In the event that U is a polygon, we get

Corollary 6.2.6. *Let U be a polygon and suppose $\lambda_N\epsilon\ge 2$. Then*

$$\left|\zeta_U(-\frac{1}{2}) - \sum_{k=0}^{2}\frac{a_k(U)}{(3-k)\sqrt{\pi}}\epsilon^{\frac{k-3}{2}} + \sum_{n=1}^{N}\frac{1}{2\sqrt{\pi}}\int_\epsilon^\infty t^{-3/2}e^{-t\lambda_n}dt\right| \le$$
$$\frac{1}{2\sqrt{\pi}}\int_0^\epsilon\Big|\frac{Z(t)-Z_2(t)}{t^{3/2}}\Big|dt + \frac{|U|^2\lambda_N}{8\pi^{5/2}N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.$$

[1] This can be seen from formula 5.4.13 on http://dlmf.nist.gov/5.4. It also follows on from the relation

$$\frac{\Gamma'(1)}{\Gamma(1)} - \frac{\Gamma'(\frac{1}{2})}{\Gamma(\frac{1}{2})} = \log 4,$$

which is formula (91) on http://mathworld.wolfram.com/GammaFunction.html.

In general it is hard to get precise values of the first several hundred Dirichlet eigenvalues. So we suppose that μ_n, $n = 1, \cdots, N$, are approximate values of λ_n. Based on Corollary 6.2.3, for example, an approximate value of the spectral determinant of a polygon U can be taken as

$$-\frac{a_0(U)}{\epsilon} - \frac{2a_1(U)}{\sqrt{\epsilon}} + a_2(U)(\gamma + \log\epsilon) + \sum_{n=1}^{N} \int_{\mu_n\epsilon}^{\infty} t^{-1}e^{-t}dt.$$

Now the error arises from two parts: one is

$$\int_0^{\epsilon} \Big|\frac{Z(t) - Z_2(t)}{t}\Big| dt + \frac{|U|^2\lambda_N}{4\pi^2 N\epsilon} e^{-\lambda_N\epsilon},$$

the other is

$$\sum_{n=1}^{N} \Big| \int_{\mu_n\epsilon}^{\lambda_n\epsilon} t^{-1}e^{-t}dt \Big|.$$

To summarize on how to apply Theorem 6.2.1 – Corollary 6.2.6 effectively, we need 1) as good quantitative short-time Dirichlet trace asymptotics as possible, and 2) high precision approximation of the first several hundred or one thousand Dirichlet eigenvalues.

6.3 Polygons

In this section we assume that U is a bounded connected open set in $\mathbb{R}^2$ with a polygonal boundary ∂U. To be clear, ∂U is polygonal if it is a finite union of pairwise disjoint connected components such that each connected component is a finitely piecewise linear Jordan curve. On can easily check that the number of edges is the same as the number of vertices whether the given polygon is simply connected or not. So we let $E_1, \ldots, E_m$ denote the edges of U, and let $P_1, \ldots, P_m$ denote the vertices of U with corresponding interior angles $\gamma_1, \ldots, \gamma_m$. For each i, let F_i be the straight line through E_i, H_i the open half-plane with boundary F_i having the same inward normal at E_i as U, W_i the infinite wedge of angle γ_i with vertex P_i such that its boundary contains the two edges adjacent to P_i, and define

$$B_i(r) = \{A \in W_i : d(A, P_i) < r\}$$

for any $r > 0$. It was conjectured in [24] that

$$\mathrm{tr}(e^{-t\Delta_U}) = \frac{|U|}{4\pi t} - \frac{|\partial U|}{8\sqrt{\pi t}} + \beta_1 + O(e^{-\beta_2/t}) \quad (t \to 0^+) \tag{6.8}$$

for some constants β_1, β_2. By exploiting the Neumann-Poincare construction of the heat kernel, a proof of this conjecture was obtained in [5, 6]. Later on, M. Kac [88] explicitly determined β_1 for the class of convex polygons without acute and right interior angles. His method was developed to a full resolution

$$\beta_1 = \sum_{i=1}^{m} \frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i} \tag{6.9}$$

by M. van den Berg and S. Srisatkunarajah [12] for all polygons. It was reported in [108] that D. B. Ray had obtained the same formula for β_1.

Obviously, good applications of Corollaries 6.2.3 and 6.2.6 need tight bounds for $|Z(t) - Z_2(t)|$, where according to (6.8) and (6.9),

$$Z_2(t) = \frac{|U|}{4\pi t} - \frac{|\partial U|}{8\sqrt{\pi t}} + \sum_{i=1}^{m} \frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i}.$$

To this end we define

$$\beta_U = \liminf_{t\to 0^+} \big(- t \log \big(\big|Z(t) - Z_2(t)\big|\big)\big),$$

which is essentially the best choice for β_2. Along with determining β_1 explicitly, M. van den Berg and S. Srisatkunarajah [12] showed that

$$\beta_U \geq \frac{(R \sin \frac{\gamma_0}{2})^2}{16}, \tag{6.10}$$

where

$$\gamma_0 = \min \gamma_i,$$

$$R = \frac{1}{2} \sup \Big\{ r : B_i(r) \cap B_j(r) = \emptyset \text{ for all } i \neq j, \bigcup_{k=1}^{m} B_k(r) \subset U \Big\}. \tag{6.11}$$

For example, if $U = S$ is a unit square, then (6.10) reads $\beta_S \geq \frac{1}{512}$. But it is not hard to use the Poisson summation formula to deduce that $\beta_S = 1$. M. van den Berg and K. Gittins [11] have posed an open problem on determining the precise form of β_U, which is a challenge beyond the scope of this thesis. Note also β_U is a spectral invariant for polygonal domains. To the best of our knowledge, except (6.10) there is no other known lower bound for β_2. The purpose of this section is to substantially improve (6.10) for β_U. To compare, our result below when applied to a unit square S gives $\beta_S \geq \frac{1}{8}$.

