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Heat Kernel Method and its Applications

Birkhäuser

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ISBN 978-3-319-26265-9 ISBN 978-3-319-26266-6 (eBook)
DOI 10.1007/978-3-319-26266-6

Library of Congress Control Number: 2015956332

Mathematics Subject Classification (2010): 35-01, 35K05, 35K08, 35K10, 35K67, 35Q91, 58-01, 58J05, 58J35, 58J37, 81Q20, 91G20, 91G30, 91G80

Springer Cham Heidelberg New York Dordrecht London

Printed on acid-free paper

Springer International Publishing AG Switzerland is part of Springer Science+Business Media (www.birkhauser-science.com)

To my wife Valentina, my son Grigori, and my parents

Preface

I am a mathematical physicist. I have been working in mathematical physics over thirty years. The primary focus of my research, until recently, has been developing advanced methods of geometric analysis and applying them to quantum theory. A financial industry practitioner might ask a natural question: "Is there anything useful a mathematical physicist can tell me?" Well, I asked myself the same question when I got an email from Michel Crouhy, the head of Research and Development at NATIXIS Corporate and Investment Bank in Paris, inviting me to present a series of lectures for the members of his group. Very soon, with the help of Olivier Croissant, I realized that one of the major problems of quantitative finance, at least in option pricing theory, is the problem of finding the solution of a partial differential equation of parabolic type called a generalized diffusion equation (or heat equation). This is exactly what I have been doing my whole life, and that was exactly the reason why Michel Crouhy asked me to explain to his quants what is the "heat kernel" and how one can compute it, at least approximately, to price options. This book grew out of these lectures. I believe it might be useful for other quants too as well as for physicists, applied mathematicians and engineers, in fact, anybody who is concerned with the need to solve parabolic partial differential equations.

The book consists of four parts: Analysis, Geometry, Perturbations and Applications. In the first part after a short review of some background material I present an introduction to partial differential equations. The second part is devoted to a short introduction to various aspects of differential geometry that will be needed later. The third part is devoted to a systematic development of effective methods for various approximation schemes for parabolic differential equations that make an extensive use of differential geometric and analytical concepts introduced earlier. The heart of the book is the development of a short-time asymptotic expansion for the heat kernel. I explain it in details and give explicit examples of some advanced calculations. We also discuss some advanced methods and extensions, including path integrals, jump diffusion and others. In the forth part I start with a short introduction to

financial mathematics, in particular, stochastic differential equations and the description of some basic models. I show that all these models, including stochastic volatility models, lead to a valuation equation for the option price, which is nothing but a second order partial differential equation of parabolic type. I demonstrate how the advanced perturbational techniques can be applied to some models of mathematical finance.

A remark about the level and the style of the presentation is in order. Since most of the time I start from scratch, the level of the presentation is necessarily uneven. I start from very elementary introductory concepts (that should be boring for a specialist) and go pretty quickly to rather advanced technical methods needed for our purposes. So, it is normal if you are bored at the beginning and lost at the end.

Also, I intentionally sacrifice rigor for clarity and accessibility for a wider audience. So, the style is rather informal. Most of the time I do not discuss and state precise conditions (which are, of course, of primary interest for pure mathematicians) under which the statements and results are valid.

I provide some references to the original papers and books that I found useful. However, the subject is so huge that it is impossible to give a more or less comprehensive review of the literature. No such attempt has been made. This book is a tutorial for non-specialists rather than a review of the area for the experts.

Socorro,
July, 2015 *Ivan Avramidi*

Acknowledgements

I would like to express my gratitude to many friends, collaborators and colleagues but I will single out just a few people who had an enormous influence on my education and my career: my PhD advisor Vladislav Khalilov, my postoctoral mentor Julius Wess as well as Thomas Branson, Peter Gilkey, Bryce De Witt, Stuart Dowker and Stephen Fulling from whom I learned a lot of material in this book. I am especially indebted to Michel Crouhy and Olivier Croissant who inspired my interest in quantitative finance and without whom this book certainly would never have been written. Most importantly, I thank my wife, Valentina, for constant support and encouragement.

Contents

Notation

$\partial_t = \frac{\partial}{\partial t}$	Partial derivative with respect to time
$\dot{S} = \partial_t S$	Dot denotes time derivative
$\partial_i = \frac{\partial}{\partial x^i}$	Partial derivative with respect to space variables
∇_i	Covariant derivative
$\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i$	Generalized covariant derivative
∇_X	Directional covariant derivative along a vector field X
∇_N	Normal derivative at the boundary
$\sim$	Asymptotic equivalence
$\binom{m}{n}$	Binomial coefficient
$\langle p, x \rangle$	Standard pairing between dual vector spaces
(f, φ)	Inner product
$\|\|f\|\| = \sqrt{(f,f)}$	Norm
$\bar{f}$	Complex conjugate
$dx = dx^1 \cdots dx^n$	Lebesgue measure on $\mathbb{R}^n$
$dx\, g^{1/2}$	Riemannian volume element
$\mathcal{D}x(\tau)$	Path integral measure
∂M	Boundary of the manifold M
$T_{(i_1,\ldots i_p)}$	Symmetrization of a tensor
$T_{[i_1,\ldots i_p]}$	Anti-symmetrization of a tensor
$[f(x,x')] = f(x,x)$	Coincidence limit of a two-point function
A^*	Adjoint operator (or Hermitian conjugate matrix)
A^T	Transposed matrix
$[X, Y]$	Lie bracket (commutator)
$x_+ = \max(x, 0)$	Nonnegative maximum function
$\delta(x)$	Dirac delta function
$\delta(x, x')$	Covariant delta function
$\delta_{ij} = \delta^{ij} = \delta^i{}_j$	Kronecker symbol
Δ	Laplacian
$\Delta(x, x')$	Van Vleck-Morette determinant
$\varepsilon_{j_1 \ldots j_{n-1}}$	Levi-Civita symbol
$\Gamma(s)$	Gamma function

$\Gamma^i{}_{jk}$	Christoffel symbols
$\theta(x)$	Heaviside step function
$\rho(X^i, X^j)$	Correlation matrix
$\sigma(x, p)$	Symbol of a partial differential operator
$\sigma(x, x')$	Synge function
$\sigma(X)$	Standard deviation
$\chi_B(x)$	Characteristic function of a set B
$\psi(x) = \Gamma'(x)/\Gamma(x)$	Digamma function
$\mathcal{A}_i$	Generalized connection
$\mathbb{C} = 0.577\ldots$	Euler's constant
$C^i{}_{jk}$	Structure constants of a Lie group
$\mathrm{Cov}(X^i, X^j)$	Covariance matrix
$d(x, x')$	Geodesic distance between x and x'
$E(X)$	Expected value
$E(X\|A)$	Conditional expected value of X given A
$f_X(x)$	Probability density function
$F_X(x)$	Cumulative distribution function
g_{ij}	Riemannian metric tensor
$g = \det g_{ij}$	Determinant of the metric
g^{ij}	Inverse matrix of the metric
$\hat{g}_{\mu\nu}$	Induced Riemannian metric on the boundary
$\hat{g} = \det \hat{g}_{\mu\nu}$	Determinant of the induced metric
$G(\lambda)$	Resolvent
$G(\lambda; x, x')$	Resolvent kernel
H^n	n-dimensional hyperbolic space
I	Identity operator
K	Gaussian curvature
L_X	Lie derivative along a vector field X
$L^2(M, \mu)$	Hilbert space of square integrable functions on a manifold M with the weight μ
N^i	Inward pointing normal vector to the boundary
$p_X(t, x; t', x')$	Conditional probability density function (transitional distribution)
$P(A)$	Probability of an event A
$P(A\|B)$	Conditional probability of an event A given B
$P = (g^i{}_{j'})$	Operator of parallel transport along the geodesic
$\mathcal{P}(x, x')$	Generalized operator of parallel transport along the geodesic
$R^i{}_{jkl}$	Riemann tensor
R_{ij}	Ricci tensor
R	Scalar curvature
$\mathcal{R}_{ij}$	Curvature of the connection $\mathcal{A}_i$
S^n	n-dimensional sphere
$SO(n)$	Special orthogonal group
$SO(1, n)$	Special pseudo-orthogonal group

$SU(n)$	Special unitary group
$U(t)$	Heat semi-group
$U(t,t')$	Heat semi-group of a time-dependent operator
$U(t;x,x')$	Heat kernel
$U(t,x;t',x')$	Heat kernel of a time-dependent operator
$\mathrm{Var}(X)$	Variance
$x=(x^1,\dots,x^n)$	Local coordinates on a manifold
$\hat{x}=(\hat{x}^1,\dots,\hat{x}^{n-1})$	Local coordinates on the boundary of a manifold
X_t	Stochastic process

Part I
Analysis

Chapter 1
Background in Analysis

Abstract In this chapter we present some of the necessary background material needed for the study of the heat kernel method, such as integral transforms, asymptotic expansions, Hamiltonian systems and the theory of operators in Hilbert spaces. We also introduce some notation used throughout the book. It can be safely skipped by a reader familiar with these subjects.

1.1 Asymptotic Expansions

First of all, we remind some definitions of asymptotic analysis [23, 30, 35, 36, 67, 64]. Let us consider two functions f and g of a real variable x. We consider the limits of these functions as x approaches some point a. We say that $f(x)$ is *infinitesimal* with respect to $g(x)$ as $x \to a$, and we write

$$f(x) = o(g(x))\,, \tag{1.1}$$

if

$$\lim_{x\to a} \frac{f(x)}{g(x)} = 0\,. \tag{1.2}$$

We say that $f(x)$ is *bounded* with respect to $g(x)$ as $x \to a$, and we write

$$f(x) = O(g(x))\,, \tag{1.3}$$

if

$$\lim_{x\to a} \frac{f(x)}{g(x)} = C\,, \tag{1.4}$$

with some constant C.

In particular, $f(x) = o(1)$ means that $f(x)$ is *infinitesimal* as $x \to a$, that is, $\lim_{x\to a} f(x) = 0$, and $f(x) = O(1)$ means that $f(x)$ is *bounded* as $x \to a$.

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_1

Finally, we write

$$f(x) \sim g(x) \tag{1.5}$$

if

$$\lim_{x \to a} \frac{f(x)}{g(x)} = 1\,, \tag{1.6}$$

Let $(\varphi_n)_{n=1}^{\infty}$ be a sequence of real valued functions such that $\varphi_n(x) \neq 0$ in a neighborhood of a and

$$\varphi_{n+1}(x) = o(\varphi_n(x))\,. \tag{1.7}$$

Such a sequence is called an *asymptotic sequence* at $x \to a$. For example, the sequence $((x-a)^n)_{n=0}^{\infty}$ is an asymptotic sequence.

Let f be a function and $(\varphi_n)_{n=1}^{\infty}$ be an asymptotic sequence as $x \to a$. We say that the function f is expanded in an *asymptotic series*, and write

$$f(x) \sim \sum_{n=1}^{\infty} a_n \varphi_n(x), \tag{1.8}$$

where a_n are constants, if for all $N \geq 0$

$$f(x) - \sum_{n=1}^{N} a_n \varphi_n(x) = o(\varphi_N(x))\,. \tag{1.9}$$

This series is called the *asymptotic expansion* of the function f with respect to the asymptotic sequence (φ_n). The function

$$R_N(x) = f(x) - \sum_{n=1}^{N} a_n \varphi_n(x) \tag{1.10}$$

is called the *remainder term* of the asymptotic series.

The condition $R_N(x) = o(\varphi_N(x))$ means, in particular, that for any fixed N

$$\lim_{x \to a} R_N(x) = 0\,. \tag{1.11}$$

However, if for some fixed x

$$\lim_{N \to \infty} R_N(x) \neq 0 \tag{1.12}$$

then the asymptotic series diverges. In general, there are three possibilities:

1. asymptotic series converges to the original function;
2. asymptotic series converges to a different function;
3. asymptotic series diverges.

One can also show that the asymptotic expansion of a function with respect to an asymptotic sequence is unique. However, two different functions can

have the same asymptotic expansion. As an example consider the asymptotic sequence

$$\varphi_n(x) = x^n, \qquad n = 0, 1, 2, \ldots, \tag{1.13}$$

as $x \to 0$. It is easy to see that the asymptotic expansion of the function $f(x) = (1 - x)^{-1}$ is given by the geometric series

$$f(x) \sim \sum_{n=0}^{\infty} x^n. \tag{1.14}$$

However, it is also not difficult to show that the function

$$g(x) = (1 - x)^{-1} + \exp\left(-\frac{1}{x^2}\right) \tag{1.15}$$

has the same asymptotic expansion as $x \to 0$.

1.2 Gaussian Integrals

First of all, we remind the fundamental one-dimensional Gaussian integral

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}\,. \tag{1.16}$$

By scaling the variable $x \to \sqrt{a}\, x$ with a positive constant $a > 0$ we also get

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\pi}\, a^{-1/2}\,. \tag{1.17}$$

Next, by shifting the variable $x \to x - b/(2a)$, with b being an arbitrary constant, we get

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2+bx} = \sqrt{\pi}\, a^{-1/2} \exp\left(\frac{b^2}{4a}\right)\,. \tag{1.18}$$

By differentiating this equation with respect to b we have, in particular,

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2+bx} x = \frac{1}{2}\sqrt{\pi}\, a^{-3/2} b \exp\left(\frac{b^2}{4a}\right), \tag{1.19}$$

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2+bx} x^2 = \frac{1}{2}\sqrt{\pi}\, a^{-3/2} \left(1+\frac{b^2}{2a}\right) \exp\left(\frac{b^2}{4a}\right). \tag{1.20}$$

By expanding both sides of eq. (1.18) in a power series in b we finally obtain the following Gaussian integrals for any non-negative integer k

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} x^{2k+1} = 0\,, \tag{1.21}$$

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} x^{2k} = \sqrt{\pi}\, \frac{(2k)!}{2^{2k} k!} a^{-k-1/2}\,. \tag{1.22}$$

Multidimensional Gaussian integrals are computed similarly. We will use the following notation throught this book. For a vector $x = (x^i) = (x^1, \ldots, x^n)$ and a covector $p = (p_i) = (p_1, \ldots, p_n)$ in $\mathbb{R}^n$ we define the standard pairing

$$\langle p, x\rangle = \sum_{i=1}^{n} p_i x^i\,. \tag{1.23}$$

Also, if $A = (A^{ij})$ is an $n \times n$ matrix, then we denote

$$\langle p, Ap\rangle = \sum_{i,j=1}^{n} p_i A^{ij} p_j\,. \tag{1.24}$$

Now, let $A = (A_{ij})$ be a real symmetric positive matrix, which means that $\langle x, Ax\rangle > 0$ for all $x \neq 0$ in $\mathbb{R}^n$. Then for any vector $B = (B_i)$ there holds

$$\int_{\mathbb{R}^n} dx\, \exp\Big(-\langle x, Ax\rangle + \langle B, x\rangle\Big) = \pi^{n/2} (\det A)^{-1/2} \exp\left(\frac{1}{4}\,\langle B, A^{-1} B\rangle\right), \tag{1.25}$$

where $dx = dx^1 \cdots dx^n$ is the standard Lebesgue (or Riemann) measure on $\mathbb{R}^n$ and $A^{-1} = (A^{ij})$ is the inverse of the matrix A. This formula can be proved by diagonalizing the matrix A and using the one-dimensional Gaussian integral (1.18).

By differentiating with respect to B_i we have

$$\int\limits_{\mathbb{R}^n} dx\ \exp\Big(-\langle x, Ax\rangle + \langle B, x\rangle\Big) x^i$$

$$= \frac{\pi^{n/2}}{2} (\det A)^{-1/2} \sum_{k=1}^{n} A^{ik} B_k \exp\left(\frac{1}{4}\ \langle B, A^{-1} B\rangle\right), \tag{1.26}$$

$$\int\limits_{\mathbb{R}^n} dx\ \exp\Big(-\langle x, Ax\rangle + \langle B, x\rangle\Big) x^i x^j \tag{1.27}$$

$$= \frac{\pi^{n/2}}{2} (\det A)^{-1/2} \left(A^{ij} + \frac{1}{2} \sum_{k,l=1}^{n} A^{ik} B_k B_l A^{lj}\right) \exp\left(\frac{1}{4}\ \langle B, A^{-1} B\rangle\right).$$

By expanding both sides of eq. (1.25) in Taylor series in B_i we also obtain

$$\int\limits_{\mathbb{R}^n} dx\ \exp\Big(-\langle x, Ax\rangle\Big)\, x^{i_1} \cdots x^{i_{2k+1}} = 0\,, \tag{1.28}$$

$$\int\limits_{\mathbb{R}^n} dx\ \exp\Big(-\langle x, Ax\rangle\Big)\, x^{i_1} \cdots x^{i_{2k}}$$

$$= \pi^{n/2} (\det A)^{-1/2}\, \frac{(2k)!}{2^{2k} k!}\, A^{(i_1\, i_2} \cdots A^{i_{2k-1}\, i_{2k})}\,, \tag{1.29}$$

where the parenthesis denote complete symmetrization over all indices included (for the definition of symmetrization see eq. (3.47) in Sec. 3.1.8), in particular,

$$\int\limits_{\mathbb{R}^n} dx\ \exp\Big(-\langle x, Ax\rangle\Big)\, x^i x^j = \frac{1}{2} \pi^{n/2} (\det A)^{-1/2}\, A^{ij}\,, \tag{1.30}$$

$$\int\limits_{\mathbb{R}^n} dx\ \exp\Big(-\langle x, Ax\rangle\Big)\, x^i x^j x^k x^l$$

$$= \frac{1}{4} \pi^{n/2} (\det A)^{-1/2} \left(A^{ij} A^{kl} + A^{ik} A^{jl} + A^{il} A^{jk}\right). \tag{1.31}$$

The beauty of Gaussian integrals is that they can be easily generalized to any dimension, even infinite dimensions. A very important property of Gaussian integrals is that the right-hand sides of the above equations do not depend on the dimension of the space $\mathbb{R}^n$, which enables one to go to the limit $n \to \infty$ and define the infinite-dimensional Gaussian *path integrals*. We will discuss this briefly in Chap. 6.

1.3 Laplace Integrals

Let S be a real-valued smooth function and φ be a complex valued smooth function on an interval $[a, b]$. We consider integrals of the form

$$F(\lambda) = \int_a^b dx\ \varphi(x) \exp\left[-\lambda S(x)\right] , \tag{1.32}$$

where λ is a large positive parameter. Such integrals appear quite often in applications; they are called *Laplace integrals*. Unfortunately, except for Gaussian integrals Laplace integrals cannot be computed exactly. Therefore, it is very important to develop systematic methods to study the asymptotics of such integrals as $\lambda \to \infty$.

It is clear that the main contribution to the integral comes from the neighborhood of the points where the function $S(x)$ is minimal. Suppose that the function S has a minimum at an interior point x_0 of the interval $[a, b]$ which implies that $a < x_0 < b$, so that $S'(x_0) = 0$. Assume, for simplicity, that $S''(x_0) \neq 0$; then $S''(x_0) > 0$. In other words, in a neighborhood of x_0 the function S has the following Taylor expansion

$$S(x) = S(x_0) + \frac{1}{2} S''(x_0)(x - x_0)^2 + O((x - x_0)^3) . \tag{1.33}$$

Such a point is called a *non-degenerate critical point*.

Then, as $\lambda \to \infty$ the main contribution to the integral comes from a small neighborhood of x_0. In this neighborhood the function φ is almost constant and can be replaced by its value at x_0. The terms of order $(x - x_0)^3$ can be neglected in the exponent and the remaining integral can be extended to the whole real line so that it becomes a standard Gaussian integral. Thus, we obtain the main term of the asymptotics as $\lambda \to \infty$

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{1/2} \left[S''(x_0)\right]^{-1/2}\ \exp\left[-\lambda S(x_0)\right] \varphi(x_0) . \tag{1.34}$$

More generally, one can prove that if the function S has a minimum only at a single non-degenerate interior critical point x_0, then as $\lambda \to \infty$ there is an asymptotic expansion

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{1/2} \left[S''(x_0)\right]^{-1/2}\ \exp\left[-\lambda S(x_0)\right] \sum_{k=0}^{\infty} a_k \lambda^{-k} , \tag{1.35}$$

where the coefficients a_k are expressed in terms of the derivatives of the functions φ and S at x_0. More precisely, the coefficients a_k of the asymptotic expansion are polynomials in the higher derivatives $S^{(k)}(x_0)$, $k \geq 3$, the

inverse of the second derivative $[S''(x_0)]^{-1}$, and linear in derivatives $\varphi^{(l)}(x_0)$, $l \geq 0$.

This can be proved as follows. First, we change the integration variable

$$x = x_0 + \lambda^{-1/2} y \,. \tag{1.36}$$

The interval of integration should be changed accordingly, so that the minimum point is now $y = 0$. Then, we expand both functions S and φ in Taylor series at x_0,

$$S(x_0 + \lambda^{-1/2} y) = S(x_0) + \frac{1}{2}\lambda^{-1} S''(x_0) y^2 + \sum_{n=3}^{\infty} \frac{S^{(n)}(x_0)}{n!} y^n \lambda^{-n/2} \,, \tag{1.37}$$

$$\varphi(x_0 + \lambda^{-1/2} y) = \sum_{n=0}^{\infty} \frac{\varphi^{(n)}(x_0)}{n!} y^n \lambda^{-n/2} \,. \tag{1.38}$$

Then the quadratic term in the exponent is of order $O(1)$ as $\lambda \to \infty$. So we leave it in the exponent and expand the exponent of the rest in a power series in powers of $\lambda^{-1/2}$. We obtain

$$F(\lambda) = \lambda^{-1/2} \exp\left[-\lambda S(x_0)\right] \int_{-(x_0-a)\sqrt{\lambda}}^{(b-x_0)\sqrt{\lambda}} dy \, \exp\left[-\frac{1}{2} S''(x_0) y^2\right] V(x_0, y, \lambda) \,, \tag{1.39}$$

where the function $V(x_0, y, \lambda)$ has the form

$$V(x_0, y, \lambda) = \sum_{k=0}^{\infty} b_k(x_0, y) \lambda^{-k/2} \,. \tag{1.40}$$

The coefficients $b_k(x_0, y)$ are polynomials in y with coefficients that are polynomial in the derivatives $S^{(k)}(x_0)$, $k \geq 3$, of the function S of order greater or equal than three and linear in all derivatives $\varphi^{(l)}(x_0)$, $l \geq 0$, of the function φ evaluated at x_0.

Next, as $\lambda \to \infty$ we extend the integration interval to the whole real line and compute the standard Gaussian integrals. The half-integer powers of λ^{-1} always come with half-integer powers of y and, therefore, vanish after integration. Finally, we get the power series (1.35) in inverse powers of λ.

Laplace integrals in higher dimensions can be evaluated similarly. Let M be a bounded connected open set in $\mathbb{R}^n$, S be some real-valued smooth function, φ be some complex-valued smooth function on M and $\lambda > 0$ be a large positive parameter. We will study the asymptotics as $\lambda \to \infty$ of the multidimensional Laplace integrals

$$F(\lambda) = \int\limits_M dx\ \varphi(x) \exp[-\lambda S(x)]\,. \tag{1.41}$$

Here and throughout this book we denote the partial derivative with respect to a variable t by

$$\partial_t = \frac{\partial}{\partial t}\,. \tag{1.42}$$

More, generally, in $\mathbb{R}^n$ we denote partial derivatives with respect to space variables x^i by

$$\partial_i = \frac{\partial}{\partial x^i}\,. \tag{1.43}$$

A point x_0 in M is called a *critical point* of the function S if

$$\partial_i S(x_0) = 0\,. \tag{1.44}$$

The $n \times n$ real symmetric matrix of second derivatives of the function S at the critical point,

$$H = (\partial_i \partial_j S(x_0))\,, \tag{1.45}$$

is called the *Hessian matrix* and its determinant is called the *Hessian*. A critical point x_0 is called *non-degenerate* if the Hessian matrix is non-degenerate at x_0, that is,

$$\det H \neq 0\,. \tag{1.46}$$

By standard analytic arguments one can show that non-degenerate critical points are *isolated*, that is, there is a neighborhood where there are no other critical points.

Let the function S have a minimum only at a single interior non-degenerate critical point x_0 in M. Then $\partial_i S(x_0) = 0$ and the Hessian matrix H is *positive definite*. Then in a neighborhood of x_0 the function S has the following Taylor expansion

$$S(x) = S(x_0) + \frac{1}{2}\,\langle (x - x_0), H(x - x_0)\rangle + O((x - x_0)^3)\,. \tag{1.47}$$

Then as $\lambda \to \infty$ the main contribution to the integral comes from a small neighborhood of the point x_0. In this neighborhood the terms of the third order in the Taylor expansion of S can be neglected. Also, since the function φ is continuous at x_0, it can be replaced by its value at x_0. Then the region of integration can be extended to the whole $\mathbb{R}^n$. By using the formula for the standard Gaussian integral (1.25) we get the leading asymptotics of the integral $F(\lambda)$ as $\lambda \to \infty$

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{n/2} (\det H)^{-1/2} \exp[-\lambda S(x_0)]\varphi(x_0)\,. \tag{1.48}$$

More generally, one can prove that if the function S has only one non-degenerate interior critical point x_0 in M, where it has the only minimum in M, then there is an asymptotic expansion as $\lambda \to \infty$

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{n/2} (\det H)^{-1/2} \exp[-\lambda S(x_0)] \sum_{k=0}^{\infty} a_k \lambda^{-k} . \tag{1.49}$$

The coefficients a_k are expressed in terms of the derivatives of the functions φ and S at the point x_0. More precisely, the coefficients a_k are polynomial in the higher derivatives $[\partial_{i_1} \cdots \partial_{i_m} S(x_0)]$, $m \geq 3$, of the function S, the inverse Hessian matrix $G = H^{-1}$, and linear in the derivatives $[\partial_{i_1} \cdots \partial_{i_l} \varphi(x_0)]$, $l \geq 0$, of the function φ evaluated at the point x_0.

The idea of the proof is the same as in the one-dimensional case and goes as follows. First, we change the integration variables

$$x^i = x_0^i + \lambda^{-1/2} y^i . \tag{1.50}$$

The region of integration should be changed accordingly, so that the minimum point is now $y = 0$. Then, we expand both functions S and φ in Taylor series at x_0,

$$S(x_0 + \lambda^{-1/2} y) = S(x_0) + \frac{1}{2}\lambda^{-1} \langle y, Hy \rangle + \sum_{m=3}^{\infty} \sum_{i_1,\ldots,i_m=1}^{n} \frac{\lambda^{-m/2}}{i_1! \cdots i_m!} [S_{i_1 \ldots i_m} y^{i_1} \cdots y^{i_m} , \tag{1.51}$$

$$\varphi(x_0 + \lambda^{-1/2} y) = \sum_{m=0}^{\infty} \sum_{i_1,\ldots,i_m=1}^{n} \frac{\lambda^{-m/2}}{i_1! \cdots i_m!} [\partial_{i_1} \cdots \partial_{i_m} \varphi(x_0)] \, y^{i_1} \cdots y^{i_m} , \tag{1.52}$$

where $S_{i_1 \ldots i_m} = \partial_{i_1} \cdots \partial_{i_m} S(x_0)$ and $\varphi_{i_1 \ldots i_m} = \partial_{i_1} \cdots \partial_{i_m} \varphi(x_0)$. Similarly to the one-dimensional case, the quadratic terms in the exponent are of order $O(1)$ as $\lambda \to \infty$. So, we leave them in the exponent and expand the exponent of the rest in a power series. Next, we extend the integration domain to the whole $\mathbb{R}^n$ and compute the standard Gaussian integrals. Finally, we get the power series (1.49) in inverse powers of λ.

Each term in the asymptotic expansion can be represented by a graph, known as a *Feynmann diagram*, as follows. We represent the derivatives $[\partial_{i_1} \cdots \partial_{i_m} S(x_0)]$, $m \geq 3$, by *vertices* with m lines attached to them. Next, we represent the inverse Hessian $G = H^{-1}$, called the *propagator*, by a line connecting two vertices. Then each term of the asymptotic expansion can be represented by an appropriate graph where the corresponding legs of the vertices are linked by propagators. For example, the following term

$$\varphi_{rst} G^{ri} G^{sj} G^{tp} S_{ijkl} G^{lm} G^{kn} S_{mnp} \tag{1.53}$$

is described by the diagram 1.1

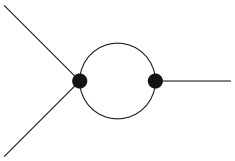


Fig. 1.1 Feynman Diagram

The coefficients a_k of the asymptotic expansion of the integral $F(\lambda)$ are *invariants* under smooth local diffeomorphisms (changes of variables) in a neighborhood of x_0 and play very important role in mathematical physics and in various applications.

1.4 Fourier Transform

First, let us recall the definition of the *Fourier transform*. Let f be a smooth function of a real variable $x \in \mathbb{R}$ that falls off sufficiently fast at infinity. Then the Fourier transform of f is a function $\hat{f}$ of a real variable $p \in \mathbb{R}$ defined by

$$\hat{f}(p) = (\mathcal{F}f)(p) = \int_{-\infty}^{\infty} dx\, e^{-ipx} f(x)\,, \tag{1.54}$$

so that

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx} \hat{f}(p)\,. \tag{1.55}$$

The Fourier transform of the derivatives is particularly simple. We have

$$(\mathcal{F}[\partial_x f(x)])(p) = ip\hat{f}(p)\,, \tag{1.56}$$

$$(\mathcal{F}[\partial_x^2 f(x)])(p) = -p^2 \hat{f}(p)\,. \tag{1.57}$$

More generally, one can show that

$$(\mathcal{F}[xf(x)])(p) = i\partial_p \hat{f}(p)\,, \tag{1.58}$$

$$(\mathcal{F}[x\partial_x f(x)])(p) = -\partial_p[p\hat{f}(p)] = -(p\partial_p + 1)\hat{f}(p)\,, \tag{1.59}$$

$$(\mathcal{F}[x\partial_x^2 f(x)])(p) = -i\partial_p[p^2\hat{f}(p)] = -i(p^2\partial_p + 2p)\hat{f}(p)\,. \tag{1.60}$$

We also note that for many functions the Fourier transform can be analytically continued in a horizontal strip near the real axis. This enables one

to define the Fourier transforms of distributions, or singular functions, which would normally diverge, by deforming the contour of integration, that is, by carefully avoiding the singularities in a specified manner. This also enables one to compute the Fourier transform by closing the contour of integration either in the upper half-plane or in the lower half-plane.

The Fourier representation of the Heaviside step function θ defined by

$$\theta(x) = \begin{cases} 1, & \text{if} \quad x > 0, \\ 0, & \text{if} \quad x \leq 0, \end{cases} \tag{1.61}$$

can be obtained as follows

$$\theta(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi i} e^{ipx} \frac{1}{p - i\varepsilon}\,, \tag{1.62}$$

where $\varepsilon > 0$ is an infinitesimal positive parameter. Indeed, for $x > 0$ the contour can be closed in the upper half plane and there is a simple pole there at $p = i\varepsilon$ with residue equal to 1. For $x < 0$ the contour can be closed in the lower half plane and since the integrand is analytic in the lower half-plane the integral vanishes. Of course, for $x = 0$ it is not defined.

It is easy to see that the derivative of the step function is equal to the delta function,

$$\partial_x \theta(x) = \delta(x)\,, \tag{1.63}$$

which immediately gives the Fourier representation of the delta function

$$\delta(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx}\,. \tag{1.64}$$

The Fourier transform can be obviously generalized to n dimensions. Let f be a function of n real variables x^j, $j = 1, \ldots, n$. Let x be the n-tuple $x = (x^1, \ldots, x^n)$. Then x is just a point in the n-dimensional Euclidean space, $x \in \mathbb{R}^n_x$. Let us introduce the *dual space* $\mathbb{R}^n_p$ whose points are n-tuples $p = (p_1, \ldots, p_n)$. Then the Fourier transform of f is a function $\hat{f}$ of real variables p_j defined by

$$\hat{f}(p) = (\mathcal{F}f)(p) = \int\limits_{\mathbb{R}^n} dx\; e^{-i\langle p,x\rangle} f(x)\,, \tag{1.65}$$

where $dx = dx^1 \ldots dx^n$, and $\langle p, x\rangle = \sum_{j=1}^n p_j x^j$. The inverse Fourier transform is then defined by

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,x\rangle} \hat{f}(p)\,. \tag{1.66}$$

The n-dimensional delta-function can be represented as the Fourier integral

$$\delta(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,x\rangle} \,. \tag{1.67}$$

1.5 Laplace Transform

Another important tool for solving differential equations is the Laplace transform. Let f be a function of a real variable $t \in (0,\infty)$. Then *Laplace transform* of the function f is a function F of a complex variable $s \in \mathbb{C}$ defined by

$$F(s) = (\mathcal{L}f)(s) = \int\limits_0^\infty dt\; e^{-st} f(t) \,. \tag{1.68}$$

We assume that the function f belongs to a class of functions that can grow at infinity not faster than an exponential. Then there is a smallest real constant γ such that Laplace transform $F(s)$ converges in the half-plane $\operatorname{Re} s > \gamma$. Then the inverse Laplace transform is defined by

$$f(t) = (\mathcal{L}^{-1}F)(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} F(s) \,. \tag{1.69}$$

where c is a sufficiently large constant, $c > \gamma$.

Laplace transform of derivatives can be easily computed by integration by parts,

$$(\mathcal{L}[\partial_t f(t)])(s) = sF(s) - f(0) \,, \tag{1.70}$$

$$(\mathcal{L}[\partial_t^2 f(t)])(s) = s^2F(s) - sf(0) - f'(0) \,. \tag{1.71}$$

Also, Laplace transform of products with polynomials can be easily computed, in particular,

$$(\mathcal{L}[tf(t)])(s) = -\partial_s F(s) \,. \tag{1.72}$$

More generally, one can show that

$$(\mathcal{L}[t\partial_t f(t)])(s) = = -(s\partial_s + 1)F(s) \,, \tag{1.73}$$

$$(\mathcal{L}[t\partial_t^2 f(t)])(s) = -(s^2\partial_s + 2s)F(s) + f(0) \,. \tag{1.74}$$

1.6 Mellin Transform

Let f be a function of a real variable t on the interval $(0, \infty)$. The *Mellin transform* of f is a function F of a complex variable $s \in \mathbb{C}$ defined by

$$F(s) = (\mathcal{M}f)(s) = \int_0^\infty dt\, t^{s-1} f(t)\,. \tag{1.75}$$

We consider the class of functions f such that there are two real numbers, a and b, such that $a < b$ and $F(s)$ is analytic in the infinite strip $a < \mathrm{Re}\, s < b$ and

$$\lim_{|\mathrm{Im} s| \to \infty} F(s) = 0\,. \tag{1.76}$$

Then the inverse Mellin transform is defined by

$$f(t) = (\mathcal{M}^{-1}F)(t) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} t^{-s} F(s)\,, \tag{1.77}$$

where c is any real number such $a < c < b$, that is, the integral is taken over a vertical line in the strip $a < \mathrm{Re}\, s < b$. The numbers a and b, which determine the region of analyticity of the Fourier transform, are determined by the rate at which the function f decreases or increases at 0 and ∞.

The Mellin transform is related to the Fourier transform as follows. Let $t = e^x$, where $t \in (0, \infty)$ and $x \in (-\infty, \infty)$. Then the Fourier transform of a function f is

$$\begin{aligned}(\mathcal{M}f(t))(s) &= \int_{-\infty}^{\infty} dx\, e^{sx} f(e^x) \\ &= [\mathcal{F}f(e^x)]\,(is)\,,\end{aligned} \tag{1.78}$$

which is nothing but the Fourier transform of the function $f(e^x)$ evaluated at $p = is$. Similarly, we have $x = \log t$, and, therefore, the Fourier transform of the function f is

$$\begin{aligned}[\mathcal{F}f(x)]\,(p) &= \int_0^\infty dt\, t^{-ip-1} f(\log t) \\ &= [\mathcal{M}f(\log t)]\,(-ip)\,,\end{aligned} \tag{1.79}$$

which is the Fourier transform of the function $f(\log t)$ evaluated at $s = -ip$. This means, in particular, that the Fourier transform of the function f is

well defined if the imaginary axis is in the strip of analyticity of the Fourier transform of the function $f(\log t)$.

The nice thing about the Fourier transform is how it behaves under homogeneous differentiation. In the strip of analyticity, $a < \mathrm{Re}\, s < b$, we obviously have

$$[\mathcal{M}(tf(t))](s) = (\mathcal{M}f)(s+1)\,. \tag{1.80}$$

Further, by integration by parts we obtain

$$[\mathcal{M}(\partial_t f(t))](s) = -(s-1)(\mathcal{M}f)(s-1)\,. \tag{1.81}$$

Therefore,

$$[\mathcal{M}(t\partial_t f(t))](s) = -s(\mathcal{M}f)(s)\,, \tag{1.82}$$

$$[\mathcal{M}(t^2\partial_t^2 f(t))](s) = s(s+1)(\mathcal{M}f)(s)\,. \tag{1.83}$$

Recall that Euler's gamma function $\Gamma(s)$ is the Fourier transform of the exponential function

$$\Gamma(s) = \int_0^\infty dt\; t^{s-1}e^{-t}\,. \tag{1.84}$$

It satisfies the functional equation

$$s\Gamma(s) = \Gamma(s+1)\,, \tag{1.85}$$

and is a meromorphic function with simple poles at non-positive real integer values $s = -k$ with residues

$$\mathrm{Res}\,\{\Gamma(s); -k\} = \frac{(-1)^k}{k!}\,. \tag{1.86}$$

In the following we shall investigate the relation of the Mellin transform with the asymptotic expansion as $t \to 0$. Let Ω be a function of a real variable t such that:

1. for any positive real number $\alpha > 0$ and any non-negative integer $N \geq 0$ the following limits vanish

$$\lim_{t\to 0,\infty} t^\alpha \partial_t^N \Omega(t) = 0\,, \tag{1.87}$$

2. for any non-negative integer $k \geq 0$ there exist the limits

$$b(k) = (-1)^k \lim_{t\to 0} \partial_t^k \Omega(t)\,. \tag{1.88}$$

That is, we assume that the function Ω has a well defined Taylor series at $t = 0$, but we do not assume that the Taylor series converges, that is, we do not assume that the function Ω is analytic at $t = 0$. We show below that

such a function has an asymptotic expansion at $t \to 0$ and the coefficients of this asymptotic expansion are determined by $b(k)$.

Let b be the rescaled Mellin transform of the function Ω defined by

$$b(s) = \frac{1}{\Gamma(-s)}(\mathcal{M}\Omega)(-s) = \frac{1}{\Gamma(-s)} \int_0^\infty dt\, t^{-s-1}\Omega(t)\,. \tag{1.89}$$

This integral converges for $\operatorname{Re} s < 0$. Now, by integrating by parts we can analytically continue it to the whole complex plane obtaining an entire function $b(s)$. In particular, for $\operatorname{Re} s < N$ we have

$$b(s) = \frac{(-1)^N}{\Gamma(-s+N)} \int_0^\infty dt\, t^{-s-1+N}\partial_t^N \Omega(t)\,, \tag{1.90}$$

where N is a positive integer. Moreover, by using the analytical properties of the gamma function we can also obtain that the values of the function $b(k)$ at the non-negative integer points $k = 0, 1, 2, \dots$, are given by the Taylor coefficients (1.88) of the function $\Omega(t)$ at $t = 0$.

Now we can invert the Mellin transformation to get

$$\Omega(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds\, t^s \Gamma(-s) b(s)\,, \tag{1.91}$$

where c is a negative constant. Next, by shifting the contour of integration to the right we obtain

$$\Omega(t) = \sum_{k=0}^{N-1} \frac{(-t)^k}{k!} b(k) + R_N(t)\,, \tag{1.92}$$

where

$$R_N(t) = \frac{1}{2\pi i} \int_{c_N-i\infty}^{c_N+i\infty} ds\, t^s \Gamma(-s) b(s)\,, \tag{1.93}$$

with $N - 1 < c_N < N$. Here $R_N(t)$ is of order $O(t^N)$ at $t \to 0$ and is smaller than the last term of the sum in this limit.

Therefore, this equation gives the asymptotic expansion of $\Omega(t)$ as $t \to 0$

$$\Omega(t) \sim \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} b(k)\,. \tag{1.94}$$

For the definition of the asymptotic expansions see Sec. 1.1. Note that this series is convergent only in the case when the remainder term $R_N(t)$ vanishes

as $N \to \infty$ in a neighborhood of the point $t = 0$. In this case the above series converges and the function $\Omega(t)$ is analytic in a neighborhood of $t = 0$. However, in general, $\Omega(t)$ is not an analytic function at the point $t = 0$. Therefore, for any small $t > 0$ the remainder term $R_N(t)$ does not vanish as $N \to \infty$ and the asymptotic expansion diverges at any finite $t \neq 0$. That is why we used the symbol $\sim$ instead of the symbol $=$ in this equation.

1.7 Derivative of Determinants

We list below some useful properties of the determinants that we will use in this book. Let A be an arbitrary $n \times n$ matrix and $B = \exp A$. We will be using quite often a very useful formula for the determinant

$$\log \det B = \operatorname{tr} A\,, \tag{1.95}$$

which can be proved by diagonalizing the matrix A. We also have

$$\frac{d}{ds} B^{-s} = -AB^{-s} \tag{1.96}$$

and, therefore,

$$\frac{d}{ds} B^{-s}\Big|_{s=0} = -A\,. \tag{1.97}$$

Thus, the above formula can be written as

$$\log \det B = -\frac{d}{ds} \operatorname{tr} B^{-s}\Big|_{s=0}\,. \tag{1.98}$$

Suppose that the matrix $A = A(t)$ depends on a parameter t. By differentiating eq. (1.95) we get another very useful equation for the derivative of a determinant

$$\frac{d}{dt} \log \det B = \operatorname{tr} \frac{d}{dt} A\,. \tag{1.99}$$

One can also show that

$$\operatorname{tr} \frac{d}{dt} A = \operatorname{tr} \left(\exp(-A) \frac{d}{dt} \exp A \right)\,. \tag{1.100}$$

Therefore, for any non-degenerate matrix $B = \exp A$ there holds

$$\begin{aligned} \frac{d}{dt} \log \det B &= \operatorname{tr} \left(B^{-1} \frac{d}{dt} B \right) \\ &= \sum_{j,k=1}^{n} B^{kj} \frac{d}{dt} B_{jk}\,, \end{aligned} \tag{1.101}$$

where $B^{-1} = (B^{kj})$ is the inverse of the matrix $B = (B_{ij})$.

1.8 Hamiltonian Systems

Let $x = (x^i)$ be a point in the Euclidean space $\mathbb{R}^m$. A system of ordinary differential equations

$$\frac{dx^i}{dt} = F^i(x)\,, \tag{1.102}$$

where the right hand side depends only on the space variables x but not on the time variable t is called an *autonomous system*. If the vector field $F^i(x)$ is smooth then such autonomous system with arbitrary initial conditions

$$x(0) = x_0\,, \tag{1.103}$$

has a unique solution $x = x(t)$, at least for sufficiently small t.

The solution of this system defines a map

$$x_0 \mapsto x(t) \tag{1.104}$$

with the Jacobian

$$J(t) = \det\left(\frac{\partial x^i(t)}{\partial x_0^j}\right). \tag{1.105}$$

It is possible to obtain an explicit formula for this Jacobian in terms of the vector field F. Applying eq. (1.101) to the Jacobian matrix (4.38) we obtain

$$\frac{d}{dt}\log J = \sum_{i,j=1}^{m} \frac{\partial x_0^j}{\partial x^i}\frac{d}{dt}\frac{\partial x^i}{\partial x_0^j}\,. \tag{1.106}$$

Next, we use the equation

$$\frac{d}{dt}\frac{\partial x^i}{\partial x_0^j} = \frac{\partial}{\partial x_0^j}\frac{dx^i}{dt} = \frac{\partial F^i}{\partial x_0^j} \tag{1.107}$$

to get

$$\frac{d}{dt}\log J = \sum_{i,j=1}^{m} \frac{\partial x_0^j}{\partial x^i}\frac{\partial F^i}{\partial x_0^j} = \sum_{i=1}^{m}\frac{\partial F^i}{\partial x^i}\,. \tag{1.108}$$

Thus, we see that the Jacobian $J(t)$ satisfies the linear differential equation

$$\left(\frac{d}{dt} - \Phi\right) J = 0\,, \tag{1.109}$$

where

$$\Phi(t) = \sum_{i=1}^{m} \frac{\partial F^i(x(t))}{\partial x^i} \,. \tag{1.110}$$

This is the *Liouville formula*. Of course, this equation can be integrated to give an explicit formula for the Jacobian

$$J(t) = J(0) \exp\left\{ \int_0^t d\tau \; \Phi(\tau) \right\} . \tag{1.111}$$

A *Hamiltonian system* is an autonomous system of a special type in even dimensional spaces, that is, for $m = 2n$. Let $x = (x^i)$ be a point in the *coordinate space* $\mathbb{R}^n_x$ and $p = (p_i)$ be a point in the dual *momentum space* $\mathbb{R}^n_p$. We put extra indices x and p on $\mathbb{R}^n$ to distinguish these spaces. Then the $2n$-dimensional space $\mathbb{R}^{2n}_{x,p} = \mathbb{R}^n_x \times \mathbb{R}^n_p$ of points (x, p) is called the *phase space*.

Let $H = H(x, p)$ be a smooth function on the phase space bounded from below, called a *Hamiltonian*. Then the system of $2n$ ordinary differential equations

$$\frac{dx^k}{dt} = \frac{\partial H(x,p)}{\partial p_k} \,, \tag{1.112}$$

$$\frac{dp_j}{dt} = -\frac{\partial H(x,p)}{\partial x^j} \,, \tag{1.113}$$

is called a *Hamiltonian system*. Obviously it is autonomous.

The solutions of the Hamiltonian system define so-called *phase trajectories* in the phase space $\mathbb{R}^{2n}_{x,p}$

$$x = x(t), \qquad p = p(t) \,. \tag{1.114}$$

The projection of the phase trajectories onto the coordinate space $\mathbb{R}^n_x$ defines the *classical trajectories* or *rays* $x = x(t)$.

Every Hamiltonian system has two very important properties. First of all, the fundamental property of a Hamiltonian system is that the Hamiltonian $H(x, p)$ is an integral of motion along the phase trajectories, that is,

$$H\left(x(t), p(t)\right) = H\left(x(0), p(0)\right) \,. \tag{1.115}$$

Indeed, it is easy to see that along the phase trajectory

$$\begin{aligned} dH(x,p) &= \sum_{i=1}^{n} \frac{\partial H(x,p)}{\partial x^i} \frac{dx^i}{dt} + \sum_{i=1}^{n} \frac{\partial H(x,p)}{\partial p_i} \frac{dp_i}{dt} \qquad (1.116) \\ &= \sum_{i=1}^{n} \frac{\partial H(x,p)}{\partial x^i} \frac{\partial H(x,p)}{\partial p_i} - \sum_{i=1}^{n} \frac{\partial H(x,p)}{\partial p_i} \frac{\partial H(x,p)}{\partial x^i} = 0 \,. \end{aligned}$$

Second, for a Hamiltonian system the quantity Φ given by (1.110) vanishes,

$$\Phi = \sum_{k=1}^{n} \frac{\partial}{\partial x^k} \frac{dx^k}{dt} + \sum_{j=1}^{n} \frac{\partial}{\partial p_j} \frac{dp_j}{dt}$$

$$= \sum_{k=1}^{n} \frac{\partial}{\partial x^k} \frac{\partial H}{\partial p_k} - \sum_{j=1}^{n} \frac{\partial}{\partial p_j} \frac{\partial H}{\partial x^j} = 0\,, \tag{1.117}$$

and therefore, the Jacobian

$$J_H(t) = \frac{\partial(x(t), p(t))}{\partial(x_0, p_0)}\,, \tag{1.118}$$

remains constant,

$$J_H(t) = J_H(0)\,. \tag{1.119}$$

This leads, in particular, to the conservation of the volume in the phase space along the phase trajectories. This property is called the *Liouville theorem*.

1.9 Hilbert Spaces

Partial differential operators act on functions. To study such operators one needs to carefully define the domain of differential operators, that is, the set of functions they are acting upon. These are functional spaces. The theory of functional spaces is pretty complicated and requires a background in functional analysis. We will take here a rather pragmatic approach and will visualize functional Hilbert spaces simply as infinite-dimensional vector spaces with an inner product.

First of all, we remind some definitions. A real (or complex) *vector space* is a set of vectors, which can be added and multiplied by numbers (called *scalars*). A collection of vectors forms a *basis* if every vector can be uniquely written as a linear combination of vectors from the collection. The number of vectors in a basis is called the *dimension* of the vector space. An *inner product* (or scalar product) is a mapping that assigns a number (f, h) to two vectors f and h. It is linear in the second argument and anti-linear in the first argument and satisfies the relation

$$(f, h) = \overline{(h, f)}\,, \tag{1.120}$$

where the bar denotes complex conjugation. The *norm* of a vector is simply the square root of the inner product of the vector with itself

$$||f|| = \sqrt{(f, f)}\,. \tag{1.121}$$

Note that the norm is non-negative $||f|| \geq 0$ and is equal to zero $||f|| = 0$ if and only if the vector is the zero vector, $f = 0$. The norm is needed to define the notion of distance and the notion of convergence.

A *Hilbert space* is a complete infinite-dimensional vector space with an inner product. The completeness simply means that Hilbert space contains the limits of all convergent sequences of vectors.

Two vectors are said to be *orthogonal* if their scalar product is equal to zero. A basis $(\varphi_n)_{n=1}^{\infty}$ is said to be *orthonormal* if it consists of mutually orthogonal unit vectors. The complex numbers

$$f_n = (\varphi_n, f) \tag{1.122}$$

are called the *components* (or *generalized Fourier coefficients*) of the vector f with respect to the basis (φ_n) and the expansion

$$f = \sum_{n=1}^{\infty} f_n \varphi_n \,, \tag{1.123}$$

is called the *generalized Fourier series*. The norm of the vector f is then

$$||f||^2 = \sum_{n=1}^{\infty} |f_n|^2 \,. \tag{1.124}$$

1.10 Functional Spaces

Let $[a, b]$ be an interval on the real line (in particular, it could be the whole real line). Then the set of real (or complex) valued functions on $[a, b]$ is a vector space. The L^2 inner product on this vector space is defined by

$$(f, h) = \int_a^b dx \, \overline{f(x)} h(x) \,; \tag{1.125}$$

then the L^2 norm is

$$||f||^2 = (f, f) = \int_a^b dx \, |f(x)|^2 \,. \tag{1.126}$$

The space $L^2([a, b])$ is the Hilbert space of *square integrable functions*, that is, complex valued functions with finite L^2 norm.

Consider the Hilbert space $L^2([-\pi, \pi])$ of real-valued square integrable functions on $[-\pi, \pi]$. Then the sequence

$$\varphi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}, \qquad n = 0, \pm 1, \pm 2, \ldots \tag{1.127}$$

forms an orthonormal basis, and for any function f the series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \varphi_n(x), \tag{1.128}$$

where

$$f_n = \int_{-\pi}^{\pi} dt\, \overline{\varphi_n(t)} f(t), \tag{1.129}$$

is nothing but the classical Fourier series. The scalars f_n are the Fourier coefficients. The Fourier series of a function in $L^2([-\pi, \pi])$ converges *almost everywhere*, but not pointwise, which means that there might be points where it does not converge to the original function.

More generally, let μ be a positive function on $[a, b]$ called the *weight*. Then the inner product can be defined by

$$(f, h) = \int_a^b dx\, \mu(x)\, \overline{f(x)} h(x)\,. \tag{1.130}$$

This defines the space $L^2([a, b], \mu)$ of square integrable functions with the measure μ.

Similarly, let M be an open set in $\mathbb{R}^n$ (in particular, M can be the whole $\mathbb{R}^n$) and μ be a positive function on M. Then the inner product can be defined by

$$(f, h) = \int_M dx\, \mu(x)\, \overline{f(x)} h(x)\,. \tag{1.131}$$

This defines the Hilbert space $L^2(M, \mu)$ of complex valued functions with finite L^2-norm.

The spaces of smooth functions are not complete and, therefore, are not Hilbert spaces. This is a simple consequence of the fact that there are convergent sequences of smooth functions whose limit is not a smooth function. The L^2 spaces of square integrable functions are obtained by adding the limits of all convergent sequences to the spaces of smooth functions. This process is called *completion*.

1.11 Self-Adjoint and Unitary Operators

A *linear operator* on a Hilbert space H is a linear map $A : H \to H$. The set of all operators on a Hilbert space forms an algebra. The product AB of the operators A and B is naturally identified with the composition of A and B. The *commutator* of two operators is defined by

$$[A, B] = AB - BA\,. \tag{1.132}$$

The algebra of operators on a Hilbert space is closed under taking commutators of operators. Two operators are said to be *commuting* if their commutator is equal to zero and *non-commuting* otherwise.

The *adjoint* of the operator A is an operator A^* such that for any vectors f and g,

$$(A^* f, g) = (f, Ag)\,. \tag{1.133}$$

An operator A is called *self-adjoint* if

$$A = A^* \tag{1.134}$$

and *anti-self-adjoint* if $A = -A^*$. It is not difficult to see that the operation of taking the adjoint has the following properties

$$(A^*)^* = A\,, \tag{1.135}$$

$$(AB)^* = B^* A^*\,. \tag{1.136}$$

By using these properties we immediately see that the operators AA^*, A^*A and $A + A^*$ are self-adjoint.