6.3.1 An improvement

As usual denote by $\rho(x)$ the distance from $x \in U$ to the boundary of U. Let $K_U(x, y; t)$ denote the Dirichlet heat kernel for U[2]. In 1981 M. van den Berg [9] established the following not feeling boundary estimate

$$|K_U(x, x; t) - \frac{1}{4\pi t}| \leq \frac{1}{\pi t} \exp(-\frac{\rho(x)^2}{2t}) \quad (x \in U,\ t > 0), \tag{6.12}$$

which served as a basic tool in [12] published in 1988. In 1989 M. van den Berg [10] obtained the following improvement (see also (5.7))

$$|K_U(x, x; t) - \frac{1}{4\pi t}| \leq \frac{2\rho(x)^2 + t}{2\pi t^2} \cdot \exp(-\frac{\rho(x)^2}{t}) \quad (x \in U,\ t > 0),$$

where the exponential factor $\rho(x)^2$ is known to be sharp for small times (e.g. [82, 156, 157]). Following the argument in [12] with (6.12) replaced by

$$|K_U(x, x; t) - \frac{1}{4\pi t}| \leq \frac{3\rho(x)^2}{2\pi t^2} \cdot \exp(-\frac{\rho(x)^2}{t}) \quad (x \in U,\ 0 < t < \rho(x)^2) \tag{6.13}$$

[2] In the previous chapter the Dirichlet heat kernel for U is denoted by $K_U^+(x, y; t)$.

will yield a natural but slight improvement of (6.10). As mentioned in §5.5, Bironneau obtained an estimate [16, Thm. 7.5] which is stronger than (6.12) but weaker than (6.13). He then used this estimate to derive an improvement [16, Thm. 7.7] of (6.10). But we should point out that the statements of Theorems 7.6 and 7.7 in [16] contain serious citing typos because R, introduced by M. van den Berg and S. Srisatkunarajah [12, (1.10)] (see also (6.11)), does not mean "half the length of its shortest edge." Actually, it is a simple exercise to show that R is never bigger than a quarter of the length of the shortest edge of the given polygon.

6.3.2 Probabilistic method

In this part we provide preliminary material of a lemma that will be used later in the next section. Let $V_0 \subset \mathbb{R}^2$ be a small open set such that it is contained in the intersection of two larger open ones $V_1, V_2 \subset \mathbb{R}^2$. Assume also

$$\rho = \rho(V_0; V_1, V_2) = \mathrm{dist}(V_0, (V_1 \cap \partial V_2) \cup (V_2 \cap \partial V_1)) > 0. \tag{6.14}$$

Let $x \in V_0$ denote an arbitrary fixed point. It is known (e.g. [123, 127, 142, 143]) that the diagonal element of the Dirichlet heat kernel $K_{V_i}(x, x; t)$ can be expressed as the probability that a continuous brownian bridge $B(\cdot)$ conditioned to $B(0) = B(t) = x$ does not leave V_i:

$$K_{V_i}(x, x; t) = \frac{1}{4\pi t}\mathrm{Prob}\{B(\tau) \in V_i, 0 \le \tau \le t | B(0) = B(t) = x\}.$$

By regarding x, t as fixed elements, $K_V(x, x; t)$ is a real-valued map on open subsets V of $\mathbb{R}^2$. For example, as any brownian bridge stays in the ambient plane, one gets

$$K_{\mathbb{R}^2}(x, x; t) = \frac{1}{4\pi t}.$$

Now let $B(\tau)$ be a continuous brownian bridge satisfying $B(0) = B(t) = x$, and stay in V_1 for all $\tau \in [0, t]$. Thus

- either $B(\tau)$ stays in V_2 for all $\tau \in [0, t]$,
- or $B(\tau)$ hits $V_1 \cap \partial V_2$ for some $\tau \in [0, t]$.

The complement of the latter case means that $B(\tau)$ never hits $V_1 \cap \partial V_2$ for any $\tau \in [0, t]$, which is equivalent to saying that $B(\tau)$ stays in $\mathbb{R}^2 \backslash (V_1 \cap \partial V_2)$ for all $\tau \in [0, t]$. Note also

$$B(x, \rho) \subset \mathbb{R}^2 \backslash (V_1 \cap \partial V_2).$$

So we have

$$K_{V_1}(x, x; t) \le K_{V_2}(x, x; t) + \Big(\frac{1}{4\pi t} - K_{B(x,\rho)}(x, x; t)\Big),$$

and by (6.13) we get

$$K_{V_1}(x, x; t) \le K_{V_2}(x, x; t) + \frac{3\rho^2}{2\pi t^2} \cdot \exp(-\frac{\rho^2}{t}) \quad (0 < t < \rho^2).$$

Swapping the positions between V_1 and V_2 yields

$$|K_{V_1}(x, x; t) - K_{V_2}(x, x; t)| \le \frac{3\rho^2}{2\pi t^2} \cdot \exp(-\frac{\rho^2}{t}) \quad (0 < t < \rho^2).$$

So we obtain

Lemma 6.3.1. *Let $V_0 \subset \mathbb{R}^2$ be an open set such that it is contained in the intersection of two larger open sets $V_1, V_2 \subset \mathbb{R}^2$. Assume also*

$$\rho = \rho(V_0; V_1, V_2) = \mathrm{dist}(V_0, (V_1 \cap \partial V_2) \cup (V_2 \cap \partial V_1)) > 0.$$

Then

$$\Big| \int_{V_0} K_{V_1}(x, x; t)dx - \int_{V_0} K_{V_2}(x, x; t)dx \Big| \leq \frac{3\rho^2}{2\pi t^2} \cdot \exp(-\frac{\rho^2}{t}) \cdot |V_0| \quad (0 < t < \rho^2).$$

We should mention that the above argument is essentially contained in [12], in which the weaker estimate (6.12) was used rather than (6.13).

6.3.3 Further improvement

Similar to the analysis in [12], suppose that the polygon U can be decomposed as the union of some pairwise disjoint subsets

$$U = \bigcup_{j=1}^{2m+1} V_0^{(j)},$$

such that over each part $V_0^{(j)}$ the integral of the diagonal Dirichlet heat kernel for $V_1 = U$ will be compared with that for certain $V_2^{(j)}$ in the manner of Lemma 6.3.1. Here (see the beginning of this section for the exact meaning of edges W_i and half-planes H_i)

- $V_2^{(j)} = W_j$ for $1 \leq j \leq m$;
- $V_2^{(j)} = H_{j-m}$ for $m + 1 \leq j \leq 2m$;
- $V_2^{(2m+1)} = \mathbb{R}^2$.

Later on we will a give specific construction of $\{V_0^{(j)}\}_{j=1}^{2m+1}$ and deduce from Lemma 6.3.1 that

$$\beta_U \geq \min_{1 \leq j \leq 2m+1} \rho(V_0^{(j)}; U, V_2^{(j)})^2. \tag{6.15}$$

To compare, M. van den Berg and S. Srisatkunarajah did not fully stick with Lemma 6.3.1, and their introduction of convex sets G_A [12, p. 125] brings some loss to (6.15). At least in the case that U is a convex polygon, we think it could be better to let G_A be U. On the other hand, they required that $\{B_j(2R)\}_{j=1}^m$ are pairwise disjoint subsets of U and set $V_0^{(j)} = B_j(R)$ for $j \leq m$, while we relax the parameters $r_1 < r_2$ so that

- (A1) $\{V_0^{(j)} = B_j(r_1)\}_{j=1}^m$ are pairwise disjoint;
- (A2) $\{B_j(r_2)\}_{j=1}^m$ are subsets of U.

Now we state and prove the main result of this section. Together with (A1) and (A2), we assume

- (A3) $\{V_0^{(j)} = C_{j-m}(\delta_0)\}_{j=m+1}^{2m}$ are pairwise disjoint for $\delta_0 \in (0, r_1 \sin(\frac{\gamma_0}{2})]$.

Here

$$C_j(\delta_0) = \{x \in U : d(x, E_j) < \delta_0,\ x \notin \cup_{i=1}^m B_i(r_1)\} \quad (j \le m).$$

Let $V_0^{(2m+1)}$ denote the complement of $\cup_{j=1}^{2m} V_0^{(j)}$ in U, and define

$$\omega = \min\{r_2 - r_1, \rho(C_1(\delta_0); U, H_1), \ldots, \rho(C_m(\delta_0); U, H_m), \delta_0\}. \tag{6.16}$$

With these assumptions available, (6.15) is a consequence of the following theorem.

Theorem 6.3.2. *Assume (A1) – (A3) and* $0 < t < \omega^2$*. Then*

$$\Big|\mathrm{tr}(e^{-t\Delta_U}) - \frac{|U|}{4\pi t} + \frac{|\partial U|}{8\sqrt{\pi t}} - \sum_{i=1}^m \frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i}\Big| \le \frac{C_U}{t^2}\exp(-\frac{\omega^2}{t})$$

with

$$C_U = \frac{3\omega^2|U|}{2\pi} + \frac{m\pi^2\omega^4}{4\gamma_0^2} + \frac{|\partial U|\omega^4}{8\pi\delta_0} + \frac{mr_1^2\omega^2}{8}.$$