An operator A is called *invertible* if there is an operator A^{-1} called the *inverse* of the operator A such that

$$AA^{-1} = A^{-1}A = I\,, \tag{1.137}$$

where I is the identity operator. The operation of taking the inverse has the following properties

$$(A^{-1})^{-1} = A\,, \tag{1.138}$$

$$(AB)^{-1} = B^{-1}A^{-1}\,, \tag{1.139}$$

$$(A^*)^{-1} = (A^{-1})^*. \tag{1.140}$$

An operator U is called *unitary* if

$$UU^* = U^*U = I\,, \tag{1.141}$$

or

$$U^{-1} = U^* . \tag{1.142}$$

Therefore, the inverse and the adjoint of a unitary operator are unitary. It is easy to see that unitary operators preserve the inner product. Indeed, for any f and g we have

$$(Uf, Ug) = (f, U^*Ug) = (f, g). \tag{1.143}$$

Every unitary operator U can be represented in the form

$$U = \exp A\,, \tag{1.144}$$

with some anti-self-adjoint operator A.

A self-adjoint operator A is called *positive* if for all $f \neq 0$

$$(f, Af) > 0\,. \tag{1.145}$$

By using the definition of the adjoint, it is easy to see that the operators AA^* and A^*A are non-negative. Indeed, for any f we have

$$(f, A^*Af) = (Af, Af) = ||Af||^2 \geq 0\,, \tag{1.146}$$

and similarly for AA^*. Also, the inverse of a positive operator is positive since for any f

$$(f, A^{-1}f) = (Ag, g) > 0\,, \tag{1.147}$$

where $g = A^{-1}f$.

An operator P is called *idempotent* if

$$P^2 = P\,. \tag{1.148}$$

A self-adjoint idempotent operator is called a *projection*. Given a vector subspace S, the *orthogonal complement* of S is the vector subspace $S_\perp$ such that every vector from S is orthogonal to every vector from $S_\perp$. For any projection operator P there is a vector subspace S it projects onto. That is, for any vector f the vector Pf is in S. More precisely,

$$Pf = \begin{cases} f & \text{if } f \text{ is in } S\,, \\ 0 & \text{if } f \text{ is in } S_\perp\,. \end{cases} \tag{1.149}$$

It is easy to see that if P is a projection operator onto a subspace S, then the operator $P_\perp = I - P$ is a projection operator onto the orthogonal complement $S_\perp$.

Let $(\varphi_n)_{n=1}^\infty$ be an orthonormal basis in H. Then every operator A can be represented by an infinite-dimensional matrix A_{kj} (called the *matrix of the operator* A with respect to the basis (φ_n)),

$$A\varphi_j = \sum_{k=1}^{\infty} A_{kj}\varphi_k \,, \tag{1.150}$$

where

$$A_{kj} = (\varphi_k, A\varphi_j) \,, \tag{1.151}$$

that is, for any function f

$$Af = \sum_{j,k=1}^{\infty} A_{kj} f_j \varphi_k \,, \tag{1.152}$$

which means that the components of the vector Af are obtained by acting with the matrix (A_{kj}) of the operator A on the vector (f_j)

$$(Af)_k = \sum_{j=1}^{\infty} A_{kj} f_j \,. \tag{1.153}$$

The matrix of the adjoint operator A^* is equal to the Hermitian conjugate of the matrix of the original operator, that is,

$$(A^*)_{jk} = \overline{A_{kj}} \,, \tag{1.154}$$

where the bar denotes complex conjugation.

The *trace* of the operator A is defined as the trace of its matrix

$$\mathrm{Tr}\, A = \sum_{k=1}^{n} (\varphi_k, A\varphi_k) = \sum_{k=1}^{n} A_{kk} \,. \tag{1.155}$$

Of course, the trace, when it exists, does not depend on the choice of the orthonormal basis. An operator A is called *trace-class* if it has a finite trace.

It is easy to see that the projection operator P on a subspace S is trace-class if the subspace S is finite-dimensional and the dimension of the subspace S is equal to the trace of the projection

$$\dim S = \mathrm{Tr}\, P \,. \tag{1.156}$$

The trace has a nice *cyclic property*, that is, if the operators A, B, AB and BA are trace class, then

$$\mathrm{Tr}\, AB = \mathrm{Tr}\, BA \,, \tag{1.157}$$

that is,

$$\mathrm{Tr}\, [A, B] = 0 \,, \tag{1.158}$$

More generally, under similar assumptions there holds

$$\mathrm{Tr}\,(ABC) = \mathrm{Tr}\,(BCA) = \mathrm{Tr}\,(CAB)\,, \tag{1.159}$$

and

$$\mathrm{Tr}\,[A, B]C = 0, \tag{1.160}$$

if either A or B commute with the operator C.

Let B be an invertible operator and A be a trace-class operator. Then the operator

$$A_B = B^{-1}AB \tag{1.161}$$

is said to be *similar* to the operator A. By using the cyclic property of the trace it is easy to see that similar operators have the same trace

$$\mathrm{Tr}\,A_B = \mathrm{Tr}\,A\,. \tag{1.162}$$

1.12 Integral Operators

An *integral operator* on the Hilbert space $L^2([a, b])$ is defined as follows. Let $K(x, x')$ be a function of two variables. Then the integral

$$(Kf)(x) = \int_a^b dx'\, K(x, x')f(x')\,, \tag{1.163}$$

defines an integral operator K on $L^2([a, b])$. The function $K(x, x')$ is called the *integral kernel* of the operator K.

Similarly, we can define multi-dimensional integral operators on the space $L^2(M, \mu)$, where M is an open set in $\mathbb{R}^n$ and μ is a positive weight function. Let $K(x, x')$ be a function of two points x and x'. Then the integral

$$(Kf)(x) = \int_M dx'\, \mu(x')\, K(x, x')f(x')\,, \tag{1.164}$$

defines an integral operator K on $L^2(M, \mu)$ with the integral kernel $K(x, x')$. Although we use the same symbol K for the operator and its integral kernel this should not cause any confusion because the meaning of the symbol is usually clear from the context.

Suppose that the integral operator K is such that its kernel has a well-defined *diagonal*

$$K^{\mathrm{diag}}(x) = K(x, x)\,. \tag{1.165}$$

Then the *trace* of the operator K can be computed as the integral of its diagonal

$$\text{Tr } K = \int\limits_M dx\, \mu(x) K(x,x)\,. \tag{1.166}$$

It is not difficult to show that the kernel of the adjoint operator K^* is

$$(K^*)(x,x') = \overline{K(x',x)}\,. \tag{1.167}$$

Therefore, the kernel of a self-adjoint operator K satisfies the symmetry relation

$$K(x,x') = \overline{K(x',x)}\,. \tag{1.168}$$

1.13 Resolvent and Spectrum

Let L be an operator on a Hilbert space. A complex number λ is called an *eigenvalue* of the operator L if there is a non-zero vector φ such that

$$L\varphi = \lambda\varphi\,. \tag{1.169}$$

The vector φ is called the *eigenvector* corresponding to the eigenvalue λ.

Note that there are infinitely many eigenvectors corresponding to an eigenvalue. One can easily show that the collection of all eigenvectors corresponding to a given eigenvalue λ forms a vector subspace called the *eigenspace*) of λ. The dimension of the eigenspace of the eigenvalue λ is called the *multiplicity* of the eigenvalue λ. An eigenvalue of multiplicity one is called *simple* (or non-degenerate). An eigenvalue of multiplicity greater than one is called *multiple* (or degenerate). The multiplicity of an eigenvalue is also called the *degree of degeneracy*.

The operator

$$G(\lambda) = (L - \lambda I)^{-1}\,, \tag{1.170}$$

where I is the identity operator is called the *resolvent* of the operator L. A complex number λ for which the resolvent $G(\lambda)$ is well defined (bounded) is called a *regular point* of L. The set of all regular points is called the *resolvent set*. The complement of the resolvent, that is, the set of complex numbers λ which are not regular, is called the *spectrum* of the operator L.

Note that every eigenvalue belongs to the spectrum but not all points in the spectrum are eigenvalues. The set of all eigenvalues is called the *point spectrum*. The remaining part of the spectrum is called the *continuous spectrum*. The continuous spectrum has far richer and more complicated structure than the point spectrum. It contains, in general, a singular part and an absolutely continuous part. We will not be concerned with such issues since in most cases of our interest the operators with have only pure point spectrum, which is, of course the simplest situation.

We list below some facts about the spectrum of special types of operators. Most of these can be easily proved.

1. The eigenvalues of self-adjoint operators are real, that is they lie on the real line.
2. The eigenvalues of unitary operators are complex numbers with modulus equal to 1, that is, they lie on the unit circle.
3. The eigenvectors corresponding to distinct eigenvalues of self-adjoint and unitary operators are mutually orthogonal.
4. The eigenvalues of positive operators are positive.
5. The eigenvalues of projections can only be either 1 or 0.

1.14 Spectral Resolution

If all eigenvalues of a self-adjoint operator are simple, that is, all eigenspaces are one-dimensional, then the set of all normalized eigenvectors forms an orthonormal basis in the Hilbert space. When the eigenvalues have multiplicities larger than one, that is, the eigenspaces are more than one-dimensional, then the eigenvectors belonging to the same eigenspace are not necessarily orthogonal, but, nevertheless, they can always be made orthonormal. Therefore, in general, there always exists an orthonormal basis consisting of eigenvectors of a self-adjoint operator.

Let $(\varphi_n)_{n=1}^{\infty}$ be such an orthonormal basis corresponding to the eigenvalues $(\lambda_n)_{n=1}^{\infty}$ of a self-adjoint operator L. Then the matrix of the operator L diagonalizes

$$(\varphi_k, L\varphi_j) = \lambda_k \delta_{kj} \,, \tag{1.171}$$

and the operator L acts simply by multiplication, that is, for any vector

$$f = \sum_{n=1}^{\infty} f_n \varphi_n \tag{1.172}$$

with some constants f_n, we have

$$Lf = \sum_{n=1}^{\infty} \lambda_n f_n \varphi_n \,. \tag{1.173}$$

This can be rephrased as follows. Let P_n be the projection operator onto the one-dimensional subspace spanned by the eigenvector φ_n. The set of all projections is complete, that is,

$$\sum_{n=1}^{\infty} P_n = I \tag{1.174}$$

and orthogonal, that is, for any $i \neq j$,

$$P_i P_j = 0\,. \tag{1.175}$$

Then the operator L can be written in the form

$$L = \sum_{n=1}^{\infty} \lambda_n P_n\,. \tag{1.176}$$

Such a representation makes sense even for non-real eigenvalues, that is, for non-self-adjoint operators.

1.15 Functions of Operators

The spectral representation (1.176) enables one to define pretty general functions of operators by

$$f(L) = \sum_{n=1}^{\infty} f(\lambda_n) P_n\,. \tag{1.177}$$

Of course, the function f and the operator L must be such that this series converges. Note that if the operator L is self-adjoint then the operator $f(L)$ is also self-adjoint and its eigenvalues are equal to $f(\lambda_n)$ with the same eigenspaces.

This gives for the resolvent of a self-adjoint operator L

$$G(\lambda) = \sum_{n=1}^{\infty} (\lambda_n - \lambda)^{-1} P_n, \tag{1.178}$$

which is well defined for any $\lambda \neq \lambda_n$ for all $n \in \mathbb{Z}_+$.

More generally, for a self-adjoint positive operator L one can define the complex power of L by

$$L^{-s} = \sum_{n=1}^{\infty} \lambda_n^{-s} P_n\,, \tag{1.179}$$

where s is a complex variable, and the exponential of L (called the *heat semigroup* of thee operator L) by

$$U(t) = \exp(-tL) = \sum_{n=1}^{\infty} e^{-t\lambda_n} P_n\,, \tag{1.180}$$

where $t > 0$. Here it is assumed that the sequence of eigenvalues λ_n is such that the above spectral series converge.

It is easy to see that powers of similar operators L and $L_B = B^{-1}LB$ (with B an invertible operator) are related by

$$L_B^n = B^{-1}L^n B. \tag{1.181}$$

More generally, the same holds for a rather general function f analytic at 0,

$$f(L_B) = B^{-1}f(L)B\,. \tag{1.182}$$

1.16 Spectral Functions

The traces of various functions of an operator L

$$\mathrm{Tr}\, f(L) = \sum_{k=1}^{\infty} f(\lambda_k) \tag{1.183}$$

define so-called *spectral functions*. They can be used to study the spectrum of the operator L. By using eq. (1.182) and the cyclic property of the trace it is easy to see that the traces of similar operators are equal,

$$\mathrm{Tr}\, f(L_B) = \mathrm{Tr}\, f(L)\,. \tag{1.184}$$

Of particular importance are the *zeta-function* and the *heat trace*. Let L be a self-adjoint positive operator with a purely point spectrum $(\lambda_k)_{k=1}^{\infty}$ (each eigenvalue repeated with multiplicity). The zeta-function $\zeta(s)$ of the operator L is defined as the trace of a complex power of L for a complex number s

$$\zeta(s) = \mathrm{Tr}\, L^{-s} = \sum_{k=1}^{\infty} \lambda_k^{-s}\,. \tag{1.185}$$

For $t > 0$ the exponential $\exp(-tL)$ of an operator L is called the *heat semigroup*. The *heat trace* is defined as the trace of the heat semigroup

$$\mathrm{Tr}\, \exp(-tL) = \sum_{k=1}^{\infty} e^{-t\lambda_k}\,. \tag{1.186}$$

We assume that the sequence of eigenvalues λ_k grows without bound as $k \to \infty$ so that the spectral sum for the heat trace converges for $t > 0$. For the zeta-function the spectral sum should be evaluated in the region of the complex plane of s where it converges, that is, for sufficiently large $\mathrm{Re}\, s$. Then the zeta-function is defined by analytical continuation to the whole complex plane.

The zeta function and the heat trace are related by the Mellin transform

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty dt\, t^{s-1}\, \mathrm{Tr}\, \exp(-tL)\,, \tag{1.187}$$

$$\mathrm{Tr}\, \exp(-tL) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds\, t^{-s} \Gamma(s)\zeta(s)\,, \tag{1.188}$$

where $\Gamma(s)$ is the gamma-function and c is a sufficiently large positive real constant.

The zeta function can be used to define another very important spectral function, namely, the *functional determinant*. Recall that the determinant of a positive matrix can be written in terms of the trace of its logarithm, (1.98). If the zeta-function $\zeta(s)$ is analytic at $s = 0$, then this equation can be used to define the *functional determinant* $\mathrm{Det}\, L$ of the operator L,

$$\mathrm{Det}\, L = \exp\left[-\zeta'(0)\right]\,, \tag{1.189}$$

where $\zeta'(s) = \frac{d}{ds}\zeta(s)$.

1.17 Heat Semigroups

1.17.1 Definition and Basic Properties

Let A be a positive operator in a Hilbert space. The operator

$$U(t) = \exp(-tA) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} t^k A^k \tag{1.190}$$

is well defined for $t > 0$. It satisfies the operator heat equation

$$(\partial_t + A)U(t) = 0 \tag{1.191}$$

with the initial condition

$$U(0) = I\,, \tag{1.192}$$

where I is the identity operator. The operator $U(t)$ satisfies the semigroup property: for any $t_1, t_2 > 0$

$$U(t_1 + t_2) = U(t_1)U(t_2)\,. \tag{1.193}$$

That is why, it is called the *heat semigroup*. It is not a group because the operator $U(t)$ does not necessarily have an inverse, since the operator $[U(t)]^{-1} = \exp(tA)$ is not well defined for $t > 0$.

We derive a very useful integral equation for the heat semigroup. Let us decompose the operator A in two parts

$$A = A_0 + sA_1\,, \tag{1.194}$$

where s is a parameter. Without going into the details we assume that in some sense the operator A_0 is "nice" (has nice properties, with known heat semigroup) and the operator A_1 is "small" compared to the operator A_0, in other words, we will treat it as a perturbation of the operator A_0 with s being a small parameter. Let $U(t) = \exp(-tA)$ be the heat semigroup of the operator A, and $U_0(t) = \exp(-tA_0)$ be the semigroup of the operator A_0. Let

$$U(t) = U_0(t)K(t)\,. \tag{1.195}$$

Then the operator K satisfies the equation

$$\partial_t K(t) = -sU_0(-t)A_1U_0(t)K(t) \tag{1.196}$$

with initial condition

$$K(0) = I\,. \tag{1.197}$$

By integrating this equation we obtain

$$K(t) = I - s\int_0^t d\tau\; U_0(-\tau)A_1U_0(\tau)K(\tau)\,, \tag{1.198}$$

and, therefore,

$$U(t) = U_0(t) - s\int_0^t d\tau\; U_0(t-\tau)A_1U(\tau)\,. \tag{1.199}$$

Similarly, we can obtain

$$U(t) = U_0(t) - s\int_0^t d\tau\; U(\tau)A_1U_0(t-\tau)\,. \tag{1.200}$$

This is a very important equation that enables one to obtain an expansion of the heat semigroup $U(t)$ in terms of the heat semigroup $U_0(t)$ and the operator A_1.

1.17.2 Duhamel's Formula and Volterra's Series

Now suppose that the operator $A = A(s)$ depends on a parameter s in such a way that the operators $A(s)$ do not necessarily commute for different values of the parameter s. Then the heat semigroup varies according to the *Duhamel's formula*

$$\partial_s U(t) = -\int_0^t d\tau\, U(t-\tau)(\partial_s A)U(\tau)\,. \tag{1.201}$$

By differentiating this equation with respect to t one can check directly that both sides of this equation satisfy the same differential equation and the same initial condition and therefore are the same.

Suppose that the operator $A(s)$ has a well defined Taylor series in s at $s = 0$. Then by repeated application of Duhamel's formula one can obtain the Taylor series for heat semigroup $\exp[-tA(s)]$ at $s = 0$. Let us assume for simplicity that

$$A(s) = A_0 + sA_1\,, \tag{1.202}$$

where A_0 is an operator with a well defined heat semigroup $U_0(t) = \exp(-tA_0)$.

Then the Duhamel formula reads

$$\partial_s U(t) = -\int_0^t d\tau\, U(t-\tau)A_1 U(\tau)\,. \tag{1.203}$$

Then by treating s as a small parameter we obtain the Taylor series for the heat semigroup $U(t) = \exp[-t(A_0 + sA_1)]$ as

$$U(t) = U_0(t) + \sum_{k=1}^{\infty}(-1)^k s^k \int_0^t d\tau_k \int_0^{\tau_k} d\tau_{k-1} \cdots \int_0^{\tau_2} d\tau_1 \tag{1.204}$$

$$\times\, U_0(t-\tau_k)A_1 U_0(\tau_k - \tau_{k-1}) \cdots U_0(\tau_2 - \tau_1)A_1 U_0(\tau_1)\,.$$

This expansion is called *Volterra series*.

Let us define an operator Ad_A that acts on operators by left commutator, that is,

$$Ad_A B = [A, B]\,. \tag{1.205}$$

The k-th power of this operator defines k-folded commutators

$$(Ad_A)^k B = \underbrace{[A, [A, \cdots, [A, B]\cdots]]}_{k}\,. \tag{1.206}$$

Let us consider an operator-valued function

$$F(t) = \exp(tA)B\exp(-tA)\,. \tag{1.207}$$

By differentiating it with respect to t we obtain the differential equation

$$\partial_t F = [A, F] = Ad_A F\,, \tag{1.208}$$

with an obvious initial condition

$$F(0) = B\,. \tag{1.209}$$

The solution of this equation is

$$F(t) = \exp(tAd_A)B\,. \tag{1.210}$$

Now, by expanding the exponential we obtain a very useful expansion

$$\begin{aligned}\exp(tA)B\exp(-tA) &= \sum_{k=0}^{\infty}\frac{t^k}{k!}(Ad_A)^k B \\ &= B + t[A,B] + \frac{1}{2}t^2[A,[A,B]] + O(t^3)\,.\end{aligned} \tag{1.211}$$

This expansion gives an approximation for the operator $F(t)$ in the case when the commutators of the operators A and B are small. In some cases this expansion may even terminate giving us a polynomial.

Now, we go back to Volterra series and define an operator

$$\begin{aligned}V(t) &= \exp(tA_0)A_1\exp(-tA_0) = \exp(tAd_{A_0})A_1 \\ &= A_1 + t[A_0,A_1] + \frac{1}{2}t^2[A_0,[A_0,A_1]] + O(t^3)\,.\end{aligned} \tag{1.212}$$

Then the Volterra series can be written in two equivalent forms

$$\begin{aligned}U(t) = U_0(t)\Bigg\{I + \sum_{k=1}^{\infty}(-1)^k s^k \int_0^t d\tau_k \int_0^{\tau_k} d\tau_{k-1}\cdots\int_0^{\tau_2} d\tau_1 \\ \times V(\tau_k)\cdots V(\tau_2)V(\tau_1)\Bigg\}\,,\end{aligned} \tag{1.213}$$

or

$$U(t) = \left\{ I + \sum_{k=1}^{\infty} (-1)^k s^k \int_0^t d\tau_k \int_0^{\tau_k} d\tau_{k-1} \cdots \int_0^{\tau_2} d\tau_1 \right.$$
$$\left. \times V(\tau_k - t) V(\tau_{k-1} - t) \cdots V(\tau_1 - t) \right\} U_0(t)\,, \quad (1.214)$$

We already have $V(\tau)$ as a power series in τ. By using this power series we obtain an expansion as $t \to 0$

$$U(t) = \left\{ I - stA_1 + \frac{t^2}{2} \left(s^2 A_1^2 + s[A_0, A_1] \right) + O(t^3) \right\} U_0(t)\,. \quad (1.215)$$

This equation can be used to compute the asymptotic expansion of the heat kernel of a differential operator A by just applying a differential operator in the brackets to the heat kernel of the operator A_0.

1.17.3 Chronological Exponent

The integration in Volterra series over $\tau_1, \ldots, \tau_k$ is restricted to the following simplex in $\mathbb{R}^k$

$$0 \le \tau_1 \le \tau_2 \le \tau_3 \le \cdots \le \tau_k \le t\,. \quad (1.216)$$

Suppose that the operators $V(t)$ commute at different times. Then by symmetrizing over the variables $\tau_1, \ldots, \tau_k$ we get

$$U(t) = U_0(t) \left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} \int_0^t d\tau_k \cdots \int_0^t d\tau_2 \int_0^t d\tau_1 \; V(\tau_k) \cdots V(\tau_1) \right\}$$
$$= U_0(t) \left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} \left(\int_0^t d\tau \; V(\tau) \right)^k \right\}$$
$$= U_0(t) \exp\left(-s \int_0^t d\tau \; V(\tau) \right)\,. \quad (1.217)$$

A similar argument can be used to rewrite the perturbation series in general case, even when the operators $V(t)$ do not commute at different times, in a very compact form. Let us define the *time-ordering operator* T as follows. Let $V(t)$ be a time dependent operator. Then the operator T orders the product of non-commuting operators $V(\tau)$ at different times according to their time arguments from left to right. That is,

$$T\left[V(\tau_2)V(\tau_1)\right] = \begin{cases} V(\tau_2)V(\tau_1) & \text{if } \tau_2 > \tau_1\,, \\ V(\tau_1)V(\tau_2) & \text{if } \tau_1 > \tau_2\,. \end{cases} \tag{1.218}$$

More generally, let $\tau_1, \ldots, \tau_k$ be such that $0 < \tau_1 < \cdots < \tau_k < t$. Then the time-ordering operator T orders the product of operators $V(\tau_1), \ldots, V(\tau_k)$ in arbitrary order to the *chronological order*, that is,

$$T\left[V(\tau_{i_k}) \cdots V(\tau_{i_1})\right] = V(\tau_k) \cdots V(\tau_1)\,. \tag{1.219}$$

Now, by using this operator we can forget that the operators $V(\tau)$ do not commute at different times and rewrite the perturbation series (1.213) in the following form

$$\begin{aligned} U(t) &= U_0(t)\left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} \int_0^t d\tau_k \cdots \int_0^t d\tau_2 \int_0^t d\tau_1\; T\left[V(\tau_k) \cdots V(\tau_1)\right] \right\} \\ &= U_0(t)\left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} T \left(\int_0^t d\tau\; V(\tau) \right)^k \right\} \\ &= U_0(t)\, T \exp\left(-s \int_0^t d\tau\; V(\tau) \right)\,. \end{aligned} \tag{1.220}$$

This expression is called the *time-ordered (or chronological) exponent*. It is defined by the above perturbation series. In other words, it means

$$\exp[-t(A_0 + sA_1)] = e^{-tA_0} T \exp\left(-s \int_0^t d\tau\; e^{\tau A_0} A_1 e^{-\tau A_0} \right) \tag{1.221}$$

Similarly, from eq. (1.214) one can obtain

$$\begin{aligned} U(t) &= T \exp\left(-s \int_0^t d\tau\; V(\tau - t) \right) U_0(t) \\ &= T \exp\left(-s \int_0^t d\tau\; V(-\tau) \right) U_0(t)\,. \end{aligned} \tag{1.222}$$

1.17.4 Campbell-Hausdorff Formula

The chronological exponent can be used, in particular, as follows. Suppose that the commutators of the operators A_0 and A_1 are small, say each commutator brings a small factor. Then one can get a power series in this parameter. For example, suppose that we neglect all higher commutators taking into account only the first commutator $[A_0, A_1]$, that is, the commutator $[A_0, A_1]$ commutes with both A_0 and A_1,

$$V(\tau) = A_1 + \tau[A_0, A_1]\,. \tag{1.223}$$

Then the operators $V(\tau)$ at different times commute with each other and, therefore, the chronological exponent becomes the usual exponent; thus, we get

$$U(t) = \exp\left(-stA_1 + s\frac{t^2}{2}[A_0, A_1]\right) U_0(t)\,, \tag{1.224}$$

what is known as a particular case of *Campbell-Hausdorff formula*. Of course, by expanding the exponent in powers of t we get the previously mentioned result up to $O(t^3)$.

1.17.5 Heat Semigroup for Time Dependent Operators

More generally, suppose that the operator $A = A(t)$ depends on time t. Then the heat semigroup $U(t, t')$ is defined by the equation

$$\partial_t U(t, t') = -A(t)U(t, t') \tag{1.225}$$

and the initial condition

$$U(t', t') = I\,. \tag{1.226}$$

It satisfies the semigroup property in the form

$$U(t, t') = U(t, t'')U(t'', t')\,. \tag{1.227}$$

In particular, this means that

$$U(t, t') = [U(t', t)]^{-1}\,. \tag{1.228}$$

By using this equation and the semigroup property (1.227) we also obtain

$$\partial_{t'} U(t, t') = U(t, t')A(t')\,. \tag{1.229}$$

The differential equations (1.225) and (1.229) are equivalent to the integral equations

$$U(t,t') = I - \int_{t'}^{t} d\tau\ A(\tau)U(\tau,t')\,, \tag{1.230}$$

$$U(t,t') = I + \int_{t'}^{t} d\tau\ U(t,\tau)A(\tau)\,. \tag{1.231}$$

Now we can solve these integral equations for $t' < t$ by the perturbation series

$$U(t,t') = I + \sum_{k=1}^{\infty}(-1)^k \int_{t'}^{t} d\tau_k \cdots \int_{t'}^{\tau_3} d\tau_2 \int_{t'}^{\tau_2} d\tau_1\ A(\tau_k)\cdots A(\tau_1)\,, \tag{1.232}$$

where the integration over $\tau_1, \ldots, \tau_k$ is restricted to the following simplex in $\mathbb{R}^k$

$$t' \le \tau_1 \le \tau_2 \le \tau_3 \le \cdots \le \tau_k \le t\,. \tag{1.233}$$

As we have explained above, if the operators $A(t)$ commute at different times, then by symmetrizing over the variables $\tau_1, \ldots, \tau_k$ we get

$$U(t,t') = \exp\left(-\int_{t'}^{t} d\tau\ A(\tau)\right)\,. \tag{1.234}$$

Of course, if the operator A does not depend on time this immediately gives

$$U(t,t') = \exp[-(t-t')A]\,. \tag{1.235}$$

In the general case, this perturbation series can be written as a chronological exponent

$$U(t,t') = T\exp\left(-\int_{t'}^{t} d\tau\ A(\tau)\right)\,. \tag{1.236}$$

Suppose that we have a situation that the operators $A(\tau)$ do not commute but their commutators are small. By assigning a small parameter to each commutator one can get from here a perturbation series in the commutators of the operators $A(\tau)$. The zero-order of such perturbation series does not have any commutators and is given by the same formula as for commuting operators. The first order will have only first commutators, the second order will have double commutators etc.

Let us consider a time-dependent operator $A(t)$ and decompose it as

$$A(t,s) = A_0(t) + sA_1(t)\,, \tag{1.237}$$

where s is a parameter. Let $U_0(t,t')$ and $U(t,t')$ be heat semigroups of the operators A_0 and A. Then, similarly to the time-independent case there are integral equations for the heat-semigroup

$$U(t,t') = U_0(t,t') - s\int_{t'}^{t} d\tau\; U_0(t,\tau)A_1(\tau)U(\tau,t')\,, \tag{1.238}$$

and

$$U(t,t') = U_0(t,t') - s\int_{t'}^{t} d\tau\; U(t,\tau)A_1(\tau)U_0(\tau,t')\,. \tag{1.239}$$

More generally, if the operator A depends on both the time t and a parameter s, that is, $A = A(t,s)$, the Duhamel formula reads

$$\partial_s U(t,t') = -\int_{t'}^{t} d\tau\; U(t,\tau)[\partial_s A(\tau)]U(\tau,t')\,. \tag{1.240}$$

Let us also derive Volterra series for a time-dependent operator. Let us assume for simplicity that

$$A(t,s) = A_0(t) + sA_1(t)\,, \tag{1.241}$$

where $A_0(t)$ is a time-dependent operator with a well defined heat semigroup $U_0(t,t')$. Now, we can use Duhamel formula repeatedly to obtain the Taylor series in s for heat semigroup $U(t,t')$ of the operator $A(t,s)$. We obtain

$$U(t,t') = U_0(t,t') + \sum_{k=1}^{\infty}(-1)^k s^k \int_{t'}^{t} d\tau_k \int_{t'}^{\tau_k} d\tau_{k-1}\cdots\int_{t'}^{\tau_2} d\tau_1 \tag{1.242}$$

$$\times\, U_0(t,\tau_k)A_1(\tau_k)U_0(\tau_k,\tau_{k-1})\cdots A_1(\tau_2)U_0(\tau_2,\tau_1)A_1(\tau_1)U_0(\tau_1,t')\,.$$

Now, let us define the operator

$$B(\tau,t) = U_0(t,\tau)A_1(\tau)U_0(\tau,t)\,. \tag{1.243}$$

Then for t close to τ we can expand both heat kernels in a power series to get

$$B(\tau,t) = A_1(\tau) - \int_\tau^t d\tau\ [A_0(\tau_1), A_1(\tau)] \tag{1.244}$$

$$+ \int_\tau^t d\tau_2 \int_\tau^{\tau_2} d\tau_1\ [A_0(\tau_2), [A_0(\tau_1), A_1(\tau)]] + O[(t-\tau)^3]\,.$$

By using these operators we can rewrite the Volterra series in the form

$$U(t,t') = \left\{ I + \sum_{k=1}^{\infty} (-1)^k s^k \int_{t'}^t d\tau_k \int_{t'}^{\tau_k} d\tau_{k-1} \cdots \int_{t'}^{\tau_2} d\tau_1 \right. \tag{1.245}$$

$$\left. \times B(\tau_k,t)B(\tau_{k-1},t)\cdots B(\tau_2,t)B(\tau_1,t) \right\} U_0(t,t')\,.$$

Up to the third order in s and $(t-t')$ we have

$$U(t,t') = \left\{ I - s\int_{t'}^t d\tau\ A_1(\tau) \right.$$

$$+ \int_{t'}^t d\tau_2 \int_{t'}^{\tau_2} d\tau_1\ \left\{ s^2 A_1(\tau_2)A_1(\tau_1) + s[A_0(\tau_2), A_1(\tau_1)] \right\}$$

$$\left. + O[(t-t')^3] \right\} U_0(t,t')\,. \tag{1.246}$$

Of course, in the case of time-independent operators this coincides with our previous result (1.215).

1.18 Notes

In this chapter we introduced some background information from analysis and fixed the notation in the form that will be useful for the rest of the book. There are many good references on the asymptotic expansions; here is the list that we found very useful [30, 23, 64, 34, 35, 37, 67]. For integral transforms see the books [16, 27]. Material on Hamiltonian systems can be found in [28, 33, 71]. A good reference on functional analysis is [24]. Some material on heat semigroups can be found in [74].

Chapter 2
Introduction to Partial Differential Equations

Abstract In this chapter we present an introduction to some methods for the solution of partial differential equations. After a short review of the first-order equations we discuss the classification of second-order equations and introduce the fundamental tools such as the resolvent and the heat kernel. We also show how to solve exactly partial differential equations in some simple cases, such as equations with constant coefficients and homogeneous equations.

2.1 First Order Partial Differential Equations

Partial differential equations are usually much more complicated than ordinary differential equations, even systems of ordinary differential equations. However, there is one class of partial differential equations that is as difficult to solve as a system of ordinary differential equations. These are linear first-order partial differential equations.

Let x^i, $i = 1, \dots, n$, be the coordinates in the Euclidean space $\mathbb{R}^n$ and $\xi^i(x)$ be a vector field in $\mathbb{R}^n$. Let f be a given smooth function in $\mathbb{R}^n$ and L be a first-order partial differential operator of the form

$$L = \sum_{i=1}^{n} \xi^i(x) \frac{\partial}{\partial x^i} \,. \tag{2.1}$$

Let us consider a partial differential equation

$$(\partial_t - L)u(t, x) = 0 \,, \tag{2.2}$$

with the initial condition

$$u(0, x) = f(x) \,. \tag{2.3}$$

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_2

The formal solution of this initial value problem is expressed in terms of the exponential of the operator L,

$$u(t,x) = \exp(tL) f(x)\,. \tag{2.4}$$

For first-order differential operators the action of such an exponent is easy to compute; indeed, it has the form

$$u(t,x) = f(\hat{x}(t,x))\,, \tag{2.5}$$

where $\hat{x}(t,x)$ is the integral curve of the vector field ξ^i passing through the point x. That is, $\hat{x}(t,x)$ is the solution of an autonomous system of ordinary differential equations

$$\frac{d\hat{x}^i}{dt} = \xi^i(\hat{x}) \tag{2.6}$$

with the initial condition

$$\hat{x}^i(0) = x^i\,. \tag{2.7}$$

It is not difficult to verify directly that the function $u(t,x)$ defined by (2.5) satisfies both the partial differential equation (2.2) and the initial condition (2.3).

2.2 Second Order Partial Differential Equations

A very wide class of models in physics, engineering or mathematical finance lead to linear second-order partial differential (or integro-differential) equations. The case of differential equations is much more important than the case of integro-differential equations. That is why, most of the time we will study second-order partial differential equations.

2.2.1 Elliptic Partial Differential Operators

We will distinguish between the time variable, t, and the space variables, x^i, $i = 1, \ldots, n$. By changing the sign of the time variable and by shifting it if necessary without loss of generality we can always assume that the time variable is positive, $t \geq 0$. The range of space variables is a more complicated issue. It depends on their precise meaning. We will assume that the space variables range in some open subset M of the Euclidean space $\mathbb{R}^n_x$ with or without boundary ∂M, which is a hypersurface in $\mathbb{R}^n$. Henceforth, we use the shorthand $x = (x^1, \ldots, x^n)$ and denote the partial derivatives with respect to the time and space variables simply by

$$\partial_t = \frac{\partial}{\partial t}\,, \qquad \partial_i = \frac{\partial}{\partial x^i}\,. \tag{2.8}$$

We will often denote the vector of all space partial derivatives by $\partial_x = (\partial_1, \dots, \partial_n)$. A second-order partial differential operator in space variables has the following general form

$$L = L(t, x, \partial_x) = -\sum_{i,j=1}^{n} \alpha^{ij}(t,x)\partial_i\partial_j + \sum_{i=1}^{n} \beta^i(t,x)\partial_i + \gamma(t,x)\,, \tag{2.9}$$

where the coefficients $\alpha^{ij}(t,x)$, are some real valued functions of space variables, and, in general, time and the coefficients $\beta^i(t,x)$ and $\gamma(t,x)$ are, in general, complex valued. We will always assume that the coefficients functions are smooth, that is, infinitely times differentiable.

Let p_i, $i = 1, \dots, n$, be some new n variables that are called *dual variables* (or *momenta*). We assume that they range from $-\infty$ to $+\infty$, that is, the vector $p = (p_1, \dots, p_n)$ is a point in the space $\mathbb{R}^n_p$. We introduce the standard Euclidean pairing of dual variables x and p by

$$\langle p, x\rangle = \sum_{i=1}^{n} p_i x^i, \tag{2.10}$$

and the Euclidean norm

$$|p| = \sqrt{\langle p, p\rangle}. \tag{2.11}$$

Also, if $A = (\alpha^{ij})$ is a matrix then we denote

$$\langle p, Ap\rangle = \sum_{i,j=1}^{n} p_i \alpha^{ij} p_j. \tag{2.12}$$

Let A denote the matrix of the coefficients of second derivatives, $A = (\alpha^{ij})$, and β be the vector of the coefficients of first derivatives, $\beta = (\beta^j)$. Then the expression

$$\sigma(t, x, p) = L(t, x, ip) = \langle p, A(t,x)p\rangle + i\,\langle p, \beta(t,x)\rangle + \gamma(t,x)\,, \tag{2.13}$$

obtained by replacing the space derivatives ∂_x by the momenta ip is called the *symbol* of the operator L and the expression

$$\sigma_L(t, x, p) = \langle p, A(t,x)p\rangle \tag{2.14}$$

is called the *leading symbol* (or the *principal symbol*) of the operator L. Here and below $i = \sqrt{-1}$ as the imaginary unit should not be confused with the index i. The meaning of the symbol i is usually clear from its role in an expression: the imaginary unit cannot appear as an index of a vector and an

index cannot appear as a coefficient in an equation. Of course, the index i is a dummy index and can be changed to any other symbol.

We will assume that for any point x in M and for any real $p \neq 0$ the leading symbol $\sigma_L(t, x, p)$ is positive definite, that is,

$$\langle p, A(t, x)p\rangle > 0\,. \tag{2.15}$$

Such operators are called *elliptic*.

Elliptic operators play a very important role in mathematics. One of the most important operators of this type is negative *Laplacian* (or *Laplace operator*), $L = -\Delta$, which (in the Euclidean space) has the form

$$\Delta = \sum_{j=1}^{n} \partial_j^2\,. \tag{2.16}$$

It is obtained by choosing the matrix $\alpha^{jk} = \delta_{jk}$ as the unit matrix, and $\beta^i = \gamma = 0$. Here

$$\delta_{jk} = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{if } j \neq k \end{cases} \tag{2.17}$$

is the so-called *Kronecker symbol*. Obviously, the symbol of negative Laplacian is simply the Euclidean square of the vector p,

$$\sigma(x, p) = |p|^2\,. \tag{2.18}$$

2.2.2 Classification of Second-Order Partial Differential Equations

There are three main classes of linear second-order partial differential equations: *elliptic*, *parabolic* and *hyperbolic*. Let L be an elliptic operator of the form (2.9) and $h = h(t, x)$ be some given function. Elliptic equations do not have any time derivatives at all; they have the form

$$L\varphi = h\,. \tag{2.19}$$

In general, if the right hand-side of the equation (that is, the function h) is equal to zero, then the equation is called *homogeneous*; otherwise, it is called *non-homogeneous*. We will consider mostly homogeneous equations.

Such equations describe static physical phenomena, such as potential theory (electrostatic and gravitational potential), elasticity theory, etc. Since there is no time derivative the elliptic equations do not need any initial conditions.

Parabolic equations have time derivative of the first order only,

$$(\partial_t + L)\,\varphi = h\,. \tag{2.20}$$

Such equations describe phenomena like heat conduction, diffusion, etc. That is why, this equation is simply called the *heat equation* or the *diffusion equation*. It is this equation that is of our primary interest in this book. Parabolic equations have to be supplemented by some *initial condition*

$$\varphi(0,x) = \varphi_0(x)\,, \tag{2.21}$$

where $\varphi_0(x)$ is a given function of the space variables x.

Hyperbolic equations have time derivatives of second order with the opposite sign to the space derivatives,

$$\left(\partial_t^2 + L\right)\varphi = h\,. \tag{2.22}$$

Such equations describe mainly propagation of waves, and are called, therefore, *wave equations*. Since the hyperbolic equations contain two time derivatives the initial conditions need to specify the initial velocity as well, that is,

$$\varphi(0,x) = \varphi_0(x)\,, \tag{2.23}$$

$$\partial_t\varphi(0,x) = \varphi_1(x)\,, \tag{2.24}$$

where φ_0 and φ_1 are some given functions of x.

2.2.3 Elliptic Equations

We list some of the most important partial differential equations of mathematical physics. Typical examples of elliptic equations are the *Poisson equation*

$$\Delta\varphi = \rho\,, \tag{2.25}$$

and the *Laplace equation*

$$\Delta\varphi = 0\,. \tag{2.26}$$

The Poisson equation describes the gravitational potential of a non-homogeneous medium with a (non-constant) mass density $\rho = \rho(x)$ or the electrostatic potential in the medium with a charge density ρ. The Laplace equation describes the potential in the vacuum.

A more general elliptic equation is the *stationary Schrödinger equation*

$$\left(-\frac{\hbar^2}{2m}\Delta + V - E\right)\varphi = 0\,. \tag{2.27}$$

The solution of this equation determines the wave function φ of a quantum particle of mass m with constant energy E moving in the space-dependent potential $V = V(x)$; here $\hbar$ is Planck constant.

Another elliptic equation of this type is the *Helmholtz equation*

$$\left(\frac{1}{k^2}\Delta + n^2\right)\varphi = 0\,. \tag{2.28}$$

This equation describes waves with wave number k in optics and acoustics in a non-homogeneous medium with the space-dependent refraction coefficient $n = n(x)$.

2.2.4 Parabolic Equations

The typical example of the parabolic equations is the *heat equation*

$$(\partial_t - \varkappa\Delta)\varphi = h\,, \tag{2.29}$$

where $\varkappa$ is a positive constant. This equation describes the distribution of heat in an isotropic material over time; the function h describes the source of the heat and the constant $\varkappa$ depends on specific characteristics of the material such as thermal conductivity, the density and heat capacity. The same equation is also called *diffusion equation*; it describes diffusion of particles with the diffusion coefficient $\varkappa$.

For complex functions one can consider a parabolic equation with "imaginary time". An equation of this type is the *non-stationary Schrödinger equation*

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\Delta - V\right)\varphi = 0\,, \tag{2.30}$$

which describes the dynamics of the wave function of a particle of mass m in a potential V in quantum mechanics.

2.2.5 Hyperbolic Equations

The typical example of a hyperbolic equation is the *d'Alambert equation*

$$\left(\frac{1}{c^2}\partial_t^2 - \Delta\right)\varphi = 0\,, \tag{2.31}$$

where c is the speed of light. This equation describes, in particular, propagation of electromagnetic waves.

A more general equation is the *Klein-Gordon equation*

$$\left(\frac{1}{c^2}\partial_t^2 - \Delta + \frac{m^2c^2}{\hbar^2}\right)\varphi = 0\,. \tag{2.32}$$

This equation describes relativistic elementary particles with mass m in quantum field theory.

2.2.6 Boundary Conditions

If the open set M has a boundary ∂M, then the above equations have to be supplemented also by some *boundary conditions*. Even if there is no boundary one has to specify the behavior of the unknown function at infinity. The choice of the boundary conditions depends, of course, on the model under consideration. Local boundary conditions have the form

$$B\varphi(t,x)\Big|_{x\in\partial M} = 0\,, \tag{2.33}$$

where B is, in general, a first-order partial differential operator in space variables

$$B = \sum_{i=1}^{n} v^i(t,x)\partial_i + u(t,x)\,, \tag{2.34}$$

where $v^i(t,x)$, $i = 1,\ldots,n$, and $u(t,x)$ are some functions of x and, in general, t, evaluated at the boundary ∂M.

The classical boundary conditions are described as follows. The *Dirichlet boundary conditions* simply set the value of the function equal to zero at the boundary, i.e. the Dirichlet boundary operator is

$$B_D = 1\,. \tag{2.35}$$

Let N^i be the inward pointing unit normal vector to the boundary ∂M. Then the *Neumann boundary conditions* require that the normal derivative of the function vanishes at the boundary, i.e. the Neumann boundary operator is

$$B_N = \sum_{i=1}^{n} N^i(x)\partial_i\,. \tag{2.36}$$

More generally, the *Robin boundary operator* is a modification of the Neumann

$$B_R = \sum_{i=1}^{n} N^i(x)\partial_i + u(x)\,, \tag{2.37}$$

where u is a smooth function.

2.2.7 Gauss Theorem

We describe briefly the *Gauss theorem* that will be needed throughout this book (for more details see Chap. 3). We denote the Cartesian coordinates in $\mathbb{R}^n$ by $x = (x^1, \dots, x^n)$. Let M be a bounded open set in $\mathbb{R}^n$ with a smooth boundary ∂M; then the boundary is an $(n-1)$-dimensional hypersurface that can be described by n equations

$$x^i = x^i(\hat{x}), \qquad i = 1, \dots, n, \tag{2.38}$$

where $\hat{x} = (\hat{x}^1, \dots, \hat{x}^{n-1})$ are the parameters that provide local coordinates for the boundary. Then the $(n-1)$ vectors

$$\frac{\partial x^j}{\partial \hat{x}^1}, \cdots, \frac{\partial x^j}{\partial \hat{x}^{n-1}} \tag{2.39}$$

are tangent to the boundary; moreover, they form a basis in the tangent space, that is, any tangent vector is a linear combination of these vectors.

At this point we need to remind the definition of the Jacobian of a coordinate transformation (see also Sec. 3.1). Let $u^1, \dots, u^m$, be m coordinates which are functions of m other variables $v^1, \dots, v^m$, that is, $u^i = u^i(v)$. Then the *Jacobian* of such a change of coordinates is defined by the determinant of the matrix $\partial u^i / \partial v^j$ and denoted by

$$\frac{\partial(u^1, \dots, u^m)}{\partial(v^1, \dots, v^m)} = \det \begin{pmatrix} \dfrac{\partial u^1}{\partial v^1} & \cdots & \dfrac{\partial u^1}{\partial v^m} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial u^m}{\partial v^1} & \cdots & \dfrac{\partial u^m}{\partial v^m} \end{pmatrix}. \tag{2.40}$$

The importance of Jacobians comes from the fact that if the Jacobian of a coordinate transformation $u^i = u^i(v)$ is not equal to zero, then this transformation is locally invertible, that is, there exists the inverse coordinate transformation $v^i = v^i(u)$; such transformations are called *local diffeomorphisms*.

Next, we define the normal vector $N = (N_i)$ to the boundary. The components of the normal vector are determined by special Jacobians. Consider the $n \times (n-1)$ matrix

$$\left(\frac{\partial x^j}{\partial \hat{x}^\mu}\right) = \begin{pmatrix} \frac{\partial x^1}{\partial \hat{x}^1} & \cdots & \frac{\partial x^1}{\partial \hat{x}^{n-1}} \\ \vdots & & \vdots \\ \frac{\partial x^i}{\partial \hat{x}^1} & \cdots & \frac{\partial x^i}{\partial \hat{x}^{n-1}} \\ \vdots & & \vdots \\ \frac{\partial x^n}{\partial \hat{x}^1} & \cdots & \frac{\partial x^n}{\partial \hat{x}^{n-1}} \end{pmatrix}. \tag{2.41}$$

Let M_i be the $(n-1)\times(n-1)$ matrix obtained by deleting the i-th row in this matrix. Then

$$N_i = (-1)^{n-i} \det M_i \,. \tag{2.42}$$

That is, it is nothing but the Jacobian

$$N_i = (-1)^{n-i} \frac{\partial(x^1, \ldots, x^{i-1}, x^{i+1}, \ldots x^n)}{\partial(\hat{x}^1, \ldots, \hat{x}^{n-1})} \,. \tag{2.43}$$

This can also be written in another form

$$N_i = \sum_{j_1,\ldots,j_{n-1}=1}^{n} \varepsilon_{j_1 \ldots j_{n-1} i} \frac{\partial x^{j_1}}{\partial \hat{x}^1} \cdots \frac{\partial x^{j_{n-1}}}{\partial \hat{x}^{n-1}} \,, \tag{2.44}$$

where $\varepsilon_{j_1 \ldots j_{n-1} i}$ is the so-called *Levi-Civita symbol* defined by (3.58) (see Sec. 3.1.10, in particular, eq. (3.67)). It is easy to see that the vector N_i is indeed orthogonal to all tangent vectors, that is,

$$N_i \frac{\partial x^i}{\partial \hat{x}^\mu} = 0, \qquad \mu = 1, \ldots, n-1. \tag{2.45}$$

Then the *Gauss divergence theorem* (which is a particular case of a more general *Stokes' theorem*) asserts that for any vector field K^i we have

$$\int\limits_M dx \, \sum_{i=1}^{n} \frac{\partial}{\partial x^i} K^i = \int\limits_{\partial M} d\hat{x} \, \sum_{i=1}^{n} N_i K^i \,. \tag{2.46}$$

This formula enables one to integrate by parts by using the equation

$$\int\limits_M dx \, \varphi \sum_{i=1}^{n} \frac{\partial}{\partial x^i} K^i = -\int\limits_M dx \, \sum_{i=1}^{n} \left(\frac{\partial}{\partial x^i}\varphi\right) K^i + \int\limits_{\partial M} d\hat{x} \, \varphi \sum_{i=1}^{n} N_i K^i \,, \tag{2.47}$$

where φ is an arbitrary smooth function. Furthermore, the formula of integration by parts is valid for the so-called *covariant derivatives*

$$\mathcal{D}_j = \partial_j + iA_j \tag{2.48}$$

where A_j is a real vector field. Indeed, it is easy to see that

$$\int_M dx\ \bar{\varphi} \sum_{j=1}^{n} \mathcal{D}_j(K^j\psi) = -\int_M dx\ \sum_{j=1}^{n} \left(\overline{\mathcal{D}_j\varphi}\right) K^j\psi + \int_{\partial M} d\hat{x}\ \bar{\varphi} \sum_{i=1}^{n} N_i K^i\psi\,, \tag{2.49}$$

2.2.8 Existence and Uniqueness of Solutions

The question arises whether there *exists* a function that satisfies the given partial differential equation and the imposed initial and boundary conditions and, if it exists, whether it is *unique*. In other words, this is the question of the existence and uniqueness of the solution. Without going into details we quote the result. Roughly speaking, this problem does indeed have a unique solution, at least for small times, if all coefficient functions are smooth and the operator L and the boundary conditions are *elliptic*. Let us just note that the classical boundary conditions (Dirichlet and Neumann) are elliptic. The ellipticity of general boundary conditions is a much more complicated issue. For a more formal result see, for example, [74, 32, 72].

In most of this book we will simplify the problem by assuming that the coefficients of the operator L as well as the boundary operator B are smooth functions of space coordinates that do not depend on time. Also, most of the time we will assume that there is no boundary. We will come back to time-dependent operators and the boundary value problems at the end of the book.

2.3 Partial Differential Operators

The definition of differential operators on functional L^2 Hilbert spaces is more complicated due to two main reasons.

First of all, not all functions are differentiable. The nicest functions are, of course, those which have continuous derivatives of all orders. Such functions are called *smooth*. However, although the sets of smooth functions form vector spaces, denoted by C^∞, these spaces are not Hilbert spaces since they are not complete. On the other hand, we need completeness to be able to use convergence, continuity and many other technical things. The remarkable fact about spaces of smooth functions is that they are *dense* subsets of the L^2 spaces. This means that every function in L^2 space can be approximated as a limit of a sequence of smooth functions. Therefore, we can define the derivatives of L^2 functions as limits of sequences of usual derivatives of smooth functions.

The other difficulty, in fact, related to the first one, in dealing with differential operators is the fact that they are *unbounded*. In particular, their spectra are unbounded and the sequence of their eigenvalues goes to infinity. This makes some of the formal constructions described above much more subtle and more difficult to handle due to the fact that some of the infinite series may diverge. So, one has to make sure at each step that everything is well-defined, all infinite series converge etc. This is one of the main differences between finite-dimensional linear algebra and functional analysis. In this book we will not care too much about such subtleties and deal with differential operators formally as if they were just some infinite-dimensional matrices. If we know what we are doing then this should not lead to any problems.

2.3.1 Adjoint Operator

Let us consider the space $L^2(M,\mu)$ of square integrable functions on some open subset M of the Euclidean space $\mathbb{R}^n$ with some weight function μ. Let us consider an elliptic second-order partial differential operator

$$L = -\sum_{i,j=1}^{n} \alpha^{ij}(x)\partial_i\partial_j + \sum_{j=1}^{n} \beta^j(x)\partial_j + \gamma(x)\,. \tag{2.50}$$

acting on smooth functions on M; as usual, we assume that the coefficients α^{ij} are real and the coefficients β^i and γ may be complex.