Proof. First applying Lemma 6.3.1 with $V_0 = V_0^{(j)}, V_1 = U$ and $V_2 = V_2^{(j)}$ for each $j \le 2m+1$, then putting them together gives

$$\Big|\mathrm{tr}(e^{-t\Delta_U}) - \sum_{i=1}^m \int_{B_i(r_1)} K_{W_i} - \sum_{j=1}^m \int_{C_j(\delta_0)} K_{H_j} - \frac{|V_0^{(2m+1)}|}{4\pi t}\Big| \le \frac{3\omega^2|U|}{2\pi t^2}\exp(-\frac{\omega^2}{t})$$

for $0 < t < \omega^2$. Here $\int_{B_i(r_1)} K_{W_i}$ is short for $\int_{B_i(r_1)} K_{W_i}(x,x;t)dx$, and $\int_{C_j(\delta_0)} K_{H_j}$ is similarly interpreted. It was shown in [12, Thm. 2] that

$$\int_{B_i(r_1)} K_{W_i} = \frac{|B_i(r_1)|}{4\pi t} - \frac{1}{2\pi t}\int_0^{r_1} e^{-\frac{z^2}{t}}\sqrt{r_1^2 - z^2}dz + \frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i} + X_i(t),$$

where one can control $X_i(t)$ by applying [12, Cor. 3] appropriately to get

$$|X_i(t)| \le \frac{\pi^2}{4\gamma_0^2}\exp(-\frac{r_1^2\sin(\frac{\gamma_0}{2})^2}{t})$$

for any $t > 0$. On the other hand, it follows from [12, (4.4)] that

$$\int_{C_j(\delta_0)} K_{H_j} = \frac{|C_j(\delta_0)|}{4\pi t} - \frac{|E_j|}{8\sqrt{\pi t}} + \frac{|E_j|}{4\pi t}\int_{\delta_0}^\infty e^{-\frac{z^2}{t}}dz + \frac{1}{2\pi t}\int_0^{\delta_0} e^{-\frac{s^2}{t}}\sqrt{r_1^2 - z^2}dz.$$

Consequently, by combining all of the above formulae, we see that, for any $0 < t < \omega^2$,

$$|\mathrm{tr}(e^{-t\Delta_U}) - \frac{|U|}{4\pi t} + \frac{|\partial U|}{8\sqrt{\pi t}} - \sum_{i=1}^m \frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i}|$$

is bounded above by

$$\frac{3\omega^2|U|}{2\pi t^2}e^{-\frac{\omega^2}{t}} + \frac{m\pi^2}{4\gamma_0^2}e^{-\frac{r_1^2\sin(\frac{\gamma_0}{2})^2}{t}} + \frac{|\partial U|}{4\pi t}\int_{\delta_0}^\infty e^{-\frac{z^2}{t}}dz + \frac{m}{2\pi t}\int_{\delta_0}^{r_1} e^{-\frac{z^2}{t}}\sqrt{r_1^2 - z^2}dz.$$

A consideration of $\omega \le \delta_0 \le r_1\sin\frac{\gamma_0}{2}$ then allows us to get

$$|Z(t) - Z_2(t)| \le (\frac{3\omega^2|U|}{2\pi t^2} + \frac{m\pi^2}{4\gamma_0^2} + \frac{|\partial U|}{8\pi\delta_0} + \frac{mr_1^2}{8t}) \cdot \exp(-\frac{\omega^2}{t}).$$

This finishes the proof simply by noting $0 < t < \omega^2$. □

We end this section with an example. Let U_n $(n \geq 4)$ denote a regular n-gon whose circumscribed circle is of radius one. Then $|U_n| = \frac{n}{2}\sin(\frac{2\pi}{n})$, $|\partial U_n| = 2n\sin(\frac{\pi}{n})$, $a_2 = a_2(U_n) = \frac{n-1}{6(n-2)}$, $\gamma_0 = \frac{(n-2)\pi}{n}$, and $R = \frac{1}{2}\sin(\frac{\pi}{n})$. We set

$$(r_1, r_2, \delta_0) = (2R, 4R, 2R\sin(\frac{\gamma_0}{2})) = (\sin(\frac{\pi}{n}), 2\sin(\frac{\pi}{n}), \frac{1}{2}\sin(\frac{2\pi}{n})) \tag{6.17}$$

to ensure that (A1) $\sim$ (A3) are satisfied. One can easily check that $\omega = \delta_0 = \frac{1}{2}\sin(\frac{2\pi}{n})$. It then follows from Theorem 6.3.2 that

$$\Big|\mathrm{tr}(e^{-t\Delta_{U_n}}) - \frac{n\sin(\frac{2\pi}{n})}{8\pi t} + \frac{n\sin(\frac{\pi}{n})}{4\sqrt{\pi t}} - \frac{n-1}{6(n-2)}\Big| \leq \frac{C_n}{t^2}\exp(-\frac{\sin^2(\frac{2\pi}{n})}{4t}) \quad (0 < t < \frac{\sin^2(\frac{2\pi}{n})}{4}),$$

where

$$\begin{aligned} C_n &= \frac{3n\sin^3(\frac{2\pi}{n})}{16\pi} + \frac{n^3\sin^4(\frac{2\pi}{n})}{64(n-2)^2} + \frac{n\sin(\frac{\pi}{n})\sin^3(\frac{2\pi}{n})}{32\pi} + \frac{n\sin^2(\frac{\pi}{n})\sin^2(\frac{2\pi}{n})}{32} \\ &\leq \frac{n\sin^3(\frac{2\pi}{n})}{6}. \end{aligned}$$

To compare, M. van den Berg and S. Srisatkunarajah ([12]) established the following bound

$$Big|\mathrm{tr}(e^{-t\Delta_{U_n}}) - \frac{|U|}{4\pi t} + \frac{|\partial U|}{8\sqrt{\pi t}} - \sum_{i=1}^{m}\frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i}\Big| \leq \Big(5m + \frac{20|U|}{R^2}\Big)\frac{1}{\gamma_0^2}\exp(-\frac{(R\sin\frac{\gamma_0}{2})^2}{16t})$$

for all $t > 0$. Taking $U = U_n$ $(n \geq 4)$ for example, one gets

$$\Big|\mathrm{tr}(e^{-t\Delta_{U_n}}) - \frac{n\sin(\frac{2\pi}{n})}{8\pi t} + \frac{n\sin(\frac{\pi}{n})}{4\sqrt{\pi t}} - \frac{n-1}{6(n-2)}\Big| \leq \widetilde{C_n}\exp(-\frac{\sin^2(\frac{2\pi}{n})}{256t})$$

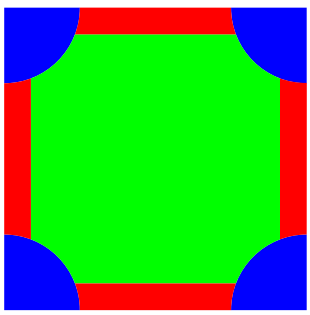
for $t > 0$, where

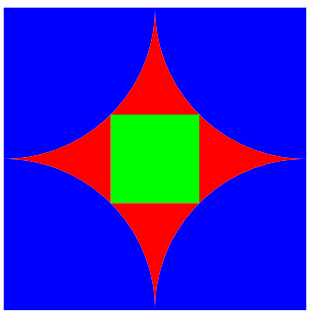
$$\widetilde{C_n} = \big(5n + 80n\coth\frac{\pi}{n}\big)\cdot\frac{n^2}{(n-2)^2\pi^2}.$$

Therefore, our small-time exponential remainder $\frac{\sin^2(\frac{2\pi}{n})}{4}$ for U_n is better than M. van den Berg and S. Srisatkunarajah's counterpart $\frac{\sin^2(\frac{2\pi}{n})}{256}$. Actually, their proof in this particular example chooses

$$(r_1, r_2, \delta_0) = (R, 2R, \frac{R}{2}\sin(\frac{\gamma_0}{2})). \tag{6.18}$$

M. van den Berg and S. Srisatkunarajah's decomposition of a square and our improvement are illustrated respectively as the following left and right pictures:





6.4 Numerical applications

We follow all of the notations introduced in the previous section. For example, we let U_n $(n \geq 4)$ denote the unit regular n-gon whose circumscribed circle is of radius one.

6.4.1 Spectral determinants

Let $N \in \mathbb{N}$, $\epsilon > 0$ be parameters such that $\frac{2}{\lambda_N} \leq \epsilon \leq \omega^2$. Note

$$\int_0^\epsilon t^{-3}\exp(-\frac{\omega^2}{t})dt = \frac{1}{\omega^4}\int_{\frac{\omega^2}{\epsilon}}^\infty ze^{-z}dz = \frac{1}{\omega^4}(1+\frac{\omega^2}{\epsilon})\exp(-\frac{\omega^2}{\epsilon}) \leq \frac{2}{\omega^2\epsilon}\exp(-\frac{\omega^2}{\epsilon}).$$

It thus follows from Corollary 6.2.3 and Theorem 6.3.2 that

$$\left|\frac{d\zeta_U}{ds}\Big|_{s=0} + \frac{|U|}{4\pi\epsilon} - \frac{|\partial U|}{4\sqrt{\pi\epsilon}} - \Big(\sum_{i=1}^m \frac{\pi^2-\gamma_i^2}{24\pi\gamma_i}\Big)(\gamma+\log\epsilon) - \sum_{k=1}^N \int_{\lambda_k\epsilon}^\infty t^{-1}e^{-t}dt\right| \leq$$
$$\frac{2C_U}{\omega^2\epsilon}\exp(-\frac{\omega^2}{\epsilon}) + \frac{|U|^2\lambda_N}{4\pi^2N\epsilon}e^{-\lambda_N\epsilon}. \tag{6.19}$$

In the event that $U = U_n$ $(n \geq 4)$ is a unit regular polygon, this yields (see §6.3.3)

$$\left|\frac{d\zeta_{U_n}}{ds}\Big|_{s=0} + \frac{n\sin(\frac{2\pi}{n})}{8\pi\epsilon} - \frac{n\sin(\frac{\pi}{n})}{2\sqrt{\pi\epsilon}} - \frac{n-1}{6(n-2)}(\gamma+\log\epsilon) - \sum_{k=1}^N \int_{\lambda_k\epsilon}^\infty t^{-1}e^{-t}dt\right| \leq$$
$$\frac{4n\sin(\frac{2\pi}{n})}{3\epsilon}\exp(-\frac{\sin^2(\frac{2\pi}{n})}{4\epsilon}) + \frac{|U|^2\lambda_N}{4\pi^2N\epsilon}e^{-\lambda_N\epsilon}. \tag{6.20}$$