The *adjoint* L^* (more precisely, the *formal adjoint*) of the operator L is defined by

$$(\varphi, L\psi) = (L^*\varphi, \psi) \tag{2.51}$$

for any smooth functions φ and ψ that vanish at the boundary together with all derivatives. Let us define a bilinear form

$$\begin{aligned} F(\varphi,\psi) &= (\varphi, L\psi) - (L^*\varphi,\psi) \\ &= \int\limits_M dx\,\mu(x)\left\{\overline{\varphi(x)}L\psi(x) - \overline{[L^*\varphi(x)]}\psi(x)\right\}. \end{aligned} \tag{2.52}$$

Then the equation (2.51) means

$$F(\varphi,\psi) = 0\,. \tag{2.53}$$

To find the adjoint operator L^* we need to integrate by parts twice. Of course, in doing so, we will get some boundary terms but because the functions vanish at the boundary together with all derivatives the boundary terms vanish. What remains is an expression for the operator L^*

$$L^* = -\sum_{i,j=1}^{n} \mu^{-1}\partial_i\partial_j\alpha^{ij}\mu - \sum_{j=1}^{n}\mu^{-1}\partial_j\bar{\beta}^j\mu + \bar{\gamma}$$
$$= -\sum_{i,j=1}^{n}\alpha^{ij}\partial_i\partial_j + \sum_{j=1}^{n}\tilde{\beta}^j\partial_j + \tilde{\gamma}\,, \tag{2.54}$$

where

$$\tilde{\beta}^j = -\bar{\beta}^j - 2\sum_{i=1}^{n}\mu^{-1}\partial_i(\mu\alpha^{ij})\,, \tag{2.55}$$

$$\tilde{\gamma} = \bar{\gamma} - \sum_{i,j=1}^{n}\mu^{-1}\partial_i\partial_j(\mu\alpha^{ij}) - \sum_{i=1}^{n}\mu^{-1}\partial_i(\mu\bar{\beta}^i)\,, \tag{2.56}$$

It is worth making a remark about our notation. When we write a differential operator in such a form, then the order of functions and derivatives does matter. It is assumed that the operators act on a function f from the left in the order they are written, for example, the first term should be understood as follows

$$\mu^{-1}\partial_i\partial_j\alpha^{ij}\mu f = \mu^{-1}\partial_i\left[\partial_j\left(\alpha^{ij}\mu f\right)\right]. \tag{2.57}$$

We study the conditions on the coefficients of this operator so that it is self-adjoint (more precisely, *formally self-adjoint*), that is, $L = L^*$. We see that the operator L is self-adjoint if the coefficient functions satisfy the following conditions

$$\beta^j + \bar{\beta}^j = -2\sum_{i=1}^{n}\mu^{-1}\partial_i(\mu\alpha^{ij})\,, \tag{2.58}$$

$$\gamma - \bar{\gamma} = -\sum_{i,j=1}^{n}\mu^{-1}\partial_i\partial_j(\mu\alpha^{ij}) - \sum_{i=1}^{n}\mu^{-1}\partial_i(\mu\bar{\beta}^i). \tag{2.59}$$

A remark has to be made here. The definition of the adjoint operator, and, therefore, of the self-adjoint operator, depends on the weight function μ. Therefore, the same operator may be self-adjoint for one weight function and not self-adjoint for another. Since most of the time the form of the operator is already given the question should be whether it is possible to find a weight function μ such that the operator becomes self-adjoint. In other words, given the functions α^{ij} and β^i the question is whether it is possible to find a function μ such that the equation (2.58) is satisfied. Obviously, such a function does not always exist.

Let us decompose the vector β^j and the scalar γ according to

$$\beta^j = B^j - \sum_{i=1}^{n} \mu^{-1}\partial_i(\mu\alpha^{ij}) - 2i\sum_{k=1}^{n} \alpha^{jk}A_k, \tag{2.60}$$

$$\gamma = Q + \sum_{i,j=1}^{n} A_i\alpha^{ij}A_j - i\sum_{i,j=1}^{n} \mu^{-1}\partial_i(\mu\alpha^{ij}A_j)\,, \tag{2.61}$$

with new real valued vectors A_i and B^i, and a scalar Q. This allows us to rewrite the operator L in a more symmetric form.

$$L = -\sum_{k,j=1}^{n} \mu^{-1}\mathcal{D}_j\mu\alpha^{jk}\mathcal{D}_k + B^j\mathcal{D}_j + Q \tag{2.62}$$

where $\mathcal{D}_j = \partial_j + iA_j$.

Now, the conditions for the operator L to be self-adjoint simply mean that Q is real and B^j vanishes

$$B^j = 0, \tag{2.63}$$

$$Q = \bar{Q}; \tag{2.64}$$

in this case

$$L = -\sum_{k,j=1}^{n} \mu^{-1}\mathcal{D}_j\mu\alpha^{jk}\mathcal{D}_k + Q. \tag{2.65}$$

Therefore, a self-adjoint operator is uniquely determined by the following data: a real symmetric non-degenerate matrix α^{ij}, a real vector A_j, a real function Q and a positive real function μ.

It turns out that the theory of elliptic second-order partial differential operators is intimately related to and can be significantly simplified in terms of Riemannian geometry. The main advantage of the machinery of Riemannian geometry is that it is invariant under general transformation of coordinates (so-called *diffeomorphisms*). A Riemannian metric naturally appears in the theory of elliptic partial differential operators as follows. Since the operator L is elliptic then the matrix α^{ij} is real, symmetric and non-degenerate. Therefore, its inverse can be identified (up to a conformal factor) with the Riemannian metric (see Chap. 3 for details, in particular, Sec. 3.15).

2.3.2 Adjoint Boundary Conditions

The adjoint operator L^* is a partial differential operator. Therefore, to specify it completely one needs to supplement it with some boundary conditions. These boundary conditions (called the *adjoint boundary conditions*) are not arbitrary and they are not necessarily the same as the boundary conditions

for the operator L. They are defined rather uniquely by the requirement that the eq. (2.53) should hold not only for functions that vanish at the boundary with all their derivatives but for functions ψ that satisfy the boundary conditions for the operator L and functions φ that satisfy the adjoint boundary conditions for the operator L^*. This defines the *adjoint boundary operator* B^* rather uniquely in terms of the boundary operator B. Then the operator L with the boundary condition B is called *self-adjoint* if not only $L^* = L$ but also $B^* = B$.

We will restrict ourselves to the case when the boundary ∂M is a smooth $(n-1)$-dimensional hypersurface. As before, for simplicity we assume that M is just a domain in the Euclidean space $\mathbb{R}^n$. To find the adjoint boundary conditions we need to compute the bilinear form $F(\varphi, \psi)$, (2.52), for arbitrary smooth functions φ and ψ. By integrating by parts and using the Gauss theorem (2.47) we get

$$F(\varphi,\psi) = \int\limits_{\partial M} d\hat{x}\ \mu\Bigg\{ \sum_{i,j=1}^{n} N_i \mu^{-1} \partial_j (\mu \alpha^{ij} \bar{\varphi}) \psi - \sum_{i,j=1}^{n} \bar{\varphi} N_i \alpha^{ij} \partial_j \psi + \sum_{i=1}^{n} N_i \beta^i \bar{\varphi} \psi \Bigg\}. \tag{2.66}$$

This can be rewritten in the following form

$$F(\varphi,\psi) = \int\limits_{\partial M} d\hat{x}\ \mu \left\{ \left(\overline{\partial_N \varphi}\right) \psi - \bar{\varphi} \partial_N \psi + \rho \bar{\varphi} \psi \right\}, \tag{2.67}$$

where (note the appearance of the matrix α^{ij} in the definition of the normal derivative)

$$\partial_N = \sum_{i,j=1}^{n} N_i \alpha^{ij} \partial_j, \tag{2.68}$$

$$\begin{aligned} \rho &= \sum_{j=1}^{n} N_j \beta^j + \sum_{k,j=1}^{n} N_j \mu^{-1} \partial_k (\mu \alpha^{kj}) \\ &= \sum_{j=1}^{n} N_j B^j - 2i \sum_{i,j=1}^{n} N_j \alpha^{jk} A_k \,. \end{aligned} \tag{2.69}$$

For a self-adjoint operator the function ρ takes the form

$$\rho = -2i \sum_{i,j=1}^{n} N_j \alpha^{jk} A_k \,. \tag{2.70}$$

Now, we see that if we choose the Dirichlet boundary conditions for ψ, that is, ψ vanishes on the boundary, then for this bilinear form to vanish we need to choose that φ also vanishes at the boundary, that is, the adjoint boundary conditions is also Dirichlet. That is, the Dirichlet boundary operators are

$$B_D = B_D^* = 1\,. \tag{2.71}$$

Another simple choice of the boundary conditions is the Neumann condition (or, more generally, Robin boundary condition), which in this case takes the form

$$(\partial_N + \varkappa)\,\psi\Big|_{x\in\partial M} = 0\,, \tag{2.72}$$

where $\varkappa$ is a smooth function. In this case for the bilinear form F to vanish we need to choose

$$(\partial_N + \bar{\varkappa} + \bar{\rho})\,\varphi\Big|_{x\in\partial M} = 0\,, \tag{2.73}$$

which defines the adjoint boundary condition to the Robin condition. That is the Robin boundary operators are

$$B_R = \partial_N + \varkappa, \tag{2.74}$$

$$B_R^* = \partial_N + \bar{\varkappa} + \bar{\rho}\,. \tag{2.75}$$

Therefore, for the operator L with Robin boundary conditions to be self-adjoint in addition to the conditions (2.63)-(2.64) the function $\varkappa$ has to satisfy the condition

$$\bar{\varkappa} - \varkappa = \rho, \tag{2.76}$$

which simply means that the imaginary part of the function $\varkappa = u + iv$ is equal to

$$v = \sum_{i,j=1}^{n} N_i \alpha^{ij} A_j\,, \tag{2.77}$$

and the real part u remains arbitrary. That is, for a self-adjoint operator (2.65) the boundary operator takes the form

$$B_R = B_R^* = \mathcal{D}_N + u, \tag{2.78}$$

where

$$\mathcal{D}_N = \sum_{k,j=1}^{n} N_k \alpha^{kj} \mathcal{D}_j, \tag{2.79}$$

and u is an arbitrary real function.

2.3.3 Spectral Theorem

We list here without proof some properties of elliptic partial differential operators on compact manifolds. We will describe the manifold theory briefly in more details in the next chapter. For now one can simply visualize a compact manifold as a bounded open subset of $\mathbb{R}^n$ with some boundary ∂M.

Let L be a self-adjoint elliptic second-order partial differential operator with smooth coefficients with some appropriate elliptic boundary conditions B (say, Dirichlet or Neumann) and with a positive leading symbol acting in the space $L^2(M,\mu)$. Then the spectral theorem asserts the following facts:

1. The spectrum of the operator L is a pure point spectrum. That is, the spectrum consists of eigenvalues only and there is no continuous spectrum.
2. The spectrum of L is real.
3. The spectrum of L is bounded from below.
4. The operator L is either positive or has only finitely many non-positive eigenvalues.
5. The eigenvalues form a non-decreasing sequence $(\lambda_k)_{k=1}^{\infty}$, that is,

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_k \le \lambda_{k+1} \le \cdots . \tag{2.80}$$

6. The eigenvalues have finite multiplicities and, therefore, the eigenspaces are finite-dimensional. That is, for each k there are only finitely many eigenvalues equal to λ_k.
7. The projections to the eigenspaces are trace-class operators and their traces are equal to the multiplicities of the eigenvalues.
8. As $k \to \infty$ the eigenvalues grow to infinity as k^2, more precisely, they have the following asymptotics

$$\lambda_k = ck^2 + O(k)\,, \tag{2.81}$$

   where c is some positive constant and $O(k)$ denotes terms of order k.
9. The eigenfunctions $(\varphi_k)_{k=1}^{\infty}$ are smooth functions that form a basis in $L^2(M,\mu)$, which can be made orthonormal, in particular,

$$\sum_{k=1}^{\infty} \varphi_k(x)\overline{\varphi_k(x')} = \delta(x,x')\,, \tag{2.82}$$

$$(\varphi_j,\varphi_k) = \delta_{jk}\,. \tag{2.83}$$

Here

$$\delta(x,x') = \mu^{-1}(x)\delta(x-x') \tag{2.84}$$

is the *invariant* (or *covariant*) delta-function and

$$\delta(x-x') = \delta(x^1-x'^1)\cdots\delta(x^n-x'^n) \tag{2.85}$$

is the n-dimensional Dirac delta-function. The extra factor $\mu^{-1}(x)$ is introduced here to compensate for the integration measure so that

$$\int_M dx\ \mu(x)\delta(x,x')f(x) = f(x')\,. \tag{2.86}$$

10. The integral kernel of the resolvent $G(\lambda) = (L-\lambda)^{-1}$ is given by

$$G(\lambda;x,x') = \sum_{k=1}^{\infty} \frac{1}{\lambda_k - \lambda}\varphi_k(x)\overline{\varphi_k(x')}\,, \tag{2.87}$$

and is a meromorphic function of λ with poles at the eigenvalues λ_k. It is self-adjoint, that is

$$\overline{G(\lambda;x,x')} = G(\bar{\lambda};x',x), \tag{2.88}$$

and satisfies the differential equations

$$[L(x,\partial_x) - \lambda]\, G(\lambda;x,x') = \delta(x,x')\,, \tag{2.89}$$

$$[L(x',\partial_{x'}) - \lambda]\, G(\lambda;x,x') = \delta(x,x')\,, \tag{2.90}$$

and the boundary conditions

$$B_x G(\lambda;x,x')\Big|_{x\in\partial M} = 0, \tag{2.91}$$

$$B_{x'} G(\lambda;x,x')\Big|_{x'\in\partial M} = 0\,. \tag{2.92}$$

2.4 Heat Kernel

2.4.1 Heat Kernel

Let us consider first a time-independent elliptic self-adjoint partial differential operator L with some boundary conditions B (either Dirichlet or Neumann). Then the integral kernel of the heat semigroup $\exp(-tL)$, called the *heat kernel*, is given by

$$U(t;x,x') = \sum_{k=1}^{\infty} e^{-t\lambda_k}\varphi_k(x)\overline{\varphi_k(x')}\,. \tag{2.93}$$

It is self-adjoint, that is,

$$\overline{U(t;x,x')} = U(t;x',x), \tag{2.94}$$

and satisfies the equations

$$[\partial_t + L(x, \partial_x)]\, U(t; x, x') = 0\,, \tag{2.95}$$

$$[\partial_t + L(x', \partial_{x'})]\, U(t; x, x') = 0\,, \tag{2.96}$$

with the initial condition

$$U(0; x, x') = \delta(x, x')\,, \tag{2.97}$$

and the boundary conditions

$$B_x U(t; x, x')\Big|_{x\in\partial M} = 0, \tag{2.98}$$

$$B_{x'} U(t; x, x')\Big|_{x'\in\partial M} = 0\,. \tag{2.99}$$

Obviously, the resolvent kernel and the heat kernel are related by the Laplace transform

$$G(\lambda; x, x') = \int_0^\infty dt\; e^{\lambda t} U(t; x, x')\,, \tag{2.100}$$

$$U(t; x, x') = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\lambda\; e^{-\lambda t} G(\lambda; x, x')\,, \tag{2.101}$$

where c is a sufficiently large negative real constant.

Let $\omega = \omega(x)$ be a smooth function. It is easy to see that the heat kernels of the operators L and $L_\omega = e^{-\omega} L e^{\omega}$ are related by

$$U(t; x, x') = e^{\omega(x)} U_\omega(t; x, x') e^{-\omega(x')}. \tag{2.102}$$

This equation can be used to find the heat kernel of an operator L in terms of the heat kernel of the operator L_ω by carefully choosing the function ω to simplify the form of the operator L_ω.

Let us consider now the more general case of an elliptic (not necessarily self-adjoint) time-dependent operator $L = L(t, x, \partial_x)$. Then we define the heat kernel as a function $U(t, x|t', x')$ that depends on two time variables, t and t', and two sets of space variables, x and x', and satisfies the differential equations

$$[\partial_t + L(t, x, \partial_x)]\, U(t, x|t', x') = 0\,, \tag{2.103}$$

$$[-\partial_{t'} + L^*(t', x', \partial_{x'})]\, U(t, x|t', x') = 0\,, \tag{2.104}$$

with the initial condition

$$U(t', x|t', x') = \delta(x, x')\,, \tag{2.105}$$

and the boundary conditions

$$B_x U(t, x|t', x')\Big|_{x\in\partial M} = 0, \tag{2.106}$$

$$B^*_{x'} U(t, x|t', x')\Big|_{x'\in\partial M} = 0\,, \tag{2.107}$$

where L^* is the operator adjoint to L and B^* is the boundary operator adjoint to B.

In the case when the operator L does not depend on time t, the heat kernel $U(t, x|t'x')$ depends on just one time variable, $t-t'$, and is related to the heat kernel introduced above by

$$U(t, x|t', x') = U(t - t'; x, x')\,, \tag{2.108}$$

We slightly abuse notation here by denoting the heat kernel in these two cases by the same symbol, but this should not cause any confusion since from the number of arguments it is always clear what function is being used.

The heat kernel $U(t, x|t', x')$ is the primary object of interest of this book. It is intimately related to the conditional probability density function (transitional distribution) $p_X(t, x; t', x')$ of a stochastic process X_t described in Chap. 7. It is the probability density function of the random variable X_t at time t given that the stochastic process X_t started with value x' at time t'.

2.4.2 Heat Kernel of Time-dependent Operators

The heat kernel for a time dependent operator $L(t)$ is defined by the chronological exponent (1.222). To be able to use that formula we have to develop some perturbation series. There are at least two kinds of perturbation theories. The simplest one is based on Volterra series for the heat semi-group described in Sec. 1.17.5. We separate a time-independent operator L_0 and treat the time-dependent part as a perturbation, that is,

$$L(t) = L_0 + \varepsilon L_1(t)\,, \tag{2.109}$$

where ε is a small parameter. Let $U_0(t; x, x')$ be the heat kernel of the time-independent operator L_0. Then by using the equation (1.246) we obtain the heat kernel of the time-dependent operator $L(t)$ up to the second order in ε and $(t - t')$,

$$U(t,x|t',x') = \Bigg\{ 1 - \varepsilon \int_{t'}^{t} d\tau \; L_1(\tau) + \int_{t'}^{t} d\tau_2 \int_{t'}^{\tau_2} d\tau_1 \; \left\{ \varepsilon^2 L_1(\tau_2) L_1(\tau_1) + \varepsilon [L_0, L_1(\tau_1)] \right\} + O[(t-t')^3, \varepsilon^3] \Bigg\} U_0(t-t';x,x') \,, \tag{2.110}$$

where the differential operators act on the first argument of the heat kernel.

Another perturbation theory can be based on the chronological exponent and the assumption that the operators $L(t)$ almost commute for different times, that is, the commutator

$$[L(\tau_1), L(\tau_2)] \tag{2.111}$$

is small. Let us define the average L_0 of the operator $L(\tau)$ by

$$L_0 = \frac{1}{(t-t')} \int_{t'}^{t} d\tau L(\tau) \,, \tag{2.112}$$

Of course, $L_0 = L_0(t,t')$ depends on t and t' as parameters. Let us fix both t and t' and define the operator

$$L_1(\tau;t,t') = L(\tau) - L_0(t,t') \,, \tag{2.113}$$

so that we have the decomposition of the operator $L(\tau)$

$$L(\tau) = L_0 + L_1(\tau) \,, \tag{2.114}$$

where we do not indicate the parameters t and t' to simplify notation.

The operator L_0 is time-independent, so we can apply the perturbation scheme described above. Let $U_0(\tau,t,t';x,x')$ be the heat kernel of the operator $L_0(t,t')$ computed with both t and t' being fixed, that is, it is the kernel of the heat semigroup $\exp[-\tau L_0(t,t')]$. Then in the zero order of the perturbation theory the heat kernel of the time-dependent operator $L(t)$ is

$$U(t,x|t',x') = U_0(t-t',t,t';x,x') \,. \tag{2.115}$$

This may give a good approximation for the heat kernel, if the commutators of the operators $L(\tau)$ at different times are small. Of course, we can also compute the correction terms to this solution by using the Volterra series (1.246).

2.4.3 Cauchy Problem

Suppose, for simplicity, that there is no boundary so that we do not have to worry about the boundary conditions. Then, if the heat kernel is known then the solution of the original *initial value problem* (also called *Cauchy problem*)

$$(\partial_t + L)V = 0\,, \tag{2.116}$$

$$V(0,x) = f(x)\,, \tag{2.117}$$

is given by

$$V(t,x) = \int\limits_M dx'\mu(x')U(t,x|0,x')f(x')\,. \tag{2.118}$$

More generally, the heat kernel enables one to solve the inhomogeneous heat equation. Let $f(x)$ and $h(t,x)$ be some given functions. Then the solution of the problem

$$(\partial_t + L)V(t,x) = h(t,x)\,, \tag{2.119}$$

$$V(0,x) = f(x)\,, \tag{2.120}$$

is given by

$$\begin{aligned} V(t,x) = &\int\limits_M dx'\mu(x')U(t,x|0,x')f(x') \\ &+ \int\limits_0^t dt' \int\limits_M dx'\mu(x')U(t,x|t',x')h(t',x')\,. \end{aligned} \tag{2.121}$$

2.4.4 Boundary Value Problem

Let us suppose now that the domain M has some smooth boundary ∂M. Then the correct setting of the problem must include some appropriate boundary conditions. Therefore, such a problem is called a *boundary value problem*. Let $L = L(t,x,\partial_x)$ be an elliptic second order partial differential operator that may depend, in general on the time variable as a parameter and is not necessarily self-adjoint. Let $B = B(t,x,\partial_x)$ be a corresponding boundary operator, either Dirichlet or Robin. Let $f = f(x)$ be a function of space coordinates, $h = h(t,x)$ and $s(t,x)$ be functions of the time and space coordinates. We are interested in the solution of the boundary value problem

$$[\partial_t + L(t,x,\partial_x)]\, V(t,x) = h(t,x)\,, \tag{2.122}$$

$$V(0,x) = f(x) \tag{2.123}$$

$$[B(t,x,\partial_x)V(t,x) - s(t,x)]\,\Big|_{x\in\partial M} = 0\,. \tag{2.124}$$

It turns out that the solution of this problem can be expressed in terms of the heat kernel via some integrals over the domain M and its boundary ∂M.

To show this we need to use the following identity. Let $\varphi = \varphi(t,x)$ and $\psi = \psi(t,x)$ be two arbitrary smooth functions. Then by integrating by parts and using the identity (2.67) one can show that

$$\begin{aligned}
&\int_0^t dt' \int_M dx'\mu(x')\Big\{\bar\varphi(t',x')\,[\partial_{t'} + L(t',x',\partial_{x'})]\,\psi(t',x') \\
&-\Big([-\partial_{t'} + L^*(t',x',\partial_{x'})]\,\bar\varphi(t',x')\Big)\psi(t',x')\Big\} \\
&= \int_M dx'\mu(x')\,[\bar\varphi(t,x')\psi(t,x') - \bar\varphi(0,x')\psi(0,x')] \\
&+ \int_0^t dt' \int_{\partial M} d\hat x'\mu(x')\Big\{\Big[(\partial_N^{x'} + \rho(t',x'))\bar\varphi(t',x')\Big]\psi(t',x') \\
&-\bar\varphi(x')\partial_N^{x'}\psi(t',x')\Big\}\,,
\end{aligned} \tag{2.125}$$

where ∂_N and ρ are defined by eqs. (2.68) and (2.69). The superscript x' on ∂_N indicates that it depends on the primed variables, t', x', and acts on x'.

Now, we choose here $\bar\varphi(t',x') = U(t,x|t',x')$ and $\psi(t',x') = V(t',x')$ and use the eqs. (2.103), (2.104), (2.105), (2.122) and (2.123) to get

$$\begin{aligned}
V(t,x) &= \int_M dx'\mu(x')U(t,x|0,x')f(x') + \int_0^t dt' \int_M dx'\mu(x')U(t,x|t',x')h(t',x') \\
&+ \int_0^t dt' \int_{\partial M} dx'\mu(x')\Big\{U(t,x|t',x')\partial_N^{x'}V(t',x') \\
&-\Big[(\partial_N^{x'} + \rho(t',x'))U(t,x|t',x')\Big]V(t',x')\Big\}\,.
\end{aligned} \tag{2.126}$$

Now, by using the boundary conditions for V, (2.124), and for the heat kernel, (2.98), (2.99), we obtain

$$V(t,x) = \int\limits_M dx' \mu(x') U(t,x|0,x') f(x') \tag{2.127}$$

$$+ \int\limits_0^t dt' \int\limits_M dx' \mu(x') U(t,x|t',x') h(t',x')$$

$$+ \int\limits_0^t dt' \int\limits_{\partial M} d\hat{x}' \mu(x') \left[K(t',x',\partial'_x) U(t,x|t',x') \right] s(t',x') \,,$$

where

$$K_D = -\partial_N - \rho, \tag{2.128}$$

for the Dirichlet boundary conditions, that is, when $B_D = 1$, and

$$K_R = 1, \tag{2.129}$$

for the Robin boundary conditions, when the boundary operator is $B_R = \partial_N + \varkappa$ with some function $\varkappa$.

Notice that for the Dirichlet boundary conditions, $B_D = 1$, the heat kernel satisfies the boundary conditions

$$U_D(t,x|t',x')\Big|_{x\in\partial M} = 0, \tag{2.130}$$

$$U_D(t,x|t',x')\Big|_{x'\in\partial M} = 0 \,, \tag{2.131}$$

and for the Robin boundary conditions, $B_R = \partial_N + \varkappa$, the heat kernel satisfies the boundary conditions

$$\left[\partial_N^x + \varkappa(t,x)\right] U_R(t,x|t',x')\Big|_{x\in\partial M} = 0, \tag{2.132}$$

$$\left[\partial_N^{x'} + \varkappa(t',x') + \rho(t',x')\right] U_R(t,x|t',x')\Big|_{x'\in\partial M} = 0 \,. \tag{2.133}$$

Therefore, although the form of the equation (2.127) does not depend on $\varkappa$, the heat kernel $U_R(t,x,t',x')$ does.

It should be clear at this point that the heat kernel is an invaluable tool in the theory of partial differential equations since it enables one to reduce the study of various problems with different initial and boundary conditions to the study of just one problem for the heat kernel. The knowledge of the heat kernel gives the complete information about an elliptic operator and the solution of all initial value and boundary value problems.

2.5 Differential Operators with Constant Coefficients

2.5.1 Ordinary Differential Equations

The Fourier transform enables one to solve differential equations with constant coefficients defined on the whole real line with regularity conditions at infinity. Let L be a linear second-order ordinary differential operator

$$L = -\alpha\partial_x^2 + \beta\partial_x + \gamma\,. \tag{2.134}$$

For simplicity, we restrict here to the case of real coefficients α, β and γ. We also assume that $\alpha > 0$. The symbol of this operator is

$$\sigma(p) = \alpha p^2 + i\beta p + \gamma\,. \tag{2.135}$$

The operator L is self-adjoint (with the weight function $\mu = 1$) if $\beta = 0$. Let λ be a complex number, $h = h(x)$ be a given function of x and $f = f(x)$ be an unknown function satisfying the differential equation

$$(L - \lambda)f = h\,, \tag{2.136}$$

and the boundary condition that f goes to zero at $x \to \pm\infty$.

Let $\hat{f}(p)$ and $\hat{h}(p)$ be the Fourier transforms of the functions f and h. Then by applying the Fourier transform to this equation we obtain an algebraic equation

$$[\sigma(p) - \lambda]\hat{f}(p) = \hat{h}(p)\,, \tag{2.137}$$

which we immediately solve

$$\hat{f}(p) = \frac{\hat{h}(p)}{\sigma(p) - \lambda}\,. \tag{2.138}$$

Finally, the solution of the original differential equation is obtained by the inverse Fourier transform

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx} \frac{\hat{h}(p)}{\sigma(p) - \lambda}\,. \tag{2.139}$$

We can now rewrite this solution in the form

$$f(x) = \int\limits_{-\infty}^{\infty} dx'\; G(\lambda; x, x')h(x')\,, \tag{2.140}$$

where

$$G(\lambda; x, x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \frac{1}{\sigma(p) - \lambda} \,. \tag{2.141}$$

The function $G(\lambda; x, x')$ obviously satisfies the equation

$$(L - \lambda) G(\lambda; x, x') = \delta(x - x') \,, \tag{2.142}$$

where $\delta(x)$ is the Dirac delta-function, and, therefore, is the kernel of the resolvent (or simply the resolvent) of the operator L.

This integral can be easily computed by the residue theory. The poles of the integrand are determined by the solutions of the equation

$$\sigma(p) - \lambda = 0 \,. \tag{2.143}$$

Obviously, the solutions are

$$p_{1,2}(\lambda) = i \left[\nu \pm D(\lambda) \right] \,, \tag{2.144}$$

where

$$\nu = -\frac{\beta}{2\alpha} \tag{2.145}$$

and

$$D(\lambda) = \frac{1}{2\alpha} \sqrt{\beta^2 + 4\alpha(\gamma - \lambda)} \,. \tag{2.146}$$

Here the square root is defined in such a way that when λ is sufficiently large and negative then the square root is positive. Also, we can always choose the branch of the square root so that $\operatorname{Im} D(\lambda) > 0$.

For the purpose of the calculation of the integral we will assume that λ has a sufficiently large negative real part, more precisely,

$$\operatorname{Re} (\gamma - \lambda) > 0 \,, \tag{2.147}$$

so that the roots $p_{1,2}(\lambda)$ are distinct and

$$\operatorname{Re} \left[\nu - D(\lambda) \right] < 0 < \operatorname{Re} \left[\nu + D(\lambda) \right] \,, \tag{2.148}$$

and, hence, p_1 is in the upper half-plane and p_2 is in the lower half-plane. Then the poles of the integrand are simple and we compute:

$$G(\lambda; x, x') = \begin{cases} \dfrac{1}{2\alpha D(\lambda)} \exp\left\{ - \left[\nu + D(\lambda) \right] (x - x') \right\} & \text{for } x > x' \,, \\ \dfrac{1}{2\alpha D(\lambda)} \exp\left\{ - \left[\nu - D(\lambda) \right] (x - x') \right\} & \text{for } x < x' \,. \end{cases} \tag{2.149}$$

This can also be written in the form

$$G(\lambda; x, x') = \frac{1}{2\alpha D(\lambda)} \Big\{ \theta(x - x') \exp\big\{ -[\nu + D(\lambda)](x - x') \big\} + \theta(x' - x) \exp\big\{ -[\nu - D(\lambda)](x - x') \big\} \Big\} . \tag{2.150}$$

Notice that if λ satisfies the condition (2.147) then the resolvent goes to zero at $x \to \pm\infty$.

For $\lambda = \gamma$ the resolvent is not well defined since one of the poles $p_2(\lambda)$ crosses the real line and the Fourier integral is not well defined. Thus the point γ is in the spectrum. More generally, the spectrum of the operator L is determined by the values of λ such that the integrand has poles for real values of p. That is, the spectrum is the curve, $\lambda = \lambda(p)$, in the complex plane of λ described by the equation

$$\lambda(p) = (\alpha p^2 + \gamma) + i\beta p , \tag{2.151}$$

where p is a real parameter. Let

$$\lambda = u + iv , \tag{2.152}$$

Then this spectral curve is described by

$$u(p) = \alpha p^2 + \gamma , \tag{2.153}$$

$$v(p) = \beta p . \tag{2.154}$$

If $\beta \neq 0$, then the spectral curve is the parabola

$$u = \frac{\alpha}{\beta^2} v^2 + \gamma . \tag{2.155}$$

Note that the resolvent cannot be analytically continued through this curve to large real positive values of λ. As $\beta \to 0$ this parabola degenerates to the interval $[\gamma, \infty)$ on the real line, so that in the case $\beta = 0$ the operator L becomes self-adjoint and the spectrum becomes real, it is just the interval $[\gamma, \infty)$. Since the operator acts on the whole real line the spectrum is obviously purely continuous. So, the operator L does not have any eigenvalues.

One could easily generalize this method to the operator (2.134) with complex constants β and γ. It is just the matter of analytic continuation of the resolvent (2.150) to the complex values of β and γ.

2.5.2 Indegro-Differential Equations

The Fourier transform can also be applied to *integro-differential equations* of a particular type which have a so called *convolution kernel*. Such equations

appear, in particular, in modeling of the jump-diffusion by a Poisson stochastic processes (see Sec. 8.5). To be specific let L be an ordinary differential operator of the form

$$L = -\alpha\partial_x^2 + \beta\partial_x + \gamma \tag{2.156}$$

with real coefficients and $\alpha > 0$, acting on functions on the real line $\mathbb{R}$. The symbol of this operator is, of course,

$$\sigma(p) = \alpha p^2 + i\beta p + \gamma\,. \tag{2.157}$$

Let K be an integral operator defined by

$$(Kf)(x) = \int_{-\infty}^{\infty} dx'\ \tilde{K}(x,x')f(x')\,. \tag{2.158}$$

Integral operators K whose integral kernels $\tilde{K}(x,x')$ depend only on the difference $x - x'$, that is,

$$\tilde{K}(x,x') = K(x-x')\,, \tag{2.159}$$

are called operators of *convolution type*; they said to have a *convolution kernel*. We assume that the operator K is such an operator. Let $\hat{K}(p)$ be the Fourier transform of the kernel $K(x)$, that is,

$$\hat{K}(p) = \int_{-\infty}^{\infty} dx\ e^{-ipx}K(x)\,, \tag{2.160}$$

so that the kernel is

$$K(x-x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')}\hat{K}(p)\,. \tag{2.161}$$

A remarkable fact about the convolution operators is that they act simply as multiplication operators on the Fourier transforms. Indeed, it is easy to show that the Fourier transform $\widehat{(Kf)}(p)$ of the function $(Kf)(x)$ is

$$\widehat{(Kf)}(p) = \hat{K}(p)\hat{f}(p)\,. \tag{2.162}$$

Let $h = h(x)$ be a given function, λ be a complex number and $f = f(x)$ be an unknown function satisfying the integro-differential equation

$$(L + K - \lambda)f = h\,. \tag{2.163}$$

Then by applying the Fourier transform to this equation we obtain a linear algebraic equation

$$[\sigma(p) + \hat{K}(p) - \lambda]\hat{f}(p) = \hat{h}(p)\,, \tag{2.164}$$

the solution of which is, of course,

$$\hat{f}(p) = \frac{\hat{h}(p)}{\sigma(p) + \hat{K}(p) - \lambda}\,. \tag{2.165}$$

Finally, the solution of the integro-differential equation is obtained by the inverse Fourier transform

$$f(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\, e^{ipx} \frac{\hat{h}(p)}{\sigma(p) + \hat{K}(p) - \lambda}\,. \tag{2.166}$$

Of course, this can be written in the form

$$f(x) = \int_{-\infty}^{\infty} dx'\, G(\lambda; x, x')h(x')\,, \tag{2.167}$$

where

$$G(\lambda; x, x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\, e^{ip(x-x')} \frac{1}{\sigma(p) + \hat{K}(p) - \lambda} \tag{2.168}$$

is the resolvent of the integro-differential operator $L + K$.

As usual, the spectrum of the operator $L + K$ is determined by the values of λ such that the integrand has poles on the real line. That is, the spectrum is the curve in the complex plane parametrized by a real parameter p

$$\lambda(p) = \sigma(p) + \hat{K}(p)\,. \tag{2.169}$$

To be specific assume that $\hat{K}(p)$ is real, which means that the kernel is symmetric, that is, $K(x) = K(-x)$. Let

$$\lambda = u + iv\,. \tag{2.170}$$

Then this spectral curve is described by

$$u(p) = \alpha p^2 + \gamma + \hat{K}(p)\,, \tag{2.171}$$

$$v(p) = \beta p\,. \tag{2.172}$$

If $\beta \neq 0$, then the spectral curve is the curve

$$u = \frac{\alpha}{\beta^2} v^2 + \gamma + \hat{K}\left(\frac{v}{\beta}\right)\,. \tag{2.173}$$

If $\beta = 0$, then the operator $L + K$ is self-adjoint and its spectrum is real. If, in addition, $\hat{K}(p)$ is bounded from below then the spectrum is the interval $[\tilde{\gamma}, \infty)$, where

$$\tilde{\gamma} = \gamma + k\,, \tag{2.174}$$

where $k = \inf \hat{K}(p)$.

Let us consider an integral operator T defined by

$$(Tf)(x) = \int\limits_{-\infty}^{\infty} dx'\, \omega(x')\,[f(x + x') - f(x)]\,, \tag{2.175}$$

where $\omega(x)$ is some probability distribution (for a review of probabitity see Sec. 7.1.1), in particular, $\omega(x)$ is non-negative and

$$\int\limits_{-\infty}^{\infty} dx\, \omega(x) = 1\,. \tag{2.176}$$

Such an operator can be called a *jump operator*. The Fourier transform of the probability distribution $\omega(x)$,

$$\hat{\omega}(p) = \int\limits_{-\infty}^{\infty} dx\, e^{-ipx}\omega(x), \tag{2.177}$$

is called the *characteristic function*. The action of the operator T can be also written as

$$(Tf)(x) = \int\limits_{-\infty}^{\infty} dx'\, \omega(x' - x)f(x') - f(x)\,. \tag{2.178}$$

Therefore, the jump operator has the form

$$T = K - I\,, \tag{2.179}$$

where I is the identity operator and K is a convolution operator with the kernel

$$K(x - x') = \omega(x' - x)\,. \tag{2.180}$$

Let us consider an integro-differential equation

$$(L + \nu T - \lambda)f = h\,, \tag{2.181}$$

where ν is a constant. Then by using the solution to the convolution integro-differential equation above we obtain

$$f(x) = \int_{-\infty}^{\infty} dx'\, G(\lambda; x, x') h(x')\,, \tag{2.182}$$

where the resolvent is now

$$G(\lambda; x, x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi}\, e^{ip(x-x')} \frac{1}{\sigma(p) + \nu\hat{\omega}(-p) - \nu - \lambda}\,. \tag{2.183}$$

2.5.3 Elliptic Partial Differential Operators

Similarly to the one-dimensional case, the multi-dimensional Fourier transform enables one to find resolvents of elliptic partial differential operators with constant coefficients. Let α^{ij} be a real non-degenerate constant symmetric positive matrix, β^j be a constant vector and γ be a constant. Let L be a linear second-order partial differential differential operator with constant coefficients of the form

$$L = -\sum_{j,k=1}^{n} \alpha^{jk} \partial_j \partial_k + \sum_{j=1}^{n} \beta^j \partial_j + \gamma\,, \tag{2.184}$$

Let A denote the matrix of the coefficients of second derivatives, $A = (\alpha^{ij})$, and β be the vector of the coefficients of first derivatives, $\beta = (\beta^j)$. Then the symbol of the operator L is given by the expression

$$\begin{aligned} \sigma(p) &= \langle p, Ap\rangle + i\,\langle p, \beta\rangle + \gamma \\ &= \sum_{j,k=1}^{n} \alpha^{jk} p_j p_k + i \sum_{j=1}^{n} \beta^j p_j + \gamma\,, \end{aligned} \tag{2.185}$$

and the leading symbol of the operator L is

$$\sigma_L(p) = \langle p, Ap\rangle = \sum_{j,k=1}^{n} \alpha^{jk} p_j p_k\,. \tag{2.186}$$

Since the leading symbol $\sigma_L(p)$ is positive definite for any real $p \neq 0$, the operator L is elliptic. The operator L is self-adjoint (with weight function $\mu = 1$) if β^i is imaginary and γ is real.

Let λ be a complex number, $h = h(x)$ be a given function of x and $f = f(x)$ be an unknown function satisfying the differential equation

$$(L - \lambda) f = h\,, \tag{2.187}$$

and the boundary condition that f goes to zero at $x \to \pm\infty$. Then by applying the Fourier transform to this equation we obtain the solution

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,x\rangle} \frac{\hat{h}(p)}{\sigma(p)-\lambda}\,. \tag{2.188}$$

This can be now written in the form

$$f(x) = \int\limits_{\mathbb{R}^n} dx'\; G(\lambda; x, x')h(x')\,, \tag{2.189}$$

where

$$G(\lambda; x, x') = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,(x-x')\rangle} \frac{1}{\sigma(p)-\lambda}\,, \tag{2.190}$$

is the resolvent of the operator L satisfying the equation

$$(L-\lambda)G(\lambda; x, x') = \delta(x-x')\,. \tag{2.191}$$

This integral can be computed as follows. Let us assume that λ has a sufficiently large negative real part so that for any real p

$$\mathrm{Re}\,(\sigma(p)-\lambda) > 0\,. \tag{2.192}$$

Then we have

$$\frac{1}{\sigma(p)-\lambda} = \int\limits_0^\infty dt\;\exp\{-t[\sigma(p)-\lambda]\}\;, \tag{2.193}$$

and, therefore, we obtain an integral representation of the resolvent

$$G(\lambda; x, x') = \int\limits_0^\infty dt\; e^{t\lambda} U(t; x, x')\,, \tag{2.194}$$

where

$$U(t; x, x') = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} \exp\{-t\sigma(p) + i\,\langle p, (x-x')\rangle\}\;. \tag{2.195}$$

Since the symbol $\sigma(p)$ is a quadratic polynomial this is a particular case of so-called *Gaussian integral* considered in Sec. 1.2. By using the eq. (1.25) we obtain

$$U(t;x,x') = (4\pi t)^{-n/2}(\det A)^{-1/2}\exp\left\{\frac{1}{2}\left\langle (x-x'), A^{-1}\beta\right\rangle\right\}$$
$$\times\exp\left\{-t\left[\gamma+\frac{1}{4}\left\langle\beta, A^{-1}\beta\right\rangle\right]\right\}$$
$$\times\exp\left\{-\frac{1}{4t}\left\langle (x-x'), A^{-1}(x-x')\right\rangle\right\}. \tag{2.196}$$

Now, by using the Fourier integral representation of the delta-function we see that

$$\lim_{t\to 0^+}(4\pi t)^{-n/2}(\det A)^{-1/2}\exp\left\{-\frac{1}{4t}\left\langle x, A^{-1}x\right\rangle\right\} = \delta(x), \tag{2.197}$$

and, therefore, the function $U(t;x,x')$ satisfies the initial condition

$$U(0;x,x') = \delta(x-x'). \tag{2.198}$$

Also, again by using the Fourier integral representation it is easy to see that the function $U(t;x,x')$ satisfies the differential equation

$$(\partial_t + L)U(t;x,x') = 0. \tag{2.199}$$

This equation is called the *heat equation* (or diffusion equation). The function $U(t;x,x')$ is the fundamental solution of the heat equation called the *heat kernel*.

To get the resolvent we need to compute the integral over t. The integral (2.194) can be computed by using the formula, which can be found in [29, 1, 68],

$$\int_0^\infty dt\, t^{-p}\exp\left(-at-\frac{b}{4t}\right) = 2^p\left(\frac{a}{b}\right)^{(p-1)/2}K_{p-1}\left(\sqrt{ab}\right), \tag{2.200}$$

where $a, b > 0$ and $K_\alpha(x)$ is the modified Bessel function of an imaginary argument of the second kind called the *Macdonald function* of order α (for details see [29]).

By using this formula, we obtain finally the resolvent

$$G(\lambda;x,x') = (4\pi)^{-n/2}(\det A)^{-1/2}\exp\left\{\frac{1}{2}\left\langle (x-x'), A^{-1}\beta\right\rangle\right\}$$
$$\times 2^{n/2}\left(\frac{a}{b}\right)^{(n-2)/2}K_{(n-2)/2}\left(\sqrt{ab}\right), \tag{2.201}$$

where

$$b = \left\langle (x - x'), A^{-1}(x - x') \right\rangle , \tag{2.202}$$

$$a = \frac{1}{4} \left\langle \beta, A^{-1}\beta \right\rangle + \gamma - \lambda . \tag{2.203}$$

This, of course, is only true for λ with sufficiently large negative real part so that

$$\mathrm{Re}\,(\lambda - \gamma) < 0 . \tag{2.204}$$

The study of the spectrum of non-self-adjoint operators is, in general, a more complicated problem. What we know for sure is that the spectrum is located in the half-plane

$$\mathrm{Re}\,(\lambda - \gamma) \geq 0 . \tag{2.205}$$

Since the operator L acts on a non-compact space we can also say that it is continuous and it does not have any eigenvalues. In the case, $\beta^i = 0$, when the operator L is self-adjoint, then the spectrum is the interval $[\gamma, \infty)$ on the real line.

2.5.4 Parabolic Partial Differential Equations

The Laplace transform naturally applies to linear differential equations with constant coefficients. We consider the space $\mathbb{R}_+ \times \mathbb{R}^n$ with time coordinate $t > 0$ and space coordinates $x = (x^i)$, $i = 1, 2, \ldots, n$; the space coordinates ranging in $-\infty < x^i < \infty$. Let $\alpha^{ij}(x)$,$i, j = 1, \ldots, n$ be a real non-degenerate symmetric positive definite matrix, $\beta^j(x)$, $j = 1, \ldots, n$, be a vector and $\gamma(x)$ be a function, which do not depend on time t. Let L be an elliptic second-order partial differential differential operator with variable coefficients of the form

$$L = -\sum_{j,k=1}^{n} \alpha^{jk}(x)\partial_j\partial_k + \sum_{j=1}^{n} \beta^j(x)\partial_j + \gamma(x) . \tag{2.206}$$

Let $h(x)$ be a function of $x \in \mathbb{R}^n$ that goes to zero at infinity. We consider a *parabolic* partial differential equation of the form

$$(\partial_t + L)f(t, x) = 0 \tag{2.207}$$

with initial condition

$$f(0, x) = h(x) . \tag{2.208}$$

As usual, we also assume that the function f vanishes at infinity.

Let $F(s; x)$ be the Laplace transform of the function $f(t, x)$ with respect to the time variable. By applying the Laplace transform to this equation we obtain an elliptic equation

$$(L + s)F(s; x) = h(x) . \tag{2.209}$$

Let $\operatorname{Re} s$ be sufficiently large. Then the operator $L+s$ is invertible. Its Green function is equal to the resolvent $G(-s;x,x')$ of the operator L evaluated at $\lambda=-s$, that is,

$$(L+s)G(-s;x,x')=\delta(x-x')\,. \tag{2.210}$$

Then the solution of the elliptic equation can be written in the form

$$F(s;x)=\int\limits_{\mathbb{R}^n} dx'\; G(-s;x,x')h(x')\,, \tag{2.211}$$

and the solution of the original problem is obtained by inverse Laplace transform

$$f(t,x)=\int\limits_{\mathbb{R}^n} dx' U(t;x,x')h(x')\,, \tag{2.212}$$

where

$$U(t;x,x')=\int\limits_{c-i\infty}^{c+i\infty}\frac{ds}{2\pi i}e^{st}G(-s;x,x')\,, \tag{2.213}$$

and c is a sufficiently large real constant. This is nothing but the *heat kernel*; it satisfies the heat equation

$$(\partial_t+L)U(t;x,x')=0 \tag{2.214}$$

and the initial condition

$$U(0;x,x')=\delta(x-x')\,. \tag{2.215}$$

Obviously, the resolvent $G(-s;x,x')$ is nothing but Laplace transform of the heat kernel

$$G(-s;x,x')=\int\limits_0^\infty dt\; e^{-st}U(t;x,x')\,. \tag{2.216}$$

Both the resolvent $G(-s;x,x')$ and the heat kernel $U(t;x,x')$ satisfy the boundary condition at infinity.

2.5.5 Ordinary Differential Equations on Half-line

The Laplace transform can also be applied to solve second-order differential equations with constant coefficients. Let L be a linear second-order differential differential operator

$$L=\alpha\partial_t^2+\beta\partial_t+\gamma\,, \tag{2.217}$$

with real coefficients α, β and γ, acting on functions of a positive real variable t, that is, on $\mathbb{R}_+$. We will assume that $\alpha \neq 0$, say $\alpha > 0$.

Let $h = h(t)$ be a known function of t and $f = f(t)$ be an unknown function satisfying the differential equation

$$Lf = h\,, \tag{2.218}$$

with some initial conditions

$$f(0) = a\,, \qquad f'(0) = b\,. \tag{2.219}$$

Let $F(s)$ and $H(s)$ be the Laplace transforms of the functions f and h. Applying the Laplace transform to this equation we get an algebraic equation

$$\sigma(s)F(s) = H(s) + \alpha(as + b) + a\beta\,, \tag{2.220}$$

where

$$\sigma(s) = \alpha s^2 + \beta s + \gamma\,. \tag{2.221}$$

Then we immediately obtain

$$F(s) = \frac{1}{\sigma(s)}\left[H(s) + \alpha(as + b) + a\beta\right]\,, \tag{2.222}$$

and, therefore, the solution of the original differential equation is obtained by the inverse Laplace transform

$$f(t) = (\mathcal{L}^{-1}F)(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} \frac{1}{\sigma(s)}\left[H(s) + \alpha(as + b) + a\beta\right]\,, \tag{2.223}$$

where c is a sufficiently large positive real constant.

We can now rewrite this solution in the form

$$f(t) = \int\limits_0^\infty dt'\; G(t, t')h(t') + \psi(t)\,, \tag{2.224}$$

where

$$G(t, t') = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s(t-t')} \frac{1}{\sigma(s)}\,, \tag{2.225}$$

and

$$\psi(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} \frac{\alpha(as + b) + a\beta}{\sigma(s)}\,. \tag{2.226}$$

These integrals can be easily computed by the residue theory. Let s_1 and s_2 be the poles of the integrand, in other words, the roots of the symbol $\sigma(s)$, that is, the solutions of the equation

$$\sigma(s) = 0\,. \tag{2.227}$$

They are given by

$$s_{1,2} = \nu \pm D\,, \tag{2.228}$$

where

$$\nu = -\frac{\beta}{2\alpha} \tag{2.229}$$

$$D = \frac{1}{2\alpha}\sqrt{\beta^2 - 4\alpha\gamma}\,. \tag{2.230}$$

Let us assume for simplicity that $D \neq 0$ so that the roots are distinct. We do not make any assumptions on whether or not they are real or complex.

Then the poles of the integrand are simple and we compute:

$$G(t,t') = \begin{cases} \dfrac{1}{2\alpha D}\Big\{\exp\left[(\nu+D)(t-t')\right] - \exp\left[(\nu-D)(t-t')\right]\Big\} & \text{for } t > t'\,, \\ 0 & \text{for } t < t'\,, \end{cases} \tag{2.231}$$

which can also be written in the form

$$G(t,t') = \theta(t-t')\frac{1}{2\alpha D}\Big\{\exp\left[(\nu+D)(t-t')\right] - \exp\left[(\nu-D)(t-t')\right]\Big\}\,, \tag{2.232}$$

where $\theta(t)$ is the step function.

Similarly, we compute the function $\psi(t)$,

$$\psi(t) = c_1 e^{(\nu+\Delta)t} + c_2 e^{(\nu-\Delta)t}\,, \tag{2.233}$$

where

$$c_1 = \frac{\alpha(\nu+D)a + \alpha b + \beta a}{2\alpha D}\,, \tag{2.234}$$

$$c_2 = -\frac{\alpha(\nu-D)a + \alpha b + \beta a}{2\alpha D}\,. \tag{2.235}$$

Of course, $\psi(t)$ is nothing but the solution of the homogeneous equation

$$Lf = 0 \tag{2.236}$$

with the initial conditions (2.219), and $G(t,t')$ is a Green function of the operator L satisfying the equation

$$LG(t,t') = \delta(t-t')\,. \tag{2.237}$$

Contrary to elliptic operators this equation alone does not define the Green function uniquely. One has to specify also some initial or some symmetry conditions. In particular, the Green function satisfying the condition

$$G(t,t') = 0 \quad \text{for} \quad t < t' \tag{2.238}$$

is called the *retarded* Green function.

2.6 Differential Operators with Linear Coefficients

The Laplace transform can be also applied for solving equation with non-constant coefficients. Let L be a second-order differential operator of the form

$$L = -(\alpha_0 + \alpha_1 x)\partial_x^2 + (\beta_0 + \beta_1 x)\partial_x + \gamma_0 + \gamma_1 x\,, \tag{2.239}$$

with coefficients that are linear functions. If $\alpha_1 \neq 0$, then the point $x_0 = -\alpha_0/\alpha_1$ is a *singular point* of the operator. That is why we assume that $\alpha_0, \alpha_1 > 0$ so that $x_0 < 0$ and consider the domain $x > 0$. Then the leading symbol of the operator L

$$\sigma_L(x,p) = (\alpha_0 + \alpha_1 x)p^2 \tag{2.240}$$

is positive definite.

For a given function h the equation

$$Lf = h \tag{2.241}$$

with the initial conditions

$$f(0) = a, \qquad b = f'(0), \tag{2.242}$$

is a second-order differential equation with non-constant coefficients. Let us apply the Laplace transform to this equation. Since the coefficients are not constants any longer we do not get an algebraic equation but rather a linear first-order differential equation with non-constant coefficients

$$[r(s)\partial_s + q(s)]\,F(s) = \tilde{H}(s)\,, \tag{2.243}$$

where $F(s)$ is the Laplace transform of the function f and

$$r(s) = \alpha_1 s^2 - \beta_1 s - \gamma_1\,, \tag{2.244}$$

$$q(s) = -\alpha_0 s^2 + (\beta_0 + 2\alpha_1)s + \gamma_0 - \beta_1\,, \tag{2.245}$$

$$\tilde{H}(s) = H(s) - \alpha_0 as - \alpha_0 b + \alpha_1 a + \beta_0 a, \tag{2.246}$$

with $H(s)$ being the Laplace transform of the function h.