For example, letting $U = U_4$ be a square of side length $\sqrt{2}$, we then have

$$\left|\frac{d\zeta_{U_4}}{ds}\Big|_{s=0} + \frac{1}{2\pi\epsilon} - \sqrt{\frac{2}{\pi\epsilon}} - \frac{\gamma+\log\epsilon}{4} - \sum_{k=1}^N \int_{\lambda_k\epsilon}^\infty t^{-1}e^{-t}dt\right| \leq \frac{16}{3\epsilon}e^{-\frac{1}{4\epsilon}} + \frac{\lambda_N}{2\pi^2N\epsilon}e^{-\lambda_N\epsilon}. \tag{6.21}$$

Note all eigenvalues of the Dirichlet Laplacian for U_4 are made up of the following set

$$\Big\{\frac{\pi^2}{2}(i^2+j^2) : i,j \in \mathbb{N}\Big\},$$

from which one can work out the first one thousand eigenvalues in non-decreasing order such as $\lambda_{1000} = 657\pi^2 \geq 6484$. Hence setting $N = 1000$ in (6.21) gives

$$\left|\frac{d\zeta_{U_4}}{ds}\Big|_{s=0} + \frac{1}{2\pi\epsilon} - \sqrt{\frac{2}{\pi\epsilon}} - \frac{\gamma+\log\epsilon}{4} - \sum_{k=1}^{1000} \int_{\lambda_k\epsilon}^\infty t^{-1}e^{-t}dt\right| \leq \frac{16}{3\epsilon}e^{-\frac{1}{4\epsilon}} + \frac{0.3285}{\epsilon}e^{-6484\epsilon}, \tag{6.22}$$

where the right-hand side as a function of $\epsilon > 0$ attains its minimal value near $\epsilon_0 = 0.006$. One can easily verify that $\frac{2}{\lambda_{1000}} \leq 0.0003 \leq \epsilon_0 = 0.006 \leq 0.25 = \omega^2$, which means in particular that we can indeed set $\epsilon = 0.006$. Thus

$$\left|\frac{d\zeta_{U_4}}{ds}\Big|_{s=0} + \frac{1}{0.012\pi} - \sqrt{\frac{1}{0.003\pi}} - \frac{\gamma+\log 0.006}{4} - \sum_{k=1}^{1000} \int_{0.006\lambda_k}^\infty t^{-1}e^{-t}dt\right| \leq 2\times 10^{-15}.$$

Finally, with the help of Matlab we get

$$\Big|\frac{d\zeta_{U_4}}{ds}\Big|_{s=0} - 0.783532455668890\Big| \leq 2\times 10^{-15} + \text{computer error}.$$

To calculate each integral $\int_{0.006\lambda_k}^{\infty} t^{-1}e^{-t}dt$, the Matlab program is accurate up to 15 digits, so the total error caused by computer program is bounded by 10^{-12}. To conclude, we have

$$\Big|\frac{d\zeta_{U_4}}{ds}\Big|_{s=0} - 0.783532455668890\Big| \leq 2\times 10^{-15} + 10^{-12}, \tag{6.23}$$

and consequently

$$\Big|\exp\big(-\frac{d\zeta_{U_4}}{ds}\Big|_{s=0}\big) - 0.456789569078052\Big| \leq 10^{-12}. \tag{6.24}$$

According to [4, (105)], the first 15 digits of the precise value of $\frac{d\zeta_{U_4}}{ds}\big|_{s=0}$ are 0.783532455668877, which agrees with (6.23).

6.4.2 Casimir energies

Let $N\in\mathbb{N}$, $\epsilon>0$ be parameters such that $\frac{2}{\lambda_N}\leq\epsilon\leq\frac{\omega^2}{3}$. Note

$$\begin{aligned}\int_0^{\epsilon} t^{-7/2}\exp(-\frac{\omega^2}{t})dt &= \frac{1}{\omega^5}\int_{\frac{\omega^2}{\epsilon}}^{\infty} z^{3/2}e^{-z}dz \leq \frac{\sqrt{\epsilon}}{\omega^6}\int_{\frac{\omega^2}{\epsilon}}^{\infty} z^2e^{-z}dz\\ &= \frac{\sqrt{\epsilon}}{\omega^6}(2+2\frac{\omega^2}{\epsilon}+\frac{\omega^4}{\epsilon^2})\exp(-\frac{\omega^2}{\epsilon}) \leq \frac{2}{\omega^2\epsilon^{3/2}}\exp(-\frac{\omega^2}{\epsilon}).\end{aligned}$$

It thus follows from Corollary 6.2.6 and Theorem 6.3.2 that

$$\begin{aligned}&\Big|\zeta_U(-\frac{1}{2}) - \frac{|U|}{12\pi^{3/2}\epsilon^{3/2}} + \frac{|\partial U|}{16\pi\epsilon} - \frac{\sum_{i=1}^m \frac{\pi^2-\gamma_i^2}{24\pi\gamma_i}}{\sqrt{\pi\epsilon}} + \sum_{k=1}^N \frac{1}{2\sqrt{\pi}}\int_{\epsilon}^{\infty} t^{-3/2}e^{-t\lambda_k}dt\Big| \leq\\ &\frac{C_U}{\sqrt{\pi}\omega^2\epsilon^{3/2}}\exp(-\frac{\omega^2}{\epsilon}) + \frac{|U|^2\lambda_N}{8\pi^{5/2}N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.\end{aligned} \tag{6.25}$$

In the event that $U=U_n$ $(n\geq 4)$ is a unit regular polygon, this yields (see §6.3.3)

$$\begin{aligned}&\Big|\zeta_{U_n}(-\frac{1}{2}) - \frac{n\sin(\frac{2\pi}{n})}{24\pi^{3/2}\epsilon^{3/2}} + \frac{n\sin(\frac{\pi}{n})}{8\pi\epsilon} - \frac{n-1}{6(n-2)\sqrt{\pi\epsilon}} + \sum_{k=1}^N \frac{1}{2\sqrt{\pi}}\int_{\epsilon}^{\infty} t^{-3/2}e^{-t\lambda_k}dt\Big| \leq\\ &\frac{2n\sin(\frac{2\pi}{n})}{3\sqrt{\pi}\epsilon^{3/2}}\exp(-\frac{\sin^2(\frac{2\pi}{n})}{4\epsilon}) + \frac{|U|^2\lambda_N}{8\pi^{5/2}N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.\end{aligned} \tag{6.26}$$

For example, letting $U=U_4$ be a square of side length $\sqrt{2}$, we then have

$$\begin{aligned}&\Big|\zeta_{U_4}(-\frac{1}{2}) - \frac{1}{6\pi^{3/2}\epsilon^{3/2}} + \frac{\sqrt{2}}{4\pi\epsilon} - \frac{1}{4\sqrt{\pi\epsilon}} + \sum_{k=1}^N \frac{1}{2\sqrt{\pi}}\int_{\epsilon}^{\infty} t^{-3/2}e^{-t\lambda_k}dt\Big| \leq\\ &\frac{8}{3\sqrt{\pi}\epsilon^{3/2}}\exp(-\frac{1}{4\epsilon}) + \frac{\lambda_N}{2\pi^{5/2}N\epsilon^{3/2}}e^{-\lambda_N\epsilon}.\end{aligned} \tag{6.27}$$

Setting $N = 980$ in (6.27) and working out $\lambda_{980} = 650\pi^2 \geq 6415$ gives

$$\left|\zeta_{U_4}(-\frac{1}{2}) - \frac{1}{6\pi^{3/2}\epsilon^{3/2}} + \frac{\sqrt{2}}{4\pi\epsilon} - \frac{1}{4\sqrt{\pi\epsilon}} + \sum_{k=1}^{980} \frac{1}{2\sqrt{\pi}} \int_{\epsilon}^{\infty} t^{-3/2} e^{-t\lambda_k} dt\right| \leq 1.51 \frac{\exp(-\frac{1}{4\epsilon})}{\epsilon^{3/2}} + \frac{0.19}{\epsilon^{3/2}} e^{-6415\epsilon},$$

where the right-hand side as a function of $\epsilon > 0$ attains its minimal value near $\epsilon_0 = 0.006$. One can easily verify that $\frac{2}{\lambda_{980}} \leq 0.0003 \leq \epsilon_0 = 0.006 \leq 0.08 \leq \frac{\omega^2}{3}$, which means in particular that we can indeed set $\epsilon = 0.006$. Thus

$$\left|\zeta_{U_4}(-\frac{1}{2}) - \frac{1}{6\pi^{3/2}0.006^{3/2}} + \frac{\sqrt{2}}{0.024\pi} - \frac{1}{4\sqrt{0.006\pi}} + \sum_{k=1}^{980} \frac{1}{2\sqrt{\pi}} \int_{0.006}^{\infty} t^{-3/2} e^{-t\lambda_k} dt\right| \leq 2 \times 10^{-14}.$$

Finally, with the help of Matlab we get

$$\left|\zeta_{U_4}(-\frac{1}{2}) - 0.058040169372028\right| \leq 2 \times 10^{-14} + \text{computer error}.$$

To calculate each integral $\frac{1}{2\sqrt{\pi}} \int_{0.006}^{\infty} t^{-3/2} e^{-t\lambda_k} dt$, the Matlab program is accurate up to 15 digits, so the total error caused by computer program is bounded by 980×10^{-15}. To conclude, we have

$$\left|\zeta_{U_4}(-\frac{1}{2}) - 0.058040169372028\right| \leq 10^{-12}, \tag{6.28}$$

which agrees with [1, Table I].

6.5 Further comments

We finish this chapter with some comments.

1) One can modify the argument in the previous section to calculate the spectral determinant and Casimir energy of an equilateral, hemi-equilateral, or isosceles right triangle with arbitrarily high precision because all of their Dirichlet eigenvalues are explicitly known (e.g. [15, 61, 107, 119, 120, 122]). We refer the reader to [1] for the same problem about the Casimir energy of these triangles with a different approach.

2) The method introduced in §6.3.3 about decomposition of polygonals can be naturally adapted to improve the estimates in [11, 13] about the short-time heat content asymptotics.

3) For the Neumann Laplacian $\Delta_U^{(-)}$ on a polygon U, it is known (see [73] and references therein) that

$$\mathrm{tr}(e^{-t\Delta_U^{(-)}}) = \frac{|U|}{4\pi t} + \frac{|\partial U|}{8\sqrt{\pi t}} + \sum_{i=1}^{m} \frac{\pi^2 - \gamma_i^2}{24\pi\gamma_i} + O(e^{-\beta_3/t}) \quad (t \to 0^+),$$

but no explicit lower bounds for β_3 have been achieved yet. This is an interesting question if one wishes to further measure certain specific values of the Neumann spectral zeta function with high precision.