This equation can be easily solved. First we define

$$\nu(s) = \exp\left(\int ds\, \frac{q(s)}{r(s)}\right) ; \tag{2.247}$$

then the solution is

$$F(s) = \frac{1}{\nu(s)} \left\{ \int ds\, \nu(s) \frac{\tilde{H}(s)}{r(s)} + c \right\} , \tag{2.248}$$

where c is an arbitrary constant that should be determined from the boundary condition

$$\lim_{\mathrm{Im}\, s \to \pm\infty} F(s) = 0 . \tag{2.249}$$

Finally, the solution of the original differential equation is obtained by the inverse Laplace transform.

There is an elegant variation of the method of the Laplace transform for such differential equations. We describe it on the example of the linear homogeneous second-order differential equation with linear coefficients

$$Lf = 0 , \tag{2.250}$$

where L is the second-order differential operator (2.239) with coefficients that are linear functions.

We represent the solution in the form

$$f(t) = \int_C \frac{ds}{2\pi i}\, e^{sx} F(s) , \tag{2.251}$$

where C is a contour of integration in the complex plane that will be specified later. Then one can show that

$$\partial_x f(x) = \int_C \frac{ds}{2\pi i}\, e^{sx} s F(s) , \tag{2.252}$$

$$\partial_x^2 f(x) = \int_C \frac{ds}{2\pi i}\, e^{sx} s^2 F(s) , \tag{2.253}$$

$$x f(x) = -\int_C \frac{ds}{2\pi i}\, e^{sx} \partial_s F(s) + \frac{1}{2\pi i}\, e^{sx} F(s) \Big|_{\partial C} , \tag{2.254}$$

$$x \partial_x f(x) = -\int_C \frac{ds}{2\pi i}\, e^{sx} \partial_s [sF(s)] + \frac{1}{2\pi i}\, e^{sx} sF(s) \Big|_{\partial C} , \tag{2.255}$$

$$x\partial_x^2 f(x) = -\int\limits_C \frac{ds}{2\pi i}\, e^{sx}\partial_s[s^2F(s)] + \frac{1}{2\pi i}\, e^{sx}s^2F(s)\Big|_{\partial C}\,, \qquad (2.256)$$

where ∂C is the boundary of the contour C.

Substituting these equations into the original equation we obtain

$$\int\limits_C \frac{ds}{2\pi i}\, e^{sx}\left[r(s)\partial_s + q(s)\right]F(s) + \frac{1}{2\pi i}\, e^{sx}\left(-\alpha_1 s^2 + \beta_1 s + \gamma_1\right)F(s)\Big|_{\partial C} = 0\,, \qquad (2.257)$$

where $r(s)$ and $q(s)$ are defined above. This equation will be satisfied if both parts are equal to zero. Thus, we obtain a first-order differential equation

$$\left[r(s)\partial_s + q(s)\right]F(s) = 0 \qquad (2.258)$$

and a boundary condition

$$\left(-\alpha_1 s^2 + \beta_1 s + \gamma_1\right)F(s)\Big|_{\partial C} = 0\,. \qquad (2.259)$$

Once the function $F(s)$ is found the function $f(x)$ is obtained by taking the inverse Laplace transform.

Notice that if the contour C is closed, then it does not have a boundary, that is, $\partial C = \emptyset$, and the second equation is satisfied automatically. If the contour C consists of one connected piece with an initial point s_0 and a final point s_1, then the boundary of the contour C consists of two points, $\partial C = \{s_0, s_1\}$, and the notation above means

$$\psi(s)\Big|_{\partial C} = \psi(s_1) - \psi(s_0). \qquad (2.260)$$

for any function ψ. This means that we could choose a contour whose endpoints are either the roots of the equation

$$-\alpha_1 s^2 + \beta_1 s + \gamma_1 = 0 \qquad (2.261)$$

or the zeros of the function $F(s)$. Notice that the contour C can go to infinity in some sector in the complex plane if $F(s)$ vanishes at infinity in that sector; it can even be an infinite contour that starts at infinity and returns to infinity (maybe in different sectors). Different contours of integration C and different arbitrary constants c in the solution of the first-order differential equation correspond to different solutions of the original second-order homogeneous differential equation. Of course, there are only two linearly independent solutions.

2.7 Homogeneous Differential Operators

Let L be a linear second-order ordinary differential operator of the form

$$L = -\alpha x^2 \partial_x^2 + \beta x \partial_x + \gamma \,, \tag{2.262}$$

with real coefficients α, β and γ, acting on functions of x with $x > 0$, that is, on half-line $\mathbb{R}_+$. We will assume that $\alpha > 0$. This operator is invariant under the rescaling $x \mapsto \lambda x$ of the variable x with an arbitrary nonzero real constant λ. Such operators are called *homogeneous*.

The leading symbol of the operator L,

$$\sigma(x,p) = \alpha x^2 p^2 \,, \tag{2.263}$$

is positive but fails to be elliptic at $x = 0$. The point $x = 0$ is a *singular point* of this operator. The function

$$\sigma^{\mathcal{M}}(s) = -\alpha s^2 - (\alpha + \beta)s + \gamma \,. \tag{2.264}$$

can be called the *Mellin symbol* of the operator L.

Let λ be a complex number, $h = h(x)$ be a given function of x and $f = f(x)$ be an unknown function satisfying the differential equation

$$(L - \lambda) f = h \,, \tag{2.265}$$

and the boundary condition

$$\lim_{x \to 0} f(x) = \lim_{x \to \infty} f(x) = 0 \,. \tag{2.266}$$

This equation can be easily solved by using the Fourier transform. Let $F(s)$ and $H(s)$ be the Fourier transforms of the functions f and h. Then by applying the Fourier transform to this equation we obtain an algebraic equation

$$\left[\sigma^{\mathcal{M}}(s) - \lambda\right] F(s) = H(s) \,. \tag{2.267}$$

Then we immediately obtain

$$F(s) = \frac{H(s)}{\sigma^{\mathcal{M}}(s) - \lambda} \,, \tag{2.268}$$

and, therefore, the solution of the original differential equation is obtained by the inverse Mellin transform

$$f(t) = (\mathcal{M}^{-1} F)(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} t^{-s} \frac{H(s)}{\sigma^{\mathcal{M}}(s) - \lambda} \,, \tag{2.269}$$

where c is a constant that will be specified below.

We can now rewrite this solution in the form

$$f(x) = \int_0^\infty \frac{dx'}{x'}\, G(\lambda; x, x') h(x')\,, \tag{2.270}$$

where

$$G(\lambda; x, x') = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \left(\frac{x}{x'}\right)^{-s} \frac{1}{\sigma^{\mathcal{M}}(s) - \lambda} \tag{2.271}$$

is the resolvent of the operator L satisfying the equation

$$(L - \lambda) G(\lambda; x, x') = x' \delta(x - x')\,. \tag{2.272}$$

This integral can be easily computed by residue theory. Let s_1 and s_2 be the roots of the Mellin symbol $\sigma^{\mathcal{M}}(s)$, that is, the solutions of the equation

$$\sigma^{\mathcal{M}}(s) = 0\,. \tag{2.273}$$

We have explicitly

$$s_{1,2} = \nu \pm D(\lambda)\,, \tag{2.274}$$

where

$$\nu = -\frac{\beta + \alpha}{2\alpha} \tag{2.275}$$

and

$$D(\lambda) = \frac{1}{2\alpha} \sqrt{(\alpha + \beta)^2 + 4\alpha(\gamma - \lambda)}\,. \tag{2.276}$$

We will assume that λ has a sufficiently large negative real part, that is,

$$\operatorname{Re}(\lambda - \gamma) < 0\,, \tag{2.277}$$

so that the roots are distinct and

$$\operatorname{Re} s_2 < 0 < \operatorname{Re} s_1\,. \tag{2.278}$$

Then the constant c in the inverse Mellin transform must satisfy $\operatorname{Re} s_2 < c < \operatorname{Re} s_1$. Further, the poles of the integrand are simple and we compute:

$$G(\lambda; x, x') = \begin{cases} \dfrac{1}{2\alpha D(\lambda)} \left(\dfrac{x}{x'}\right)^{-\nu - D} & \text{for } x > x'\,, \\ \dfrac{1}{2\alpha D(\lambda)} \left(\dfrac{x}{x'}\right)^{-\nu + D} & \text{for } x < x'\,. \end{cases} \tag{2.279}$$

This can also be written in the form

$$G(\lambda; x, x') = \frac{1}{2\alpha D(\lambda)} \left\{ \theta(x - x') \left(\frac{x}{x'} \right)^{-\nu - D} + \theta(x' - x) \left(\frac{x}{x'} \right)^{-\nu + D} \right\} . \tag{2.280}$$

Notice that the resolvent goes to zero as $x \to 0$ and $x \to \infty$.

2.8 Notes

In this chapter we gave an introduction to the theory of linear partial differential equations at a rather elementary level. The literature on partial differential equations is huge. There are plenty of books at any level, from a very applied one to an advanced graduate level. Here is a list (that is in no way exhausting) of some good references that we found useful [76, 75, 31, 72, 74, 57].

Part II
Geometry

Chapter 3
Introduction to Differential Geometry

Abstract In this chapter we give a brief introduction to basic concepts of differential geometry. This is a huge subject and we will only introduce background material necessary for the study of the heat kernel on Riemannian manifolds. A wide range of books on differential geometry at various levels of difficulty is listed in the bibliography.

3.1 Differentiable Manifolds

3.1.1 Basic Definitions

A manifold is a general space that looks locally like a Euclidean space of the same dimension at each point. This enables one to develop the differential and integral calculus on manifolds called *geometric* (or *global*) analysis. Historically, the subject arose from the development of the theory of curves and surfaces in Euclidean space. So, when studying manifolds it is always helpful to visualize them, say, as surfaces in the Euclidean space.

A *manifold* M of dimension n is a space that can be locally smoothly deformed everywhere to an open set of the Euclidean space $\mathbb{R}^n$. A *smooth manifold* M of dimension n is covered by a family of overlapping *local coordinate systems* assigning n coordinates $x = (x^1, \dots, x^n)$ to a point p in M. Different sets of local coordinates of the point p are related by *diffeomorphisms*, that is, bijective smooth maps described by some smooth *transition functions*

$$x'^i = f^i(x)\,, \qquad i = 1, \dots, n\,. \tag{3.1}$$

The matrix of partial derivatives

$$\left(\frac{\partial x'^i}{\partial x^j}\right) \tag{3.2}$$

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_3

is called the *Jacobian matrix*, and the determinant of the Jacobian matrix

$$J = \det\left(\frac{\partial x'^i}{\partial x^j}\right) \tag{3.3}$$

is called the *Jacobian*. It is a standard fact from the multivariable calculus that the Jacobian matrix of a diffeomorphism is non-degenerate with a non-zero Jacobian $J \neq 0$. If the Jacobian is positive then the coordinate systems have the same *orientation*. If it is possible to choose local coordinate systems on a manifold such that they all have the same orientation then the manifold is said to be *orientable*.

A *submanifold* S of a manifold M is a subset of M that is itself a manifold. The difference of dimensions $k = (\dim M - \dim S)$ is called the *codimension* of the submanifold S. A submanifold of dimension 1 is a curve. A submanifold of co-dimension 1 is called a *hypersurface*; hypersurfaces are $(n-1)$-dimensional submanifolds.

A simple example of a manifold is the *sphere* S^n of radius a which can be realized as a hypersurface in the Euclidean space $\mathbb{R}^{n+1}$ described by the locus of points whose coordinates satisfy

$$(x^1)^2 + \cdots + (x^n)^2 + (x^{n+1})^2 = a^2\,. \tag{3.4}$$

Another example is the *hyperbolic space* H^n of pseudo-radius a which can be realized as a hypersurface in $\mathbb{R}^{n+1}$ described by

$$(x^1)^2 + \cdots + (x^n)^2 - (x^{n+1})^2 = -a^2\,. \tag{3.5}$$

A fundamental fact about manifolds (*Whitney theorem*) says that every n-dimensional manifold can be realized as a smooth submanifold of $\mathbb{R}^{2n+1}$. Such a realization is called an *embedding*. Thus, every manifold is a submanifold of a Euclidean space. However, there are many properties of manifolds that do not depend on its embedding in a Euclidean space. Such properties are called *intrinsic*.

3.1.2 Vector Fields

Let us consider a curve in M described in some local coordinate system (x^i) by

$$x^i = x^i(t)\,, \qquad t \in [a, b]\,. \tag{3.6}$$

The *velocity vector* is described in these coordinates by

$$(\dot{x}^i) = \left(\dot{x}^1, \ldots, \dot{x}^n\right)\,, \tag{3.7}$$

where the dot denotes the derivative with respect to the parameter t. Let (x'^j) be another local coordinate system. Then the velocity vectors in these coordinates are related by the *chain rule*

$$\dot{x}'^i = \sum_{j=1}^{n} \frac{\partial x'^i}{\partial x^j} \dot{x}^j \,. \tag{3.8}$$

Of course, the velocity vector to a curve in $\mathbb{R}^n$ is tangent to it. This motivates the following definition. A *tangent vector* at a point p_0 of a manifold M is a map that assigns to each local coordinate system an ordered n-tuple $(v^i) = (v^1, \ldots, v^n)$ that transforms under the change of local coordinates according to

$$v'^i = \sum_{j=1}^{n} \left(\frac{\partial x'^i}{\partial x^j} \right) (p_0) v^j \,. \tag{3.9}$$

The set of all tangent vectors at a point p in the manifold M forms a real vector space T_pM called the *tangent space* to M at p. A *vector field* v on a manifold M is a smooth assignment of a tangent vector $v(p)$ to each point p in M. In local coordinates a vector field is described by an n-tuple $(v^j(x))$ of smooth functions.

Each vector field $v^j(x)$ on a manifold M defines a one-parameter group of diffeomorphisms $\varphi_t : M \to M$ such that through any point x of the manifold M passes a curve $\varphi_t(x)$ such that the tangent vector to the curve at each point is equal to the vector field v, that is,

$$\frac{d\varphi_t(x)}{dt} = v(\varphi_t(x)) \,, \tag{3.10}$$

and

$$\varphi_0(x) = x \,. \tag{3.11}$$

The diffeomorphisms φ_t are called the *flow* generated by the vector field v and the curves $\varphi_t(x)$, $t \in [a, b]$, are called the *integral curves* of the vector field v.

In local coordinates the integral curve passing through the point x_0 is the solution of the system of ordinary first-order differential equations

$$\frac{dx^j}{dt} = v^j(x) \,, \qquad j = 1, \ldots, n, \tag{3.12}$$

with the initial conditions

$$x^j(0) = x_0^j \,. \tag{3.13}$$

It is not difficult to solve this equation for small t as a Taylor series in t; we obtain

$$\varphi_t^i(x) = x^i + t v^i(x) + O(t^2) \,. \tag{3.14}$$

3.1.3 Covector Fields

Let f be a function on a manifold M. Under a change of local coordinates $x'^j = x'^j(x)$ the partial derivatives $\partial_i f = \partial f/\partial x^i$ of the function f transform according to

$$\partial'_j f = \sum_{i=1}^{n} \frac{\partial x^i}{\partial x'^j} \partial_i f \,, \tag{3.15}$$

which is again nothing but the chain rule. Note that the matrix $\left(\frac{\partial x^i}{\partial x'^j}\right)$ is inverse to the Jacobian matrix (3.2).

This motivates the following definition. A *covector* at a point p_0 of a manifold M is a map that assigns to each local coordinate system an ordered n-tuple $(\alpha_i) = (\alpha_1, \ldots, \alpha_n)$ that transforms under the change of local coordinates according to

$$\alpha'_j = \sum_{j=1}^{n} \left(\frac{\partial x^i}{\partial x'^j}\right)(p_0)\alpha_i \,. \tag{3.16}$$

The set of all covectors at a point p in the manifold M forms a real vector space $T_p^* M$ called the *cotangent space* to M at p. A *covector field* or a *one-form* α on a manifold M is a smooth assignment of a covector $\alpha(p)$ to each point p in M. In local coordinates a one-form is described by an n-tuple $(\alpha_j(x))$ of smooth functions.

There is a natural *pairing* (or *duality*) between the tangent and cotangent spaces. This means that there is a natural assignment of a real number to a covector α and a vector v defined by

$$\langle \alpha, v \rangle = \sum_{i=1}^{n} \alpha_i v^i \,. \tag{3.17}$$

The importance of this pairing is the fact that this number is an invariant, that is, it does not change under diffeomorphisms.

We want to draw the attention to the use of indices (subscripts and superscripts) above. In differential geometry upper indices (superscripts) and lower indices (subscripts) play different roles: upper indices are used to denote components of vectors and are called *contravariant indices*) and lower indices are used to denote components of covectors and are called *covariant indices*).

3.1.4 Riemannian Metric

A positive definite inner product in the tangent space is defined with the help of a a symmetric positive definite matrix, g_{ij}, called the *metric*,

$$(v, w) = \sum_{i,j=1}^{n} g_{ij} v^i w^j \,. \tag{3.18}$$

Its inverse,

$$(g^{ij}) = (g_{ij})^{-1} \tag{3.19}$$

defines then the inner product in the cotangent space by

$$(\alpha, \beta) = \sum_{i,j=1}^{n} g^{ij} \alpha_i \beta_j \,. \tag{3.20}$$

The metric enables one to define naturally the *length* (or the *norm*) of vectors and covectors by

$$||v|| = \sqrt{(v, v)}\,, \tag{3.21}$$

$$||\alpha|| = \sqrt{(\alpha, \alpha)}\,. \tag{3.22}$$

The metric is also used to establish an isomorphism between tangent and cotangent spaces. Each vector v defines a covector called the *covariant version* of the vector v by

$$v_i = \sum_{j=1}^{n} g_{ij} v^j \,. \tag{3.23}$$

This operation is called *lowering the index* of a vector. Therefore, we can denote the components of the covector corresponding to a vector v by the same symbol and call them the *covariant components* of the vector. Similarly, given a covector α we can define a vector (the *contravariant version* of the covector α) such that

$$\alpha^i = \sum_{j=1}^{n} g^{ij} \alpha_j \,. \tag{3.24}$$

This operation is called *raising the index* of a covector. The components of the vector corresponding to a covector α are denoted by the same symbol and are called the *contravariant components* of the covector.

A *Riemannian metric* on a manifold M is a differentiable assignment of a positive definite inner product in each tangent space T_pM to the manifold at each point p. A manifold with a Riemannian metric on it is called the *Riemannian manifold*.

By requiring the inner product to be diffeomorphism invariant we find that the components of the metric tensor transform under the local diffeomorphisms as follows

$$g'_{ij}(x') = \sum_{k,l=1}^{n} \frac{\partial x^k}{\partial x'^i} \frac{\partial x^l}{\partial x'^j} g_{kl}(x)\,, \tag{3.25}$$

$$g'^{ij}(x') = \sum_{k,l=1}^{n} \frac{\partial x'^i}{\partial x^k} \frac{\partial x'^j}{\partial x^l} g^{kl}(x)\,. \tag{3.26}$$

For example, the standard metric on the sphere S^n and the hyperbolic space H^n in the local coordinates defined by eqs. (3.4) and (3.5) is given by

$$g_{ij}^{S^n} = \delta_{ij} + \frac{x^i x^j}{a^2 - |x|^2}\,, \tag{3.27}$$

$$g_{ij}^{H^n} = \delta_{ij} - \frac{x^i x^j}{a^2 + |x|^2}\,, \tag{3.28}$$

where

$$|x| = \sqrt{\sum_{i=1}^{n} (x^i)^2}\,. \tag{3.29}$$

Notice that formally the metric on the sphere S^n is obtained from the metric on the hyperbolic space H^n by replacing $a \to ia$; this reflects a deep fundamental *duality* between these manifolds. That is why the hyperbolic space is also called a *pseudo-sphere* and the parameter a of H^n is called the *pseudo-radius*.

3.1.5 Arc Length

The Riemannian metric $g_{ij}(x)$ determines the *interval* (or the *distance*), ds, between infinitesimaly close points x and $x + dx$ by

$$ds^2 = \sum_{i,j=1}^{n} g_{ij}(x)\, dx^i\, dx^j\,. \tag{3.30}$$

More precisely, let x and x' be two points on a manifold M and γ be a smooth curve connecting these points described locally by $x^i(\tau)$, where $\tau \in [0, t]$, so that $x(0) = x'$ and $x(t) = x$. The *tangent vector* to the curve γ is defined by

$$\dot{x}^i(\tau) = \frac{dx^i}{d\tau}\,. \tag{3.31}$$

Here and everywhere below the dot denotes the derivative with respect to τ.

Therefore,

$$ds = ||\dot{x}(\tau)||\, d\tau\,, \tag{3.32}$$

where $||\dot{x}||$ is the norm of the tangent vector, and the *length of the curve* γ is defined as

$$l(\gamma) = \int_0^t d\tau \, ||\dot{x}(\tau)|| \, . \tag{3.33}$$

Of course, here the metric $g_{ij} = g_{ij}(x(\tau))$ is evaluated along the curve γ. Notice that the length of the curve does not depend on the parametrization of the curve, that is, it is reparametrization invariant.

3.1.6 Riemannian Volume Element

We introduce the notation for the determinant of the metric (which we will use all the time)

$$g = \det g_{ij} \, . \tag{3.34}$$

Although this function does not have any indices it is not a scalar! Indeed, by taking the determinant of the eq. (3.25) we obtain

$$\sqrt{g'(x')} = J(x)\sqrt{g(x)} \, , \tag{3.35}$$

where

$$J(x) = \det \left(\frac{\partial x^k}{\partial x'^i} \right) \, . \tag{3.36}$$

A scalar function f does not change under the change of coordinates

$$f'(x') = f(x) \, . \tag{3.37}$$

Therefore, the determinant of the metric is not a scalar.

A function that transforms like (3.35) is called a *scalar density* of weight 1. Recall that the standard integration volume element $dx = dx^1 \cdots dx^n$ in $\mathbb{R}^n$ transforms under the local diffeomorphisms as

$$dx' = \det \left(\frac{\partial x'^k}{\partial x^i} \right) dx \, . \tag{3.38}$$

Obviously, the matrix $\left(\frac{\partial x'^k}{\partial x^i} \right)$ is the inverse of the matrix $\left(\frac{\partial x^k}{\partial x'^i} \right)$. Therefore, the quantity

$$d\,\mathrm{vol}\,(x) = \sqrt{g(x)} \, dx \tag{3.39}$$

remains invariant under the change of coordinates. This quantity is called *Riemannian volume element.*

3.1.7 Tensor Fields

A *tensor* of type (p, q) at a point p_0 of a manifold M is a map that assigns to each local coordinate system a collection of numbers $T^{i_1\dots i_p}_{j_1\dots j_q}$, where each index ranges from 1 to n, that transforms under the change of local coordinates according to

$$T'^{i_1\dots i_p}_{j_1\dots j_q} = \sum_{k_1,\dots,k_p=1}^{n} \sum_{l_1,\dots,l_q=1}^{n} \frac{\partial x'^{i_1}}{\partial x^{k_1}} \cdots \frac{\partial x'^{i_p}}{\partial x^{k_p}} \frac{\partial x^{l_1}}{\partial x'^{l_q}} \cdots \frac{\partial x^{j_1}}{\partial x'^{j_q}} T^{k_1\dots k_p}_{l_1\dots l_q} . \quad (3.40)$$

A *tensor field* of type (p, q) on a manifold M is a smooth assignment of a tensor of type (p, q) to each point p in M. In local coordinates a tensor field of type (p, q) is described by a collection of smooth functions $T^{k_1\dots k_p}_{l_1\dots l_q}(x)$.

The number $r = p + q$ is called the *rank of the tensor* of type (p, q). Such a tensor is said to be p times contravariant and q times covariant.

More generally, a function φ that transforms under the change of coordinates according to

$$\varphi(x') = [J(x)]^w \varphi(x) \quad (3.41)$$

with some real parameter w, is called a *scalar density of weight* w. One can easily show that for any covariant tensor of rank 2, A_{ij}, the determinant $\det A_{ij}$ is a scalar density of weight 2 and for any contravariant tensor of rank 2, B^{ij}, the determinant $\det B^{ij}$ is a scalar density of weight (-2). To obtain true scalars from such determinants one needs to multiply them by the corresponding power of the determinant of the metric to cancel the Jacobian, that is, the quantities

$$g^{-1} \det A_{ij} = \frac{\det A_{ij}}{\det g_{ij}}, \qquad g \det B^{ij} = (\det g_{ij}) \det B^{ij} \quad (3.42)$$

are scalars. Notice that for a tensor $C^i{}_j$ of a type $(1, 1)$ the determinant $\det C^i_j$ is a proper scalar.

3.1.8 Permutations of Tensors

One of the most important tensor operation is the *permutation*. Let $\mathbb{Z}_p = \{1, \dots, p\}$ be the set of p integers. A *permutation* φ is simply a transformation (bijective map) of this set which maps every integer $i \in \mathbb{Z}_p$ to the integer $\varphi(i)$. The identity permutation is obviously such a permutation that for any integer i, $\varphi(i) = i$. The inverse of a permutation and the product of two permutations are defined in an obvious manner.

Then the set of all permutations of the set $\mathbb{Z}_p$ forms a group S_p called the *symmetric group* of order p. One can easily show that the number of different

permutations that form the symmetric group is

$$|S_p| = p! \,. \tag{3.43}$$

A permutation that exchanges the order of only two elements is called an *elementary permutation* (or a *transposition*). Every permutation can be realized as a product of elementary permutations. A permutation that can be realized by an even number of elementary permutations is called an *even permutation*. A permutation that can be realized by an odd number of elementary permutations is called an *odd permutation*. The *sign of a permutation* φ, denoted by $\mathrm{sign}(\varphi)$ is then defined by

$$\mathrm{sign}(\varphi) = \begin{cases} +1, \text{ if } \varphi \text{ is even}, \\ -1, \text{ if } \varphi \text{ is odd}\,. \end{cases} \tag{3.44}$$

Let $T_{i_1 \ldots i_p}$ be a covariant tensor of type $(0, p)$. Then every permutation φ in the symmetric group S_p defines a new tensor $\varphi(T)$, called a *permutation of the tensor* T, by

$$\varphi(T)_{i_1 \ldots i_p} = T_{i_{\varphi(1)} \ldots i_{\varphi(p)}} \,. \tag{3.45}$$

The *symmetrization* of the tensor T is defined by

$$\mathrm{Sym}(T) = \frac{1}{p!} \sum_{\varphi \in S_p} \varphi(T) \,, \tag{3.46}$$

where we sum over all permutations. The symmetrization is also denoted by parenthesis. The components of the symmetrized tensor $\mathrm{Sym}(T)$ are given by

$$T_{(i_1 \ldots i_p)} = \frac{1}{p!} \sum_{\varphi \in S_p} T_{i_{\varphi(1)} \ldots i_{\varphi(p)}} \,. \tag{3.47}$$

The *anti-symmetrization* of the tensor T is defined by

$$\mathrm{Alt}(T) = \frac{1}{p!} \sum_{\varphi \in S_p} \mathrm{sign}\,(\varphi) \varphi(T) \,. \tag{3.48}$$

The anti-symmetrization is also denoted by square brackets. The components of the anti-symmetrized tensor $\mathrm{Alt}(T)$ are given by

$$T_{[i_1 \ldots i_p]} = \frac{1}{p!} \sum_{\varphi \in S_p} \mathrm{sign}\,(\varphi) T_{i_{\varphi(1)} \ldots i_{\varphi(p)}} \,. \tag{3.49}$$

The symmetrization and the antisymmetrization of a tensor A of rank $p = 2$ are given by

$$A_{(ij)} = \frac{1}{2}(A_{ij} + A_{ji})\,, \tag{3.50}$$

$$A_{[ij]} = \frac{1}{2}(A_{ij} - A_{ji})\,. \tag{3.51}$$

Similarly, for a tensor B of rank $p = 3$ the above definition gives

$$B_{(ijk)} = \frac{1}{6}(B_{ijk} + B_{jki} + B_{kij} + B_{jik} + B_{kji} + B_{ikj})\,, \tag{3.52}$$

$$B_{[ijk]} = \frac{1}{6}(B_{ijk} + B_{jki} + B_{kij} - B_{jik} - B_{kji} - B_{ikj})\,. \tag{3.53}$$

A tensor T is called *symmetric* if for any permutation $\varphi \in S_p$

$$\varphi(T) = T\,. \tag{3.54}$$

and *anti-symmetric* if for any permutation $\varphi \in S_p$

$$\varphi(T) = \text{sign}\,(\varphi)T\,. \tag{3.55}$$

An anti-symmetric tensor of type $(0, p)$ is called a *p-form*.

Similarly one can define permutations of contravariant tensors of type $(p, 0)$.

3.1.9 Einstein Summation Convention

As we move on there are more and more summation symbols when dealing with tensor components in local coordinates. In differential geometry there is a very convenient way to deal with this problem that is called *Einstein summation convention*.

Here are the main points.

1. In any expression there are two types of indices: *free indices* and *repeated indices*. A free index appears only once in an expression; it is assumed to take all possible values from 1 to n.
2. The position (that is, up or down) of each free index in all terms in an equation must be the same.
3. Every repeated index appears twice in an expression. It is assumed that there is a summation over each repeated pair of indices from 1 to n. The summation over a pair of repeated indices in an expression is called the *contraction* of indices.
4. Repeated indices are *dummy indices*: they can be replaced by any other letter (not already used in the expression) without changing the meaning of the expression.

5. Indices cannot be repeated on the same level. That is, in a pair of repeated indices one index is in the upper position and another is in the lower position.
6. There cannot be indices occuring three or more times in any expression.

As an example, consider a tensor equation

$$B^{ij} = A^{ij}{}_{kl} v^k w^l \,. \tag{3.56}$$

Here i and j are free indices and k and l are repeated indices; a summation over k and l from 1 to n is implicitly assumed but not written explicitly, that is, this equation actually means

$$B^{ij} = \sum_{k,l=1}^{n} A^{ij}{}_{kl} v^k w^l \,. \tag{3.57}$$

From now on we will be using the Einstein summation convention.

3.1.10 Levi-Civita Symbol

The completely anti-symmetric *Levi-Civita symbol* (or the *alternating symbol*) is defined by

$$\varepsilon^{i_1 \dots i_n} = \varepsilon_{i_1 \dots i_n} = \begin{cases} 1 & \text{if } (i_1, \dots, i_n) \text{ is an even permutation of } (1, \dots, n), \\ -1 & \text{if } (i_1, \dots, i_n) \text{ is an odd permutation of } (1, \dots, n), \\ 0 & \text{otherwise.} \end{cases} \tag{3.58}$$

It is easy to see that

$$\varepsilon_{i_1 \dots i_n} = n! \delta^1_{[i_1} \cdots \delta^n_{i_n]}, \tag{3.59}$$

$$\varepsilon^{i_1 \dots i_n} = n! \delta^{[i_1}_1 \cdots \delta^{i_n]}_n \,, \tag{3.60}$$

where δ^i_j is the Kronecker symbol defined by (2.17). By using these equations one can compute the product of the Levi-Civita symbols

$$\varepsilon^{j_1 \dots j_n} \varepsilon_{i_1 \dots i_n} = n! \delta^{j_1}_{[i_1} \cdots \delta^{j_n}_{i_n]}. \tag{3.61}$$

Moreover, one can show that the contraction of the product of the Levi-Civita symbols over k indices is equal to

$$\varepsilon^{j_1 \dots j_{n-k} m_1 \dots m_k} \varepsilon_{i_1 \dots i_{n-k} m_1 \dots m_k} = k!(n-k)! \delta^{j_1}_{[i_1} \cdots \delta^{j_{n-k}}_{i_{n-k}]}. \tag{3.62}$$

The determinant of a $n \times n$ matrix $A = (A^i{}_j)$ is defined by

$$\det A = \sum_{\varphi \in S_n} \operatorname{sign}(\varphi) A^1{}_{\varphi(1)} \cdots A^n{}_{\varphi(n)} \,. \tag{3.63}$$

By using the Levi-Civita symbol it can be written in one of the following forms

$$\begin{aligned} \det A &= \varepsilon^{i_1 \ldots i_n} A^1{}_{i_1} \ldots A^n{}_{i_n} \\ &= \varepsilon_{j_1 \ldots j_n} A^{j_1}{}_1 \ldots A^{j_n}{}_n \\ &= \frac{1}{n!} \varepsilon^{i_1 \ldots i_n} \varepsilon_{j_1 \ldots j_n} A^{j_1}{}_{i_1} \ldots A^{j_n}{}_{i_n} \,. \end{aligned} \tag{3.64}$$

It is important to understand that the Levi-Civita symbols are not tensors, but rather tensor densities. It is easy to see that the proper tensors (more precisely, pseudo-tensors) are obtained by multiplying them by the factors $g^{1/2}$ and $g^{-1/2}$,

$$E_{i_1 \ldots i_n} = g^{1/2} \varepsilon_{i_1 \ldots i_n} \,, \tag{3.65}$$

$$E^{i_1 \ldots i_n} = g^{-1/2} \varepsilon^{i_1 \ldots i_n} \,. \tag{3.66}$$

Furthermore, there is a generalization of the cross product of vectors in $\mathbb{R}^3$ to n dimensions. A collection of $(n-1)$ vectors $e_{(1)}, \ldots e_{(n-1)}$ naturally defines a covector N_i (which can be called the *n-dimensional cross product* of these vectors) by

$$N_i = g^{1/2} \varepsilon_{j_1 \ldots j_{n-1} i} e^{j_1}_{(1)} \cdots e^{j_{n-1}}_{(n-1)} \,. \tag{3.67}$$

We placed the label μ of the vectors $e^i_{(\mu)}$, which runs over $\mu = 1, \ldots, n-1$, in parenthesis in order not to confuse it with the vector index i which runs over $i = 1, \ldots, n$.

We consider $n \times (n-1)$ matrix $(e^i_{(\mu)})$ with n rows and $(n-1)$ columns. Let M_i be the $(n-1) \times (n-1)$ matrix obtained by deleting the i-th row in this matrix. Then

$$N_i = (-1)^{n-i} g^{1/2} \det M_i \,. \tag{3.68}$$

This vector is orthogonal to all vectors $e_{(1)}, \ldots, e_{(n-1)}$, that is,

$$N_i e^i_{(\mu)} = 0 \,, \qquad \mu = 1, \ldots, (n-1). \tag{3.69}$$

By using the properties of the Levi-Civita symbol one can also show that its norm

$$||N|| = \sqrt{g^{ij} N_i N_j} \tag{3.70}$$

is equal to the volume of the parallelepiped spanned by the vectors $e_{(1)}, \ldots, e_{(n-1)}$, that is,

$$||N|| = \sqrt{\det\,(A_{\mu\nu})}, \tag{3.71}$$

where

$$A_{\mu\nu} = (e_{(\mu)}, e_{(\nu)}) = g_{ij} e^i_{(\mu)} e^j_{(\nu)}. \tag{3.72}$$

is the $(n-1)\times(n-1)$ matrix of inner products of these vectors. Of course, if the vectors $e_{(1)}, \ldots, e_{(n-1)}$ are linearly dependent this volume vanishes and, therefore, $N_i = 0$.

3.1.11 Lie Derivative

Let v be a vector field on a manifold M and $\varphi_t : M \to M$ be the flow generated by v. *Lie derivative* with respect to the vector field v measures the rate of change of geometric objects, such as tensors, along the flow generated by v. It is defined as follows.

Lie derivative of a scalar function f is nothing but the directional derivative along the vector field v, that is,

$$L_v f = v^i \partial_i f \,. \tag{3.73}$$

Lie derivative of a vector field w with respect to the vector field v is the vector field $L_v w$ defined by

$$(L_v w)^i = v^j \partial_j w^i - w^j \partial_j v^i \,. \tag{3.74}$$

The expression

$$[v, w]^i = v^j \partial_j w^i - w^j \partial_j v^i \tag{3.75}$$

is called *Lie bracket* of the vector fields v and w; notice that it is anti-symmetric

$$[v, w] = -[w, v] \,. \tag{3.76}$$

Lie derivative of a 1-form α with respect to the vector field v is a 1-form $L_v\alpha$ defined by

$$(L_v \alpha)_i = v^j \partial_j \alpha_i + \alpha_j \partial_i v^j \,. \tag{3.77}$$

Lie derivative of a tensor field T of type (p, q) with respect to a vector field v is a tensor $L_v T$ of type (p, q) defined by

$$\begin{aligned}(L_v T)^{k_1\ldots k_p}_{i_1\ldots i_q} &= v^j \partial_j T^{k_1\ldots k_p}_{i_1\ldots i_q} + T^{k_1\ldots k_p}_{j i_2\ldots i_q} \partial_{i_1} v^j + \cdots + T^{k_1\ldots k_p}_{i_1\ldots i_{q-1} j} \partial_{i_q} v^j \\ &\quad - T^{j k_2\ldots k_p}_{i_1 i_2\ldots i_q} \partial_j v^{k_1} - \cdots - T^{k_1\ldots k_{p-1} j}_{i_1\ldots i_q} \partial_j v^{k_p} \,. \end{aligned} \tag{3.78}$$

If the Lie derivative of a tensor T with respect to a vector field v vanishes then the tensor T does not change along the flow of the vector field v; we say that the tensor T is *invariant* under the vector field v.

3.2 Connection

3.2.1 Covariant Derivative

As we have seen, local coordinates play only an auxiliary role in differential geometry. The choice of local coordinates is rather arbitrary. That is why, one of the main problems in developing analysis on manifolds is to construct a calculus which is invariant under the change of coordinates. This means that the usual partial derivatives (which are not invariant) have to be replaced by new derivative operators which transform covariantly under diffeomorphisms. Such operators are called *covariant derivatives*.

To define covariant derivatives of tensors we need a new object called *affine connection* $\Gamma^i{}_{jk}$. Then the covariant derivative of vector fields v^i and covector fields α_i is defined by

$$\nabla_j v^i = \partial_j v^i + \Gamma^i{}_{kj} v^k \,, \tag{3.79}$$

$$\nabla_j \alpha_i = \partial_j \alpha_i - \Gamma^k{}_{ij} \alpha_k \,. \tag{3.80}$$

More generally, the covariant derivative of a tensor field T of type (p, q) is defined by

$$\begin{aligned} \nabla_j T^{i_1 \dots i_p}_{k_1 \dots k_q} = \partial_j T^{i_1 \dots i_p}_{k_1 \dots k_q} + \Gamma^{i_1}{}_{mj} T^{m i_1 \dots i_p}_{k_1 \dots k_q} + \dots + \Gamma^{i_p}{}_{mj} T^{i_1 \dots i_{p-1} m}_{k_1 \dots k_q} \\ - \Gamma^m{}_{i_1 j} T^{i_1 \dots i_p}_{m k_2 \dots k_q} - \dots - \Gamma^m{}_{i_q j} T^{i_1 \dots i_p}_{k_1 \dots k_{q-1} m} \,. \end{aligned} \tag{3.81}$$

The covariant derivative is also denoted by a semi-colon, that is,

$$\nabla_i v^j = v^j{}_{;i} \,. \tag{3.82}$$

We should warn the reader that our notation differs slightly from the notation used in mathematical literature, where the quantity $\nabla_i v^j$ is often denoted by $(\nabla_{e_i} v)^j$, with $e_i = \partial_i$ being the coordinate basis in the tangent space.

Even though affine connection has one upper index and two lower indices it is not a $(1, 2)$ tensor! It does not transform as a tensor under diffeomorphisms. It is transformed rather in a very special way which guarantees that the covariant derivative of a tensor of type (p, q) is a tensor of type $(p, q + 1)$. However, the anti-symmetric part of the affine connection,

$$T^i{}_{jk} = \Gamma^i{}_{jk} - \Gamma^i{}_{kj} = 0, \tag{3.83}$$

defines a tensor of type $(1, 2)$ called the *torsion*. The affine connection is called *torsion-free* (or *symmetric*) if its torsion vanishes, that is,

$$\Gamma^i{}_{jk} - \Gamma^i{}_{kj} = 0 \,. \tag{3.84}$$

The connection is called *compatible* with the metric g_{ij} if the covariant derivative of the metric vanishes, that is,

$$\nabla_j g_{ik} = \partial_j g_{ik} - \Gamma^m{}_{ij} g_{mk} - \Gamma^m{}_{kj} g_{im} = 0\,. \tag{3.85}$$

An affine connection that is torsion-free and compatible with the metric is called *Levi-Civita connection*.

It is not difficult to show that each Riemannian manifold has a unique Levi-Civita connection given by so-called *Christoffel symbols*

$$\Gamma^i{}_{jk} = \frac{1}{2} g^{im} \left(\partial_j g_{mk} + \partial_k g_{jm} - \partial_m g_{jk}\right)\,. \tag{3.86}$$

There is a very useful formula for the contraction of the Christoffel symbols, which can be obtained as follows. By multiplying eq. (3.85) by g^{ik} and using the fact that g^{ik} is the inverse of the matrix g_{im}, we get

$$\Gamma^j{}_{ij} = \frac{1}{2} g^{jk} \partial_i g_{jk}\,. \tag{3.87}$$

By using eqs. (1.101) and (3.87) one can now express it in terms of the derivative of the determinant of the metric,

$$\Gamma^j{}_{ij} = \frac{1}{2} g^{-1} \partial_i g = g^{-1/2} \partial_i g^{1/2}\,. \tag{3.88}$$

This leads, in particular, to a very useful formula for the divergence of a vector field

$$\nabla_i K^i = g^{-1/2} \partial_i \left(g^{1/2} K^i\right)\,. \tag{3.89}$$

Now, one can also show that the Levi-Civita connection satisfies the usual rules of integration by parts. In particular, for any tensor fields that vanish (together with their derivatives) on the boundary of a manifold M there holds

$$\int\limits_M dx\, g^{1/2} A^i \nabla_i f = -\int_M dx\, g^{1/2} (\nabla_i A^i) f\,, \tag{3.90}$$

$$\int\limits_M dx\, g^{1/2} B^{ij} \nabla_i v_j = -\int_M dx\, g^{1/2} (\nabla_i B^{ij}) v_j\,. \tag{3.91}$$

3.2.2 Parallel Transport

Let T be a tensor field and v be a vector field on a manifold M. Then the *directional derivative* of the tensor field T along the vector field v is defined by

$$\nabla_v T = v^i \nabla_i T \,. \tag{3.92}$$

Let x and x' be two points on a manifold M and γ be a smooth curve connecting these points described locally by $x^i = x^i(\tau)$, where $\tau \in [0,t]$, so that $x(0) = x'$ and $x(t) = x$. We say that a tensor T is *parallel transported* along the curve γ (or, simply, *parallel* along γ) if it satisfies the linear differential equation along the curve γ

$$\dot{x}^i \nabla_i T = 0 \,. \tag{3.93}$$

In particular, for a vector field u^i the equation of parallel transport has the form

$$\dot{x}^i \nabla_i u^j = \dot{x}^i \partial_i u^j + \Gamma^j{}_{ik} \dot{x}^i u^k = 0 \,. \tag{3.94}$$

Now, by noting that

$$\dot{x}^i \partial_i = \frac{d}{d\tau} \tag{3.95}$$

we get the ordinary differential equation

$$\frac{du^j}{d\tau} = -A^j{}_k u^k \,. \tag{3.96}$$

where

$$A^j{}_k = \Gamma^j{}_{ik}(x(\tau)) \dot{x}^i \,. \tag{3.97}$$

The solution of this equation at the point x has the form

$$u_\gamma{}^i(x,x') = P_\gamma{}^i{}_j(x,x') u^j(x') \,, \tag{3.98}$$

where the matrix $P_\gamma = (P_\gamma{}^i{}_j)$ is defined by

$$P_\gamma = \exp\left(- \int_0^t d\tau \; A(\tau) \right) \,. \tag{3.99}$$

The matrix $P_\gamma(x,x')$ is called the *operator of parallel transport* of a vector field along the curve γ from the point x' to the point x.

One can easily compute the determinant of the matrix P_γ. By using eq. (1.95) we have

$$\log \det P_\gamma = - \int_0^t d\tau \;\; \mathrm{tr}\, A(\tau) \,. \tag{3.100}$$

Now, from the eqs. (3.88) and (3.97) we get

$$\mathrm{tr}\, A = \Gamma^j{}_{ij} \dot{x}^i = g^{-1/2} \dot{x}^i \partial_i g^{1/2} = \frac{d}{d\tau} \log \left[g^{1/2}(x(\tau)) \right] \,. \tag{3.101}$$

Therefore, we obtain

$$\log \det P_\gamma(x,x') = -\log \left[g^{1/2}(x(\tau))\right]\Big|_0^t = \log \frac{g^{1/2}(x')}{g^{1/2}(x)}\,. \tag{3.102}$$

Thus, finally

$$\det P_\gamma(x,x') = g^{-1/2}(x)g^{1/2}(x')\,. \tag{3.103}$$

It is easy to see that the operator of parallel transport satisfies the matrix differential equation

$$\dot{x}^i \nabla_i P_\gamma = 0 \tag{3.104}$$

with the initial condition

$$P_\gamma\big|_{t=0} = I\,, \tag{3.105}$$

where I is the unit matrix.

Note that the operator of parallel transport P_γ depends on the curve γ. Also, even though for $t = 0$ the matrix $P_\gamma(x,x')$ is equal to the unit matrix, $P_\gamma(x,x')|_{t=0} = I$, in general, the curve γ could be a closed curve such that $x = x(t) = x(0) = x'$ for $t \neq 0$; for such a curve the matrix $P_\gamma(x,x)$ for $x = x'$ is not equal to the unit matrix. This is different for a special class of curves called geodesics that we will discuss later.

The operators of parallel transport of tensor fields are defined similarly. For example, the equation of parallel transport of covectors has the form

$$\frac{du_j}{d\tau} = A^k{}_j u_k\,. \tag{3.106}$$

The solution of this equation at the point x has the form

$$u_{\gamma i}(x,x') = \tilde{P}_\gamma{}^j{}_i(x,x')u_j(x')\,, \tag{3.107}$$

where the matrix $\tilde{P}_\gamma = (\tilde{P}_\gamma{}^i{}_j)$ is defined by

$$\tilde{P}_\gamma = \exp\left(\int_0^t d\tau\ A(\tau)\right)\,. \tag{3.108}$$

Note that

$$\tilde{P}_\gamma = (P_\gamma)^{-1}\ . \tag{3.109}$$

By using the matrices P_γ and $\tilde{P}_\gamma$ one can define the parallel transport of an arbitrary tensor. For example, the parallel transport of a tensor $T^i{}_j$ of type $(1,1)$ is defined by

$$T_\gamma{}^i{}_k(x,x') = \tilde{P}_{\gamma k}{}^m(x,x')P_\gamma{}^i{}_j(x,x')T^j{}_m(x')\,. \tag{3.110}$$

Note that, in general, if the tensor field T is not parallel along the curve γ, then the value $T(x)$ of the tensor field T at the point x is different from the value $T_\gamma(x,x')$ obtained by the parallel transport along the curve γ from the point x' .

3.2.3 Geodesics

Let γ be a smooth curve on a manifold M described locally by $x^i = x^i(\tau)$, with $\tau \in [0, t]$. The curve γ is called a *geodesic* if the tangent vector $\dot{x}$ satisfies the equation

$$\dot{x}^j \nabla_j \dot{x}^i = f(\tau)\dot{x}^i, \tag{3.111}$$

with some function $f(\tau)$. The form of the function f does depend on the parametrization, in general. It is easy to show that given a geodesic γ there always exists a parametrization such that $f = 0$, that is, the tangent vector to the geodesic is transported parallel along γ,

$$\dot{x}^j \nabla_j \dot{x}^i = 0. \tag{3.112}$$

Such a parametrization is called *affine* and the parameter τ is called an *affine parameter*. In more detail, the coordinates of the geodesics $x^i(\tau)$ satisfy the non-linear second-order ordinary differential equation

$$\ddot{x}^i + \Gamma^i{}_{jk}\dot{x}^k\dot{x}^j = 0\,, \tag{3.113}$$

where $\Gamma^i{}_{jk} = \Gamma^i{}_{jk}(x(\tau))$ are evaluated along the geodesic.

A very important fact about the geodesics is that any two sufficiently close points, x and x', can be connected by a single geodesic. Another fact that is often used as a definition of the geodesic is that the geodesic is the *shortest curve* between the points x and x'. The distance between the points x and x' along the geodesics is called the *geodesic distance*. It is denoted simply by $d(x, x')$.

An immediate consequence of the definition of the geodesic is that the norm of the tangent vector $||\dot{x}||$ in affine parametrization is conserved along the geodesic; it is just a constant, which can be set to one by a reparametrization. This simply follows from the fact that the connection is compatible with the metric, that is, $\nabla_k g_{ij} = 0$, and the tangent vector is parallel along the geodesic, that is,

$$\dot{x}^k \nabla_k ||\dot{x}||^2 = 0\,. \tag{3.114}$$

Therefore, the length of the geodesic is

$$d(x, x') = t||\dot{x}||\,, \tag{3.115}$$

where $||\dot{x}||$ can be evaluated at any point along the geodesic.

3.3 Curvature

3.3.1 Riemann Tensor

Since the covariant derivatives are invariant differential operators, then the commutators of covariant derivatives are also invariant. It is not difficult to compute the commutator of covariant derivatives of a vector field to obtain

$$[\nabla_k, \nabla_l]v^i = R^i{}_{jkl}v^j\,, \tag{3.116}$$

where

$$R^i{}_{jkl} = \partial_k\Gamma^i{}_{jl} - \partial_l\Gamma^i{}_{jk} + \Gamma^i{}_{mk}\Gamma^m{}_{jl} - \Gamma^i{}_{ml}\Gamma^m{}_{jk}\,. \tag{3.117}$$

Since the left-hand side of this equation is a tensor, then the right hand side must also be a tensor. This means that the quantity $R^i{}_{jkl}$ is, in fact, a tensor of type $(1,3)$ called the *Riemann curvature tensor*.

Similarly, we have

$$[\nabla_i, \nabla_j]\alpha_k = -R^l{}_{kij}\alpha_l\,, \tag{3.118}$$

and, more generally,

$$[\nabla_i, \nabla_j]T^{j_1\cdots j_p}_{k_1\ldots k_q} = \sum_{m=1}^{p} R^{j_m}{}_{lij}T^{j_1\cdots j_{m-1}lj_{m+1}\cdots j_p}_{k_1\ldots k_q} - \sum_{n=1}^{q} R^l{}_{k_nij}T^{j_1\cdots j_p}_{k_1\ldots k_{n-1}lk_nk_q}\,. \tag{3.119}$$

These relations are called the *Ricci identities*.

As we noted above since Christoffel symbols are not a tensor they do not determine the extent to which a manifold is not just a Euclidean space. This is measured rather by the curvature tensor. We say that a manifold is *flat* if the curvature is equal to zero; otherwise, it is called *curved*.

3.3.2 Properties of Riemann Tensor

By using the definition of the Riemann tensor one can show that it has the following symmetry properties

$$R_{ijkl} = -R_{ijlk}\,, \tag{3.120}$$

$$R_{ijkl} = -R_{jikl}\,, \tag{3.121}$$

$$R_{ijkl} = R_{klij}\,, \tag{3.122}$$

where $R_{ijkl} = g_{im}R^m{}_{jkl}$. That is, it is anti-symmetric in the first two indices and in the last wo indices and is symmetric under the exchange of these pairs

of indices. Further, one can also show that it satisfies the identity

$$R^i{}_{jkl} + R^i{}_{klj} + R^i{}_{ljk} = 0\,. \tag{3.123}$$

The Riemann tensor defines the *sectional curvature* $K(u,v)$ in the plane spanned by two unit vectors u and v by

$$K(u,v) = R_{ijkl}u^i u^k v^j v^l\,. \tag{3.124}$$

By contraction of Riemann tensor one can define new tensors, the *Ricci tensor*

$$R_{ij} = R^k{}_{ikj} = g^{mk}R_{mikj}\,, \tag{3.125}$$

and the *scalar curvature*

$$R = g^{ij}R_{ij} = g^{ij}R^k{}_{ikj}\,. \tag{3.126}$$

It is not difficult to see that the Ricci tensor is symmetric,

$$R_{ij} = R_{ji}\,. \tag{3.127}$$

By using the symmetry properties of the Riemann tensor one can show that the number of algebraically independent components of Riemann tensor is equal to

$$N = \frac{n^2(n^2-1)}{12}\,. \tag{3.128}$$

In dimension $n = 2$ the Riemann tensor has only one independent component, that is, $N = 1$, determined by the scalar curvature

$$R^{ij}{}_{kl} = \frac{1}{2}R\left(\delta^i{}_k\delta^j{}_l - \delta^i{}_l\delta^j{}_k\right)\,, \tag{3.129}$$

so that

$$R_{ij} = \frac{1}{2}Rg_{ij}\,. \tag{3.130}$$

In dimension $n = 3$ the Riemann tensor has six independent components, that is, $N = 6$, determined by the Ricci tensor R_{ij},

$$\begin{aligned} R^{ij}{}_{kl} &= R^i{}_k\delta^j{}_l - R^i{}_l\delta^j{}_k + R^j{}_l\delta^i{}_k - R^j{}_k\delta^i{}_l \\ &\quad + \frac{1}{2}R\left(\delta^i{}_k\delta^j{}_l - \delta^i{}_l\delta^j{}_k\right)\,. \end{aligned} \tag{3.131}$$

By using the *Jacobi identity* for the commutators

$$[\nabla_i,[\nabla_j,\nabla_k] + [\nabla_j,[\nabla_k,\nabla_i] + [\nabla_k,[\nabla_i,\nabla_j] = 0 \tag{3.132}$$

one can show that the Riemann tensor satisfies the following differential identities

$$\nabla_m R^{ij}{}_{kl} + \nabla_k R^{ij}{}_{lm} + \nabla_l R^{ij}{}_{mk} = 0\,, \tag{3.133}$$

called *Bianchi identities*. By contraction of these identities we obtain further

$$\nabla_i R^{ij}{}_{kl} = \nabla_k R^j{}_l - \nabla_l R^j{}_k\,, \tag{3.134}$$

and, further,

$$\nabla_i R^i{}_j = \frac{1}{2}\nabla_j R\,. \tag{3.135}$$

Finally, for $n > 2$ one can define the *Weyl tensor*

$$C^{ij}{}_{kl} = R^{ij}{}_{kl} - \frac{4}{n-2} R^{[i}{}_{[k}\delta^{j]}{}_{l]} + \frac{2}{(n-1)(n-2)} R\delta^{[i}{}_{[k}\delta^{j]}{}_{l]}\,. \tag{3.136}$$

Here and everywhere below the square brackets mean the anti-symmetrization over the indices included, for example,

$$A_{[ij]} = \frac{1}{2}\left(A_{ij} - A_{ji}\right)\,. \tag{3.137}$$

The Weyl tensor has the same symmetry properties as the Riemann tensor and all its contractions vanish, that is,

$$C^i{}_{jik} = 0\,. \tag{3.138}$$

The Weyl tensor measures the anisotropy of the metric in the following sense. If the Weyl tensor is equal to zero, then there exist local coordinates and a scalar function $\omega(x)$ such that the metric has the form

$$g_{ij}(x) = e^{\omega(x)}\delta_{ij}\,. \tag{3.139}$$

Such metrics are called *conformally flat*.