4) How to determine the first few hundreds Dirichlet eigenvalues with high precision for an arbitrary bounded but not necessarily polygonal planar region remains a challenging problem.

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List of notation

$\mathbb{N}$: set of natural numbers
$\mathbb{R}$: set of real numbers
$\mathbb{R}^+$: set of positive real numbers
$\mathbb{C}$: set of complex numbers
$\mathbb{S}^{d-1}$: unit sphere in $\mathbb{R}^d$
i: imaginary unit
∂_x^α: partial differential operator, $\partial_x^\alpha = (\frac{\partial}{\partial x_1})^{\alpha_1} \cdots (\frac{\partial}{\partial x_d})^{\alpha_d}$
D_x^α: partial differential operator, $D_x^\alpha = (-\mathrm{i}\frac{\partial}{\partial x_1})^{\alpha_1} \cdots (-\mathrm{i}\frac{\partial}{\partial x_d})^{\alpha_d}$
Δ: Laplace operator, $\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}$
$\mathscr{S}(\mathbb{R}^d)$: Schwartz space of rapidly decreasing functions on $\mathbb{R}^d$
$\mathscr{S}'(\mathbb{R}^d)$: space of tempered distributions on $\mathbb{R}^d$
$\mathscr{F}$: Fourier transform on $\mathscr{S}(\mathbb{R}^d)$ or $\mathscr{S}'(\mathbb{R}^d)$
$\mathscr{F}^{-1}$: inverse Fourier transform on $\mathscr{S}(\mathbb{R}^d)$ or $\mathscr{S}'(\mathbb{R}^d)$
γ: Euler-Mascheroni constant (or Clifford module structure)
U: Euclidean domain
$|U|$: volume of U
∂U: boundary of U
$|\partial U|$: surface area of U
$C^\infty(U)$: space of smooth functions on U
$C_c^\infty(U)$: space of compactly supported smooth functions on U
$L^2(U)$: space of square integrable functions on U
$C_c^\infty(U;\mathbb{C}^N)$: N-fold direct sum of $C_c^\infty(U)$
$L^2(U;\mathbb{C}^N)$: N-fold direct sum of $L^2(U)$
$\mathscr{D}'(U)$: space of distributions on U
K_U: Dirichlet heat kernel for U (Chapter 6)
$K_U^{(+)}$: Dirichlet heat kernel for U (Chapter 5)
$K_U^{(-)}$: Neumann heat kernel for U
ζ_U: spectral zeta function for U
$\Gamma(\cdot)$: Gamma function
$B(\cdot,\cdot)$: Beta function
J_φ: Jacobian matrix of $\varphi : \mathbb{R}^d \to \mathbb{R}^d$
H_f: Hessian matrix of $f : \mathbb{R}^d \to \mathbb{C}$
$\mathrm{Mat}(r,\mathbb{C})$: set of complex-valued matrices of size $r \times r$

$\mathrm{Re}(s)$: real part of $s \in \mathbb{C}$
T: transpose of a matrix
P: partial differential operator on a Euclidean domain (Chapter 2)
$\sigma_{\mathrm{Full}}(P)$: full symbol of P
$\sigma_m(P)$: principal symbol of an m-th order operator P
$\langle \cdot, \cdot \rangle$: inner product or dual
Id: identity operator
Tr: trace of an endomorphism
tr: trace of a trace class operator
$\mathrm{supp}(\cdot)$: support of an function
$\mathrm{Dom}(\cdot)$: domain of an operator
M: d-dimensional smooth or Riemannian manifold
TM: tangent bundle of M
T^*M: cotangent bundle of M
T_1^*M: unit cotangent bundle of a Riemannian manifold M
T_xM: tangent space at $x \in M$
T_x^*M: cotangent space at $x \in M$
(M, g): M is a Riemannian manifold with metric g
∇: Levi-Civita connection on TM (or a connection on a vector bundle)
$(x^1, \ldots, x^d)$: local coordinates of M
Γ_{ij}^k: Christoffel symbols
$\Psi^m(M)$: space of pseudo-differential operators of order m on M
$\Psi_{\mathrm{cl}}^m(M)$: space of classical pseudo-differential operators of order m on M
$\Psi_{\mathrm{cl}}^\infty(M)$: space of classical pseudo-differential operators on M
σ_A: principal symbol of $A \in \Psi_{\mathrm{cl}}^\infty(M)$
$\sigma_A^{(0)}$: principal symbol of $A \in \Psi_{\mathrm{cl}}^\infty(M)$
$\mathrm{Sub}(A)$: sub-principal symbol of $A \in \Psi_{\mathrm{cl}}^\infty(M)$
E: complex vector bundle over M of rank r
$C^\infty(M; \mathrm{End}(E))$: space of smooth endomorphisms of E
$\nabla, \widehat{\nabla}, \widetilde{\nabla}$: connections on a vector bundle
$\Psi_{\mathrm{cl}}^m(M; E)$: space of classical pseudo-differential operators of order m acting on sections of E
$\Psi_{\mathrm{cl}}^\infty(M; E)$: space of classical pseudo-differential operators acting on sections of E