A Riemannian manifold M is called a *symmetric space* if (in addition to some global topological conditions) the curvature is covariantly constant, that is,

$$\nabla_j R^i{}_{klm} = 0\,. \tag{3.140}$$

This equation leads to profound algebraical consequences that enable one to find the heat kernel on symmetric spaces. This will be studied in a later chapter.

3.4 Geometry of Two-dimensional Manifolds

3.4.1 Gauss Curvature

Let us specify the above machinery for two-dimensional manifolds, $n = \dim M = 2$. In this case the tensor indices run only over two values, 1 and 2. The curvature tensor has just one independent component, K, called the *Gauss curvature*. It is defined as follows. Because of the symmetries of the curvature tensor it can only have the form

$$R^{ij}{}_{kl} = K\left(\delta^i{}_k\delta^j{}_l - \delta^i{}_l\delta^j{}_k\right)\,, \tag{3.141}$$

where K is a scalar function. The Ricci tensor and the scalar curvature are then

$$R^i{}_j = K\delta^i{}_j\,, \tag{3.142}$$

$$R = 2K\,. \tag{3.143}$$

That is, Gauss curvature is just one half of the scalar curvature, and the only independent non-zero components of the Riemann tensor and the Ricci tensor are

$$R^{12}{}_{12} = R^1{}_1 = R^2{}_2 = K\,. \tag{3.144}$$

We give below explicit formulas for Gauss curvature in various coordinate systems.

Let us consider first a coordinate system such that the metric is given by

$$ds^2 = A^2(dx^1)^2 + B^2(dx^2)^2\,, \tag{3.145}$$

where A and B are some functions of x^1 and x^2. Such coordinate system is called *orthogonal*.

The components of the metric are

$$g_{11} = A^2, \qquad g_{22} = B^2, \qquad g_{12} = 0\,. \tag{3.146}$$

First, we compute the components of the inverse metric

$$g^{11} = \frac{1}{A^2}, \qquad g^{22} = \frac{1}{B^2}, \qquad g^{12} = 0\,. \tag{3.147}$$

Next, we compute Christoffel symbols; we obtain

$$\Gamma^1{}_{11} = \frac{\partial_1 A}{A}\,, \tag{3.148}$$

$$\Gamma^1{}_{12} = \frac{\partial_2 A}{A}\,, \tag{3.149}$$

$$\Gamma^1{}_{22} = -\frac{B\partial_1 B}{A^2}\,, \tag{3.150}$$

$$\Gamma^2{}_{11} = -\frac{A\partial_2 A}{B^2}\,, \tag{3.151}$$

$$\Gamma^2{}_{12} = \frac{\partial_1 B}{B}\,, \tag{3.152}$$

$$\Gamma^2{}_{22} = \frac{\partial_2 B}{B}\,, \tag{3.153}$$

where, as usual, $\partial_i = \partial/\partial x^i$. Recall that Christoffel coefficients are symmetric in low indices, so $\Gamma^i{}_{12} = \Gamma^i{}_{21}$.

The only non-zero component of the curvature is given by

$$\begin{aligned} R^1{}_{212} = {} & \partial_1 \Gamma^1{}_{22} - \partial_2 \Gamma^1{}_{21} \\ & + \Gamma^1{}_{11}\Gamma^1{}_{22} - \Gamma^1{}_{12}\Gamma^1{}_{21} + \Gamma^1{}_{21}\Gamma^2{}_{22} - \Gamma^1{}_{22}\Gamma^2{}_{21}\,. \end{aligned} \tag{3.154}$$

By using the Christoffel coefficients we compute

$$R^1{}_{212} = -\frac{B}{A^2}\partial_1^2 B - \frac{1}{A}\partial_2^2 A + \frac{B}{A^3}(\partial_1 A)(\partial_1 B) + \frac{1}{AB}(\partial_2 A)(\partial_2 B)\,. \tag{3.155}$$

Finally, by raising the second index

$$R^{12}{}_{12} = \frac{1}{B^2} R^1{}_{212}\,, \tag{3.156}$$

we get the Gauss curvature which can be written in a slightly more compact symmetric form

$$K = -\frac{1}{AB}\left\{\partial_1\left(\frac{1}{A}\partial_1 B\right) + \partial_2\left(\frac{1}{B}\partial_2 A\right)\right\}\,. \tag{3.157}$$

One can show that every two-dimensional manifold is conformally flat, that is, there always exists a coordinate system in which the metric has the form

$$ds^2 = e^{2\omega}\left(dx^2 + dy^2\right)\,, \tag{3.158}$$

where ω is a function of x and y; such coordinate system is called *conformal*. In this case $A = B = e^{\omega}$, therefore, Christoffel symbols take the form

$$\Gamma^1{}_{11} = \Gamma^2{}_{12} = -\Gamma^1{}_{22} = \partial_1\omega\,, \tag{3.159}$$

$$\Gamma^2{}_{22} = \Gamma^1{}_{12} = -\Gamma^2{}_{11} = \partial_2\omega\,, \tag{3.160}$$

and the Gauss curvature is

$$K = -e^{-2\omega}\left(\partial_x^2 + \partial_y^2\right)\omega\,. \tag{3.161}$$

In the so-called *geodesic polar coordinates* the metric has the form

$$ds^2 = dr^2 + f^2\,d\theta^2\,, \tag{3.162}$$

where f is some function of r and θ. In these coordinates $A = 1$ and $B = f$, so the above formula for the Gauss curvature gives

$$K = -\frac{1}{f}\partial_r^2 f\,. \tag{3.163}$$

3.4.2 Two-dimensional Constant Curvature Manifolds

A very important class of manifolds consists of manifolds with constant curvature. In dimension two there are just three types of such manifolds, the *sphere*, S^2, with positive constant curvature, $K > 0$, the *hyperbolic plane*, H^2, (also called *pseudo-sphere*) with negative constant curvature, $K < 0$, and the Euclidean space $\mathbb{R}^2$ with $K = 0$. The positive real number

$$a = \frac{1}{\sqrt{|K|}} \tag{3.164}$$

is called the *radius* of the sphere for $K > 0$ and the *pseudo-radius* of the hyperbolic plane H^2 for $K < 0$. Of course, formally the Euclidean space $\mathbb{R}^2$ corresponds to the limit $a \to \infty$.

Let

$$\omega = -\log\left[1 - \frac{K}{4}(x^2 + y^2)\right]\,. \tag{3.165}$$

Then it is easy to compute

$$\left(\partial_x^2 + \partial_y^2\right)\omega = -Ke^{2\omega}\,. \tag{3.166}$$

Therefore, all manifolds of constant curvature can be described in conformal coordinates by the metric (3.158)

$$ds^2 = \frac{dx^2 + dy^2}{\left[1 + \frac{K}{4}(x^2 + y^2)\right]^2}\,. \tag{3.167}$$

Here, in the case $K > 0$ or $K = 0$ the coordinates x, y range over the whole plane, $-\infty < x, y < \infty$, while in the case $K < 0$ they range over the disk

$$x^2 + y^2 < 4a^2 \,. \tag{3.168}$$

For $K < 0$ this metric is called the *Poincaré disk model* of the hyperbolic plane.

By introducing polar coordinates

$$x = \rho \cos\theta \,, \qquad y = \rho \sin\theta \,, \tag{3.169}$$

where $0 \leq \theta < 2\pi$, this metric takes in the form

$$ds^2 = \frac{d\rho^2 + \rho^2 d\theta^2}{\left(1 + \dfrac{K}{4}\rho^2\right)^2} \,. \tag{3.170}$$

Here the radial coordinate ρ ranges over $0 \leq \rho < \infty$ for $K \geq 0$ and over $0 \leq \rho < 2a$ for $K < 0$.

Notice that for both S^2 and H^2 in the limit of large radius, $a \to \infty$, the curvature vanishes and the metric approaches the standard Euclidean metric

$$ds^2 = dx^2 + dy^2 \,, \tag{3.171}$$

or in polar coordinates

$$ds^2 = d\rho^2 + \rho^2 d\theta^2 \,. \tag{3.172}$$

The sphere S^2 can also be described in geodesic polar coordinates by the metric

$$ds^2 = dr^2 + a^2 \sin^2\left(\frac{r}{a}\right) d\theta^2 \,, \tag{3.173}$$

where r is defined by

$$r = 2a \cot^{-1}\left(\frac{\rho}{2a}\right) \,; \tag{3.174}$$

then r ranges over $0 \leq r \leq a\pi$.

The hyperbolic plane H^2 can be described in geodesic polar coordinates by the metric (called the *Lobachevsky metric*)

$$ds^2 = dr^2 + a^2 \sinh^2\left(\frac{r}{a}\right) d\theta^2 \,, \tag{3.175}$$

where r is defined by

$$\begin{aligned} r &= 2a \tanh^{-1}\left(\frac{\rho}{2a}\right) \\ &= a \log \frac{2a + \rho}{2a - \rho} \,, \end{aligned} \tag{3.176}$$

so that r ranges over $0 \leq r < \infty$.

Notice the *duality* between the sphere and the hyperbolic plane. The expressions for the metric for the hyperbolic plane can be obtained by those for the sphere by the formal transformation $a \mapsto ia$.

Another popular model for the hyperbolic plane is the so-called *Poincaré upper half-plane model* with the metric

$$ds^2 = a^2 \frac{du^2 + dv^2}{v^2}\,. \tag{3.177}$$

where

$$u = \frac{4ay}{(x+2a)^2 + y^2}\,, \tag{3.178}$$

$$v = \frac{4a^2 - x^2 - y^2}{(x+2a)^2 + y^2}\,, \tag{3.179}$$

so that $-\infty < u < \infty$ and $0 \leq v < \infty$.

This metric also has locally conformal form (3.161) with $\omega = -\log(v/a)$. By using eq. (3.161) it is easy to see that indeed $K = -e^{-2\omega}\partial_v^2 w = -1/a^2$. Next, the Christoffel coefficients are

$$\Gamma^1{}_{11} = \Gamma^2{}_{12} = \Gamma^1{}_{22} = 0\,, \tag{3.180}$$

$$\Gamma^2{}_{22} = \Gamma^1{}_{12} = -\Gamma^2{}_{11} = -\frac{1}{v}\,. \tag{3.181}$$

By using the eqs. (3.180) and (3.181) we get the equations of geodesics

$$\ddot{u} - \frac{2}{v}\dot{u}\dot{v} = 0 \tag{3.182}$$

$$\ddot{v} + \frac{1}{v}\dot{u}^2 - \frac{1}{v}\dot{v}^2 = 0\,. \tag{3.183}$$

First of all, by multiplying eq. (3.182) by $\dot{u}$ and eq. (3.183) by $\dot{v}$ and summing these equations we get

$$\dot{u}\ddot{u} + \dot{v}\ddot{v} - \frac{1}{v}(\dot{u}^2 + \dot{v}^2) = \frac{v^2}{2}\frac{d}{dt}\left[\frac{1}{v^2}(\dot{u}^2 + \dot{v}^2)\right] = 0, \tag{3.184}$$

which means that

$$\frac{1}{v^2}(\dot{u}^2 + \dot{v}^2) = \frac{1}{a^2}\,. \tag{3.185}$$

Here the integration constant has been chosen so that the norm of the tangent vector is equal to $||\dot{x}|| = 1$; such parametrization is called *natural*. Recall that in this parametrization the parameter t is the arc length of the geodesic.

Next, from eq. (3.182) we get

$$\dot{u} = c_1 v^2 \,, \tag{3.186}$$

where c_1 is an integration constant. If $c_1 = 0$ then $\dot{u} = 0$ and, therefore, $u = u_0$, where u_0 is a constant. Then eq. (3.183) can be easily integrated to give $\dot{v} = c_3 v$. By using eq. (3.185) we find that $c_3^2 = 1/a^2$, so $c_3 = \pm 1/a$. The sign $\pm$ here corresponds to the direction of time, so we choose it so that $\dot{v} > 0$. Therefore,

$$v = a e^{t/a}. \tag{3.187}$$

This is nothing but a vertical line in the plane

$$u = u_0, \qquad v = a e^{t/a} \,, \tag{3.188}$$

Now, assume that $c_1 \neq 0$. Then assuming $\dot{u} > 0$ one can restrict to $c_1 > 0$. Moreover, we define a new parameter $c = 1/(ac_1)$. Then, by substituting (3.186) into (3.185) we get

$$\dot{v} = \pm \frac{1}{ac} v \sqrt{c^2 - v^2} \,. \tag{3.189}$$

This equation can be easily integrated

$$v = \frac{c}{\cosh\,(t/a)} \,, \tag{3.190}$$

where the integration constant has been chosen to satisfy the initial condition $v(0) = c$; the parameter t ranges over $-\infty < t < \infty$. Now, one can integrate eqs. (3.186) to get finally

$$u = b + c \tanh\,(t/a) \,, \tag{3.191}$$

where b is an integration constant. By rewriting this equation in the non-parametrized form

$$(u - b)^2 + v^2 = c^2 \,, \tag{3.192}$$

we see that the geodesics are nothing but semicircles centered on the real line (u-axis).

Given any two points $x = (u, v)$ and $x' = (u', v')$ in the hyperbolic plane H^2 there is only one geodesic joining them, that is the parameters b and c are determined by the coordinates (u, v) and (u', v')

$$b = \frac{1}{2} \left\{ u + u' + \frac{v^2 - v'^2}{u - u'} \right\} \,, \tag{3.193}$$

$$c = \frac{1}{2} \left\{ (u - u')^2 + 2v^2 + 2v'^2 + \frac{(v^2 - v'^2)^2}{(u - u')^2} \right\}^{1/2} \,. \tag{3.194}$$

Now let

$$h = 1 + \frac{(u-u')^2 + (v-v')^2}{2vv'} \,. \tag{3.195}$$

Then, by using the above formulas for the geodesics one can show that

$$h = \cosh(t-t') \,. \tag{3.196}$$

Recall that t is the natural parameter; therefore, the geodesic distance between the points $x = x(t)$ and $x' = x(t')$ is equal to $d(x,x') = t - t'$ and is given by

$$\begin{aligned} d(x,x') &= a \cosh^{-1} h \\ &= a \log\left(h + \sqrt{h^2-1}\right) \,. \end{aligned} \tag{3.197}$$

3.5 Killing Vectors

The Lie derivative of the metric tensor g_{ij} along a vector field ξ is

$$\begin{aligned} (L_\xi g)_{ij} &= \xi^k \partial_k g_{ij} + g_{ik}\partial_j \xi^k + g_{kj}\partial_i \xi^k \\ &= \nabla_i \xi_j + \nabla_j \xi_i \,. \end{aligned} \tag{3.198}$$

If the metric remains invariant under the flow generated by the vector field ξ, then the vector field ξ is called a *Killing vector field* and its flow is called an *isometry*. In other words, given a metric g_{ij} Killing vector fields ξ^i are solutions of the linear first-order partial differential equations

$$\nabla_i \xi_j + \nabla_j \xi_i = 0 \,. \tag{3.199}$$

The existence of Killing vector fields indicates some symmetries of the metric. The more symmetric the metric is the more Killing vectors it has. For a given dimension n the maximal number of linearly independent Killing vectors is $n(n+1)/2$. The metrics that posses that many symmetries are called *maximally symmetric spaces*. As an example, the manifolds $\mathbb{R}^n$, S^n and H^n are all maximally symmetric spaces.

By using this equation it is not difficult to compute higher derivatives of Killing vectors. First of all, we immediately see that

$$\nabla_i \xi^i = 0 \,. \tag{3.200}$$

Also, by differentiating eq. (3.199) and commuting derivatives we obtain

$$\nabla_k \nabla_i \xi_j + \nabla_j \nabla_k \xi_i = R^l{}_{ikj} \xi_l \,. \tag{3.201}$$

Now, by symmetrizing over the indices i, k, and using the eq. (3.199) we get

$$(\nabla_k\nabla_i + \nabla_i\nabla_k)\,\xi_j = (R^l{}_{ikj} + R^l{}_{kij})\xi_l\,. \tag{3.202}$$

By combining this equation with the commutator

$$(\nabla_k\nabla_i - \nabla_i\nabla_k)\,\xi_j = -R^l{}_{jki}\xi_l\,, \tag{3.203}$$

and using the curvature identity (3.123) we obtain

$$\nabla_k\nabla_i\xi^j = -R^j{}_{ilk}\xi^l\,, \tag{3.204}$$

in particular, this means

$$\Delta\xi^j = -R^j{}_l\xi^l\,, \tag{3.205}$$

where Δ is the Laplacian

$$\Delta = g^{ij}\nabla_i\nabla_j\,. \tag{3.206}$$

By using the eq. (3.199) it is not difficult to show that every Killing vector ξ commutes with the Laplacian, that is,

$$[\xi, \Delta] = 0\,. \tag{3.207}$$

3.6 Synge Function

3.6.1 Definition and Basic Properties

In this section we follow our papers [4, 10]. For more details the reader is advised to consult these papers. Let x' be a fixed point in a manifold M. Then there is a sufficiently small neighborhood of x' such that each point x in this neighborhood can be connected with the point x' by a single geodesic $x = x(\tau)$, with an affine parameter $\tau \in [0, t]$ so that $x(0) = x'$ and $x(t) = x$ and the tangent vector $\dot{x}(\tau)$. In the following we denote indices of tensors in the tangent space at the point x' by prime Latin letters. The derivatives with respect to coordinates x'^i will be denoted by prime indices as well. Finally, the prime indices are raised and lowered by the metric $g_{i'j'}(x')$ at the point x'. This should not cause any confusion.

The *Synge function* is defined as half of the square of the geodesic distance [73, 26]

$$\sigma(x, x') = \frac{1}{2}d^2(x, x')\,. \tag{3.208}$$

It can also be written in the form

$$\sigma(x, x') = \frac{1}{2}t\int_0^t d\tau\, g_{ij}\dot{x}^i\dot{x}^j\,, \tag{3.209}$$

where all functions in the integrand are evaluated at the point τ. The Synge function is a first example of the so-called *two-point geometric objects*. More precisely, it is a *bi-scalar* function that behaves like a scalar at both points x and x'. This function is a very powerful tool in Riemannian geometry that completely determines the local geometry of the manifold.

We will only consider sufficiently small regions in the manifold. Then all two-points functions will be single-valued smooth functions of the coordinates of the points x and x' whose derivatives have well-defined limits as $x \to x'$. We will call the limit as $x \to x'$ the *coincidence limit* and denote it simply by square brackets, that is,

$$[f(x,x')] = \lim_{x\to x'} f(x,x')\,. \tag{3.210}$$

The value of a two-point quantity in the coincident limit will be also called the *diagonal value* (or simply the *diagonal*). In particular, it is clear that the coincidence limit of the Synge function itself vanishes,

$$[\sigma] = 0\,. \tag{3.211}$$

Alternatively, we can define the Synge function as the solution of certain differential equation with some initial conditions. To derive this equation we need to compute the derivatives of the function σ. To compute the derivative $\nabla_i\sigma$ of the function $\sigma(x,x')$ with respect to x we fix the point x' and let the point x depend on a parameter ε, that is, we consider a one-parameter family of geodesics $x^i = x^i(\tau,\varepsilon)$ such that the initial point $x^i(0,\varepsilon) = x^{i\prime}$ is fixed. Let us denote

$$h^i(\tau) = \frac{\partial x^i(\tau,\varepsilon)}{\partial\varepsilon}\Big|_{\varepsilon=0}\,. \tag{3.212}$$

Since the point x' is fixed, we have

$$h^i(0) = 0\,. \tag{3.213}$$

Then we will compute $\nabla_i\sigma$ by evaluating

$$\frac{\partial\sigma}{\partial\varepsilon}\Big|_{\varepsilon=0} = h^i(t)\nabla_i\sigma\,. \tag{3.214}$$

Now, substituting this into the equation (3.209) we get

$$\begin{aligned}\frac{\partial\sigma}{\partial\varepsilon}\Big|_{\varepsilon=0} &= \frac{1}{2}t\int_0^t d\tau\left[2g_{ij}\dot{x}^i\frac{\partial\dot{x}^j}{\partial\varepsilon} + \frac{\partial g_{ij}}{\partial\varepsilon}\dot{x}^i\dot{x}^j\right]_{\varepsilon=0}\\ &= \frac{1}{2}t\int_0^t d\tau\left[2g_{ij}\dot{x}^i\frac{dh^j}{d\tau} + h^k\partial_k g_{ij}\dot{x}^i\dot{x}^j\right]_{\varepsilon=0}\,.\end{aligned} \tag{3.215}$$

Next, by integrating by parts in the first term we get

$$\frac{\partial\sigma}{\partial\varepsilon}\Big|_{\varepsilon=0} = t\left[g_{ij}\dot{x}^i h^j\Big|_0^t\right]_{\varepsilon=0} \tag{3.216}$$
$$+t\int_0^t d\tau\left[-g_{ij}\ddot{x}^i h^j - \partial_k g_{ij}\dot{x}^k\dot{x}^i h^j + \frac{1}{2}\partial_k g_{ij}\dot{x}^i\dot{x}^j h^k\right]_{\varepsilon=0},$$

which can be written in the form

$$\frac{\partial\sigma}{\partial\varepsilon}\Big|_{\varepsilon=0} = t\left[g_{ij}\dot{x}^i h^j\Big|_0^t\right]_{\varepsilon=0} - t\int_0^t d\tau\left[\ddot{x}^i + \Gamma^i{}_{lj}\dot{x}^l\dot{x}^j\right]g_{ik}h^k\Big|_{\varepsilon=0}.$$

Now, since $x = x(\tau,\varepsilon)$ is a geodesic, the second term vanishes, and by recalling that $h^j(0) = 0$ we are left with

$$\frac{\partial\sigma}{\partial\varepsilon}\Big|_{\varepsilon=0} = t g_{ij}(x)\dot{x}^i(t)h^j(t)\,, \tag{3.217}$$

which means that

$$\nabla_j\sigma = t g_{ij}(x)\dot{x}^i(t)\,. \tag{3.218}$$

Similarly, one can obtain the derivative of σ with respect to x',

$$\nabla_{j'}\sigma = -t g_{i'j'}(x')\dot{x}^i(0)\,. \tag{3.219}$$

Thus the first derivatives of the Synge function are proportional to the tangent vectors to the geodesic at the points x and x' respectively pointing in the opposite directions. The norm of these tangent vectors is the same and is equal to the length of the geodesic (that is, the geodesic distance)

$$g^{ij}(\nabla_i\sigma)(\nabla_j\sigma) = g^{i'j'}(\nabla_{i'}\sigma)(\nabla_{j'}\sigma) = t^2||\dot{x}||^2 = d^2\,. \tag{3.220}$$

This means that the coincidence limits of the first derivatives also vanish

$$[\nabla_i\sigma] = [\nabla_{i'}\sigma] = 0\,. \tag{3.221}$$

In other words, the Synge function satisfies the first-order differential equations

$$\sigma = \frac{1}{2}g^{ij}(\nabla_i\sigma)(\nabla_j\sigma), \tag{3.222}$$

$$\sigma = \frac{1}{2}g^{i'j'}(\nabla_{i'}\sigma)(\nabla_{j'}\sigma)\,, \tag{3.223}$$

with the initial conditions (3.221). These equations are also called "eiconal" equations.

3.6.2 Derivatives of Synge Function

We will use the notation for the covariant derivatives of the Synge function with respect to x and x', following [73], by just adding indices to σ, for example,

$$\sigma_i = \nabla_i \sigma \,, \tag{3.224}$$

$$\sigma_{i'} = \nabla_{i'} \sigma \,, \tag{3.225}$$

$$\sigma_{ij} = \nabla_j \nabla_i \sigma \,, \tag{3.226}$$

$$\sigma_{j'i} = \nabla_i \nabla_{j'} \sigma \,, \tag{3.227}$$

$$\sigma_{j'ik} = \nabla_k \nabla_i \nabla_{j'} \sigma \,. \tag{3.228}$$

With this notation the vectors

$$\frac{\sigma^i}{\sqrt{2\sigma}} \,, \qquad \frac{\sigma^{i'}}{\sqrt{2\sigma}} \tag{3.229}$$

are the unit tangent vectors to the geodesic at the points x and x' pointing in opposite directions.

Note that the derivatives with respect to x always commute with derivatives with respect to x', that is,

$$\nabla_i \nabla_{j'} = \nabla_{j'} \nabla_i \,. \tag{3.230}$$

Also, since σ is a scalar, the first two derivatives of σ always commute, that is,

$$\sigma_{ij} = \sigma_{ji} \,, \qquad \sigma_{ij'} = \sigma_{j'i} \,. \tag{3.231}$$

Let us also introduce a first order differential operator that will be extensively used below

$$D = \sigma^i \nabla_i \,. \tag{3.232}$$

It is clear that it is nothing but the derivative along the geodesic connecting the points x and x'. Then the equation (3.222) takes the form

$$D\sigma = 2\sigma \,. \tag{3.233}$$

By differentiating the equations (3.222) and (3.223) one can get new useful equations,

$$\sigma_j = \sigma_{ji} \sigma^i \,, \tag{3.234}$$

$$\sigma_{j'} = \sigma_{j'i} \sigma^i \,. \tag{3.235}$$

By taking the coincidence limit in this equations we see that the coincidence limit of the second derivatives are determined by the metric

$$[\sigma_{ij}] = g_{ij}\,, \tag{3.236}$$

$$[\sigma_{i'j'}] = g_{ij}\,, \tag{3.237}$$

$$[\sigma_{i'j}] = -g_{ij}\,. \tag{3.238}$$

The negative sign for the mixed derivatives comes from the fact that the vectors σ_i and $\sigma_{i'}$ point in opposite directions (see eqs. (3.218) and (3.219)).

By using the operator D these equations can be rewritten in the form

$$D\sigma^i = \sigma^i\,, \tag{3.239}$$

$$D\sigma^{j'} = \sigma^{j'}\,. \tag{3.240}$$

Let us define the matrices $\xi = (\xi^i{}_j)$ and $\eta = (\eta^{i'}{}_j)$ by

$$\xi^i{}_j = \sigma^i{}_j\,, \tag{3.241}$$

$$\eta^{i'}{}_j = \sigma^{i'}{}_j\,. \tag{3.242}$$

Then, the above equations take the form

$$\xi^i{}_j\sigma^j = \sigma^i\,, \tag{3.243}$$

$$\sigma_i\xi^i{}_j = \sigma_j\,, \tag{3.244}$$

$$\eta^{i'}{}_j\sigma^j = \sigma^{i'}\,, \tag{3.245}$$

$$\sigma_{i'}\eta^{i'}{}_j = \sigma_j\,. \tag{3.246}$$

It is also easy to see from the definition of the matrix η that it satisfies the equation

$$\nabla_k\eta^{i'}{}_j = \nabla_j\eta^{i'}{}_k\,. \tag{3.247}$$

Now, by differentiating the equations (3.234) and (3.235) we get further important equations

$$\sigma_{jk} = \sigma_{jik}\sigma^i + \sigma_{ji}\sigma^i{}_k\,, \tag{3.248}$$

$$\sigma_{j'k} = \sigma_{j'ik}\sigma^i + \sigma_{j'i}\sigma^i{}_k\,. \tag{3.249}$$

Note that

$$\sigma_{j'ik} = \sigma_{j'ki}\,. \tag{3.250}$$

Also, by commuting covariant derivatives we have

$$\begin{aligned}\sigma_{jik} &= \nabla_k\nabla_i\sigma_j = \nabla_i\nabla_k\sigma_j - R^m{}_{jki}\sigma_m \\ &= \sigma_{jki} - R^m{}_{jki}\sigma_m\,.\end{aligned} \tag{3.251}$$

Therefore, the last two equations above, (3.248) and (3.249), can be written in the form

$$\sigma^i \nabla_i \sigma^j{}_k + R^j{}_{ikm} \sigma^i \sigma^m + \sigma^j{}_i \sigma^i{}_k - \sigma^j{}_k = 0\,, \tag{3.252}$$

$$\sigma^i \nabla_i \sigma^{j'}{}_k + \sigma^{j'}{}_i \sigma^i{}_k - \sigma^{j'}{}_k = 0\,. \tag{3.253}$$

Now, let us define another matrix $K = (K^i{}_j)$ (do not confuse this matrix with the Gaussian curvature!) by

$$K^i{}_j = R^i{}_{kjl} \sigma^k \sigma^l\,. \tag{3.254}$$

Then from the equations (3.252) and (3.253) we get the following equations for the matrices ξ and η

$$D\xi + \xi(\xi - I) + K = 0\,, \tag{3.255}$$

$$D\eta + \eta(\xi - I) = 0\,, \tag{3.256}$$

where $I = (\delta^i{}_j)$ is the unit matrix.

One can easily show that the coincidence limits of third derivatives of the Synge function vanish, that is,

$$[\sigma_{ijk}] = [\sigma_{i'jk}] = 0\,. \tag{3.257}$$

Therefore, the initial conditions for the matrices ξ and η are

$$[\xi] = I\,, \qquad [\nabla_i \xi] = 0\,, \tag{3.258}$$

$$[\eta] = -I\,, \qquad [\nabla_i \eta] = 0\,. \tag{3.259}$$

Finally, we introduce the inverse of the matrix η,

$$\gamma = \eta^{-1}\,, \tag{3.260}$$

so that it satisfies the equations

$$\gamma^i{}_{j'} \eta^{j'}{}_k = \delta^i{}_k\,, \tag{3.261}$$

$$\eta^{j'}{}_i \gamma^i{}_{k'} = \delta^{j'}{}_{k'}\,. \tag{3.262}$$

By using the definition of the matrix γ as the inverse of the matrix η and the equation (3.247) one can show that it satisfies the equation

$$\gamma^k{}_{l'} \nabla_k \gamma^i{}_{j'} = \gamma^k{}_{j'} \nabla_k \gamma^i{}_{l'}\,. \tag{3.263}$$

Then it is easy to show that it satisfies also the equations

$$\gamma^{i}{}_{j'}\sigma^{j'} = \sigma^{i}\,, \tag{3.264}$$

$$\gamma^{i}{}_{j'}\sigma_{i} = \sigma_{j'}\,. \tag{3.265}$$

Moreover, one can obtain a second-order equation for the matrix γ only. First, we express the matrix ξ in terms of the matrix γ from eq. (3.256)

$$\xi = I - \gamma D\eta\,. \tag{3.266}$$

Now, since $\eta = \gamma^{-1}$ we get

$$D\eta = -\eta(D\gamma)\eta\,, \tag{3.267}$$

and, therefore,

$$\xi = I + (D\gamma)\eta\,. \tag{3.268}$$

Then by substituting this equation into eq. (3.255) we obtain the following equation for the matrix γ

$$\left(D^2 + D + K\right)\gamma = 0\,. \tag{3.269}$$

The initial condition for the matrix γ is

$$[\gamma] = -I\,, \qquad [\nabla_i\gamma] = 0\,. \tag{3.270}$$

It is this equation that is the most important ingredient in our approach. It is the most convenient basis to find all of two-point quantities since all those quantities are expressible in terms of γ. We will see below that since this equation is linear it has a unique solution which is easy to find in form of a covariant Taylor series. Moreover, this equation can be solved exactly in symmetric spaces when the curvature tensor is covariantly constant.

We will need below the following rule for commuting the operators D and $\gamma^{j'}{}_{k}\nabla_j$

$$\gamma^{j}{}_{k'}\nabla_j D = (D+I)\gamma^{j}{}_{k'}\nabla_j + \gamma^{j}{}_{k'}\sigma^{i}[\nabla_j, \nabla_i]\,. \tag{3.271}$$

Indeed, we compute

$$\begin{aligned}
\gamma^{j}{}_{k'}\nabla_j D &= \gamma^{j}{}_{k'}\sigma^{i}\nabla_j\nabla_i + \gamma^{j}{}_{k'}\sigma^{i}{}_{j}\nabla_i \\
&= \gamma^{j}{}_{k'}D\nabla_j + \gamma^{j}{}_{k'}\sigma^{i}[\nabla_j, \nabla_i] + \gamma^{j}{}_{k'}\sigma^{i}{}_{j}\nabla_i \\
&= \left(D\gamma^{j}{}_{k'} + \xi^{j}{}_{i}\gamma^{i}{}_{k'} - (D\gamma^{j}{}_{k'})\right)\nabla_j + \gamma^{j}{}_{k'}\sigma^{i}[\nabla_j, \nabla_i] \\
&= (D+I)\gamma^{j}{}_{k'}\nabla_j + \gamma^{j}{}_{k'}\sigma^{i}[\nabla_j, \nabla_i]\,.
\end{aligned} \tag{3.272}$$

Here in the last equation we used the equation (3.268).

3.6.3 Van Vleck-Morette Determinant

Next, we define a two-point quantity $\Delta(x, x')$ called *Van Vleck-Morette determinant*

$$\Delta(x, x') = g^{-1/2}(x) \det\, (-\sigma_{ij'}(x, x'))\, g^{-1/2}(x')\,. \tag{3.273}$$

Recall that $g = \det g_{ij}$ denotes the determinant of the metric. It is very convenient to use the following exponential parametrization of the Van-Vleck-Morette determinant

$$\Delta = e^{2\zeta}\,, \tag{3.274}$$

where

$$\zeta(x, x') = \frac{1}{2} \log \det\, (-\sigma_{ij'}(x, x')) - \frac{1}{4} \log\, (g(x)g(x'))\,. \tag{3.275}$$

Note that

$$\sigma_{ij'} = g_{j'k'} \eta^{k'}{}_{i}\,. \tag{3.276}$$

Therefore,

$$\det\, (-\sigma_{ij'}) = g(x') \det (-\eta) = g(x') \det (-\gamma)^{-1}\,. \tag{3.277}$$

Thus, the Van-Vleck-Morette determinant can be expressed in terms of the matrices η and γ

$$\Delta(x, x') = g^{-1/2}(x) \det (-\eta) g^{1/2}(x') = g^{-1/2}(x) \det (-\gamma)^{-1} g^{1/2}(x')\,. \tag{3.278}$$

As we noted above determinants of tensors are not scalars but rather scalar densities. The matrix of mixed second derivatives of Synge function, $\sigma_{ij'}$, is not a tensor but rather a bi-covector that transforms as a covector at the point x as well as at the point x'. Therefore, the determinant $\det (-\sigma_{ij'})$ is not a scalar but a bi-scalar density of weight 1 at the point x and at the point x'. This is precisely the reason why we needed to multiply this determinant by the corresponding powers of the determinant of the metric. Then the quantity $\Delta(x, x')$ is a bi-scalar.

We will need the derivative of the Van-Vleck-Morette determinant. By using the eq. (1.101) we find (to avoid confusion we stress that Δ^{-1} below means just the reciprocal of the Van Vleck-Morette determinant Δ)

$$\begin{aligned}\Delta^{-1}\nabla_i\Delta &= \partial_i \log\left(g^{-1/2}\det(-\eta)\right)\\ &= \operatorname{tr}\gamma\partial_i\eta - g^{-1/2}\partial_i g^{1/2}\\ &= \gamma^k{}_{j'}\partial_i\eta^{j'}{}_k - \Gamma^k{}_{ik}\\ &= \gamma^k{}_{j'}\nabla_i\eta^{j'}{}_k\\ &= \operatorname{tr}\gamma\nabla_i\eta\,. \end{aligned} \tag{3.279}$$

This is a very useful equation. First of all, by multiplying it with σ^i we get

$$\Delta^{-1}D\Delta = \operatorname{tr}\gamma D\eta\,. \tag{3.280}$$

Now, by taking the trace of the eq. (3.266) we find

$$\operatorname{tr}\gamma D\eta = n - \sigma^i{}_i\,. \tag{3.281}$$

Thus, we see that the Van-Vleck-Morette determinant satisfies the following linear differential equation

$$D\Delta = (n - \sigma^i{}_i)\Delta\,, \tag{3.282}$$

and its square root satisfies the equation

$$D\Delta^{1/2} = \frac{1}{2}(n - \sigma^i{}_i)\Delta^{1/2}\,. \tag{3.283}$$

The coincidence limit of the Van-Vleck-Morette determinant is determined by the coincidence limit of the matrix η; so

$$[\Delta] = 1\,. \tag{3.284}$$

In terms of the function ζ the equation (3.283) takes a simpler form

$$D\zeta = \frac{1}{2}(n - \sigma^i{}_i)\,. \tag{3.285}$$

We will need this equation to study the heat kernel on Riemannian manifolds.

Second, by using eq. (3.247) we get another equation for Δ from eq. (3.279)

$$\Delta^{-1}\nabla_i\Delta = \gamma^k{}_{j'}\nabla_k\eta^{j'}{}_i\,, \tag{3.286}$$

which can be written in the form

$$\gamma^k{}_{j'}\nabla_k\left(\Delta^{-1}\eta^{j'}{}_i\right) = 0\,. \tag{3.287}$$

3.7 Operator of Parallel Transport

3.7.1 Definition and Basic Properties

Let $g^{i}{}_{j'}(x,x')$ be the operator of parallel transport of vector fields along the geodesic $x = x(\tau)$, $\tau \in [0,t]$, connecting the points x' and x such that $x(0) = x'$ and $x(t) = x$. Recall that if the points x' and x are sufficiently close to each other then the geodesic is a smooth curve without self-intersection so that for any $t \neq 0$, $x = x(t) \neq x(0) = x'$. That is, the coincidence limit $x \to x'$ is equivalent to the limit $t \to 0$. This is not so for a general curve which is not necessarily a geodesic. That is why, the operator of parallel transport $g^{i}{}_{j'}(x,x')$ along the geodesic depends only on the coordinates of the points x and x'. It is a *bi-vector*, which means that it is a vector at the point x and a covector at the point x'.

Recall that the matrix of the operator of parallel transport satisfies the equation of parallel transport which can be written in the form

$$Dg^{i}{}_{j'} = 0\,, \tag{3.288}$$

with the initial condition

$$[g^{i}{}_{j'}] = \delta^{i}{}_{j}\,. \tag{3.289}$$

By differentiating the equation (3.288) and taking the coincidence limit it is easy to see that the coincidence limit of the derivative of the operator of parallel transport vanishes

$$[\nabla_k g^{i}{}_{j'}] = 0\,. \tag{3.290}$$

Recall also that the derivatives of the Synge function, σ^{i} and $\sigma^{i'}$, are proportional to the tangent vectors to the geodesic at the points x and x' respectively pointing in opposite directions. Since the tangent vector to the geodesic is transported parallel along the geodesic and these two vectors have the same norm we obviously have the following useful relation

$$\sigma^{i} = -g^{i}{}_{j'}\sigma^{j'}\,. \tag{3.291}$$

The operator of parallel transport of covector fields is obtained by lowering the first index and raising the second index

$$g_{i}{}^{j'} = g_{im}g^{m}{}_{k'}g^{k'j'}\,. \tag{3.292}$$

This also means that these matrices are related by

$$g^{m}{}_{j'}g_{m}{}^{i'} = \delta^{i'}{}_{j'}\,, \qquad g^{i}{}_{m'}g_{j}{}^{m'} = \delta^{i}{}_{j}\,, \tag{3.293}$$

$$g_{ij}g^{i}{}_{k'}g^{j}{}_{l'} = g_{k'l'}\,, \qquad g_{i'j'}g_{k}{}^{i'}g_{l}{}^{j'} = g_{kl}\,. \tag{3.294}$$

The last property means, in particular, that the operator of parallel transport preserves the metric, that is, the norm of vectors.

Let $P = (g^{i}{}_{j'})$ be the matrix of the operator of parallel transport. Then, by using the determinant of the operator of parallel transport (3.103),

$$\det P(x, x') = g^{-1/2}(x) g^{1/2}(x'), \tag{3.295}$$

one can express Van Vleck-Morette determinant in the form

$$\Delta = \det \left(-P^{-1}\gamma\right)^{-1} , \tag{3.296}$$

which means

$$\zeta = -\frac{1}{2} \log \det \left(-P^{-1}\gamma\right) . \tag{3.297}$$

We will use this equation to calculate ζ, and, hence, Δ by computing the matrix γ first from the eq. (3.269).

3.7.2 Derivatives of the Operator of Parallel Transport

We derive an equation for the parallel transport operator. Let $P = (g^{i}{}_{j'})$ be the matrix of the operator of parallel transport; it satisfies the equation

$$DP = 0 . \tag{3.298}$$

Now, by applying the operator $\gamma^{j}{}_{k'}\nabla_j$ to this equation and using eq. (3.271) we obtain

$$(D + I)\gamma^{j}{}_{k'}\nabla_j P + \gamma^{j}{}_{k'}\sigma^{i}[\nabla_j, \nabla_i]P = 0 . \tag{3.299}$$

Next, by multiplying this equation by P^{-1} and recalling that the matrix P commutes with the operator D we obtain

$$(D + I)\mathcal{G}_{k'} = -\gamma^{j}{}_{k'}\mathcal{B}_j , \tag{3.300}$$

where

$$\mathcal{G}_{k'} = \gamma^{j}{}_{k'} P^{-1}\nabla_j P \tag{3.301}$$

and

$$\mathcal{B}_j = \sigma^{i} P^{-1}[\nabla_j, \nabla_i]P . \tag{3.302}$$

The initial condition for the matrix $\mathcal{G}_{i'}$ is

$$[\mathcal{G}_{i'}] = 0 . \tag{3.303}$$

More explicitly, the components of the matrices $\mathcal{G}_{k'} = \left(\mathcal{G}^{i'}{}_{j'k'}\right)$ and $\mathcal{B}_j = \left(\mathcal{B}^{i'}{}_{k'j}\right)$ are given by

$$\mathcal{G}^{i'}{}_{j'k'} = \gamma^{m}{}_{k'} g_{l}{}^{i'} \nabla_m g^{l}{}_{j'} \,, \tag{3.304}$$

$$\mathcal{B}^{i'}{}_{k'j} = g_{n}{}^{i'} g^{l}{}_{k'} R^{n}{}_{ljm} \sigma^{m} \,. \tag{3.305}$$

Note that the matrix $\mathcal{G}_{i'}$ is a scalar at the point x (since it does not have any unprimed indices) and a tensor of rank 3 at the point x'.

3.7.3 Generalized Operator of Parallel Transport

Now, let us consider a vector field $\mathcal{A}_i$ and let

$$\mathcal{R}_{ij} = \partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i \,. \tag{3.306}$$

Note that in three dimensions the dual of $\mathcal{R}$ is nothing but the curl of the vector $\mathcal{A}$. Let $x = x(\tau)$, $\tau \in [0, t]$, be a geodesic connecting the points x' and x so that $x(0) = x'$ and $x(t) = x$. We define the *generalized covariant derivative*

$$\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i \,, \tag{3.307}$$

and the corresponding generalized operator of differentiation along the geodesic

$$D^{\mathcal{A}} = \sigma^i \nabla_i^{\mathcal{A}} \,. \tag{3.308}$$

We define the *generalized operator of parallel transport* $\mathcal{P}(x, x')$, which is a two-point scalar function, as the solution of the equation

$$D^{\mathcal{A}} \mathcal{P} = 0 \,, \tag{3.309}$$

with the initial condition

$$[\mathcal{P}] = 1 \,. \tag{3.310}$$

Obviously, this solution is given by

$$\mathcal{P}(x, x') = \exp\left(- \int_0^t d\tau \; \dot{x}^i \mathcal{A}_i(x(\tau)) \right) \,. \tag{3.311}$$

and has the following symmetry property

$$\mathcal{P}(x', x) = \mathcal{P}^{-1}(x, x') \,. \tag{3.312}$$

We will call the vector field $\mathcal{A}_i$ a *generalized connection* and the tensor $\mathcal{R}_{ij}$ its *generalized curvature*. Strictly speaking such a vector field defines a connection only if it is purely imaginary (or, more generally, if it is anti-Hermitian matrix-valued). If the vector field $\mathcal{A}_i$ is real (and not matrix valued) it does not define a connection; that is why, we call it a generalized connection rather

than simply a connection. If the vector field $\mathcal{A}_i$ is not a connection, then the generalized operator of parallel transport *is not unitary* (does not preserve the norm), that is,

$$\mathcal{P}^*\mathcal{P} \neq 1\,. \tag{3.313}$$

It is unitary if $\mathcal{A}_i$ is purely imaginary. Another manifestation of this is that the generalized covariant derivative *does not satisfy the usual rules of integration by parts* similar to (3.91).

In a fashion very similar to the one used to derive the eq. (3.300) we obtain the equation

$$(D+I)\hat{\mathcal{A}}_{i'} = -\gamma^{j}{}_{i'}\mathcal{L}_j\,, \tag{3.314}$$

where

$$\hat{\mathcal{A}}_{i'} = \gamma^{m}{}_{i'}\mathcal{P}^{-1}\nabla^{\mathcal{A}}_{m}\mathcal{P}\,, \tag{3.315}$$

and

$$\mathcal{L}_j = \mathcal{R}_{jm}\sigma^m\,, \tag{3.316}$$

with the initial condition

$$[\hat{\mathcal{A}}_{i'}] = 0\,. \tag{3.317}$$

3.8 Covariant Expansions of Two-Point Functions

The primary goal of this book is to develop an approximate solution for the heat kernel $U(t;x,x')$ for small time t and for the point x close to the point x', more precisely, we want to find an asymptotic expansion of the heat kernel as $t\to 0$ and $x\to x'$ (see Chap. 5). To do this we will need to expand all two-point functions in a covariant Taylor series. The coefficients of such Taylor series are determined by the coincidence limits of the derivatives of the two-point functions such as the Synge function $\sigma=\sigma(x,x')$, the Van Vleck-Morette determinant $\Delta=\Delta(x,x')$ and the operator of parallel transport $\mathcal{P}=\mathcal{P}(x,x')$. That is why, we need to develop an effective method for the calculation of these coincidence limits.

3.8.1 Coincidence Limits of Higher-Order Derivatives

We show that the coincidence limits of higher order *symmetrized* derivatives of order $n\geq 2$ of the vectors σ^i and $\sigma^{i'}$ vanish,

$$[\nabla_{(i_1}\cdots\nabla_{i_n)}\sigma^j] = [\nabla_{(i_1}\cdots\nabla_{i_n)}\sigma^{j'}] = 0\,. \tag{3.318}$$

Recall that the parenthesis denote the complete symmetrization over all included indices.

First of all, we recall the coincidence limits of the first and second derivatives of the Synge function

$$[\sigma^{j'}] = [\sigma^{j}] = 0\,, \tag{3.319}$$

$$[\sigma^{i}{}_{j}] = -[\sigma^{i'}{}_{j}] = \delta^{i}{}_{j}\,. \tag{3.320}$$

Next, by differentiating the basic eq. (3.234) twice (or, equivalently, by differentiating the eq. (3.248)) we get

$$\sigma^{j}{}_{kl} = \sigma^{i}\sigma^{j}{}_{ikl} + \sigma^{i}{}_{l}\sigma^{j}{}_{ik} + \sigma^{i}{}_{k}\sigma^{j}{}_{il} + \sigma^{j}{}_{i}\sigma^{i}{}_{kl}\,. \tag{3.321}$$

Now, by taking the coincidence limit of this equation we have

$$[\sigma^{j}{}_{lk}] + [\sigma^{j}{}_{kl}] = 0\,, \tag{3.322}$$

that is, the coincidence limit of the symmetrized second derivative of the vector σ^{i} vanishes

$$[\nabla_{(i_1}\nabla_{i_2)}\sigma^{j}] = 0\,. \tag{3.323}$$

We can prove the above assertion by induction. Suppose that (3.318) is true for $n = 2, 3, \ldots, k$. We want to prove that then it will be true for $n = k+1$ as well meaning that it is true for any n. We take the $(k+1)$-th derivative of the equation (3.248) and symmetrize all derivatives to get

$$\nabla_{(i_1}\cdots\nabla_{i_{k+1})}\sigma^{j} = \sum_{m=0}^{k+1}\binom{k+1}{m}\left(\nabla_{(i_1}\cdots\nabla_{i_m}\sigma^{i}\right)\left(\nabla_{i_{m+1}}\cdots\nabla_{i_{k+1})}\nabla_{i}\sigma^{j}\right)\,. \tag{3.324}$$

Now, by taking the coincidence limit and using the known coincidence limits of the first two derivatives (3.319)-(3.320) we obtain from this equation

$$\begin{aligned}(k+1)&[\nabla_{(i_1}\cdots\nabla_{i_{k+1})}\sigma^{j}] \\ &= -\sum_{m=2}^{k}\binom{k+1}{m}\left[\nabla_{(i_1}\cdots\nabla_{i_m}\sigma^{i}\right]\left[\nabla_{i_{m+1}}\cdots\nabla_{i_k+1)}\nabla_{i}\sigma^{j}\right]\,.\end{aligned} \tag{3.325}$$

Now, by the induction hypothesis all the terms on the right hand side vanish and, therefore, the left side vanishes as well, which proves the assertion.

In exactly the same way one can prove that the coincidence limits of the symmetrized derivatives of the vector $\sigma^{j'}$ also vanish.

Let us consider a two-point function f which is parallel along the geodesic, that is, it satisfies the equation

$$Df = \sigma^{i}\nabla_{i}f = 0\,, \tag{3.326}$$

and has a finite coincidence limit $[f]$. Note that f could also be a matrix-valued function like the operator of parallel transport. Then one can show that its higher order *symmetrized* derivatives of order $n \geq 1$ have vanishing coincidence limits

$$[\nabla_{(i_1} \cdots \nabla_{i_n)} f] = 0\,. \tag{3.327}$$

Indeed by taking the $(n+1)$-th symmetrized derivative of the equation (3.326) we get

$$\sum_{m=0}^{n+1} \binom{n+1}{m} \left(\nabla_{(i_1} \cdots \nabla_{i_m} \sigma^i\right) \left(\nabla_{i_{m+1}} \cdots \nabla_{i_{n+1})} \nabla_i f\right) = 0\,. \tag{3.328}$$

Now, by taking the coincidence limit and using the coincidence limit of the Synge function we see that only one term survives in this sum, namely, $m = 1$, that is, the term with one derivative of σ^i giving the eq. (3.327).

By using this general result we obtain that the coincidence limits of higher order symmetrized derivatives of order $n \geq 1$ of the operators of parallel transport vanish

$$[\nabla_{(i_1} \cdots \nabla_{i_n)} g^j{}_{k'}] = 0\,, \tag{3.329}$$

$$[\nabla^{\mathcal{A}}_{(i_1} \cdots \nabla^{\mathcal{A}}_{i_n)} \mathcal{P}] = 0\,. \tag{3.330}$$

The proof with the operators $\nabla^{\mathcal{A}}$ instead of the operators ∇ is exactly the same.

3.8.2 Covariant Taylor Series

We need to develop a method that allows one to approximate a function in a neighborhood of a given point in a Riemannian manifold. In the Euclidean space such an approximation is given by Taylor series. However, we cannot apply Taylor series to the curved manifold directly since its form depends on the local coordinate system, that is, for different coordinates one gets different expansions. We would like to have rather a *covariant* method that does not depend on the local coordinates. We describe in this section such a method that we call *covariant Taylor series*.

Let us consider a scalar function $f(x)$ on a Riemannian manifold. Let us fix a point x' and consider a sufficiently small neighborhood of this point so that an arbitrary point x can be connected to the fixed point x' by a single geodesic. Let $x = x(\tau)$ be the geodesic connecting the points x' and x with an affine parameter τ so that $x(0) = x'$ and $x(t) = x$. Each geodesic emanating from the point x' is parametrized by the tangent vector $\dot{x}^i(0)$ to the geodesic at the point x'. Let us fix a geodesic and consider the values of the function f along this geodesic. Then it becomes a function of the affine parameter τ,

that is, $f(x(\tau))$. Then we can expand it in the Taylor series in t at $\tau = 0$

$$f(x(t)) = \sum_{n=0}^{\infty} \frac{1}{n!} t^n \left[\frac{d^n}{d\tau^n} f(x(\tau)) \right]_{\tau=0} . \tag{3.331}$$

Now, we recall that

$$\frac{d}{d\tau} = \dot{x}^i(\tau) \nabla_i \,, \qquad \sigma^{i'} = -t\dot{x}^i(0) \,, \tag{3.332}$$

and use the equation of geodesic, $\dot{x}^i \nabla_i \dot{x}^j = 0$ to obtain

$$f(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sigma^{i'_1} \cdots \sigma^{i'_n} \left[\nabla_{(i_1} \cdots \nabla_{i_k)} f \right] (x') \,, \tag{3.333}$$

where the coincidence limit is evaluated at the point x'. This is the covariant Taylor series for scalar functions.

Now we show that it is nothing but an expansion in eigenfunctions of the operator D. We construct a complete set of eigenfunctions of the operator D as follows. From the equation for the tangent vector

$$D\sigma^{i'} = \sigma^{i'} \tag{3.334}$$

we see that $\sigma^{i'}$ is an eigenfunction of the operator D with the eigenvalue equal to 1. Recall also that this eigenfunction is *scalar* at the point x (and a vector at the point x'). Now, we define the scalar eigenfunctions $|n\rangle$, $(n = 0, 1, 2, \dots)$, by

$$|0\rangle = 1 \tag{3.335}$$

$$|n\rangle = |i'_1 \cdots i'_n\rangle = \frac{(-1)^n}{n!} \sigma^{i'_1} \cdots \sigma^{i'_n} \,. \tag{3.336}$$

Then, obviously,

$$D|n\rangle = n|n\rangle \,. \tag{3.337}$$

Similarly, the equation for the operator of parallel transport

$$Dg^i{}_{j'} = 0 \tag{3.338}$$

means that $g^i{}_{j'}$ is an eigenvector of the operator D with the eigenvalue equal to 0. By combining these functions we can construct now tensor eigenfunctions with any positive integer eigenvalue for any tensor type. The tensor eigenfunctions are obtained by adding a factor in form of parallel displacement operators. For example, vector eigenfunctions with the eigenvalue equal to n are given by

$$\frac{(-1)^n}{n!} g^k{}_{l'} \sigma^{i'_1} \cdots \sigma^{i'_n} \,. \tag{3.339}$$

Note also that by adding the factor $\mathcal{P}$ we get the eigenfunctions of the operator $D^{\mathcal{A}}$,

$$D^{\mathcal{A}}\mathcal{P}|n\rangle = n\mathcal{P}|n\rangle\,. \tag{3.340}$$

Let us define also the dual functions $\langle m|$ as operators acting on functions as

$$\langle m|f\rangle = \langle i_1\cdots i_m|f\rangle = \left[\nabla_{(i_1}\cdots\nabla_{i_m)}f\right]\,, \tag{3.341}$$

in other words, the operator $\langle m|$ maps a function to the coincidence limit of its symmetrized covariant derivative evaluated at the point $x = x'$.

By using the properties (3.318) and (3.320) of the vectors $\sigma^{j'}$ it is not difficult to see that these operators satisfy the following duality property

$$\langle m|n\rangle = \delta_{mn}\delta^{i_1\cdots i_n}_{j_1\cdots j_n}\,, \tag{3.342}$$

where

$$\delta^{i_1\cdots i_n}_{j_1\cdots j_n} = \delta^{i_1}_{(j_1}\cdots\delta^{i_n}_{j_n)}\,. \tag{3.343}$$

Now it is almost obvious that our set of eigenfunctions is complete due to the fact that there is no non-zero function that is "orthogonal" to all eigenfunctions $|n\rangle$. In other words, a function which is equal to zero at $x = x'$ together with all symmetrized covariant derivatives at $x = x'$ is identically equal to zero. Of course, we restrict ourselves here to functions which are analytic in the neighborhood of the point x'. The completeness property can be expressed in the form

$$\sum_{n=0}^{\infty}|n\rangle\langle n| = I\,, \tag{3.344}$$

where I is the identity operator.

By using this relation the covariant Taylor series for any scalar field f is obtained as follows

$$f = \sum_{n=0}^{\infty}|n\rangle\langle n|f\rangle \tag{3.345}$$

$$= \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}f\right](x')\,. \tag{3.346}$$

By multiplying this with operators of parallel transport (as many as needed) we obtain covariant Taylor series for an arbitrary tensor field. For example, for a vector field v^i we have

$$v^j = g^j{}_{k'}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}v^k\right](x')\,. \tag{3.347}$$

We also mention a more general expansion

$$f = \mathcal{P}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}\mathcal{P}^{-1}f\right](x')$$
$$= \mathcal{P}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla^{\mathcal{A}}_{(i_1}\cdots\nabla^{\mathcal{A}}_{i_n)}f\right](x'), \tag{3.348}$$

which can be obtained from eq. (3.330).

3.8.3 Normal Coordinates

In order to study non-local properties of functions another type of covariant expansion is needed, namely, Fourier transform. Similarly to Taylor expansion Fourier transform is defined with respect to a particular coordinate system, and, therefore, depends on the choice of the local coordinates. This makes the usual Fourier transform not suitable for curved manifolds. Again, we want to define an expansion that would be *covariant*, that is, the same in all coordinate systems.

We should make a remark here. First, we defined all two-point functions in a sufficiently small neighborhood of a fixed point x'. In such a neighborhood these functions are well-defined single-valued smooth functions of the coordinates of the points x and x'. In a general manifold it could happen though that when the point x moves away from the point x' that it can be connected by more than one geodesic with the point x'. At such points Van Vleck-Morette determinant vanishes, $\Delta(x, x') = 0$. If this happens then the points x and x' are called the *conjugate points*. This has also to do with the injectivity of the so-called *exponential mapping*. The radius of the largest geodesic ball such that the exponential mapping is injective inside the ball is called the *injectivity radius* at the point x'. The smallest injectivity radius at all points is then called the *injectivity radius of the manifold*. For smooth compact manifolds the injectivity radius is positive, that is, at every point there is a sufficiently small geodesic ball such that the exponential mapping is injective and all two-point functions are well defined. Thus, strictly speaking we can only integrate over a sufficiently small geodesic ball of a radius smaller than the injectivity radius of the manifold. This, of course, presents a difficulty. However, for our purposes it will not cause any complications since we will be only interested in asymptotic expansions, and the error of replacing the region of integration by the whole manifold will be exponentially small. Alternatively, we could just assume that the manifold M is *homeomorphic* (that is, topologically equivalent) to the Euclidean space $\mathbb{R}^n$ and every two points can be connected by only one geodesic. This is so, for example, on manifolds with sufficiently large negative curvature like hyperbolic spaces. This means, in other words, that the injectivity radius is infinite, and all

two-point functions are well defined on the whole manifold. In this case, the integral defining covariant Fourier transform is well defined.

The key observation we make now is that the vectors $\sigma^{i'} = \sigma^{i'}(x, x')$ themselves can be taken as new coordinates of the point x instead of x^j; these coordinates are called the *normal coordinates* of the point x at the point x'. Indeed, the Jacobian matrix of this transformation of coordinates

$$d\sigma^{i'} = \eta^{i'}{}_j dx^j \tag{3.349}$$

is exactly the matrix

$$\eta^{i'}{}_j = \frac{\partial \sigma^{i'}}{\partial x^j}\,, \tag{3.350}$$

and the Jacobian is expressed in terms of the Van Vleck-Morette determinant,

$$\det\left[-\eta^{i'}{}_j(x, x')\right] = g^{1/2}(x) g^{-1/2}(x') \Delta(x, x')\,. \tag{3.351}$$

Therefore, for sufficiently close points x and x' the Jacobian is not equal to zero. For the volume element in this coordinates we have then

$$g^{1/2}(x) dx^1 \cdots dx^n = \Delta^{-1}(x, x') g^{1/2}(x') d\sigma^{1'} \cdots d\sigma^{n'}\,. \tag{3.352}$$

The derivatives with respect to the normal coordinates are related with the usual ones similarly

$$\frac{\partial}{\partial \sigma^{i'}} = \gamma^j{}_{i'} \frac{\partial}{\partial x^j}\,, \tag{3.353}$$

where $\gamma^j{}_{i'}$ is the inverse of the matrix $\sigma^{i'}{}_j$. Similar relation holds for covariant derivatives too.

We define covariant Fourier transform of a scalar function f by considering it as a function of the coordinates $\sigma^{i'}$ and using the usual Fourier transform (multiplied by the factor $g^{1/2}(x')$)

$$\hat{f}(k) = \int\limits_M dx\; g^{1/2}(x) \Delta(x, x') e^{ip(x)} f(x)\,, \tag{3.354}$$

where

$$p(x) = p_{j'} \sigma^{j'}(x, x')\,, \tag{3.355}$$

and $p_{j'}$ is a covector at the point x'. The inverse Fourier transform is given then as usual

$$f(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} g^{-1/2}(x') e^{-ip(x)} \hat{f}(p)\,, \tag{3.356}$$

where $dp = dp_{1'} \ldots dp_{n'}$, and the integration goes over the whole cotangent space at x'.

This means, in particular, that covariant Fourier integral representation of the scalar delta-function has the form

$$\delta(x,y) = \Delta(x,x') \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} g^{-1/2}(x') e^{ip(y)-ip(x)}\,, \tag{3.357}$$

which can also be written in the symmetric form

$$\delta(x,y) = \Delta^{1/2}(x,x')\Delta^{1/2}(y,x') \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} g^{-1/2}(x') e^{ip(y)-ip(x)}\,. \tag{3.358}$$

The usefulness of the covariant Fourier transform comes from the fact that, similar to the usual Fourier transform, it allows to compute derivatives very easily

$$\nabla_l f(x) = -i\,\eta^{m'}{}_l \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} g^{-1/2}(x') e^{-ip(x)} p_{m'} \hat{f}(k)\,. \tag{3.359}$$

Covariant Fourier transform of tensors is defined similarly. First, we parallel transport a tensor to the point x' to make it a scalar at the point x (and a tensor at the point x') and then we apply covariant Fourier transform to the scalar field. For example, for a vector field v^j we have

$$\hat{v}^{l'}(p) = \int\limits_M dx\; g^{1/2}(x) \Delta(x,x') e^{ip(x)} g_m{}^{l'} v^m(x)\,, \tag{3.360}$$

and

$$v^m(x) = g^m{}_{l'} \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} g^{-1/2}(x') e^{-ip(x)} \hat{v}^{l'}(p)\,. \tag{3.361}$$

3.8.4 Covariant Taylor Series of Two-Point Functions

We will need to compute the two-point functions constructed from the derivatives of Synge functions and the operator of parallel transport introduced in this and the previous sections. The only way to compute these quantities is in the form of the covariant Taylor series.

Let $\eta = (\eta^{i'}{}_j)$ be the matrix $\eta^{i'}{}_j = \sigma^{i'}{}_j$, (3.242), and $\gamma = \eta^{-1} = (\gamma^i_{j'})$ be its inverse, (3.260). The basis for all further calculations is the equation (3.269) for the matrix γ. To solve it, let us introduce the matrix

$$\bar{\gamma} = P^{-1}\gamma + I\,, \tag{3.362}$$

where $P = (g^i{}_{j'})$ is the matrix of the operator of parallel transport and I is the identity matrix. Since the operator of parallel transport P satisfies the equation (3.298) it commutes with the operator D. Therefore, by multiplying the equation (3.269) by P^{-1} we see that the matrix $\bar{\gamma}$ satisfies the equation

$$(D^2 + D + \bar{K})\bar{\gamma} = \bar{K}\,, \tag{3.363}$$

with the initial condition

$$[\bar{\gamma}] = 0\,. \tag{3.364}$$

Here $\bar{K} = (K^{i'}{}_{j'})$ is the matrix defined by

$$\bar{K} = P^{-1}KP\,, \tag{3.365}$$

where $K = (K^{i}{}_{j})$ is given by $K^{i}{}_{j} = R^{i}{}_{kjl}\sigma^{k}\sigma^{l}$, (3.254), that is,

$$\bar{K}^{i'}{}_{j'} = R^{i'}{}_{k'j'l'}\sigma^{k'}\sigma^{l'}\,. \tag{3.366}$$

The equation (3.363) can be solved formally by

$$\bar{\gamma} = \left(D^2 + D + \bar{K}\right)^{-1}\bar{K}\,. \tag{3.367}$$

The inverse operator here is computed as follows

$$\begin{aligned}\left(D^2 + D + \bar{K}\right)^{-1} &= \left\{(D^2 + D)\left[I + (D^2 + D)^{-1}\bar{K}\right]\right\}^{-1} \\ &= \left[I + (D^2 + D)^{-1}\bar{K}\right]^{-1}(D^2 + D)^{-1} \\ &= \sum_{n=0}^{\infty}(-1)^n\left\{(D^2 + D)^{-1}\bar{K}\right\}^n(D^2 + D)^{-1}\,. \end{aligned} \tag{3.368}$$

Therefore, we obtain

$$\bar{\gamma} = \sum_{n=1}^{\infty}(-1)^{n+1}\left\{(D^2 + D)^{-1}\bar{K}\right\}^n\,. \tag{3.369}$$

Next, one can obtain the covariant Taylor series of the matrix K defined by (3.254)

$$K = P\sum_{n=2}^{\infty}\frac{(-1)^n}{(n-2)!}K_{(n)}P^{-1}\,, \tag{3.370}$$

where

$$K_{(n)} = \left(K_{(n)}{}^{i'}{}_{j'}\right) \tag{3.371}$$

are matrices defined by

$$K_{(n)}{}^{i'}{}_{j'} = K^{i'}{}_{j'l'_1\cdots l'_n}\sigma^{l'_1}\cdots\sigma^{l'_n}\,, \tag{3.372}$$

with tensor coefficients given by

$$K^{i}{}_{jl_1\cdots l_n} = \nabla_{(l_1}\cdots\nabla_{l_{n-2}}R^{i}{}_{l_{n-1}|j|l_n)}\,. \tag{3.373}$$

Here, as usual, the parenthesis denote complete symmetrization over all indices included except those separated by the vertical lines.

Notice that the the action of the inverse operator $(D^2+D)^{-1}$ on a function f with the zero coincidence limit, that is, such that $[f] = 0$, is well defined and can be represented by the spectral sum

$$(D^2 + D)^{-1} f = \sum_{n=1}^{\infty} \frac{1}{n(n+1)} |n\rangle\langle n|f\rangle \,. \tag{3.374}$$

By using this representation one can finally obtain the solution

$$\begin{aligned} \gamma &= P(-I + \bar{\gamma}) \\ &= P\left(-I + \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \gamma_{(n)}\right) , \end{aligned} \tag{3.375}$$

where the matrix coefficients $\gamma_{(n)}$ are given by

$$\gamma_{(n)} = \sum_{k=1}^{[n/2]} (-1)^{k+1} \sum_{\substack{n_1,\cdots,n_k \geq 2 \\ n_1+\cdots+n_k=n}} N^{-1}(n_1, \cdots, n_k) K_{(n_k)} K_{(n_{k-1})} \cdots K_{(n_2)} K_{(n_1)} \,. \tag{3.376}$$

Here $[x]$ denotes the integer part of the real number x, and $N(n_1, \ldots, n_k)$ is a combinatorial coefficient defined by

$$\begin{aligned} N(n_1, \cdots, n_k) = \frac{(n+1)}{(n-1)!} (n_1 - 2)! \cdots (n_k - 2)! \\ \times n_1(n_1+1)(n_1+n_2)(n_1+n_2+1) \cdots \\ \cdots (n_1 + \cdots + n_{k-1})(n_1 + \cdots + n_{k-1} + 1) \,. \end{aligned} \tag{3.377}$$

The summation in the internal sum goes over k integers $n_1, \ldots, n_k$ greater or equal than 2 whose sum is equal to n. For the details of this derivation see [4, 10] where this result was first obtained.

We see that the matrices

$$\gamma_{(n)} = \left(\gamma_{(n)}{}^{i'}{}_{j'}\right) \tag{3.378}$$

have the form

$$\gamma_{(n)}{}^{i'}{}_{j'} = \gamma^{i'}{}_{j' l'_1 \cdots l'_n} \sigma^{l'_1} \cdots \sigma^{l'_n} \,, \tag{3.379}$$

with tensor coefficients determined by the above equation. Now one can write down Taylor coefficients of the matrix γ, as many as needed. For example, some first ones are [10]

$$\gamma^{i}{}_{jk_1k_2} = \frac{1}{3}R^{i}{}_{(k_1|j|k_2)}\,, \tag{3.380}$$

$$\gamma^{i}{}_{jk_1k_2k_3} = \frac{1}{2}\nabla_{(k_1}R^{i}{}_{k_2|j|k_3)}\,, \tag{3.381}$$

$$\gamma^{i}{}_{jk_1k_2k_3k_4} = \frac{3}{5}\nabla_{(k_1k_2}R^{i}{}_{k_3|j|k_4)} - \frac{1}{5}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|j|k_4)}\,. \tag{3.382}$$

Using this solution for the matrix γ one can easily calculate all other two-point functions. For example, for the matrix $\eta = \gamma^{-1}$ we obtain

$$\begin{aligned}\eta &= (-I+\bar{\gamma})^{-1}P^{-1}\\ &= \left(-I+\sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\eta_{(n)}\right)P^{-1}\,,\end{aligned} \tag{3.383}$$

where

$$\eta_{(n)} = -\sum_{k=1}^{[n/2]}\sum_{\substack{n_1,\cdots,n_k\geq 2\\ n_1+\cdots+n_k=n}}\frac{n!}{n_1!\cdots n_k!}\gamma_{n_k}\cdots\gamma_{n_1}\,. \tag{3.384}$$

Thus the matrices

$$\eta_{(n)} = \left(\eta_{(n)}{}^{i'}{}_{j'}\right)\,, \tag{3.385}$$

have the form

$$\eta_{(n)}{}^{i'}{}_{j'} = \eta^{i'}{}_{j'k'_1\cdots k'_n}\sigma^{k'_1}\cdots\sigma^{k'_n}\,, \tag{3.386}$$

with tensor coefficients determined by the above formula. A couple of first coefficients are given by [10]

$$\eta^{i}{}_{jk_1k_2} = -\frac{1}{3}R^{i}{}_{(k_1|j|k_2)}\,, \tag{3.387}$$

$$\eta^{i}{}_{jk_1k_2k_3} = -\frac{1}{2}\nabla_{(k_1}R^{i}{}_{k_2|j|k_3)}\,, \tag{3.388}$$

$$\eta^{i}{}_{jk_1k_2k_3k_4} = -\frac{3}{5}\nabla_{(k_1}\nabla_{k_2}R^{i}{}_{k_3|j|k_4)} - \frac{7}{15}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|j|k_4)}\,, \tag{3.389}$$

which are obtained by using eqs. (3.380)-(3.382).

Similarly, we can obtain the matrix $\xi = (\xi^{i}{}_{j})$ defined by $\xi^{i}{}_{j} = \sigma^{i}{}_{j}$, (3.241). From the equation (3.268) we have

$$\xi = I + P(D\bar{\gamma})\eta\,. \tag{3.390}$$

Now by using the equation (3.337) we have obviously

$$D\gamma_{(n)} = n\gamma_{(n)}\,, \tag{3.391}$$

and, therefore,

$$D\bar{\gamma} = \sum_{n=2}^{\infty} \frac{(-1)^n}{(n-1)!} \gamma_{(n)} \,, \tag{3.392}$$

Thus, we obtain for the matrix ξ

$$\xi = I + P \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \xi_{(n)} P^{-1} \,, \tag{3.393}$$

where the matrix coefficients, $\xi_{(n)} = \left({\xi_{(n)}}^{i'}{}_{j'} \right)$, with

$${\xi_{(n)}}^{i'}{}_{j'} = {\xi^{i'}}_{j' k'_1 \cdots k'_n} \sigma^{k'_1} \cdots \sigma^{k'_n} \,, \tag{3.394}$$

are expressed in terms of $\gamma_{(n)}$. For example, the first three ones are

$$\xi_{(2)} = -2\gamma_{(2)} \,, \tag{3.395}$$

$$\xi_{(3)} = -3\gamma_{(3)} \,, \tag{3.396}$$

$$\xi_{(4)} = -4\gamma_{(4)} - 12\gamma_{(2)}^2 \,. \tag{3.397}$$

By using the above results (3.380)-(3.382) for the coefficients $\gamma_{(n)}$ we obtain

$${\xi^i}_{jk_1k_2} = -\frac{2}{3} R^i{}_{(k_1|j|k_2)} \,, \tag{3.398}$$

$${\xi^i}_{jk_1k_2k_3} = -\frac{3}{2} \nabla_{(k_1} R^i{}_{k_2|j|k_3)} \,, \tag{3.399}$$

$${\xi^i}_{jk_1k_2k_3k_4} = -\frac{12}{5} \nabla_{(k_1k_2} R^i{}_{k_3|j|k_4)} - \frac{8}{15} R^i{}_{(k_1|m|k_2} R^m{}_{k_3|j|k_4)} \,. \tag{3.400}$$

Now, by using the equation (3.297) we compute the logarithm of the Van Vleck-Morette determinant

$$\zeta = \frac{1}{2} \log \Delta = -\frac{1}{2} \log \det \, (I - \bar{\gamma}) \tag{3.401}$$

in terms of the matrices $\gamma_{(n)}$ as follows

$$\zeta = -\frac{1}{2} \sum_{k=0}^{\infty} \frac{1}{k} \operatorname{tr} \bar{\gamma}^k \,, \tag{3.402}$$

which can be presented as the series

$$\zeta = \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \zeta_{(n)} \tag{3.403}$$

with the coefficients

$$\zeta_{(n)} = \sum_{k=1}^{[n/2]} \frac{1}{2k} \sum_{\substack{n_1,\cdots,n_k\geq 2 \\ n_1+\cdots+n_k=n}} \frac{n!}{n_1!\cdots n_k!} \operatorname{tr}\left(\gamma_{(n_1)}\cdots\gamma_{(n_k)}\right) . \tag{3.404}$$

These coefficients have the form

$$\zeta_{(n)} = \zeta_{i'_1\cdots i'_n}\sigma^{i'_1}\cdots\sigma^{i'_n} \tag{3.405}$$

with the tensor coefficients determined by the above equation. In particular, by using eqs. (3.380)-(3.382) we get a couple of first coefficients

$$\zeta_{k_1k_2} = \frac{1}{6}R_{k_1k_2}, \tag{3.406}$$

$$\zeta_{k_1k_2k_3} = \frac{1}{4}\nabla_{(k_1}R_{k_2k_3)}, \tag{3.407}$$

$$\zeta_{k_1k_2k_3k_4} = \frac{3}{10}\nabla_{(k_1}\nabla_{k_2}R_{k_3k_4)} + \frac{1}{15}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|i|k_4)} . \tag{3.408}$$

We will need the Taylor expansion of the square root of the Van Vleck-Morette determinant $\Delta^{1/2}$

$$\Delta^{1/2} = 1 + \sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\Delta^{1/2}_{(n)} , \tag{3.409}$$

where

$$\Delta^{1/2}_{(n)} = \Delta^{1/2}_{i'_1\cdots i'_n}\sigma^{i'_1}\cdots\sigma^{i'_n} . \tag{3.410}$$

It can be easily obtained from the function ζ by taking the exponent, $\Delta = e^{\zeta}$, and expanding in powers of $\zeta_{(n)}$. Omitting the details, we list a couple first coefficients

$$\Delta^{1/2}_{k_1k_2} = \frac{1}{6}R_{k_1k_2}, \tag{3.411}$$

$$\Delta^{1/2}_{k_1k_2k_3} = \frac{1}{4}\nabla_{(k_1}R_{k_2k_3)}, \tag{3.412}$$

$$\begin{aligned}\Delta^{1/2}_{k_1k_2k_3k_4} = {} & \frac{3}{10}\nabla_{(k_1}\nabla_{k_2}R_{k_3k_4)} + \frac{1}{15}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|i|k_4)} \\ & + \frac{1}{12}R_{(k_1k_2}R_{k_3k_4)} .\end{aligned} \tag{3.413}$$

Finally, we compute Taylor series for the derivative of the operator of parallel transport, more precisely, the matrix $\mathcal{G}_{l'} = \left(\mathcal{G}^{i'}{}_{j'l'}\right)$, defined by eq. (3.301). In order to do this we expand first the matrix $\mathcal{B}_m = \left(\mathcal{B}^{i'}{}_{j'm}\right)$ defined by eq. (3.305) in covariant Taylor series; we obtain

$$\mathcal{B}^{i'}{}_{j'm} = g_m{}^{l'} \sum_{n=1}^{\infty} \frac{(-1)^n}{(n-1)!} \mathcal{B}^{i'}{}_{j'l'k'_1\cdots k'_n} \sigma^{k'_1} \cdots \sigma^{k'_n} , \tag{3.414}$$

where

$$\mathcal{B}^{i}{}_{jmk_1\cdots k_n} = \nabla_{(k_1} \cdots \nabla_{k_{n-1}} R^{i}{}_{|jm|k_n)} . \tag{3.415}$$

Next, we find the formal operator solution of the eq. (3.300)

$$\mathcal{G}^{i'}{}_{j'l'} = -(D+I)^{-1} \mathcal{B}^{i'}{}_{j'm} \gamma^{m}{}_{l'} . \tag{3.416}$$

Now, by defining the inverse operator in form of the spectral sum

$$(D+I)^{-1} = \sum_{n=0}^{\infty} \frac{1}{n+1} |n\rangle\langle n| \tag{3.417}$$

we obtain the Taylor series

$$\mathcal{G}^{i'}{}_{j'm'} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \mathcal{G}^{i'}{}_{j'm'k'_1\cdots k'_n} \sigma^{k'_1} \cdots \sigma^{k'_n} , \tag{3.418}$$

with the tensor coefficients given by (see the papers [4, 10])

$$\mathcal{G}^{i}{}_{jmk_1\cdots k_n} = \frac{n}{n+1} \left\{ \mathcal{B}^{i}{}_{jmk_1\cdots k_n} - \sum_{p=1}^{n-2} \binom{n-1}{p-1} \mathcal{B}^{i}{}_{jl(k_1\cdots k_p} \gamma^{l}{}_{|m|k_{p+1}\cdots k_n)} \right\} . \tag{3.419}$$

We list here the first three coefficients from our papers [4, 10]

$$\mathcal{G}^{i}{}_{jmk_1} = \frac{1}{2} R^{i}{}_{jmk_1} , \tag{3.420}$$

$$\mathcal{G}^{i}{}_{jmk_1k_2} = \frac{2}{3} \nabla_{(k_1} R^{i}{}_{j|m|k_2)} , \tag{3.421}$$

$$\mathcal{G}^{i}{}_{jmk_1k_2k_3} = \frac{3}{4} \nabla_{(k_1} \nabla_{k_2} R^{i}{}_{j|m|k_3)} - \frac{1}{4} R^{i}{}_{jl(k_1} R^{l}{}_{k_2|m|k_3)} . \tag{3.422}$$

Similarly, we can compute the Taylor expansion of the derivative of the generalized operator of parallel transport, more precisely, the vector $\hat{\mathcal{A}}_{i'}$ defined by (3.315). First, we expand the vector $\mathcal{L}_j$ defined by (3.316) in the Taylor series; we find

$$\mathcal{L}_j = g_j{}^{k'} \sum_{n=1}^{\infty} \frac{(-1)^n}{(n-1)!} \mathcal{R}_{k'i'_1\cdots i'_n} \sigma^{i'_1} \cdots \sigma^{i'_n} , \tag{3.423}$$

where

$$\mathcal{R}^k{}_{i_1\cdots i_n} = \nabla_{(i_1} \cdots \nabla_{i_{n-1}} \mathcal{R}^k{}_{i_n)} . \tag{3.424}$$

Next, we find the formal operator solution of the eq.(3.314)

$$\hat{\mathcal{A}}_{i'} = -\left(D + I\right)^{-1} \mathcal{L}_j \gamma^j{}_{i'} . \tag{3.425}$$

Now, by defining the inverse operator by (3.417) we obtain the Taylor series

$$\hat{\mathcal{A}}_{j'} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \mathcal{A}_{j'i'_1\cdots i'_n} \sigma^{i'_1} \cdots \sigma^{i'_n} , \tag{3.426}$$

with the coefficients (see the papers [4, 10])

$$\mathcal{A}_{ji_1\cdots i_n} = \frac{n}{n+1} \left\{ \mathcal{R}_{ji_1\cdots i_n} - \sum_{k=1}^{n-2} \binom{n-1}{k-1} \mathcal{R}_{l(i_1\cdots i_k} \gamma^l{}_{|j|i_{k+1}\cdots i_n)} \right\} . \tag{3.427}$$

We list below some low-order coefficients from the papers [4, 10]

$$\mathcal{A}_{mk_1} = \frac{1}{2} \mathcal{R}^i{}_{mk_1} , \tag{3.428}$$

$$\mathcal{A}_{mk_1k_2} = \frac{2}{3} \nabla_{(k_1} \mathcal{R}_{|m|k_2)} , \tag{3.429}$$

$$\mathcal{A}_{mk_1k_2k_3} = \frac{3}{4} \nabla_{(k_1} \nabla_{k_2} \mathcal{R}_{|m|k_3)} - \frac{1}{4} \mathcal{R}_{l(k_1} R^l{}_{k_2|m|k_3)} . \tag{3.430}$$

3.8.5 Two-point Functions in Symmetric Spaces

Thus, we have calculated Taylor series of all two-point functions needed for the computation of heat kernel asymptotics. In some particular cases Taylor series can be summed up giving an exact formula. For example, one can easily sum up all terms without derivatives of curvatures, i.e. in the case when

$$\nabla_m R^i{}_{jkl} = 0 . \tag{3.431}$$

Recall that such manifolds are called *symmetric spaces*.

Neglecting all terms with derivatives of curvatures we find from the Taylor series (3.375) for the matrix γ that all odd order coefficients (3.376) vanish,

$$\gamma_{(2m+1)} = 0 , \tag{3.432}$$

and the even order coefficients (3.376) are just powers of the matrix $\bar{K}$,

$$\gamma_{(2m)} = \frac{(-1)^{m+1}}{2m+1}\bar{K}^m\,. \tag{3.433}$$

Therefore, the Taylor series (3.375) can be summed up giving a closed formula for the matrix γ, (3.362),

$$\gamma = -P\frac{\sin\sqrt{\bar{K}}}{\sqrt{\bar{K}}}\,. \tag{3.434}$$

All other two-point functions are easily computed by using this result. First, we obtain

$$\eta = -\frac{\sqrt{\bar{K}}}{\sin\sqrt{\bar{K}}}P^{-1}\,, \tag{3.435}$$

and

$$\Delta = \det\frac{\sqrt{\bar{K}}}{\sin\sqrt{\bar{K}}}\,. \tag{3.436}$$

Next, by using eq. (3.240) or, more generally, (3.337) we see that

$$D\bar{K} = 2\bar{K}\,. \tag{3.437}$$

By using this property one can show that the operator D, when applied to functions of the matrix $\bar{K}$, is equivalent to

$$Df(\bar{K}) = 2\bar{K}\frac{\partial}{\partial\bar{K}}f(\bar{K})\,. \tag{3.438}$$

Therefore, by using the eq. (3.434) we obtain

$$D\gamma = P\left(\frac{\sin\sqrt{\bar{K}}}{\sqrt{\bar{K}}} - \cos\sqrt{\bar{K}}\right). \tag{3.439}$$

To compute the matrix ξ we use the equation $\xi = I + (D\gamma)\eta$, (3.268). Then by using eq. (3.439) and (3.435) we obtain

$$\xi = I + P\left(\sqrt{\bar{K}}\cot\sqrt{\bar{K}} - I\right)P^{-1}\,. \tag{3.440}$$

We can also sum up the Taylor series (3.414) for the matrix $\mathcal{G}^{i'}{}_{j'm'}$ to obtain a closed formula. However, it is easier to obtain it directly from the equation (3.300), which in the case of symmetric spaces takes the form

$$(D+I)\mathcal{G}^{i'}{}_{j'm'} = g_p{}^{l'}\gamma^p{}_{m'}R^{i'}{}_{j'l'k'}\sigma^{k'}\,. \tag{3.441}$$

The solution of this equation has the form

$$\mathcal{G}^{i'}{}_{j'm'} = -R^{i'}{}_{j'l'k'}\sigma^{k'}H^{l'}{}_{m'}\,, \tag{3.442}$$

where $H = (H^{l'}{}_{m'})$ is a matrix that satisfies the equation

$$(D+2)H^{l'}{}_{m'} = -g_p{}^{l'}\gamma^p{}_{m'}\,, \tag{3.443}$$

or in the matrix form

$$(D+2)H = \frac{\sin\sqrt{\bar{K}}}{\sqrt{\bar{K}}}\,. \tag{3.444}$$

The solution of this equation which satisfies the initial condition $[\mathcal{G}^{i'}{}_{j'm'}] = 0$ has the form

$$H = \frac{I - \cos\sqrt{\bar{K}}}{\bar{K}}\,. \tag{3.445}$$

Similarly, we can compute the derivative of the generalized operator of parallel transport $\hat{\mathcal{A}}_{m'}$ defined by (3.315) in symmetric spaces with the additional restriction

$$\nabla_i \mathcal{R}_{jk} = 0\,. \tag{3.446}$$

The equation (3.314) in symmetric spaces takes the form

$$(D+I)\hat{\mathcal{A}}_{m'} = g_p{}^{l'}\gamma^p{}_{m'}\mathcal{R}_{l'k'}\sigma^{k'}\,. \tag{3.447}$$

The solution of this equation has the form

$$\hat{\mathcal{A}}_{m'} = -\mathcal{R}_{l'k'}\sigma^{k'}H^{l'}{}_{m'}\,, \tag{3.448}$$

with the same matrix H given by (3.445).

These formulas may be useful in the discussion of the heat kernel for covariantly constant background. Let us apply these formulas to the case of the maximally symmetric spaces of constant curvature. These are spheres and hyperbolic spaces with the curvature tensor given by

$$R^i{}_{jkl} = \Lambda(\delta^i{}_k g_{jl} - \delta^i{}_l g_{jk})\,, \tag{3.449}$$

where Λ is a constant. If $\Lambda > 0$ then this symmetric space is a sphere S^n, if $\Lambda < 0$, it is the hyperbolic space H^n. The Ricci tensor and the scalar curvature are easily computed

$$R_{ij} = (n-1)\Lambda g_{ij}, \tag{3.450}$$

$$R = n(n-1)\Lambda\,. \tag{3.451}$$

The matrix $\bar{K}$ in this case has the form

$$\bar{K}^{i'}{}_{j'} = 2\Lambda\sigma\Pi^{i'}{}_{j'}\,, \tag{3.452}$$

where $\mathit{\Pi} = (\mathit{\Pi}^{i'}{}_{j'})$ is an orthogonal projection to the plane orthogonal to the vector $\sigma^{i'}$ defined by

$$\mathit{\Pi}^{i'}{}_{j'} = \delta^{i'}_{j'} - \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}\,. \tag{3.453}$$

Indeed, it is not difficult to check that

$$\mathit{\Pi}^2 = \mathit{\Pi}, \tag{3.454}$$

and

$$\mathit{\Pi}^{j'}{}_{i'}\sigma^{i'} = \sigma_{j'}\mathit{\Pi}^{j'}{}_{i'} = 0\,. \tag{3.455}$$

Obviously, the trace of the projection $\mathit{\Pi}$ is

$$\operatorname{tr}\mathit{\Pi} = n - \frac{\sigma^i\sigma_i}{2\sigma} = n-1\,. \tag{3.456}$$

Therefore, the matrix $\bar{K}$ has the eigenvalue $2\mathit{\Lambda}\sigma$ with multiplicity $(n-1)$ and the eigenvalue 0 with multiplicity 1.

Using this projection we can easily compute any function of the matrix $\bar{K}$ as follows

$$f(\bar{K}) = f(0)(I - \mathit{\Pi}) + f(2\mathit{\Lambda}\sigma)\mathit{\Pi}\,. \tag{3.457}$$

Therefore, the trace and the determinant of a function of the matrix $\bar{K}$ are

$$\operatorname{tr} f(\bar{K}) = f(0) + (n-1)f(2\mathit{\Lambda}\sigma)\,, \tag{3.458}$$

$$\det f(\bar{K}) = f(0)\left(f(2\mathit{\Lambda}\sigma)\right)^{n-1}\,. \tag{3.459}$$

Thus the formal expressions obtained above for arbitrary symmetric spaces take a more explicit form. For the matrices γ, η, ξ and H we obtain from eqs. (3.434), (3.435), (3.440) and (3.445)

$$\gamma^{l}{}_{j'} = g^{l}{}_{i'}\left\{-\delta^{i'}{}_{j'}\mathit{\Phi} + \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}(\mathit{\Phi}-1)\right\}\,, \tag{3.460}$$

$$\eta^{i'}{}_{l} = g_{l}{}^{j'}\left\{-\delta^{i'}{}_{j'}\frac{1}{\mathit{\Phi}} + \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}\left(\frac{1}{\mathit{\Phi}}-1\right)\right\}\,, \tag{3.461}$$

$$\xi^{i}{}_{j} = \delta^{i}{}_{j}(1+F) - \frac{\sigma^i\sigma_j}{2\sigma}F\,, \tag{3.462}$$

$$H^{i'}{}_{j'} = \delta^{i'}{}_{j'}\mathit{\Psi} + \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}\left(\frac{1}{2} - \mathit{\Psi}\right)\,, \tag{3.463}$$

where

$$\Phi = \frac{\sinh\sqrt{-2\Lambda\sigma}}{\sqrt{-2\Lambda\sigma}}\,, \tag{3.464}$$

$$F = \sqrt{-2\Lambda\sigma}\coth\left(\sqrt{-2\Lambda\sigma}\right) - 1\,, \tag{3.465}$$

$$\Psi = \frac{1 - \cosh\sqrt{-2\Lambda\sigma}}{2\Lambda\sigma}\,. \tag{3.466}$$

Also, by using eq. (3.459) we obtain from (3.436) the Van Vleck-Morette determinant

$$\Delta = \frac{1}{\Phi^{n-1}}\,, \tag{3.467}$$

so that

$$\zeta = -\frac{n-1}{2}\log\Phi\,. \tag{3.468}$$

An important fact to realize is that for hyperbolic space, when $\Lambda < 0$, given any two points x and x' at a finite distance the Van Vleck-Morette determinant is equal to neither zero nor infinity.

Recall that the trace of the matrix ξ determines the Laplacian of the Synge function σ, therefore, we obtain

$$\nabla^i\nabla_i\sigma = \sigma^i{}_i = n + (n-1)F\,. \tag{3.469}$$

A useful property of the operator D is that when acting on scalar functions that depend only on σ it takes the form

$$Df(\sigma) = 2\sigma\frac{\partial}{\partial\sigma}f(\sigma)\,. \tag{3.470}$$

Then it is easy to check that

$$F = D\log\Phi\,. \tag{3.471}$$

Further, by using eqs. (3.442) and (3.448) we easily obtain the derivatives of the operators of parallel transport

$$\mathcal{G}^{i'}{}_{j'm'} = -\Psi R^{i'}{}_{j'm'k'}\sigma^{k'}\,, \tag{3.472}$$

$$\hat{\mathcal{A}}_{m'} = -\Psi\mathcal{R}_{m'k'}\sigma^{k'}\,. \tag{3.473}$$

We will need the Laplacian of the square root of Van Vleck-Morette determinant. First of all, when Laplacian acts of a scalar function that depends only on σ it takes a very simple form

$$\nabla^i\nabla_i f(\sigma) = \left(2\sigma\frac{\partial^2}{\partial\sigma^2} + \sigma^i{}_i\frac{\partial}{\partial\sigma}\right)f(\sigma)\,. \tag{3.474}$$

Let r be the geodesic distance between the points x and x'; then

$$\sigma = \frac{1}{2} r^2 \tag{3.475}$$

and

$$\nabla^i \nabla_i f(r) = \left\{ \frac{\partial^2}{\partial r^2} + (n-1)\sqrt{-\Lambda} \coth\left(r\sqrt{-\Lambda}\right) \frac{\partial}{\partial r} \right\} f(r) \,. \tag{3.476}$$

Now, by using the eqs. (3.467), (3.464), (3.469) and (3.465) we obtain

$$\Delta^{-1/2} \nabla^i \nabla_i \Delta^{1/2} = \frac{(n-1)}{2} \Lambda \left\{ \frac{(n-3)}{2} \left[\coth^2\left(r\sqrt{-\Lambda}\right) + \frac{1}{\Lambda r^2} \right] + 1 \right\} . \tag{3.477}$$

A very important observation is that for $n = 3$ this equation gives

$$\nabla^i \nabla_i \Delta^{1/2} = \Lambda \Delta^{1/2} \,, \tag{3.478}$$

that is, the function $\Delta^{1/2}$ is the eigenfunction of the Laplacian with the eigenvalue Λ, which is equal to $\frac{1}{6}R$ for $n = 3$.

3.9 Parallel Orthonormal Frame

Let x' be a fixed point in a manifold M and let us consider a sufficiently small neighborhood of x'. Then every point x in this neighborhood can be connected with the point x' by a unique geodesic. Let ${e_a}^{i'}$, $a = 1, \ldots, n$, be an orthonormal basis of vectors in the tangent space at the point x', that is,

$$g_{i'j'} {e_a}^{i'} {e_b}^{j'} = \delta_{ab} \,. \tag{3.479}$$

Such basis is called an *orthonormal frame*. We will use small Latin letters from the beginning of the alphabet, $a, b, c, \ldots$, to denote frame indices. Of course, they range over $1, \ldots, n$. Let ${e^a}_{i'}$ be the *dual orthonormal frame* of covectors in the cotangent space at the point x', which means that

$${e^b}_{i'} {e_a}^{i'} = {\delta^b}_a \,. \tag{3.480}$$

We extend the local orthonormal frame at the fixed point x' to a local orthonormal frame at the point x by parallel transport

$${e_a}^i = {g^i}_{j'} {e_a}^{j'} \,, \tag{3.481}$$

$${e^a}_i = {g_i}^{j'} {e^a}_{j'} \,, \tag{3.482}$$

where $g^{i}{}_{j'}$ is the operator of parallel transport of vectors along the geodesic from the point x' to the point x. Of course, the frame $e_a{}^i$ at the point x depends on the fixed point x' as a parameter. We will call such a frame *parallel*.

Here and everywhere below the coordinate indices of the tangent space at the point x' are denoted by primed letters. They are raised and lowered by the metric tensor $g_{i'j'}$ at the point x'. The derivatives with respect to x' will be denoted by primed indices as well.

The parameters of the geodesic connecting the points x and x', namely the unit tangent vector at the point x' and the length of the geodesic, (or, equivalently, the tangent vector at the point x' with the norm equal to the length of the geodesic), provide normal coordinate system near x'. Let $\sigma(x, x')$ be the Synge function. It is equal to one-half the square of the geodesic distance between the points x and x'. As we have seen earlier the derivatives $\sigma_i = \sigma_{;i}$ and $\sigma_{i'} = \sigma_{;j'}$ are the tangent vectors to the geodesic connecting the points x and x' at the points x and x' respectively pointing in opposite directions.

We define the frame components of tensors by projecting them onto the orthonormal frame, for example,

$$R^a{}_{bcd} = R^i{}_{jkl} e^a{}_i e_b{}^j e_c{}^k e_d{}^l \,. \tag{3.483}$$

Since our frame is parallel along geodesics it should be clear that the frame components of a covariantly constant tensor are simply constant.

Now, let us define the quantities

$$y^a = e^a{}_i \sigma^i = -e^a{}_{j'} \sigma^{j'} \,, \tag{3.484}$$

so that

$$\sigma^i = e_a{}^i y^a \qquad \text{and} \qquad \sigma^{i'} = -e_a{}^{i'} y^a \,. \tag{3.485}$$

Notice that $y^a = 0$ at $x = x'$. Further, we have the Jacobian matrix of the change of variables $x \mapsto y$,

$$\frac{\partial y^a}{\partial x^j} = -e^a{}_{i'} \eta^{i'}{}_j \,, \tag{3.486}$$

where $\eta^{i'}{}_j = \nabla_j \sigma^{i'}$. Therefore, the Jacobian is proportional to the Van Vleck determinant $\Delta(x, x')$ and is non-degenerate. Thus, the geometric parameters y^a provide a local coordinate system, which is called the *normal coordinates*.

3.10 Lie Groups

We briefly list here for the reference the definitions and some facts about Lie groups. For a more detailed (and precise) treatment the reader is referred

to the literature on the theory of Lie groups listed in the bibliography, for example, [44, 43, 50, 15].

A *group* G is a set of elements with an associative composition law, $*$, called the *group multiplication*, such that for any two elements x and y another element $z = x * y$ is defined. The multiplication sign $*$ is usually omitted and one simply writes $z = xy$. The product is supposed to be associative, that is, for any three elements x, y and z there holds

$$(xy)z = x(yz). \tag{3.487}$$

It is supposed that there exists an element e, called the *identity element* such that for any x

$$xe = ex = x\,. \tag{3.488}$$

Finally, every element is supposed to have an *inverse*, that is, for any element x there exists an element x^{-1} such that

$$x^{-1}x = xx^{-1} = e. \tag{3.489}$$

A group G is called *Abelian* (or commutative) if for any two elements x and y

$$xy = yx. \tag{3.490}$$

A subset H of elements of the group G is called a *subgroup* if it is itself a group with the same composition law. In particular, it contains the identity element and is closed under the group multiplication, that is, the products of any elements of H as well as their inverses belong to H. A subgroup H of a group G is called *invariant* if for any element x in G and for any element y in H the element xyx^{-1} belongs to H. A mapping $\varphi : G \to K$ from a group G to a group K is called a *homomorphism* if for any two elements $x, y \in G$

$$\varphi(xy) = \varphi(x)\varphi(y)\,. \tag{3.491}$$

In particular,

$$\varphi(x^{-1}) = [\varphi(x)]^{-1}\,, \tag{3.492}$$

$$\varphi(e_G) = e_K\,. \tag{3.493}$$

A group G is *finite* if it has finitely many elements. Infinite groups can be *discrete* or *continuous*. The elements of a continuous group can be parametrized by a set of continuous real parameters, called the local coordinates. That is, an element x is represented by local coordinates x^i, where $i = 1, \ldots, n$. If the number n of coordinates is finite then the group is called *finite dimensional* and the number n is called the *dimension* of the group.

The multiplication map and the inversion map are defined then by some functions

$$(xy)^i = F^i(x, y), \qquad (x^{-1})^i = f^i(x)\,. \tag{3.494}$$

A *Lie group* is a continuous group whose multiplication map and the inversion map are represented by analytic functions. These functions are, of course, not arbitrary but have to satisfy important identities that guarantee the properties (3.487), (3.488) and (3.489).

A curve $x(t)$ with a real parameter t on the Lie group G is called a *one-parameter subgroup* of G if for any t, s

$$x(t+s) = x(t)x(s), \tag{3.495}$$

$$x(0) = e, \tag{3.496}$$

$$x(-t) = [x(t)]^{-1}. \tag{3.497}$$

3.11 Lie Algebras

A *Lie algebra* $\mathfrak{g}$ is a vector space with an additional operation, called the *Lie bracket*. That is, for any two vectors X and Y another vector $Z = [X, Y]$ is defined. The Lie bracket is supposed to be bilinear (linear in each argument), anti-symmetric, that is,

$$[X, Y] = -[Y, X] \tag{3.498}$$

for any X and Y, and also to satisfy the cyclic identity (called the *Jacobi identity*)

$$[X, [Y, Z] + [Y, [Z, X] + [Z, [X, Y] = 0 \tag{3.499}$$

for any X, Y, Z. A Lie algebra is called real or complex depending on the nature of the scalars. The dimension of the Lie algebra is equal to its dimension as a vector space.

A typical example of a Lie algebra is the set of $n \times n$ square matrices, or, more generally, the vector space of operators on a Hilbert space, with the Lie bracket identified with the commutator of the operators

$$[X, Y] = XY - YX. \tag{3.500}$$

It is not difficult to see that all the conditions of the Lie bracket, including the Jacobi identity, are satisfied. That is why, one often simply calls the Lie bracket the *commutator*. In fact, it turns out that an arbitrary finite-dimensional Lie algebra is isomorphic to a Lie algebra of matrices.

A Lie algebra $\mathfrak{g}$ is called *Abelian* if all commutators of all vectors vanish. A subspace A of a Lie algebra L is a *Lie subalgebra* if it is closed under the Lie bracket, that is, if the commutator of any two vectors in the subalgebra remains in the subalgebra. A subspace J of a Lie algebra $\mathfrak{g}$ is an *ideal* if the commutator of any vector from J and any vector from the algebra $\mathfrak{g}$ remains in the ideal. Obviously, every ideal is a subalgebra. The maximal ideal N commuting with the whole algebra is called the *center* of the Lie algebra.

The elements of the center obviously commute with all elements of the Lie algebra.

A Lie algebra $\mathfrak{g}$ is called *nilpotent*, more precisely, *n-step nilpotent*, if there is a positive integer n such that there is at least one nonvanishing commutator of order n and all commutators of order higher than n vanish, that is, for any m vectors $X_1, \ldots, X_m$ with $m > n$

$$[X_m, \cdots [X_2, X_1] \cdots] = 0\,. \tag{3.501}$$

Let T_i, $a = 1, \ldots, n$, be a basis in the Lie algebra $\mathfrak{g}$. Then the vectors T_i are called the *generators* of the algebra. The generators must satisfy the *commutation relations*

$$[T_i, T_j] = \sum_{c=1}^{n} C^k{}_{ij} T_k\,, \tag{3.502}$$

where $C^i{}_{jk}$ are some real constants called the *structure constants* of the Lie algebra. The structure constants are anti-symmetric in the last two indices

$$C^i{}_{jk} = -C^i{}_{kj}\,, \tag{3.503}$$

and satisfy the conditions

$$\sum_{m=1}^{n} \left(C^i{}_{jm} C^m{}_{kl} + C^i{}_{km} C^m{}_{lj} + C^i{}_{lm} C^m{}_{jk} \right) = 0\,, \tag{3.504}$$

which are a direct consequence of the Jacobi identity. These identities impose severe restriction on the structure of the Lie algebra. The structure constants completely determine the Lie algebra (up to a linear transformation of the basis) and allows the complete classification of all Lie algebras.

Every Lie group G naturally defines a Lie algebra as follows. Let us assume that the local coordinates on the Lie group are chosen so that the coordinates of the identity element are equal to zero, that is, $(e^j) = (0, \ldots, 0)$. Let us define the numbers

$$C^i{}_{jk} = \left(\frac{\partial^2}{\partial x^j \partial y^k} - \frac{\partial^2}{\partial x^j \partial y^k} \right) F^i(x, y)\Big|_{x,y=0}\,. \tag{3.505}$$

These numbers are obviously antisymmetric in lower indices. Also, by using the identities for the group multiplication map one can show that they satisfy the identities (3.504). Therefore, these constants define a specific Lie algebra $\mathfrak{g}$ associated with the Lie group G.

A linear map $\rho : \mathfrak{g} \to \mathfrak{h}$ from a Lie algebra $\mathfrak{g}$ to the Lie algebra $\mathfrak{h}$ is a *homomorphism* if for any $X, Y \in \mathfrak{g}$,

$$\rho([X, Y]) = [\rho(X), \rho(Y)]\,. \tag{3.506}$$

A *representation* of the Lie algebra $\mathfrak{g}$ is a homomorphism

$$\rho : \mathfrak{g} \to \text{Mat}\,(N, \mathbb{R}) \tag{3.507}$$

so that every element X of the Lie algebra is represented by a $N \times N$ matrix $\rho(X)$ and the Lie bracket is represented by the commutator of these matrices. Here N can be, in general, an arbitrary positive integer, not necessarily equal to the dimension of the Lie algebra n.

Let C_i denote the real $n \times n$ matrices with the entries determined by the structure constants $(C_i)^j{}_k = C^i{}_{jk}$. Then the Jacobi identities (3.504) can be written in the form

$$[C_i, C_j] = \sum_{k=1}^{n} C^k{}_{ij} C_k \,. \tag{3.508}$$

This identity defines the Lie algebra $\mathfrak{g}$ of the Lie group G in *adjoint representation*. The matrices C_i are called the *generators* of the adjoint representation of the Lie algebra.

In adjoint representation an element $X = \sum_{i=1}^{n} X^i T_i$ is represented by the matrix

$$C(X) = \sum_{i=1}^{n} X^i C_i \,. \tag{3.509}$$

The *Killing form* on a Lie algebra is a symmetric bilinear form defined by

$$B(X, Y) = \text{tr}\, C(X) C(Y) = - \sum_{i,j=1}^{n} \gamma_{ij} X^i Y^j, \tag{3.510}$$

where

$$\gamma_{ij} = - \text{tr}\, C_i C_j = - \sum_{k,l=1}^{n} C^l{}_{ik} C^k{}_{jl} \,. \tag{3.511}$$

One can show that the Killing form satisfies the identity, for any X, Y, Z,

$$B([X, Y], Z) + B(Y, [X, Z]) = 0 \,. \tag{3.512}$$

This follows directly from the Jacobi identity (3.499).

A Lie algebra is called *semi-simple* if the Killing form, that is, the matrix $\gamma = (\gamma_{ij})$, is non-degenerate. In this case the matrix γ_{ij} is also called the *Cartan metric*. We will denote the inverse of the matrix γ by $\gamma^{-1} = (\gamma^{ij})$. The maximal Abelian subalgebra of a semi-simple Lie algebra is called *Cartan subalgebra*. A semi-simple Lie algebra is called *simple* if there is a basis such that the matrix γ is proportional to the unit matrix. A Lie algebra is *compact* if the matrix γ is positive definite. For compact semi-simple algebras the the generators of the adjoint representation have the following property

$$C_i^T = -\gamma C_i \gamma^{-1} \tag{3.513}$$

and are, therefore, traceless

$$\operatorname{tr} C_i = \sum_{j=1}^{n} C^j{}_{ij} = 0\,. \tag{3.514}$$

Let us consider a matrix representation of the Lie algebra $\mathfrak{g}$ so that the Lie bracket is determined by the commutator of matrices (3.500). Then one can define the matrix T^2 (called the *Casimir operator* (or invariant) of the representation) by

$$T^2 = \sum_{i,j=1}^{n} \gamma^{ij} T_i T_j\,. \tag{3.515}$$

It is easy to show that the Casimir operator commutes with all elements of the Lie algebra, that is,

$$[T_i, T^2] = 0\,. \tag{3.516}$$

In adjoint representation it is defined by

$$C^2 = \sum_{i,j=1}^{n} \gamma^{ij} C_i C_j\,. \tag{3.517}$$

3.12 Matrix Lie Groups

Most important examples of Lie groups are the groups of matrices. The set of all *real invertible* $n \times n$ matrices $GL(n, \mathbb{R})$ forms a group under the law of matrix multiplication called the *general linear* Lie group. The identity is obviously the unit matrix I. The Lie algebra $\mathfrak{gl}(n, \mathbb{R})$ of $GL(n, \mathbb{R})$ is the set of all real $n \times n$ matrices $\operatorname{Mat}(n, \mathbb{R})$. The dimension of this group is equal to the number of the matrix elements:

$$\dim GL(n, \mathbb{R}) = n^2. \tag{3.518}$$

Notice that if X is a matrix in the Lie algebra then the matrix $\exp(X)$ belongs to its Lie group. In some sense the non-linear relations on the Lie group are translated to linear equations on its Lie algebra, in particular, by using the relation

$$\det(\exp X) = \exp(\operatorname{tr} X)\,. \tag{3.519}$$

That is why, it is much easier to count the number of independent entries in the Lie algebra than in the Lie group.

The set of all real invertible matrices $n \times n$ matrices with unit determinant $SL(n, \mathbb{R})$ forms a subgroup of $GL(n, \mathbb{R})$ called the *special linear group*. If the determinant of $\exp X$ is equal to one then by the above formula the trace of X must be zero,

$$\operatorname{tr} X = 0\,. \tag{3.520}$$

That is why, its Lie algebra $\mathfrak{sl}(n,\mathbb{R})$ is the set of all *real* $n \times n$ *traceless* matrices. Since there is only one constraint the dimension of the special linear group is

$$\dim SL(n,\mathbb{R}) = n^2 - 1. \tag{3.521}$$

A real matrix A is called *orthogonal* if

$$A^T A = I\,, \tag{3.522}$$

or

$$A^T = A^{-1}\,. \tag{3.523}$$

In particular, this means that the determinant of an orthogonal matrix can be equal to $+1$ or -1. It is not difficult to see that the product of orthogonal matrices is an orthogonal matrix. Also, the product of matrices with unit determinant is a matrix with unit determinant. Therefore, the set of all real orthogonal matrices with unit determinant $SO(n)$ forms a subgroup of $GL(n,\mathbb{R})$ called the *special orthogonal group*. Notice that if the matrix $A = \exp X$ is orthogonal then $A^T = \exp(X^T) = \exp(-X) = A^{-1}$, and, therefore, the matrix X must be anti-symmetric. Thus, the Lie algebra $\mathfrak{so}(n)$ is the set of all *real* $n \times n$ *anti-symmetric* matrices. Such a matrix has zeros on the diagonal and the only independent entries are in its upper triangular part. The number of entries in the upper triangular part is $n(n-1)/2$. Therefore, the dimension of the special orthogonal group is

$$\dim SO(n) = \frac{n(n-1)}{2}. \tag{3.524}$$

More generally, let η be a $n \times n$ diagonal matrix with -1 and $+1$ on the diagonal, that is,

$$\eta = \text{diag}\,(-1, 1, \ldots, 1)\,. \tag{3.525}$$

A real matrix A is called *pseudo-orthogonal* if

$$A^T \eta A = \eta\,, \tag{3.526}$$

or (note that $\eta^{-1} = \eta$)

$$A^T = \eta A^{-1} \eta^{-1}\,. \tag{3.527}$$

It is not difficult to see that the product of pseudo-orthogonal matrices is a pseudo-orthogonal matrix. Therefore, the set of all real pseudo-orthogonal $n \times n$ matrices with unit determinant $SO(1, n-1)$ forms a subgroup of $GL(n,\mathbb{R})$ called the *special pseudo-orthogonal group*. The Lie algebra $\mathfrak{so}(1, n-1)$ is the set of all real $n \times n$ matrices satisfying the relation

$$X^T = -\eta X \eta^{-1}\,. \tag{3.528}$$

The dimension of the special pseudo-orthogonal group is

$$\dim SO(1,n-1) = \dim SO(n) = \frac{n(n-1)}{2}. \tag{3.529}$$

Similarly, one can define the groups of complex matrices $GL(n,\mathbb{C})$ and $SL(n,\mathbb{C})$ and their Lie algebras $\mathfrak{gl}(n,\mathbb{C})$ and $\mathfrak{sl}(n,\mathbb{C})$ Obviously,

$$\dim GL(n,\mathbb{C}) = 2n^2 \tag{3.530}$$

and

$$\dim SL(n,\mathbb{C}) = 2(n^2-1). \tag{3.531}$$

A complex matrix A is called *unitary* if

$$A^*A = I\,, \tag{3.532}$$

or

$$A^* = A^{-1}, \tag{3.533}$$

where $A^* = \overline{A^T}$ is the Hermitian conjugate combining the transposition with complex conjugation. It is easy to see that the product of unitary matrices is unitary. Therefore, the set of all complex $n \times n$ unitary matrices with unit determinant $SU(n)$ forms a subgroup of $GL(n,\mathbb{C})$ called the *special unitary group*. Notice that if the matrix $A = \exp X$ is unitary then $A^* = \exp(X^*) = \exp(-X) = A^{-1}$, and, therefore, the matrix X must be anti-Hermitian,

$$X^* = -X\,. \tag{3.534}$$

Also, since $\det \exp X = \exp \operatorname{tr} X = 1$ it must be traceless. Thus, the Lie algebra $\mathfrak{su}(n)$ is the set of all *complex* $n \times n$ *anti-Hermitian traceless* matrices. Such a matrix has imaginary entries on the diagonal whose sum is equal to zero and the other independent entries are in its upper triangular part. The number of real entries in the upper triangular part is $n(n-1)$. Therefore, the dimension of the special unitary group is

$$\dim SU(n) = n - 1 + n(n-1) = n^2 - 1. \tag{3.535}$$

3.13 Geometry of Lie Groups

It turns out that Lie groups are smooth (and particularly nice) manifolds. We briefly describe some of the properties of Lie groups that we will use later in the book.

Let G be a Lie group of dimension n. Let x^i, $i = 1,\dots,n$, be local coordinates on G with the origin at the identity element I of the group. Let $F(x,y)$ be the group multiplication map and $\varphi(x) = x^{-1}$ be the inverse map. They satisfy the identities

$$F^i(x,0) = F^i(0,x) = x^i\,, \tag{3.536}$$
$$F^i(x,\varphi(x)) = F^i(\varphi(x),x) = 0\,, \tag{3.537}$$
$$F^i(x,F(y,z)) = F^i(F(x,y),z)\,. \tag{3.538}$$

Next, we introduce real $n \times n$ matrices $L = (L^i{}_j)$ and $R = (R^i{}_j)$ by

$$Y^i{}_j(x) = \frac{\partial}{\partial y^j} F^i(y,x)\Big|_{y=0}\,, \tag{3.539}$$

$$X^i{}_j(x) = \frac{\partial}{\partial y^j} F^i(x,y)\Big|_{y=0}\,. \tag{3.540}$$

By differentiating the identities (3.539)-(3.538) one can show

$$X(0) = Y(0) = I\,, \tag{3.541}$$

where I is the unit matrix. Therefore, these matrices are invertible, at least in the neighborhood of the identity.

Now, by differentiating the basic identity (3.538) one can obtain

$$Y^k{}_i \partial_k Y^m{}_j - Y^k{}_j \partial_k Y^m{}_i = -C^l{}_{ij} Y^m{}_l\,, \tag{3.542}$$
$$X^k{}_i \partial_k X^m{}_j - X^k{}_j \partial_k X^m{}_i = C^l{}_{ij} X^m{}_l\,, \tag{3.543}$$

where $C^i{}_{jk}$ are the structure constants of the group defined by (3.505).

These identities can be rewritten in the coordinate free form by introducing the vector fields

$$Y_i = Y^k{}_i \partial_k\,, \qquad X_i = X^k{}_i \partial_k\,. \tag{3.544}$$

Then they take the form

$$[Y_i, Y_j] = -C^k{}_{ij} Y_k\,, \tag{3.545}$$
$$[X_i, X_j] = C^k{}_{ij} X_k\,. \tag{3.546}$$

Moreover, one can show that the vector fields X_a and Y_b commute

$$[Y_i, X_j] = 0\,. \tag{3.547}$$

The vector fields Y_i are called the *left-invariant* vector fields and the vector fields X_i are called the *right-invariant* vector fields.

The matrices X and Y take especially simple form in a special coordinate system called *canonical coordinates*. In these coordinates

$$x^i = Y^i{}_j(x) x^j = X^i{}_j(x) x^j\,. \tag{3.548}$$

Differentiating these equations and using the algebra of the left- and right-invariant vector fields one can obtain the following differential equation for

the matrices X and Y

$$\left[x^i\partial_i - C(x) + I\right] Y^{-1} = I\,, \tag{3.549}$$

$$\left[x^i\partial_i + C(x) + I\right] X^{-1} = I\,. \tag{3.550}$$

where $C(x)$ is a matrix defined by

$$C(x) = C_i x^i\,, \tag{3.551}$$

and $C_i = (C^j{}_{ik})$ are the generators of the adjoint representation. The solution of these equations is

$$Y = \frac{C}{\exp(C) - \mathbb{I}} = \exp[-C/2]\frac{C/2}{\sinh\left(C/2\right)}\,, \tag{3.552}$$

$$X = \frac{C}{\mathbb{I} - \exp(-C)} = \exp[C/2]\frac{C/2}{\sinh\left(C/2\right)}\,, \tag{3.553}$$

where we denoted $C = C(x)$ for simplicity.

Now, suppose that there exists a symmetric non-degenerate matrix $\gamma = (\gamma_{ij})$ such that

$$\gamma_{jk}C^k{}_{im} + \gamma_{mk}C^k{}_{ij} = 0\,; \tag{3.554}$$

this simply means that the matrices γC_i are anti-symmetric or

$$C_i^T = -\gamma C_i \gamma^{-1}\,, \tag{3.555}$$

where $\gamma^{-1} = (\gamma^{ij})$ is the matrix inverse to the matrix $\gamma = (\gamma_{ij})$. One can show that for semi-simple group such matrix, called the *Cartan metric*, always exists and can be defined, for example, by

$$\gamma_{ij} = -C^k{}_{im}C^m{}_{jk}\,. \tag{3.556}$$

Moreover, for compact semisimple groups it is, in addition, positive definite; and for compact simple group it is proportional to the Euclidean metric.

Then every semi-simple Lie group has a natural Riemannian metric of the form

$$g^{ij} = \gamma^{ab}X^i{}_a X^j{}_b = \gamma^{ab}Y^i{}_a Y^j{}_b\,. \tag{3.557}$$

Therefore, both the left-invariant vector fields and the right-invariant vector fields provide (different) orthonormal frames. Moreover, the fundamental fact about the Lie groups is that both the left-invariant vector fields and the right-invariant vector fields are Killing vectors of the metric defined above. That is, the metric is invariant under the isometries defined by these vector fields called the left and the right action on the group. That is why, it is called the *bi-invariant metric*.

By using the properties of the vectors X_i and Y_i one can compute the Riemann curvature tensor of this metric

$$R^{ijkl} = R^{abcd} X^i{}_a X^j{}_b X^k{}_c X^l{}_d = R^{abcd} Y^i{}_a Y^j{}_b Y^k{}_c Y^l{}_d \,, \tag{3.558}$$

where

$$R^a{}_{bcd} = \frac{1}{4} C^a{}_{bf} C^f{}_{cd} \tag{3.559}$$

are the frame components of the Riemann tensor. Note that the frame indices like a, b, c, d, are raised and lowered by the matrix γ_{ab} and its inverse γ^{ab} and the coordinate indices like i, j, k, l, are raised and lowered by the metric g_{ij} and its inverse g^{ij}.

Moreover, one can also show that the curvature tensor is covariantly constant

$$\nabla_m R_{ijkl} = 0 \,. \tag{3.560}$$

The frame components of the Ricci tensor are

$$R_{ab} = -\frac{1}{4} C^d{}_{ac} C^c{}_{bd} \,, \tag{3.561}$$

and the scalar curvature is

$$R = -\frac{1}{4} \gamma^{ab} C^d{}_{ac} C^c{}_{bd} \,. \tag{3.562}$$

Finally, the scalar Laplacian is simply

$$\Delta = \gamma^{ij} X_i X_j = \gamma^{ij} Y_i Y_j \,. \tag{3.563}$$

On semi-simple Lie groups one can compute the basic two-point geometric quantities like the Synge function $\sigma(x, x')$ and the Van Vleck-Morette determinant $\Delta(x, x')$ exactly. In canonical coordinates with the origin at the point x' they have the form

$$\sigma(x, x') = \frac{1}{2} \langle x, \gamma x \rangle = \frac{1}{2} \gamma_{ij} x^i x^j \,, \tag{3.564}$$

$$\Delta(x, x') = \det \left(\frac{C(x)/2}{\sinh [C(x)/2]} \right) . \tag{3.565}$$

Now, one can show that the function $\Delta^{1/2}$ is an eigenfunction of the Laplacian with the eigenvalue equal to $R/6$,

$$\Delta \Delta^{1/2}(x, x') = \frac{1}{6} R \Delta^{1/2}(x, x') \,. \tag{3.566}$$

Of course, here one should not confuse the Laplacian Δ with the Van Vleck-Morette determinant $\Delta(x, x')$.

3.14 Geometry of Symmetric Spaces

3.14.1 Algebraic Structure of Curvature Tensor

Symmetric spaces (more precisely, locally symmetric spaces) are very special manifolds with a metric whose Riemann curvature tensor $R^i{}_{jkl}$ is covariantly constant,

$$\nabla_i R^j{}_{klm} = 0\,. \tag{3.567}$$

By taking the commutator of second covariant derivatives of the Riemann tensor we get

$$R^{ij}{}_{km}R^k{}_{nlp} - R^{ij}{}_{kn}R^k{}_{mlp} + R^{ij}{}_{kl}R^k{}_{pmn} - R^{ij}{}_{kp}R^k{}_{lmn} = 0\,. \tag{3.568}$$

This condition imposes rather strict constraints on the possible algebraic structure of the curvature tensor.

We will also assume that the manifold under consideration is *simply connected* and *complete*. This means, roughly speaking, that each closed loop in M can be continuously deformed to a point and that the manifold M does not have a boundary. Such manifold is called a *globally symmetric space* (or simply symmetric space).

A symmetric space is said to be *compact*, *non-compact* or *Euclidean* if all sectional curvatures are positive, negative or zero. A product of a compact symmetric space and a non-compact symmetric space is called a *semi-simple* symmetric space.

A generic symmetric space is the product of a Euclidean space and a semi-simple symmetric space. A symmetric space is *irreducible* if it is not a product of symmetric spaces of low dimension. A generic semi-simple symmetric space is the product of irreducible symmetric spaces.

For a semi-simple symmetric space the frame components of the curvature tensor (in the parallel orthonormal frame) can be presented in the form [8, 12]

$$R_{abcd} = -\beta_{\mu\nu}E^\mu{}_{ab}E^\mu{}_{cd}\,, \tag{3.569}$$

where $\beta_{\mu\nu}$ is a symmetric nondegenerate $p \times p$ matrix, with indices running over $\mu, \nu = 1, 2, \ldots, p$, and $E^\mu{}_{ab}$ is a collection of p anti-symmetric 2-tensors. We introduce here a new type of indices, namely Greek indices, which will run over $1, 2, \ldots, p$, where p is some integer $p \leq n(n-1)/2$. The matrix $\beta = (\beta_{\mu\nu})$ and its inverse, $\beta^{-1} = (\beta^{\mu\nu})$, will be used to raise and to lower the Greek indices. Note that the matrix β is negative definite for compact symmetric spaces and positive definite for non-compact symmetric spaces. For a general space it is indefinite. That is why, in our case it will be positive definite.

Next, we define $n \times n$ matrices $D_\mu = (D^a{}_{\mu b})$, where

$$D^a{}_{\mu b} = \delta^{ca}\beta_{\mu\nu}E^\nu{}_{cb}\,. \tag{3.570}$$

Then the curvature tensor can be written as

$$R^a{}_{bcd} = -D^a{}_{\mu b} E^\mu{}_{cd}\,, \tag{3.571}$$

$$R^a{}_b{}^c{}_d = -\beta^{\mu\nu} D^a{}_{\mu b} D^c{}_{\nu d}\,, \tag{3.572}$$

and the Ricci tensor and the scalar curvature are

$$R^a{}_b = \beta^{\mu\nu} D^a{}_{\mu c} D^c{}_{\nu b}, \tag{3.573}$$

$$R = \beta^{\mu\nu} D^a{}_{\mu c} D^c{}_{\nu a}\,. \tag{3.574}$$

Also, we have identically,

$$D^a{}_{\mu[b} E^\mu{}_{cd]} = 0\,. \tag{3.575}$$

The matrices D_μ are traceless and generate the *holonomy algebra*, $\mathfrak{h}$,

$$[D_\mu, D_\nu] = F^\alpha{}_{\mu\nu} D_\alpha\,, \tag{3.576}$$

where $F^\alpha{}_{\mu\nu}$ are the structure constants of the holonomy group. The structure constants of the holonomy group define the $p \times p$ matrices F_μ, by $(F_\mu)^\alpha{}_\beta = F^\alpha{}_{\mu\beta}$, which generate the adjoint representation of the holonomy algebra,

$$[F_\mu, F_\nu] = F^\alpha{}_{\mu\nu} F_\alpha\,. \tag{3.577}$$

For symmetric spaces the introduced quantities satisfy additional algebraic constraints. The most important consequence of the eq. (3.568) is the equation [8, 12]

$$E^\mu{}_{ac} D^c{}_{\alpha b} - E^\mu{}_{bc} D^c{}_{\alpha a} = F^\mu{}_{\alpha\beta} E^\beta{}_{ab}\,. \tag{3.578}$$

Next, by using the eqs. (3.576) and (3.578) one can prove that the matrix $\beta = (\beta_{\mu\nu})$ and the matrices F_α satisfy the equation

$$(F_\alpha)^T = -\beta F_\alpha \beta^{-1}\,, \tag{3.579}$$

which means, in particular, that the matrices F_α are traceless.

Now, we introduce a new type of indices, the capital Latin indices, $A, B, C, \ldots$, which split according to $A = (a, \mu)$ and run from 1 to $N = p+n$. We define new quantities $C^A{}_{BC}$ by

$$C^\mu{}_{ab} = E^\mu{}_{ab}, \tag{3.580}$$

$$C^a{}_{\mu b} = -C^a{}_{b\mu} = D^a{}_{\mu b}, \tag{3.581}$$

$$C^\mu{}_{\alpha\beta} = F^\mu{}_{\alpha\beta}\,, \tag{3.582}$$

all other components being zero, and new $N \times N$ matrices C_A so that $(C_A)^B{}_C = C^B{}_{AC}$.

Then by using the eqs. (3.575), (3.576), (3.577) and (3.578) one can show that the quantities $C^A{}_{BC}$ satisfy the Jacobi identities

$$C^A{}_{B[C}C^C{}_{DE]} = 0\,, \tag{3.583}$$

which means that the matrices C_A satisfy the commutation relations

$$[C_A, C_B] = C^C{}_{AB}C_C\,, \tag{3.584}$$

and generate the adjoint representation of some Lie algebra $\mathfrak{g}$ with the structure constants $C^A{}_{BC}$. Note that the holonomy algebra $\mathfrak{h}$ is a subalgebra of the algebra $\mathfrak{g}$.

Next, we define a symmetric nondegenerate $N \times N$ matrix $\gamma = (\gamma_{AB})$

$$\gamma = (\gamma_{AB}) = \begin{pmatrix} \delta_{ab} & 0 \\ 0 & -\beta_{ik} \end{pmatrix}. \tag{3.585}$$

This matrix and its inverse $\gamma^{-1} = (\gamma^{AB})$ will be used to lower and to raise the capital Latin indices. Then, by using the eq. (3.578) one can show that the matrix γ and the matrices C_A satisfy the equation

$$(C_A)^T = -\gamma C_A \gamma^{-1}\,, \tag{3.586}$$

which means, in particular, that the matrices C_A are traceless; thus the algebra $\mathfrak{g}$ is compact.

3.14.2 Killing Vectors Fields

The Killing vector fields ξ_i are defined by the equation

$$\nabla_a \xi_b + \nabla_b \xi_a = 0\,. \tag{3.587}$$

By differentiating this equation, commuting derivatives and using the curvature identities we obtain

$$\nabla_a \nabla_b \xi^c = -R^c{}_{bda}\xi^d\,. \tag{3.588}$$

This enables one to obtain (by induction) all derivatives of Killing vectors

$$\nabla_{a_{2k}} \cdots \nabla_{a_1} \xi^b = (-1)^k R^b{}_{a_1 c_1 a_2} R^{c_1}{}_{a_3 c_2 a_4} \cdots R^{c_{k-1}}{}_{a_{2k-1} c_k a_{2k}} \xi^{c_k}\,, \tag{3.589}$$

$$\nabla_{a_{2k+1}} \cdots \nabla_{a_1} \xi^b = (-1)^k R^b{}_{a_1 c_1 a_2} R^{c_1}{}_{a_3 c_2 a_4} \cdots R^{c_{k-1}}{}_{a_{2k-1} c_k a_{2k}} \nabla_{a_{2k+1}} \xi^{c_k}\,. \tag{3.590}$$

These derivatives determine all coefficients of the covariant Taylor series for the Killing vectors and allows one to compute them explicitly in a closed form. Let $K = (K^a{}_b)$ be a matrix defined by

$$K^{ab} = R^a{}_c{}^b{}_d y^c y^d = \beta^{\mu\nu} D^a{}_{\mu c} y^c D^b{}_{\nu d} y^d \,, \tag{3.591}$$

and $N = (N^a{}_b)$ and $M = (M^a{}_b)$ be the matrices defined by

$$N = \cosh\sqrt{-K}, \tag{3.592}$$

$$M = \frac{\sinh\sqrt{-K}}{\sqrt{-K}}. \tag{3.593}$$

Then by summing the covariant Taylor series we obtain Killing vectors in a symmetric space computed in our papers [8, 12]

$$\xi^a(x) = N^a{}_b(y)\xi^b(x') + M^a{}_b(y) y^c \xi^b{}_{;c}(x') \,. \tag{3.594}$$

Thus, Killing vector fields at any point x are determined by their values $\xi^a(x')$ and the values of their derivatives $\xi^a{}_{;c}(x')$ at the fixed point x'.

One can show that there are $N = n+p$ linearly independent Killing vector fields, and, therefore, there is a basis $(\xi_A{}^i) = (P_a{}^i, L_\mu{}^i)$ defined by [8, 12]

$$P_a{}^i = e_b{}^i N^b{}_a \,, \tag{3.595}$$

$$L_\mu{}^i = -e_b{}^i M^b{}_a y^c D^a{}_{\mu c} \,. \tag{3.596}$$

3.14.3 Lie Derivatives

The Lie derivatives of scalar fields along Killing vector fields are first-order differential operators $(\mathcal{L}_A) = (\mathcal{L}_a, \mathcal{L}_\mu)$ defined by

$$\mathcal{L}_A = \xi_A{}^i \partial_i \,. \tag{3.597}$$

These operators take particularly simple form in normal coordinates. Let $T = (T^a{}_b)$ be a matrix defined by

$$T = \sqrt{-K}\coth\sqrt{-K} \,. \tag{3.598}$$

Then

$$\mathcal{L}_a = T^b{}_a(y)\frac{\partial}{\partial y^b} \,, \tag{3.599}$$

$$\mathcal{L}_\mu = -D^b{}_{\mu a} y^a \frac{\partial}{\partial y^b} \,. \tag{3.600}$$

The fundamental fact about the Lie derivatives $\mathcal{L}_A$ is that they satisfy the commutation relations [8, 12]

$$[\mathcal{L}_A, \mathcal{L}_B] = C^C{}_{AB}\mathcal{L}_C\,, \tag{3.601}$$

and generate the *isometry algebra* of the symmetric space M. For semi-simple symmetric spaces the isometry algebra is isomorphic to the Lie algebra $\mathfrak{g}$ defined above. Furthermore, the operators $\mathcal{L}_\mu$ form a Lie algebra

$$[\mathcal{L}_\mu, \mathcal{L}_\nu] = F^\alpha{}_{\mu\nu}\mathcal{L}_\alpha\,, \tag{3.602}$$

called the *isotropy subalgebra*; for semi-simple symmetric spaces the isotropy subalgebra is isomorphic to the holonomy algebra $\mathfrak{h}$ defined above.

Killing vector fields satisfy many important identities. By using one of them,

$$\gamma^{AB}\xi_A{}^i\xi_B{}^j = g^{ij}\,, \tag{3.603}$$

we see that the scalar Laplacian Δ can be expressed in terms of Lie derivatives by

$$\Delta = \gamma^{AB}\mathcal{L}_A\mathcal{L}_B\,. \tag{3.604}$$

Then one can easily show that Laplacian commutes with Lie derivatives

$$[\mathcal{L}_A, \Delta] = 0\,. \tag{3.605}$$

3.15 Geometric Interpretation of Partial Differential Operators

The theory of second-order elliptic partial differential operators on manifolds is closely related with Riemannian geometry. The advantage of using geometric language for studying partial differential equations consists in the fact that operators like Laplacian are natural operators which are defined in terms of intrinsic geometry of the manifold, and, therefore, are invariant under diffeomorphisms, that is, under changes of local coordinates. Therefore, one can apply the whole machinery of differential geometry, which makes the study of partial differential operators much more efficient.

3.15.1 Laplace Type Operators

Let M be a n-dimensional manifold with local coordinates x^i, $i = 1, \ldots, n$. Let L be an elliptic second-order partial differential operator acting on the smooth functions on M. Such operator has a general form

$$L = -\alpha^{ij}(x)\partial_i\partial_j + \beta^j(x)\partial_j + \gamma(x), \tag{3.606}$$

where $\alpha^{ij}(x)$ is a real symmetric positive matrix valued function. Therefore, this matrix can be identified with the Riemannian metric, that is, we denote

$$g^{ij} = \alpha^{ij} \tag{3.607}$$

and the entries of the inverse matrix $(g^{ij})^{-1}$ by g_{ij}. As usual, we denote by g the determinant of the metric, $g = \det g_{ij}$.

The *Laplacian* Δ is an invariant second-order partial differential operator acting on tensor fields on M defined by

$$\Delta = g^{ij}\nabla_i\nabla_j\,. \tag{3.608}$$

The *scalar Laplacian* (or *Laplace-Beltrami operator*) Δ is an invariant second-order partial differential operator defined by the above equation acting on smooth functions on M. By using explicit formulas for Christoffel symbols, in particular, the eq. (3.88) one can obtain for scalar Laplacian the following expression in local coordinates

$$\begin{aligned}\Delta &= g^{ij}\partial_i\partial_j + \Gamma^j\partial_j \\ &= g^{-1/2}\partial_i g^{1/2} g^{ij}\partial_j\,,\end{aligned} \tag{3.609}$$

where

$$\Gamma^j = g^{-1/2}\partial_i\left(g^{1/2}g^{ij}\right)\,. \tag{3.610}$$

Recall that when we write an operator in such form then it is assumed that it acts on a function f in the following way

$$\Delta f = g^{-1/2}\partial_i\left(g^{1/2}g^{ij}\partial_j f\right)\,. \tag{3.611}$$

Now, the operator L can be rewritten in the form (compare to Sec. 2.3.1)

$$L = -g^{-1/2}\left(\partial_i + \mathcal{A}_i\right) g^{1/2} g^{ij}\left(\partial_j + \mathcal{A}_j\right) + Q\,, \tag{3.612}$$

where

$$\mathcal{A}_i = -\frac{1}{2}g_{ij}\left(\beta^j + \Gamma^j\right)\,, \tag{3.613}$$

$$Q = \gamma + g^{ij}\mathcal{A}_i\mathcal{A}_j + g^{-1/2}\partial_i\left(g^{1/2}g^{ij}\mathcal{A}_j\right)\,. \tag{3.614}$$

Furthermore, by using the covariant derivatives this operator can be written in the form

$$L = -\left(\nabla_i + \mathcal{A}_i\right) g^{ij}\left(\nabla_j + \mathcal{A}_j\right) + Q, \tag{3.615}$$

also

$$Q = \gamma + g^{ij}\mathcal{A}_i\mathcal{A}_j + g^{ij}\nabla_i\mathcal{A}_j\,. \tag{3.616}$$

Notice that the operator L is a sum of the Laplacian and a first order operator,

$$L = -\Delta - 2g^{ij}\mathcal{A}_i\nabla_j + \gamma\,. \tag{3.617}$$

We call the vector $\mathcal{A}_i$ the generalized connection and the tensor

$$\mathcal{R}_{ij} = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i \tag{3.618}$$

the generalized curvature. Obviously, if $\mathcal{A}_i$ is a gradient, that is,

$$\mathcal{A}_i = \partial_i\psi, \tag{3.619}$$

for some function ψ, then the generalized curvature vanishes.

$$\mathcal{R}_{ij} = 0\,, \tag{3.620}$$

Therefore, the generalized curvature measures the extent to which the vector field $\mathcal{A}_i$ is not a gradient.

Finally, by using the *generalized covariant derivative*

$$\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i \tag{3.621}$$

the operator L takes a very simple form

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q\,. \tag{3.622}$$

Because of a similarity with the Laplacian, $\Delta = g^{ij}\nabla_i\nabla_j$, such operators are called *Laplace type operators*.

We can rewrite the operator L in the form

$$L = e^{\omega}L_{\omega}e^{-\omega}, \tag{3.623}$$

where ω is a smooth function and $L_{\omega} = e^{-\omega}Le^{\omega}$ is some other operator specified below. It is easy to see that

$$e^{-\omega}\nabla_i e^{\omega} = \nabla_i + \omega_i\,, \tag{3.624}$$

where $\omega_i = \nabla_i\omega$. Therefore, the operator $L_{\omega} = e^{-\omega}Le^{\omega}$ is obtained from the operator $L = L(x, \partial_x)$ simply by replacing the derivatives

$$\partial_i \mapsto \partial_i + \omega_i\,, \tag{3.625}$$

that is,

$$L_{\omega}(x, \partial) = L(x, \partial_i + \omega_i)\,, \tag{3.626}$$

that is,

$$L_{\omega} = -\left(\nabla_i + \mathcal{A}_i^{\omega}\right)g^{ij}\left(\nabla_j + \mathcal{A}_j^{\omega}\right) + Q\,, \tag{3.627}$$

where

$$\mathcal{A}_j^\omega = \mathcal{A}_j + \nabla_j \omega \,. \tag{3.628}$$

The map

$$\mathcal{A}_j \mapsto \mathcal{A}_j^\omega = \mathcal{A}_j + \nabla_j \omega \tag{3.629}$$

is called a *gauge transformation*. Notice that the generalized curvature is *gauge invariant*,

$$\mathcal{R}_{ij}^\omega = \mathcal{R}_{ij}. \tag{3.630}$$

The gauge transformation can be used to simplify the form of the operator L. In particular, it can be used to compensate for any gradient like terms in the vector field $\mathcal{A}_i$. This means that even though $\nabla_i \mathcal{A}^i \neq 0$ one can try to find a function ω so that

$$g^{ij} \nabla_i \mathcal{A}_j^\omega = 0. \tag{3.631}$$

Such a function is a solution of the differential equation

$$\Delta \omega = -g^{ij} \nabla_i \mathcal{A}_j. \tag{3.632}$$

This is an example of a *gauge condition*.

Also, we call the map $L \mapsto L_\omega = e^{-\omega} L e^{\omega}$ a *similarity transformation* and two operators related by a similarity transformation *similar operators*. Similar operators have many common properties, in particular, they are *isospectral*, that is, they have the same spectrum.

3.15.2 Self-adjoint Operators

The definition of the adjoint operator, and, therefore, of the self-adjoint operator, depends on the space it is acting on. We consider Laplace type operators acting in the space $L^2(M, \mu)$ with some positive smooth weight function μ on M that we will parametrize by a function ω,

$$\mu = g^{1/2} e^{-2\omega} \,. \tag{3.633}$$

Therefore, the same operator may be self-adjoint for one weight function and not self-adjoint for another. Since the covariant derivatives enable to integrate by parts with the Riemannian volume element $g^{1/2}$, then by using the eq. (3.615) it is easy to compute the formal adjoint of the operator L

$$L^* = -\left(\nabla_i - \bar{\mathcal{A}}_i - 2\omega_i\right) g^{ij} \left(\nabla_j - \bar{\mathcal{A}}_j - 2\omega_j\right) + \bar{Q}, \tag{3.634}$$

where $\omega_i = \nabla_i \omega$.

Thus, the operator L is self-adjoint if

$$\mathcal{A}_i + \bar{\mathcal{A}}_i = -2\omega_i, \tag{3.635}$$

that is, if the real part of the generalized connection $\mathcal{A}_i$ is equal to

$$\operatorname{Re}\mathcal{A}_i = -\omega_i, \tag{3.636}$$

which is only possible if

$$\operatorname{Re}\mathcal{R}_{ij} = 0, \tag{3.637}$$

and the imaginary part remains arbitrary. Of course, what we really mean here is *formally self-adjoint*, since we do not discuss the boundary conditions. Thus, in general, the quantity $\operatorname{Re}\mathcal{R}_{ij}$ measures the extent to which the operator L is non-self-adjoint.

By denoting the imaginary part of the generalized connection $\mathcal{A}_j$ by A_j,

$$\mathcal{A}_j = iA_j - \omega_j, \tag{3.638}$$

we obtain a general form of a self-adjoint second-order operator

$$L = -g^{kj}(\nabla_k + iA_k - \omega_i)(\nabla_j + iA_j - \omega_j) + Q\,. \tag{3.639}$$

Such an operator is similar to the operator

$$L_\omega = -g^{kj}(\nabla_k + iA_k)(\nabla_j + iA_j) + Q\,. \tag{3.640}$$

It is important to realize the following. There is a generalization of Laplace type operators which have complex matrix-valued coefficients and act on complex vector-valued functions. Then the vector $\mathcal{A}_i$ is also a complex matrix-valued vector. If this vector is anti-Hermitian, then it describes so-called connection on a vector bundle and the Laplace type operator (3.622) is self-adjoint. For a scalar Laplace type operator this is only possible if the scalar functions it is acting on are complex and the vector $\mathcal{A}_i$ is *purely imaginary*. In other words, a real-valued scalar vector $\mathcal{A}_i$ does not define a true connection. That is why, we call it a *generalized connection*.

3.16 Notes

In this chapter we built a geometric foundation for the treatment of the singularly perturbed parabolic partial differential equations. There is a large body of literature on differential geometry. We find the following books very useful [59, 71, 54, 40, 28, 33, 65]. An excellent introduction to the Synge function is the Synge's book [73]. The material on the derivatives of the Synge's function and the covariant Taylor series is taken from our papers [4, 14, 13]. A good introduction to Lie groups can be found in the references [50, 15, 43, 44, 33, 26]. The material on symmetric spaces is taken from our papers [8, 12].

Part III
Perturbations

Chapter 4
Singular Perturbations

Abstract In this chapter we introduce the basic principles of the singular perturbation techniques to study the semiclassical asymptotics and apply them to obtain the asymptotic expansion of the heat equation.

4.1 Motivation

Various problems of mathematical physics lead to so called *singularly perturbed partial differential equations*. These are linear equations which contain a small parameter as a coefficient at highest derivatives. A typical example is Schrödinger equation in quantum mechanics with Planck constant as a small parameter. In order to construct approximate solutions of such equations one has to use asymptotic methods, which are called *semi-classical (or WKB) approximation*. In this chapter we will follow mainly the book [60, 37].

This method can be applied to a wide range of problems, such as study of singularities of fundamental solutions of partial differential equations, asymptotics of Cauchy problems with fast oscillating initial conditions, high-frequency (short-wave) asymptotics of diffraction problems, asymptotics of eigenvalues and eigenfunctions of partial differential operators (spectral asymptotics), spectral geometry etc. We will explain in this book how this method can be applied to obtain approximate asymptotic solutions of the heat equation, which is of our primary interest.

Semi-classical approximation is based on a deep physical principle, namely, the duality between waves and particles, between quantum mechanics and classical mechanics, between electrodynamics and geometric optics. The mathematical basis for this duality is provided by Fourier transform. The wave (quantum) aspects of the problem are described by partial differential equations and the particle (classical) aspects of the problem are described by a system of ordinary differential equations.

Recall the Schrödinger equation (2.30)

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_4

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta - V(x)\right)\psi = 0\,, \tag{4.1}$$

This is a typical singularly perturbed partial differential equation since the Planck constant $\hbar$ is considered a small parameter. The approximate solutions of this equation as $\hbar \to 0$ are called the *semi-classical asymptotics*.

Many other equations of mathematical physics have similar form, in particular, Maxwell equations, Dirac equation, Helmholtz equation, equations of elasticity theory, etc.

4.2 Semiclassical Approximation

In this section we describe the standard semi-classical approximation applied to the evolution equation of Schrödinger type. In the next section we will modify it slightly to apply it to the heat equation, which is what we need.

4.2.1 Semi-classical Ansatz

Let $x = (x^i)$ be a point in $\mathbb{R}^n_x$. Let us consider a linear elliptic second-order partial differential operator acting on functions on $\mathbb{R}^n_x$ of the form

$$L(x,\partial) = -\alpha^{jk}(x)\partial_j\partial_k + \beta^j(x)\partial_j + \gamma(x)\,, \tag{4.2}$$

with some non-constant coefficients. We assume that all coefficient functions are smooth and go to some constant values at infinity. We also assume that the matrix $A = (\alpha^{ij}(x))$ is positive definite and bounded for all x. Let $p = (p_i)$ be the *dual momenta* that take values in $\mathbb{R}^n_p$ and $\mathbb{R}^{2n}_{x,p} = \mathbb{R}^n_x \times \mathbb{R}^n_p$ be the *phase space*. As usual, we introduce the vector $\beta = (\beta^i)$ and the natural pairing $\langle p, \beta\rangle = p_i\beta^i$. Then the symbol of the operator L is

$$\sigma(x,p) = \langle p, Ap\rangle + i\,\langle p,\beta\rangle + \gamma\,. \tag{4.3}$$

Let $\varepsilon > 0$ be a small positive parameter. Let us rescale all derivatives by the small parameter ε, that is, we replace

$$\partial_i \mapsto \varepsilon\partial_i\,. \tag{4.4}$$

Then the operator

$$L(x,\varepsilon\partial) = -\varepsilon^2\alpha^{jk}(x)\partial_j\partial_k + \varepsilon\beta^j(x)\partial_j + \gamma(x)\,, \tag{4.5}$$

is a *singularly perturbed partial differential operator*.

In a more general case, we can also assume that the coefficients $\alpha^{ij}(x,\varepsilon)$, $\beta^j(x,\varepsilon)$, and $\gamma(x,\varepsilon)$ depend on the small parameter in such a way that they have well-defined limits as $\varepsilon \to 0$; we could assume, for example, that they have a well defined Taylor series in ε and $\alpha^{ij}(x,0)$ is positive definite and bounded for all x.

Let us consider the singularly perturbed evolution equation

$$[-i\varepsilon\partial_t + L(x,\varepsilon\partial)]\,\varphi = 0\,, \tag{4.6}$$

with some fast oscillating initial conditions

$$\varphi(0,x) = \varphi_0(x)\exp\left[\frac{i}{\varepsilon}S_0(x)\right]\,, \tag{4.7}$$

where $S_0(x)$ is a given real-valued function and φ_0 is a complex-valued function. Such initial condition with small ε describes a localized wave packet.

For operators with constant coefficients this equation has the following *plane wave* solution

$$\varphi(t,x) = \exp\left\{\frac{i}{\varepsilon}\left[-\sigma(p)t + \langle p,x\rangle\right]\right\}\,, \tag{4.8}$$

where $\sigma(p)$ is the symbol of the operator L (it does not depend on x for operators with constant coefficients). Notice that the phase here is a linear function of both t and x.

The main idea of the semi-classical approximation for operators with non-constant coefficients is to replace this plane wave in the limit $\varepsilon \to 0$ by a *distorted plane wave*

$$\exp\left\{\frac{i}{\varepsilon}S(t,x)\right\}\,, \tag{4.9}$$

where $S(t,x)$ is some function called the *action*. We will see soon that it is indeed the action of a mechanical system associated to the equation (4.6).

More precisely, one looks for the solution of the equation (4.6) as $\varepsilon \to 0$ in form of the following *semi-classical asymptotic ansatz*

$$\varphi(t,x) \sim \exp\left\{\frac{i}{\varepsilon}S(t,x)\right\}\sum_{k=0}^{\infty}(-i\varepsilon)^k a_k(t,x)\,, \tag{4.10}$$

with some undetermined function S and the undetermined coefficients a_k. The leading asymptotics as $\varepsilon \to 0$ of the solution of the evolution equation (4.6) is

$$\varphi(t,x) \sim \exp\left\{\frac{i}{\varepsilon}S(t,x)\right\}a_0(t,x)\,. \tag{4.11}$$

Then the algorithm for determining the function S and the coefficients a_k is rather simple. One just substitutes the ansatz (4.10) in the differential

equation (4.6) and equates to zero the coefficients at ε^k. Then for $k = 0$ one gets a non-linear *first-order* partial differential equation for the function S, called *Hamilton-Jacobi equation*. To solve this equation one introduces the corresponding *equations of characteristics* (a system of ordinary differential equations) called the *Hamiltonian system*. Then one solves the Hamiltonian system (in principle) and finds the action S. Second, for $k \geq 1$ one gets a system of differential recursion relations for a_k, called the *transport equations*, and finds as many coefficients a_k as needed.

4.2.2 Hamilton-Jacobi Equation

We assume for simplicity that the coefficients of the operator L do not depend on ε. Then we have the following *commutation formula*

$$\exp\left(-\frac{i}{\varepsilon}S\right)\left[-i\varepsilon\partial_t + L(x, \varepsilon\partial)\right]\exp\left(\frac{i}{\varepsilon}S\right) = L_0 + (-i\varepsilon)L_1 + (-i\varepsilon)^2 L_2\,, \tag{4.12}$$

where L_0 is a function

$$L_0 = \dot{S} + \sigma(x, \partial_x S)\,, \tag{4.13}$$

L_1 is a first-order differential operator

$$L_1 = \partial_t + \left(2\alpha^{jk}S_j + i\beta^k\right)\partial_k + \alpha^{jk}S_{jk}\,, \tag{4.14}$$

and L_2 is a second-order differential operator

$$L_2 = \alpha^{kj}\partial_k\partial_j\,. \tag{4.15}$$

Here the dot denotes the time derivative, $\dot{S} = \partial_t S$, $\sigma(x, p)$ is the symbol of the operator L, and

$$\partial_x S = (\partial_j S) \tag{4.16}$$

is the gradient vector of the function S. Here and everywhere below each additional index of S denotes the partial derivative with respect to the coordinates x^i, for example,

$$S_i = \partial_i S\,, \qquad S_{ij} = \partial_i\partial_j S\,. \tag{4.17}$$

Therefore, to satisfy eq. (4.6) in the leading order in the parameter ε the action S has to satisfy a non-linear first-order partial differential equation

$$\partial_t S + \sigma\left(x, \partial_x S\right) = 0\,, \tag{4.18}$$

or, in more detail,

$$\partial_t S + \alpha^{jk}(x)(\partial_j S)(\partial_k S) + i\beta^j(x)\partial_j S + \gamma(x) = 0\,. \tag{4.19}$$

This equation is called the *Hamilton-Jacobi equation* (or the *characteristic equation*). Moreover, from the initial condition (4.7) we also obtain the initial condition for the action

$$S(0,x) = S_0(x)\,. \tag{4.20}$$

Since we want the action S to be a real function we should assume that the symbol $\sigma(x,p)$ is real, which means that the coefficient β^j must be imaginary; we assume in this section that this is indeed the case.

Alternatively, we could assume that this coefficient $\beta^j = \beta^j(x,\varepsilon)$ depends on ε in such a way that $\beta^j(x,0) = 0$. Then the action has to satisfy the equation

$$\partial_t S + \alpha^{jk}(x)(\partial_j S)(\partial_k S) + \gamma(x) = 0\,. \tag{4.21}$$

One can go even further and assume that the function $\gamma(x,\varepsilon)$ also depends on ε is such a way that $\gamma(x,0) = 0$. Then the Hamilton-Jacobi equation takes the form

$$\partial_t S + \alpha^{jk}(x)(\partial_j S)(\partial_k S) = 0\,. \tag{4.22}$$

In particular, Hamilton-Jacobi equation for the Schrödinger equation (4.1) in quantum mechanics is

$$\partial_t S + \frac{1}{2m}\delta^{ij}(\partial_i S)(\partial_j S) + V(x) = 0\,, \tag{4.23}$$

which is an equation of classical mechanics for a particle of mass m moving in the potential $V = V(x)$.

4.2.3 Hamiltonian System

Now, let

$$\frac{\partial S}{\partial x^i} = p_i\,. \tag{4.24}$$

Then from the Hamilton-Jacobi equation (4.18) we have

$$\frac{\partial S}{\partial t} = -\sigma(x,p)\,. \tag{4.25}$$

A fundamental result of analysis of partial differential equations is that the integration of a *first-order* nonlinear *partial* differential equation (4.18) can be reduced to the integration of a Hamiltonian system with the *Hamiltonian* $\sigma(x,p)$,

$$\frac{dx^k}{d\tau} = \frac{\partial\sigma(x,p)}{\partial p_k} = 2\alpha^{jk}(x)p_j + i\beta^k(x), \tag{4.26}$$

$$\frac{dp^j}{d\tau} = -\frac{\partial\sigma(x,p)}{\partial x^j} = -p_i p_k \partial_j \alpha^{ik}(x) - ip_k \partial_j \beta^k(x) - \partial_j \gamma(x)\,. \tag{4.27}$$

For example, for the Schrödinger equation (4.1) for a *quantum particle* of mass m in a potential V the Hamiltonian has the form

$$\sigma(x,p) = \frac{|p|^2}{2m} + V(x)\,, \tag{4.28}$$

where $|p|^2 = \delta^{ij}p_i p_j$, and the Hamiltonian system

$$\frac{dx^i}{d\tau} = \frac{p_i}{m}, \tag{4.29}$$

$$\frac{dp_i}{d\tau} = -\frac{\partial V(x)}{\partial x^i}, \tag{4.30}$$

describes a *classical* particle of mass m in a potential V.

We impose the initial (or, rather, boundary) conditions in the following way. We fix a final time t and a point x and look for solutions $x(\tau)$ that start at some point x_0 and reach the point x at the time $\tau = t$. The solutions of the Hamiltonian system define so-called *phase trajectories* in the phase space $\mathbb{R}^{2n}_{x,p}$ $(x(\tau), p(\tau))$. Of course, the solution also depends on t and the final point x as parameters. That is why, we will sometimes indicate this explicitly by writing $(x(\tau;t,x), p(\tau;t,x))$. The projection of the phase trajectories onto the coordinate space $\mathbb{R}^n_x$ defines the *coordinate trajectories* (or *rays*) $x(\tau;t,x)$.

At the initial time the momenta have to satisfy the consistency condition (4.24). Thus, the full boundary conditions are now

$$x^i(t) = x^i(t;t,x) = x^i\,, \tag{4.31}$$

$$p_i(0) = p_i(0;t,x) = \frac{\partial S_0(x)}{\partial x^j}\,. \tag{4.32}$$

The starting point x_0 is not fixed but is rather a function of t and x,

$$x_0 = x_0(t,x) = x(0;t,x)\,. \tag{4.33}$$

Obviously,

$$x_0(0,x) = x(0;0,x) = x\,. \tag{4.34}$$

We observe that the solution of the Hamiltonian system defines a map

$$(x,p) \mapsto (x(\tau), p(\tau))\,. \tag{4.35}$$

As we saw earlier (see eq. (1.119)) the Liouville theorem ensures that the Jacobian of this map remains constant (and, therefore, non-zero) along the phase trajectories. This means that the map (4.35) is invertible and the phase trajectories $(x(\tau), p(\tau))$ define a family of smooth curves in the phase space $\mathbb{R}^{2n}_{x,p}$ without intersections; they define a nice *phase space flow*.

In contrary, the coordinate trajectories $x(\tau)$ in the coordinate space $\mathbb{R}^n_x$ do not form a nice flow; they may intersect, touch and collect at a single point (called a *focal point*), forming so called *caustics*. To clarify this we note that the solution $x(\tau; t, x)$ of the Hamiltonian system (4.26)-(4.27) also defines a map

$$x_0 \mapsto x\,, \tag{4.36}$$

as well as the inverse map

$$x \mapsto x_0(t, x)\,. \tag{4.37}$$

The Jacobian of this map is

$$J(t,x) = \det\left(\frac{\partial x^i}{\partial x_0^j}\right) = \left[\det\left(\frac{\partial x_0^i(t,x)}{\partial x^j}\right)\right]^{-1}. \tag{4.38}$$

Note that since $x_0(0, x) = x$, then the Jacobian has the following initial condition

$$J(0, x) = 1\,. \tag{4.39}$$

If the Jacobian is not equal to zero, $J(t, x) \neq 0$, then the map $x \mapsto x_0(t, x)$ is a local diffeomorphism. This is indeed so for small t. But there is no reason why this must be so for all t. The *focal points* are exactly the points along the trajectory $x(\tau)$ such that the Jacobian vanishes

$$J(t, x) = 0\,, \tag{4.40}$$

which means that the map $x \mapsto x_0(t, x)$ fails to be an even local diffeomorphism. The *caustics* are the sets of focal points. As a consequence, the semi-classical approximation breaks down at caustics.

Now, the solution of the Hamilton-Jacobi equation is obtained as follows. From the eqs. (4.24) and (4.25) we have for the action

$$dS = \langle p, dx\rangle - \sigma(x, p)dt\,. \tag{4.41}$$

Thus, along the phase trajectories the action varies according to

$$dS = \left[\left\langle p, \frac{dx}{dt}\right\rangle - \sigma(x, p)\right] dt\,. \tag{4.42}$$

This enables one to obtain the solution of Hamilton-Jacobi equation simply by integrating from 0 to t

$$S(t,x) = S_0(x_0(t,x)) + \int_0^t d\tau \left[\left\langle p(\tau), \frac{dx(\tau)}{d\tau} \right\rangle - \sigma\left(x(\tau), p(\tau)\right) \right], \quad (4.43)$$

where the integral is taken along the phase trajectory, that is, $x(\tau) = x(\tau; t, x)$ and $p(\tau) = p(\tau; t, x)$ is the solution of the Hamiltonian system.

Recall the fundamental property of the Hamiltonian system that the Hamiltonian $\sigma(x,p)$ is an integral of motion along the phase trajectories, that is,

$$\sigma\left(x(\tau), p(\tau)\right) = \sigma\left(x(0;t,x), p(0;t,x)\right) = \sigma\left(x_0(t,x), \partial_x S_0(x)\right) . \quad (4.44)$$

Therefore, the equation (4.43) can be simplified to

$$S(t,x) = S_0(x_0(t,x)) - t\sigma\left(x_0(t,x), \partial_x S_0(x)\right) + \int_0^t \left\langle p(\tau), \frac{dx(\tau)}{d\tau} \right\rangle d\tau . \quad (4.45)$$

4.2.4 Transport Equations

To compute the coefficients a_k of the asymptotic expansion (4.10) one needs to find the corresponding differential equations. By substituting the semiclassical ansatz (4.10) into the equation (4.6) and using the commutation formula (4.12) we obtain the equation for the coefficients a_k

$$L_1 a_0 = 0 , \quad (4.46)$$

$$L_1 a_k = -L_2 a_{k-1} , \qquad k = 1, 2, \ldots . \quad (4.47)$$

These are first-order ordinary differential equations along the phase trajectory; that is why they are called *transport equations*. The initial conditions for these coefficients are obtained from the initial condition (4.7) and have the form

$$a_0(0,x) = \varphi_0(x), \quad (4.48)$$

$$a_k(0,x) = 0 , \qquad k = 1, 2, \ldots . \quad (4.49)$$

Recall that the operator L_1 is

$$L_1 = \partial_t + \left(2\alpha^{jk} S_j + i\beta^k\right) \partial_k + \alpha^{jk} S_{jk} . \quad (4.50)$$

Now, by noting that along the phase trajectory $x = x(t)$ we have

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{dx^k}{dt} \frac{\partial}{\partial x^k} = \partial_t + \left(2\alpha^{jk} S_j + i\beta^k\right) \partial_k , \quad (4.51)$$

we can rewrite the operator L_1 as

$$L_1 = \frac{d}{dt} + \alpha^{jk} S_{jk} \,. \tag{4.52}$$

Next, we derive an equation for the Jacobian $J(t)$, (4.38). By applying the Liouville formula (1.109) to the first equation (4.26) of our Hamiltonian system with $p_i = S_i = \partial_i S$, we obtain that the Jacobian $J = J(t)$ (4.38) satisfies the transport equation

$$\left(\frac{d}{dt} - 2\alpha^{ij} S_{ij} - 2N \right) J = 0 \,, \tag{4.53}$$

where

$$N = S_k \partial_j \alpha^{jk} + i \frac{1}{2} \partial_j \beta^j \,. \tag{4.54}$$

This means that

$$\alpha^{ij} S_{ij} = J^{-1/2} \left(\frac{d}{dt} - N \right) J^{1/2} \,, \tag{4.55}$$

and, therefore, the operator L_1, (4.52), can now be written in the form

$$L_1 = J^{-1/2} \left(\frac{d}{dt} - N \right) J^{1/2} \,. \tag{4.56}$$

By using this form of the operator L_1 the transport equation (4.46) with the initial condition (4.48) can be now integrated along the phase trajectories to obtain

$$a_0(t,x) = \varphi_0(x) J^{-1/2}(t,x) \exp \left\{ \int_0^t d\tau \; N(\tau) \right\} \,, \tag{4.57}$$

where

$$N(\tau) = p_k(\tau) \partial_j \alpha^{jk}(x(\tau)) + i \frac{1}{2} \partial_j \beta^j (x(\tau)) \,. \tag{4.58}$$

To find the higher order coefficients a_k, $k \geq 1$, we rewrite the transport equations (4.47) in the integral form

$$\begin{aligned} a_k(t,x) = & -J^{-1/2}(t,x) \exp \left\{ \int_0^t ds N(s) \right\} \\ & \times \int_0^t d\tau \; \exp \left\{ - \int_0^\tau ds N(s) \right\} J^{1/2}(\tau,x) L_2 a_{k-1}(\tau,x) \,. \end{aligned} \tag{4.59}$$

This can be finally written in a more compact form

$$a_k(t,x) = -\int_0^t d\tau \, \left(\frac{J(\tau,x)}{J(t,x)}\right)^{1/2} \exp\left\{\int_\tau^t ds N(s)\right\} L_2 a_{k-1}(\tau,x)\,. \tag{4.60}$$

This recursion allows to compute (in principle) all coefficients a_k, $k = 1, 2, \ldots$.

4.3 Singularly Perturbed Heat Equation

The method of semi-classical approximation was developed initially for (and is usually applied to) hyperbolic equations describing the wave propagation. However, a slight modification of this method can be also applied to get the approximate solutions of singularly perturbed parabolic equations such as the heat equation. The problem of our primary interest is finding approximate solutions of singularly perturbed heat equation. Let $L(x,\partial)$ be an elliptic second-order partial differential operator of the type considered above,

$$L = -\alpha^{ij}(x)\partial_i\partial_j + \beta^i(x)\partial_i + \gamma(x)\,, \tag{4.61}$$

acting on functions in $\mathbb{R}^n$.

Let $\varepsilon > 0$ be a small parameter and let us consider the following singularly perturbed heat equation

$$[\varepsilon\partial_t + L(x, \varepsilon\partial_x)]\, U(t;x,x') = 0\,, \tag{4.62}$$

with the initial conditions

$$U(0;x,x') = \delta(x-x')\,. \tag{4.63}$$

4.3.1 Asymptotic Ansatz

Then applying the general method described in the previous section we look for a solution in the form of an asymptotic series

$$U(t;x,x') \sim \varepsilon^{-n/2} \exp\left\{-\frac{1}{\varepsilon}S(t;x,x')\right\} \sum_{k=0}^{\infty} \varepsilon^k b_k(t;x,x')\,. \tag{4.64}$$

We introduce an extra factor $\varepsilon^{-n/2}$ to satisfy the initial condition. The leading asymptotics of the heat kernel is

$$U(t;x,x') \sim \varepsilon^{-n/2} \exp\left\{-\frac{1}{\varepsilon}S(t;x,x')\right\} b_0(t;x,x')\,. \tag{4.65}$$

Thus the initial condition for the function S should be such that as $t \to 0$

$$\lim_{t\to 0} \varepsilon^{-n/2} \exp\left\{-\frac{1}{\varepsilon} S(t;x,x')\right\} b_0(t;x,x') = \delta(x-x')\,. \tag{4.66}$$

Now, we recall eq. (2.197). One can modify it for the exponential of a more general function as follows. Let $\Phi = \Phi(x,x')$ be a real two-point function such that

$$\Phi(x,x') > 0 \qquad \text{for} \qquad x \neq x'\,, \tag{4.67}$$

and

$$\Phi(x,x') = 0 \qquad \text{if and only if} \qquad x = x'\,. \tag{4.68}$$

Further, we assume that $\Phi(x,x')$ is an analytic function of x (so that there is Taylor series) in the neighborhood of x' such that

$$\partial_i \Phi(x,x')\Big|_{x=x'} = \partial_{j'} \Phi(x,x')\Big|_{x=x'} = 0\,, \tag{4.69}$$

and that it has a non-degenerate *Hessian*, that is,

$$\det\left[-\partial_i \partial_{j'} \Phi(x,x')\right]\Big|_{x=x'} \neq 0\,. \tag{4.70}$$

Here, as usual $\partial_{i'} = \partial/\partial x'^j$ denotes partial derivatives with respect to the primed variables x'^i. In other words, the function $\Phi(x,x')$ has a non-degenerate absolute minimum at x' equal to zero.

Then eq. (2.197) can be generalized as

$$\lim_{t\to 0} (4\pi t)^{-n/2} \det\left[-\partial_i \partial_{j'} \Phi(x,x')\right]^{1/2} \exp\left\{-\frac{1}{2t}\Phi(x,x')\right\} = \delta(x-x')\,. \tag{4.71}$$

Moreover, such equation still holds if the function $\Phi(t,x,x')$ is an analytic function of t such that the function $\Phi_0(x,x') = \Phi(0,x,x')$ satisfies the conditions above and

$$\partial_t \Phi(0,x,x')\Big|_{x=x'} = 0\,. \tag{4.72}$$

This means that the functions S and b_0 should have the following asymptotics as $t \to 0$

$$S(t;x,x') = \frac{1}{2t}\Phi(x,x') + O(1)\,, \tag{4.73}$$

$$b_0(t;x,x') = (4\pi t)^{-n/2} \det\left[-\partial_i \partial_{j'} \Phi(x,x')\right]^{1/2} + O\left(t^{-n/2+1}\right)\,, \tag{4.74}$$

where Φ is a function satisfying the conditions above. Recall that in the case when the operator L is self-adjoint, the heat kernel and, therefore, the function S and all the coefficients b_k are symmetric in x and x'.

4.3.2 Hamilton-Jacobi Equation and Hamiltonian System

We will need the commutation formula

$$\exp\left(\frac{1}{\varepsilon}S\right)\left[\varepsilon\partial_t + L(x,\varepsilon\partial_x)\right]\exp\left(-\frac{1}{\varepsilon}S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 T_2\,, \tag{4.75}$$

where T_0 is a function,

$$T_0 = -\dot{S} - \alpha^{ij}S_iS_j - \beta^j S_j + \gamma\,, \tag{4.76}$$

T_1 is a first order partial differential operator

$$T_1 = \partial_t + \left(\beta^i + 2\alpha^{ij}S_j\right)\partial_i + \alpha^{ij}S_{ij}\,, \tag{4.77}$$

and T_2 is a second-order differential operator

$$T_2 = -\alpha^{ij}\partial_i\partial_j\,. \tag{4.78}$$

By substituting the asymptotic ansatz into the heat equation and using the above commutation formula we see that the function T_0 must be equal to zero. Thus, we obtain the equation for the function S (*Hamilton-Jacobi equation*)

$$\partial_t S + H(x,\partial_x S) = 0\,, \tag{4.79}$$

where

$$H(x,p) = \alpha^{ij}(x)p_ip_j + \beta^j(x)p_j - \gamma(x)\,. \tag{4.80}$$

Notice that now the Hamiltonian $H(x,p)$ is not equal to the symbol $\sigma(x,p)$ of the operator L.

The solution of Hamilton-Jacobi equation can be obtained as follows. Let us introduce the corresponding Hamiltonian system

$$\frac{dx^i}{d\tau} = \frac{\partial H(x,p)}{\partial p^i} = 2\alpha^{ij}(x)p_j + \beta^i(x)\,, \tag{4.81}$$

$$\frac{dp_k}{d\tau} = -\frac{\partial H(x,p)}{\partial x^k} = -\partial_k\alpha^{ij}(x)p_ip_j - \partial_k\beta^j(x)p_j + \partial_k\gamma(x)\,. \tag{4.82}$$

Let $(x(\tau),p(\tau))$ be the solution of this system with the following boundary conditions

$$x(0) = x'\,, \qquad x(t) = x\,. \tag{4.83}$$

The initial condition for the momentum is then determined from the eq. (4.81)

$$p_j(0) = \frac{1}{2}\alpha_{ji}(x')\left[\dot{x}^i(0) - \beta^i(x')\right]\,, \tag{4.84}$$

where, as usual, the dot denotes the derivative with respect to τ and $A^{-1} = (\alpha_{ij})$ is the matrix inverse to the matrix $A = (\alpha^{ij})$. This boundary value problem has a unique solution, at least when the points x and x' are close to each other. Of course, $x(\tau)$ and $p(\tau)$ depend on t, x, and x' as parameters, that is, more precisely, we should write

$$x = x(\tau; t, x, x'), \qquad p = p(\tau; t, x, x')\,. \tag{4.85}$$

In particular, the coordinate function satisfies the identities

$$x(0; t, x, x') = x'\,, \qquad x(t; t, x, x') = x\,. \tag{4.86}$$

4.3.3 Action

Let us define

$$S(t; x, x') = \int_0^t d\tau \ \left[\left\langle p(\tau), \frac{dx(\tau)}{d\tau} \right\rangle - H(x(\tau), p(\tau)) \right]. \tag{4.87}$$

By using the Hamiltonian equation (4.81) we can express the velocities $\dot{x}$ in terms of the momenta to get

$$S(t; x, x') = \int_0^t d\tau \ \Big\{ \big\langle p(\tau), A(x(\tau))p(\tau) \big\rangle + \gamma(x(\tau)) \Big\}, \tag{4.88}$$

where A is the matrix defined by $A = (\alpha^{ij})$ and the integral is taken along the phase trajectory. Alternatively, we can express the momenta p in terms of the velocities $\dot{x}$ to get

$$\begin{aligned} S(t; x, x') = \int_0^t d\tau \ \Bigg[& \frac{1}{4} \left\langle \frac{dx(\tau)}{d\tau}, A^{-1}(x(\tau)) \frac{dx(\tau)}{d\tau} \right\rangle \\ & - \frac{1}{2} \left\langle \beta(x(\tau)), A^{-1}(x(\tau)) \frac{dx(\tau)}{d\tau} \right\rangle \\ & + \frac{1}{4} \left\langle \beta(x(\tau)), A^{-1}(x(\tau)) \beta(x(\tau)) \right\rangle + \gamma(x(\tau)) \Bigg], \end{aligned} \tag{4.89}$$

where $A^{-1} = (\alpha_{ij})$ is the matrix inverse to the matrix $A = (\alpha^{ij})$.

Then one can show that

$$\frac{\partial S(t;x,x')}{\partial x^i} = p_i(t;t,x,x')\,, \tag{4.90}$$

$$\frac{\partial S(t;x,x')}{\partial x'^i} = -p_i(0;t,x,x')\,, \tag{4.91}$$

and that $S(t;x,x')$ satisfies Hamilton-Jacobi equation (4.79). It also satisfies Hamilton-Jacobi equation with respect to the coordinates x', that is,

$$-\partial_t S + H(x', \partial_{x'} S) = 0\,. \tag{4.92}$$

Another important property of the function S consists in the following. Let us define the determinant

$$Z(t;x,x') = \det\left[-\partial_i \partial_{j'} S(t;x,x')\right]. \tag{4.93}$$

Let us denote the derivatives of the function S with respect to x and x' just by adding indices, primed or non-primed, that is,

$$S_i = \partial_i S\,, \qquad S_{ij} = \partial_i \partial_j S\,, \qquad S_{ij'} = \partial_i \partial_{j'} S\,, \qquad S_{ijk'} = \partial_i \partial_j \partial_{k'} S\,. \tag{4.94}$$

Then by differentiating Hamilton-Jacobi equation with respect to x and x' we obtain

$$\partial_t S_{k'm} + 2(\partial_m \alpha^{ij}) S_i S_{jk'} + 2\alpha^{ij}(S_i S_{k'jm} + S_{k'j} S_{im}) + (\partial_m \beta^i) S_{k'i} + \beta^i S_{k'im} = 0\,. \tag{4.95}$$

Let $B^{k'm}$ be the inverse of the matrix $S_{k'm}$. By using the formula (1.101) for the derivative of the determinant we notice that

$$\partial_t Z = B^{k'm}(\partial_t S_{k'm}) Z \tag{4.96}$$

and

$$\partial_i Z = B^{k'm} S_{k'mi} Z\,. \tag{4.97}$$

Now, by multiplying eq. (4.95) by $B^{k'm}$ and contracting the indices k' and m we obtain the *continuity equation* for the determinant Z

$$\left\{\partial_t + (2\alpha^{ij} S_j + \beta^j)\partial_i + 2\alpha^{ij} S_{ij} + 2(\partial_i \alpha^{ij}) S_j + (\partial_i \beta^i)\right\} Z = 0\,. \tag{4.98}$$

By using this equation we obtain now the equation for the square root $Z^{1/2}$

$$\left\{\partial_t + (2\alpha^{ij} S_j + \beta^j)\partial_i + \alpha^{ij} S_{ij} + (\partial_i \alpha^{ij}) S_j + \frac{1}{2}(\partial_i \beta^i)\right\} Z^{1/2} = 0 \tag{4.99}$$

that we will need below.

4.3.4 Transport Equations

Now, by substituting the asymptotic ansatz (4.64) into the heat equation (4.62) and using the commutation formula (4.75) we obtain the recurrence relations (*transport equations*) for the coefficients b_k for $k = 0, 1, \ldots,$

$$T_1 b_0 = 0, \tag{4.100}$$

$$T_1 b_k = -T_2 b_{k-1}\,. \tag{4.101}$$

Now, it should be clear that the differential operator T_1, (4.77), has the form

$$T_1 = \frac{d}{dt} + \alpha^{ij} S_{ij}\,, \tag{4.102}$$

where $S_{ij} = \partial_i \partial_j S$ and d/dt is the total derivative (along the trajectories of the Hamiltonian system) of a function that depends on t and x, that is,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{dx^i}{dt}\frac{\partial}{\partial x^i}\,. \tag{4.103}$$

By using the transport operator T_1, (4.102), the equation (4.99) can be written as

$$(T_1 + M) Z^{1/2} = 0, \tag{4.104}$$

where

$$M = (\partial_i \alpha^{ij}) S_j + \frac{1}{2}(\partial_i \beta^i)\,. \tag{4.105}$$

This means that

$$\alpha^{ij} S_{ij} = Z^{1/2}\left(\frac{d}{dt} + M\right) Z^{-1/2}\,, \tag{4.106}$$

and, therefore, the operator T_1, (4.102), can now be written in the form

$$T_1 = Z^{1/2}\left(\frac{d}{dt} - M\right) Z^{-1/2}\,. \tag{4.107}$$

Thus, by integrating the transport equation (4.100) we get the coefficient b_0

$$b_0(t; x, x') = (2\pi)^{-n/2} Z^{1/2}(t; x, x') \exp\left\{\int_0^t d\tau M(\tau; x, x')\right\}\,. \tag{4.108}$$

The normalization factor is chosen here in such a way to satisfy the initial condition (4.74). The higher-order coefficients b_k can be computed similarly.

Finally, the leading asymptotics of the singularly perturbed heat kernel as $\varepsilon \to 0$ has the form

$$U(t;x,x') \sim (2\pi\varepsilon)^{-n/2} Z^{1/2}(t;x,x') \exp\left\{ -\frac{1}{\varepsilon} S(t;x,x') + \int_0^t d\tau M(\tau;x,x') \right\}. \tag{4.109}$$

To find the higher-order coefficients b_k for $k \geq 1$ it is useful to rewrite the recurrence relations (4.101) in the form

$$b_k(t;x,x') = -\int_0^t d\tau \left(\frac{Z(t;x,x')}{Z(\tau,x,x')} \right)^{1/2} \exp\left\{ \int_\tau^t ds M(s;x,x') \right\} \times T_2 b_{k-1}(\tau;x,x') \,. \tag{4.110}$$

This recursion allows to compute (in principle) all coefficients b_k, $k = 1, 2, \ldots$.

In the next chapter we will develop a similar technique for the calculation of the short-time asymptotic expansion of the heat kernel as $t \to 0$. In principle we could use the above method, but we will describe another method, which is much more geometrical, systematic and very powerful. It has been used to compute not just the leading asymptotics but also some higher-order coefficients of the expansion.

4.3.5 Operators with Constant Coefficients

To get an idea of the solution let us consider the simplest case when all coefficients of the operator L are constant. Then the solution of the Hamiltonian system (4.81)-(4.82) satisfying the initial conditions (4.83), (4.84) is

$$x^i(\tau) = \frac{(x^i - x'^i)}{t} \tau + x'^i \,, \tag{4.111}$$

$$p_i(\tau) = \frac{1}{2} \alpha_{ij} \left(\frac{x^j - x'^j}{t} - \beta^i \right). \tag{4.112}$$

Recall that α_{ij} denotes the entries of the matrix $A^{-1} = (\alpha_{ij})$ inverse to the matrix $A = (\alpha^{ij})$.

Then the action S is computed from eq. (4.88)

$$S(t;x,x') = \frac{1}{4t} \left\langle (x - x'), A^{-1}(x - x') \right\rangle - \frac{1}{2} \left\langle \beta, A^{-1}(x - x') \right\rangle + \left[\frac{1}{4} \left\langle \beta, A^{-1}\beta \right\rangle + \gamma \right] t \,. \tag{4.113}$$

It is easy to check directly that it satisfies Hamilton-Jacobi equation. By using this function we can compute the determinant Z, (4.93), to get

$$Z(t,x,x') = (2t)^{-n}(\det A)^{-1}\,. \tag{4.114}$$

The function M, defined by (4.105), in this case vanishes.

Thus, the leading asymptotics of the singularly perturbed heat kernel as $\varepsilon \to 0$ has the form

$$U(t;x,x') \sim (4\pi\varepsilon t)^{-n/2}\,(\det A)^{-1/2} \exp\left\{-\frac{1}{4\varepsilon t}\left\langle (x-x'), A^{-1}(x-x')\right\rangle\right\} \\ \times \exp\left\{-\frac{1}{\varepsilon}\left[-\frac{1}{2}\left\langle \beta, A^{-1}(x-x')\right\rangle + \left(\frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle + \gamma\right)t\right]\right\}. \tag{4.115}$$

Of course, this coincides with the exact solution (2.196) obtained by Fourier transform. In this simple case all higher order coefficients vanish, $b_k = 0$, for $k \geq 1$.

4.3.6 Quadratic Hamiltonians

Notice that the heat kernel of operators with constant coefficients (4.115), also (2.196), is *Gaussian*, that is, it is an exponential of a quadratic polynomial of the coordinates, that is, it has the form

$$U(t;x,x') = f(t)\exp\left\{\,\langle \Psi_1(t), x\rangle + \langle \Psi_2(t), x'\rangle\,\right\} \\ \times \exp\left\{\,\langle x, \Phi_1(t)x\rangle + \langle x, \Phi_2(t)x'\rangle + \langle x', \Phi_3(t)x'\rangle\,\right\}, \tag{4.116}$$

where f is a function, $\Phi_i(t)$ are matrix-valued functions and $\Psi_i(t)$ are some vector-valued functions of t. It turns out that this is a rather general feature of a wider class of operators with linear Hamiltonian systems (4.81)-(4.82). This is the class of operators such that the coefficients α^{ij} are constant, the functions $\beta^i(x)$ are linear in x and the coefficient $\gamma(x)$ is quadratic polynomial in x, that is,

$$\alpha^{ij}(x) = A^{ij}\,, \tag{4.117}$$

$$\beta^i(x) = \tilde{B}^i + \tilde{C}^i{}_j x^j\,, \tag{4.118}$$

$$\gamma(x) = \tilde{G} + \tilde{E}_i x^i + \tilde{D}_{ij} x^i x^j\,. \tag{4.119}$$

That is, the operator L has the form

$$\tilde{L} = -A^{ij}\partial_i\partial_j + (\tilde{B}^i + \tilde{C}^i{}_j x^j)\partial_i + \tilde{G} + \tilde{E}_i x^i + \tilde{D}_{ij} x^i x^j\,. \tag{4.120}$$

This case includes such important particular cases as harmonic oscillator and constant magnetic field. Notice that both the matrices A and $\tilde{D}$ are symmetric

by definition, that is,

$$A^T = A, \qquad \tilde{D}^T = \tilde{D}\,. \tag{4.121}$$

Here and below T denotes the transposition of matrices. Moreover, for the operator L to be elliptic the matrix $A = (\alpha^{ij})$ must be positive and, therefore, invertible. The corresponding Hamiltonian $\tilde{H}(x,p)$, (4.80), is quadratic in momenta and coordinates. As a result, this system can be solved exactly, which gives the action and finally the heat kernel.

The action of such operators on Gaussian functions like (4.117) just multiplies them by a polynomial leaving the exponential intact. This enables one to choose the quadratic polynomial in the exponential, that is, the functions $f(t)$, $\Phi_i(t)$ and $\Psi(t)$ such that it satisfies the heat equation and the initial condition. We will see many cases like this throughout the book.

However, we will do it directly, but will rather first simplify the problem as follows. Let us define a new operator

$$L = e^{-\omega}\tilde{L}e^{\omega}\,. \tag{4.122}$$

One can use this transformation to simplify the operator L. The transformed operator L reads

$$\begin{aligned} L = &-A^{ij}\partial_i\partial_j + (B^i + C^i{}_j x^j - 2A^{ij}\omega_j)\partial_i + G + E_i x^i + + D_{ij}x^i x^j \\ &+(B^i + C^i{}_j x^j)\omega_i - A^{ij}\omega_i\omega_j - A^{ij}\omega_{ij}\,, \end{aligned} \tag{4.123}$$

where $\omega_i = \partial_i\omega$ and $\omega_{ij} = \partial_i\partial_j\omega$. In particular, it is easy to see that if $\omega(x)$ is a quadratic polynomial then the form of the operator does not change. More precisely, let

$$\omega(x) = V_i x^i + W_{ij}x^i x^j\,, \tag{4.124}$$

where $V = (V_i)$ is a vector and $W = (W_{ij})$ is a symmetric matrix. Then

$$L = -A^{ij}\partial_i\partial_j + (B^i + C^i{}_j x^j)\partial_i + G + E_i x^i + D_{ij}x^i x^j\,, \tag{4.125}$$

where

$$B = \tilde{B} - 2AV\,, \tag{4.126}$$

$$C = \tilde{C} - 4AW\,, \tag{4.127}$$

$$G = \tilde{G} + \langle\tilde{B}, V\rangle - \langle V, AV\rangle - 2\,\mathrm{tr}\,AW\,, \tag{4.128}$$

$$E = \tilde{E} + C^T V + 2W\tilde{B} - 4WAV\,, \tag{4.129}$$

$$D = \tilde{D} + \tilde{C}^T W + W\tilde{C} - 4WAW\,. \tag{4.130}$$

Therefore, the function ω can be chosen to simplify the form of the operator L, for example, to cancel the coefficient B and the symmetric part of the coefficient $A^{-1}C$ by choosing

$$V = \frac{1}{2} A^{-1} \tilde{B} \,, \tag{4.131}$$

$$W = \frac{1}{8} \left[A^{-1} \tilde{C} + \tilde{C}^T A^{-1} \right] . \tag{4.132}$$

We will assume that this choice has been made so that

$$\omega(x) = \frac{1}{2} \langle \tilde{B}, A^{-1} x \rangle + \frac{1}{4} \langle x, A^{-1} \tilde{C} x \rangle \,, \tag{4.133}$$

and

$$L = -A^{ij} \partial_i \partial_j + C^i{}_j x^j \partial_i + G + E_i x^i + D_{ij} x^i x^j \,, \tag{4.134}$$

with

$$C = \frac{1}{2} \left(\tilde{C} - A \tilde{C}^T A^{-1} \right) , \tag{4.135}$$

$$G = \tilde{G} + \frac{1}{4} \langle \tilde{B}, A^{-1} \tilde{B} \rangle - \frac{1}{2} \operatorname{tr} \tilde{C} \,, \tag{4.136}$$

$$E = \tilde{E} + \frac{1}{2} \tilde{C}^T A^{-1} \tilde{B} \,, \tag{4.137}$$

$$D = \tilde{D} + \frac{1}{16} \left[3 \tilde{C}^T A^{-1} \tilde{C} + (\tilde{C}^T)^2 A^{-1} + A^{-1} \tilde{C}^2 - A^{-1} \tilde{C} A \tilde{C}^T A^{-1} \right] . \tag{4.138}$$

Notice that now the matrix CA is anti-symmetric, that is,

$$C^T = -A^{-1} C A. \tag{4.139}$$

In particular, this means that the matrix C is traceless,

$$\operatorname{tr} C = 0 \,. \tag{4.140}$$

Now, we notice that (4.122) is nothing but a similarity transformation; therefore, the heat kernel $\tilde{U}(t; x, x')$ of the operator $\tilde{L}$ is easily computed in terms of the heat kernel $U(t; x, x')$ of the operator L,

$$\tilde{U}(t; x, x') = \exp \{ \omega(x) - \omega(x') \} \, U(t; x, x') \,. \tag{4.141}$$

The Hamiltonian $H(x, p)$, (4.80), corresponding to the operator L has the form

$$H(x, p) = \langle p, Ap \rangle + \langle p, Cx \rangle - G - \langle E, x \rangle - \langle x, Dx \rangle \,, \tag{4.142}$$

and the Hamiltonian system is linear. It is convenient to introduce the vectors $x = (x^i)$ and $p = (p_i)$. Then the Hamiltonian system can be written in the

matrix form,

$$\frac{dx}{d\tau} = Cx + 2Ap\,, \tag{4.143}$$

$$\frac{dp}{d\tau} = E + 2Dx + A^{-1}CAp\,. \tag{4.144}$$

The solution of this system can be obtained as follows. First of all, we look for a constant solution (x_0, p_0). Then, of course, we have

$$Cx_0 + 2Ap_0 = 0\,, \tag{4.145}$$

$$2Dx_0 + A^{-1}CAp_0 = -E\,. \tag{4.146}$$

This system has a non-trivial solution if the matrix $C^2 - 4AD$ is invertible. We will assume that this is the case. We will find it convenient to define a new matrix ρ as the square root of the matrix AD

$$\rho = 2\sqrt{AD}\,, \tag{4.147}$$

and a matrix

$$J = C^2 - \rho^2\,. \tag{4.148}$$

Then the solution is given by

$$x_0 = 2J^{-1}AE\,, \tag{4.149}$$

$$p_0 = -A^{-1}CJ^{-1}AE. \tag{4.150}$$

Now we define new variables (y, q) by

$$y = x - x_0\,, \tag{4.151}$$

$$q = A(p - p_0)\,. \tag{4.152}$$

Then the Hamiltonian system becomes

$$\frac{dy}{d\tau} = Cy + 2q\,, \tag{4.153}$$

$$\frac{dq}{d\tau} = \frac{1}{2}\rho^2 y + Cq\,. \tag{4.154}$$

Now, let us introduce the $2n$ vector

$$\mathcal{Y} = \begin{pmatrix} y \\ q \end{pmatrix}, \tag{4.155}$$

and the $2n \times 2n$ matrix

$$\mathcal{F} = \begin{pmatrix} C & 2I \\ \frac{1}{2}\rho^2 & C \end{pmatrix}, \tag{4.156}$$

where I is the $n \times n$ unit matrix. It will be convenient to introduce the matrices

$$\mathcal{I} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \tag{4.157}$$

$$\mathcal{D} = \begin{pmatrix} 0 & 2I \\ \frac{1}{2}\rho^2 & 0 \end{pmatrix}, \tag{4.158}$$

so that

$$\mathcal{F} = C\mathcal{I} + \mathcal{D}. \tag{4.159}$$

Then the Hamiltonian system takes the form

$$\frac{d\mathcal{Y}}{d\tau} = \mathcal{F}\mathcal{Y}\,. \tag{4.160}$$

This is a linear equation with constant coefficients; its solution reads

$$\mathcal{Y}(\tau) = \exp(\tau\mathcal{F})\,\mathcal{Y}(0)\,. \tag{4.161}$$

Further calculation is significantly simplified if one assumes that the matrices C and AD (or C and ρ) commute, that is,

$$C\rho = \rho C. \tag{4.162}$$

Then the matrices $C\mathcal{I}$ and $\mathcal{D}$ commute as well and we have

$$\exp(\tau\mathcal{F}) = e^{\tau C}\exp(\tau\mathcal{D})\,, \tag{4.163}$$

Now we need to compute exponential of the matrix $\mathcal{D}$. It is easy to see that

$$\mathcal{D}^2 = \rho^2\mathcal{I}. \tag{4.164}$$

Therefore,

$$\mathcal{D}^{2n} = \rho^{2n}\mathcal{I} \tag{4.165}$$

and

$$\mathcal{D}^{2n+1} = \rho^{2n}\mathcal{D}\,, \tag{4.166}$$

which enables one to compute the exponential

$$\exp(\tau\mathcal{D}) = \cosh(\tau\rho)\,\mathcal{I} + \frac{\sinh(\tau\rho)}{\rho}\mathcal{D}. \tag{4.167}$$

Therefore, the solution (with the initial condition $y(0) = y' = x' - x_0$) becomes

$$y(\tau) = e^{\tau C} \cosh(\tau\rho) y' + 2e^{\tau C} \frac{\sinh(\tau\rho)}{\rho} q(0)\,, \tag{4.168}$$

$$q(\tau) = \frac{1}{2} e^{\tau C} \rho \sinh(\tau\rho)\, y' + e^{\tau C} \cosh(\tau\rho) q(0)\,. \tag{4.169}$$

Next, the initial condition for the momentum $q(0)$ should be chosen to satisfy the boundary condition $y(t) = x - x_0$. That is, $q(0)$ is determined by

$$q(0) = e^{-tC} \frac{\rho}{2\sinh(t\rho)} y - \frac{1}{2}\rho \coth(t\rho) y'\,. \tag{4.170}$$

This finally gives our trajectory

$$y(\tau) = e^{-(t-\tau)C} \frac{\sinh(\tau\rho)}{\sinh(t\rho)} y + e^{\tau C} \frac{\sinh[(t-\tau)\rho]}{\sinh(t\rho)} y'\,, \tag{4.171}$$

$$q(\tau) = e^{-(t-\tau)C} \frac{\rho\cosh(\tau\rho)}{2\sinh(t\rho)} y - e^{\tau C} \frac{\rho\cosh[(t-\tau)\rho]}{2\sinh(t\rho)} y'\,. \tag{4.172}$$

Now we can compute the boundary values of the momenta as well

$$q(0) = e^{-tC} \frac{\rho}{2\sinh(t\rho)} y - \frac{1}{2}\rho \coth(t\rho) y', \tag{4.173}$$

$$q(t) = \frac{1}{2}\rho \coth(t\rho) y - e^{-tC} \frac{\rho}{2\sinh(t\rho)} y'\,. \tag{4.174}$$

As expected $q(t)$ is obtained from $q(0)$ by reversing the sign of t, $t \mapsto -t$, and replacing y and y'. The dynamics of the original variables is obtained by

$$x(\tau) = x_0 + y(\tau)\,, \tag{4.175}$$

$$p(\tau) = p_0 + A^{-1} q(\tau)\,. \tag{4.176}$$

Recall that the Hamiltonian is an integral of motion, that is,

$$H(x(\tau), p(\tau)) = H(x', p(0)) = H(x, p(t))\,. \tag{4.177}$$

Now the action $S = S(t; x, x')$ can be obtained from the eq. (4.88)

$$S(t; x, x') = \int_0^t d\tau \left\{ \langle p(\tau), Ap(\tau)\rangle + \langle x(\tau), Dx(\tau)\rangle + \langle E, x(\tau)\rangle + G \right\}. \tag{4.178}$$

By using the eqs. (4.175), (4.176), we obtain

$$S(t; x, x') = tS_0 + S_1(x, x') + S_2(t; x, x')\,, \tag{4.179}$$

where

$$S_0 = \langle p_0, Ap_0\rangle + \langle x_0, Dx_0\rangle + \langle E, x_0\rangle + G$$
$$= G + \left\langle E, J^{-1}AE\right\rangle , \tag{4.180}$$

$$S_1(x,x') = \int_0^t d\tau \left\{2\langle p_0, q(\tau)\rangle + 2\langle x_0, Dy(\tau)\rangle + \langle E, y(\tau)\rangle\right\}, \tag{4.181}$$

$$S_2(t;x,x') = \int_0^t d\tau \left\{\left\langle q(\tau), A^{-1}q(\tau)\right\rangle + \frac{1}{4}\left\langle y(\tau), A^{-1}\rho^2 y(\tau)\right\rangle\right\}. \tag{4.182}$$

The function S_1 is computed by using eq. (4.153) as follows

$$S_1(x,x') = \int_0^t d\tau \left\langle p_0, \frac{dy(\tau)}{d\tau}\right\rangle = \langle p_0, (x-x')\rangle$$
$$= \left\langle E, J^{-1}C(x-x')\right\rangle . \tag{4.183}$$

Finally, by using eqs. (4.171) and (4.172) we can compute the quadratic part. After a long but straightforward calculation we obtain

$$S_2(t;x,x') = \frac{1}{2}\left\langle (x-x_0), A^{-1}\frac{\rho}{\sinh(t\rho)}\left[\cosh(t\rho) - e^{tC}\right](x'-x_0)\right\rangle$$
$$+\frac{1}{4}\left\langle (x-x'), A^{-1}\rho\coth(t\rho)(x-x')\right\rangle. \tag{4.184}$$

Now, by using the value $x_0 = 2J^{-1}AE$ we can represent the action in the form

$$S(t;x,x') = tG + \left\langle E, J^{-1}\left\{t + 4J^{-1}\frac{\rho}{\sinh(t\rho)}\left[\cosh(t\rho) - \cosh(tC)\right]\right\}AE\right\rangle$$
$$-2\left\langle E, J^{-1}\frac{\rho}{\sinh(t\rho)}[\cosh(t\rho) - \cosh(tC)](x+x')\right\rangle$$
$$+\left\langle E, J^{-1}\left[C - 2\frac{\rho}{\sinh(t\rho)}\sinh(tC)\right](x-x')\right\rangle$$
$$+\frac{1}{2}\left\langle x, A^{-1}\frac{\rho}{\sinh(t\rho)}\left[\cosh(t\rho) - e^{tC}\right]x'\right\rangle$$
$$+\frac{1}{4}\left\langle (x-x'), A^{-1}\rho\coth(t\rho)(x-x')\right\rangle . \tag{4.185}$$

Note that as $t \to 0$, the action S takes a form similar to the one for operators with constant coefficients, that is,

$$S(t;x,x') \sim \frac{1}{4t}\left\langle (x-x'), A^{-1}(x-x')\right\rangle , \tag{4.186}$$

where we neglected the terms of order $O(1)$ as $t \to 0$.

Now we can compute the determinant Z (4.93)

$$Z = \det\left\{ A^{-1} e^{tC} \frac{\rho}{2\sinh(t\rho)} \right\}. \tag{4.187}$$

By using eq. (1.95) we get

$$\det e^{tC} = e^{t\,\mathrm{tr}\, C} = 1 , \tag{4.188}$$

and, therefore, we obtain from eq. (4.187)

$$Z(t) = (2t)^{-n} (\det A)^{-1} \det\left(\frac{\sinh(t\rho)}{t\rho} \right)^{-1} . \tag{4.189}$$

We also notice that the quantity M, (4.105), vanishes since

$$M = \frac{1}{2}\partial_i \beta^i = \frac{1}{2} C^i{}_i = \frac{1}{2}\,\mathrm{tr}\, C = 0 . \tag{4.190}$$

This already gives the first coefficient of the heat kernel asymptotics

$$b_0(t) = (4\pi t)^{-n/2} (\det A)^{-1/2} \det\left(\frac{\sinh(t\rho)}{t\rho} \right)^{-1/2} . \tag{4.191}$$

As we see it does not depend on the coordinates. Thus the leading asymptotics of the singularly perturbed heat kernel as $\varepsilon \to 0$ has the form

$$U(t;x,x') \sim (4\pi\varepsilon t)^{-n/2} (\det A)^{-1/2} \det\left(\frac{\sinh(t\rho)}{t\rho} \right)^{-1/2} \times \exp\left\{ -\frac{1}{\varepsilon} S(t;x,x') \right\} . \tag{4.192}$$

The original heat kernel $\tilde{U}(t;x,x')$ of the operator $\tilde{L}$ is then given by multiplying by the overall factor $\exp\{\omega(x) - \omega(x')\}$, (4.141), given by eq. (4.133).

Note that the case of constant coefficients can be obtained from this result by substituting $\tilde{C} = \tilde{E} = \tilde{D} = 0$ and $\tilde{G} = \gamma$, which means $C = E = D = 0$ and $G = \gamma + \frac{1}{4}\langle \tilde{B}, A^{-1}\tilde{B}\rangle$, and taking the limit $\rho \to 0$. It is not difficult to see that the leading asymptotics of the heat kernel does indeed coincide with the case of constant coefficients (4.115) and the exact solution obtained by the Fourier transform (2.196).

Notice that there is a well defined limit $C \to 0$. We just need to substitute $C = 0$ and $J = -\rho^2$. For a future reference we write the result for the action for the case of harmonic oscillator when $C = E = G = 0$ and $\rho = 2\sqrt{AD}$,

$$S(t;x,x') = \frac{1}{2}\left\langle x, A^{-1}\rho\tanh\left(\frac{t\rho}{2}\right)x'\right\rangle + \frac{1}{4}\left\langle (x-x'), A^{-1}\rho\coth(t\rho)(x-x')\right\rangle . \tag{4.193}$$

This is not so in the degenerate case when $J = 0$, that is, when

$$\rho^2 = 4AD = C^2 . \tag{4.194}$$

The limit $J \to 0$ is not well defined. Again, for the future reference let us solve this case as well. Although it is possible to do it in general, we will make one additional assumption, namely, that $E = 0$, just to simplify the formulas. In this case the Hamilton equations (4.143), (4.144), take the form

$$\frac{dx}{d\tau} = Cx + 2Ap , \tag{4.195}$$

$$\frac{dp}{d\tau} = \frac{1}{2}A^{-1}C^2x + A^{-1}CAp . \tag{4.196}$$

We will exclude the trivial case when $C = 0$ and assume that the matrix C is non-degenerate. In particular, this means that the dimension n is even. These equations can be simplified by introducing new momenta

$$q = Ap + \frac{1}{2}Cx ; \tag{4.197}$$

then

$$\frac{dx}{d\tau} = 2q , \tag{4.198}$$

$$\frac{dq}{d\tau} = 2Cq . \tag{4.199}$$

The solution of these equations can be easily found

$$x(\tau) = x' + \frac{e^{2\tau C} - I}{C}q(0) , \tag{4.200}$$

$$q(\tau) = e^{2\tau C}q(0) . \tag{4.201}$$

Now, we choose $q(0)$ to satisfy the terminal condition $x(t) = x$, that is,

$$q(0) = C\left(e^{2tC} - I\right)^{-1}(x - x') . \tag{4.202}$$

Thus, the solution with the correct boundary conditions is

$$x(\tau) = x' + \frac{1}{2}\frac{e^{(2\tau-t)C} - e^{-tC}}{\sinh(tC)}(x - x')\,, \tag{4.203}$$

$$q(\tau) = \frac{1}{2}e^{(2\tau-t)C}\frac{C}{\sinh(tC)}(x - x')\,. \tag{4.204}$$

The boundary values of the momentum are

$$q(0) = \frac{1}{2}C\frac{e^{-tC}}{\sinh(tC)}(x - x') \tag{4.205}$$

$$q(t) = \frac{1}{2}C\frac{e^{tC}}{\sinh(tC)}(x - x')\,. \tag{4.206}$$

Now, the action is computed from eq. (4.89); by using eq. (4.198) we obtain

$$S(t; x, x') = \int_0^t d\tau\ \left\{\langle q(\tau), Aq(\tau)\rangle + \left\langle x(\tau), A^{-1}Cq(\tau)\right\rangle\right\}\,. \tag{4.207}$$

By using the solution (4.203), (4.204), we obtain

$$S(t; x, x') = \frac{1}{2}\left\langle x', A^{-1}Cx\right\rangle + \frac{1}{4}\left\langle (x - x'), A^{-1}C\coth(tC)(x - x')\right\rangle\,. \tag{4.208}$$

Notice that this formula is correct even in the limit $C \to 0$. Formally, it can be obtained from the general formula (4.185) by setting $G = E = 0$ and $\rho = C$. When comparing these two particular cases, that is, eqs. (4.193) and (4.208), recall that the matrix $A^{-1}\rho$ is symmetric and the matrix $A^{-1}C$ is antisymmetric.

We will develop alternative more powerful methods that can be applied to such operators in Chapt 6.

4.4 Singular Perturbations of Time-dependent Operators

The method described in the previous section can be generalized to a time-dependent operator

$$L = -\alpha^{ij}(t, x)\partial_i\partial_j + \beta^i(t, x)\partial_i + \gamma(t, x)\,, \tag{4.209}$$

where now all coefficients are functions of both t and x. Let $\varepsilon > 0$ be a small parameter and let us consider the following singularly perturbed heat equation

$$[\varepsilon\partial_t + L(t, x, \varepsilon\partial_x)]\, U(t, x|t', x') = 0\,, \tag{4.210}$$

with the initial condition

$$U(t', x|t', x') = \delta(x - x')\,. \tag{4.211}$$

We need to assume that the coefficients of the operator are smooth functions of τ in an interval $t' \le \tau \le t$ and that the operator is elliptic at all times.

The asymptotic expansion of the heat kernel as $\varepsilon \to 0$ has the form

$$U(t, x|t', x') \sim \varepsilon^{-n/2} \exp\left\{-\frac{1}{\varepsilon} S(t, x|t', x')\right\} \sum_{k=0}^{\infty} \varepsilon^k b_k(t, x|t', x')\,. \tag{4.212}$$

Almost all equations of Sec. 4.3 are valid in this case as well without any change. The only difference is that the Hamiltonian

$$H(t, x, p) = \alpha^{ij}(t, x) p_i p_j + \beta^j(t, x) p_j - \gamma(t, x) \tag{4.213}$$

depends explicitly on time and, therefore, the energy is not conserved along the phase trajectories.

Let $x(\tau)$ be the solution of the corresponding Hamiltonian system with initial conditions

$$x(t') = x'\,, \qquad x(t) = x\,. \tag{4.214}$$

Of course, $x(\tau) = x(\tau; t, t', x, x')$ depends on t, t', x, x' as parameters. Then the leading asymptotics of the heat kernel is

$$\begin{aligned} U(t, x|t', x') \sim\ & (2\pi\varepsilon)^{-n/2} Z^{1/2}(t, x|t', x') \\ & \times \exp\left\{-\frac{1}{\varepsilon} S(t, x|t', x') + \int_{t'}^{t} d\tau\ M(\tau)\right\}\,, \end{aligned} \tag{4.215}$$

where

$$\begin{aligned} S(t, x|t', x') = \int_{t'}^{t} d\tau\ \Bigg[& \frac{1}{4} \left\langle \frac{dx(\tau)}{d\tau}, A^{-1}(\tau, x(\tau)) \frac{dx(\tau)}{d\tau} \right\rangle \\ & - \frac{1}{2} \left\langle \beta(\tau, x(\tau)), A^{-1}(\tau, x(\tau)) \frac{dx(\tau)}{d\tau} \right\rangle \\ & + \frac{1}{4} \left\langle \beta(\tau, x(\tau)), A^{-1}(\tau, x(\tau)) \beta(\tau, x(\tau)) \right\rangle + \gamma(\tau, x(\tau)) \Bigg]\,, \end{aligned} \tag{4.216}$$

$$Z(t, x|t', x') = \det\left[-\partial_i \partial_{j'} S(t, x|t', x')\right]\,, \tag{4.217}$$

$$M(\tau) = \left[\partial_i \alpha^{ij}(\tau, x(\tau))\right] \partial_j S(t, x|t', x') + \frac{1}{2} \partial_i \beta^i(\tau, x(\tau))\,. \tag{4.218}$$

4.5 Notes

In this chapter we presented the theory of singular perturbation, in particular, the method of semi-classical approximation. An excellent introduction to these topics can be found in the books [60, 37]. Other useful references are [25, 58, 64, 67, 23, 36].

Chapter 5
Heat Kernel Asymptotics

Abstract This is the main chapter of the book describing the crucial ingredients of the heat kernel method. It is an enhanced version of the singular perturbation method described in the previous chapter due to a heavy use of geometric techniques. The main goal is to compute the short-time asymptotic expansion of the heat kernel and the corresponding expansion of the Green function.

5.1 Asymptotic Ansatz

We follow here [4, 10]. As we have seen before every elliptic second-order partial differential operator can be defined in geometric terms, which enables one to use powerful geometric methods in the study of analytic problems, like the heat kernel asymptotics.

Let M be an n-dimensional manifold without boundary. Let L be an elliptic second-order partial differential operator acting on smooth functions on M. Then in some local coordinates it must have the form (3.606)

$$L = -\alpha^{ij}(x)\partial_i\partial_j + \beta^j(x)\partial_j + \gamma(x)\,. \tag{5.1}$$

As we saw in Chap. 3 such an operator can be expressed entirely in terms of geometric quantities: a Riemannian metric

$$g^{ij} = \alpha^{ij}\,, \tag{5.2}$$

a generalized connection

$$\mathcal{A}_i = -\frac{1}{2}g_{ij}g^{-1/2}\partial_k\left(g^{1/2}g^{jk}\right) - \frac{1}{2}g_{ij}\beta^j\,, \tag{5.3}$$

and a scalar function Q (which plays the role of a potential)

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_5

$$Q = g^{-1/2}\partial_i \left(g^{1/2} g^{ij} \mathcal{A}_j\right) + g^{ij}\mathcal{A}_i\mathcal{A}_j + \gamma \tag{5.4}$$

$$= -\frac{1}{2} g^{-1/2}\partial_i\partial_k \left(g^{1/2} g^{ki}\right) + \frac{1}{4} g^{-1} g_{ij}\partial_k \left(g^{1/2} g^{ki}\right) \partial_m \left(g^{1/2} g^{mi}\right)$$

$$+\frac{1}{2}\beta^i g_{ij} g^{-1/2}\partial_k \left(g^{1/2} g^{kj}\right) - \frac{1}{2} g^{-1/2}\partial_i \left(g^{1/2}\beta^i\right) + \frac{1}{4} g_{ij}\beta^i\beta^j + \gamma\,.$$

Recall that (g^{ij}) is the inverse of the matrix (g_{ij}) and $g = \det g_{ij}$. Notice that for operators with constant coefficients

$$\mathcal{A}_i = -\frac{1}{2} g_{ij}\beta^j\,, \tag{5.5}$$

$$Q = \frac{1}{4} g_{ij}\beta^i\beta^j + \gamma\,. \tag{5.6}$$

The metric enables one to define then the Hilbert space $L^2(M, g^{1/2})$ with the standard Riemannian weight function $\mu = g^{1/2}$. Then the operator L can be written in terms of covariant derivatives, (3.617),

$$\begin{aligned} L &= -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q \\ &= -g^{ij}(\nabla_i + \mathcal{A}_i)(\nabla_j + \mathcal{A}_j) + Q \\ &= -g^{-1/2}(\partial_i + \mathcal{A}_i) g^{1/2} g^{ij} (\partial_j + \mathcal{A}_j) + Q\,, \end{aligned} \tag{5.7}$$

where ∇_i is the covariant derivative and

$$\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i \tag{5.8}$$

is the generalized covariant derivative. The adjoint of the operator L is

$$\begin{aligned} L^* &= -g^{ij}(\nabla_i - \bar{\mathcal{A}}_i)(\nabla_j - \bar{\mathcal{A}}_j) + \bar{Q} \\ &= -g^{-1/2}(\partial_i - \bar{\mathcal{A}}_i) g^{1/2} g^{ij} (\partial_j - \bar{\mathcal{A}}_j) + \bar{Q}\,. \end{aligned} \tag{5.9}$$

Therefore, if the connection $\mathcal{A}_i$ is purely imaginary and the potential Q is real then the operator L is self-adjoint.

The heat kernel $U(t; x, x')$ is the fundamental solution of the heat equation, that is, it is required to satisfy the equations

$$(\partial_t + L_x) U(t; x, x') = 0\,, \tag{5.10}$$

$$(\partial_t + L^*_{x'}) U(t; x, x') = 0\,, \tag{5.11}$$

and the initial condition

$$U(0; x, x') = \delta(x, x')\,, \tag{5.12}$$

where $\delta(x,x')$ is the covariant delta-function defined by

$$\delta(x,x') = g^{-1/4}(x)\delta(x-x')g^{-1/4}(x')\,. \tag{5.13}$$

The extra factors of $g(x)$ are inserted here (in a symmetric way) to satisfy the definition of the delta-function in the curved manifold

$$\int\limits_M dx\; g^{1/2}(x)\delta(x,x')f(x) = f(x')\,. \tag{5.14}$$

Under such a definition the heat kernel is a biscalar, that is, a scalar at both points x and x'. In the usual definition with the standard delta-function, the heat kernel is a bi-scalar density. In geometry it is always natural and preferable to work with invariant objects. That is why, we define the heat kernel in such a way. Therefore, one should be careful when comparing the formulas of the previous chapters to this one—they differ by factors like $g^{-1/4}(x)g^{-1/4}(x')$.

For example, for operators with constant coefficients, when α^{ij}, β^i and γ, and, hence, g_{ij}, $\mathcal{A}_i$ and Q are constant, the heat kernel has the form (compare with eq. (4.115) and (2.196))

$$\begin{aligned} U(t;x,x') = (4\pi t)^{-n/2}\exp\left\{-\frac{1}{4t}g_{ij}(x^i-x'^i)(x^j-x'^j)\right\} \\ \times\exp\left\{-\mathcal{A}_i(x^i-x'^i)\right\}e^{-Qt}\,. \end{aligned} \tag{5.15}$$

Notice the absence of the factor $g^{1/2}$. Now, if $g_{ij}=\delta_{ij}$ and $\mathcal{A}_i = Q = 0$ then we get the heat kernel of the classical Laplacian $L = -\delta^{ij}\partial_i\partial_j$ in flat Euclidean space $\mathbb{R}^n$,

$$U(t;x,x') = (4\pi t)^{-n/2}\exp\left(-\frac{|x-x'|^2}{4t}\right)\,, \tag{5.16}$$

where $|x-x'| = \sqrt{\delta_{ij}(x^i-x'^i)(x^j-x'^j)}$.

In general, one can show that for $t>0$ the heat kernel $U(t;x,x')$ is a smooth function of time t and the coordinates of both points x and x'. Our primary goal in this book is to compute the heat kernel. Unfortunately, it is impossible, in general, to do it exactly. Therefore, it is crucial to develop some methods for computation of the heat kernel at least in some approximation. This chapter is devoted to one of such approximations, namely, the calculation of the asymptotic expansion of the heat kernel for short times, as $t\to 0$. Some other, more advanced methods, will be discussed in Chap. 6.

Of course, to compute asymptotic expansion of the heat kernel we could use the methods of singular perturbations discussed in Chap. 4. Then applying the general method described in the Chap. 4 to the operator $L(x,\varepsilon\partial)$ we look for a solution in the form of an asymptotic series

$$U(t;x,x') \sim \varepsilon^{-n/2} g^{-1/4}(x) g^{-1/4}(x') \exp\left\{-\frac{1}{\varepsilon} S(t;x,x')\right\} \sum_{k=0}^{\infty} \varepsilon^k b_k(t;x,x')\,. \tag{5.17}$$

This correctly reproduced the initial condition. So, our main idea is now to exhibit an asymptotic factor that reproduces the initial data on the curved manifold. Since we are looking for the asymptotic expansion as $t \to 0$, we can use the asymptotic form of the function S and the coefficients b_k (see eqs. (4.73) and (4.74))

$$S(t;x,x') \sim \frac{1}{2t}\Phi(x,x') + \sum_{k=0}^{\infty} t^k S_k(x,x')\,, \tag{5.18}$$

$$b_k(t;x,x') \sim (4\pi t)^{-n/2} \det\left[-\partial_i \partial_{j'} \Phi(x,x')\right]^{1/2} \sum_{l=0}^{\infty} t^l b_{kl}(x,x')\,, \tag{5.19}$$

to get a new expansion

$$U(t;x,x') \sim \varepsilon^{-n/2}(4\pi t)^{-n/2} g^{-1/4}(x) \det\left[-\partial_i \partial_{j'} \Phi(x,x')\right]^{1/2} g^{-1/4}(x') \times \exp\left\{-\frac{1}{2\varepsilon t}\Phi(x,x')\right\} \sum_{k=0}^{\infty} \varepsilon^k t^k c_k(x,x')\,, \tag{5.20}$$

where Φ and c_k are some undetermined functions.

The main drawback of the whole framework of Chap. 4 is that it is not covariant (since we introduced a small parameter ε at partial derivatives ∂ and not covariant derivatives ∇). Therefore, we modify it slightly by considering the singularly perturbed operator of the form

$$L_\varepsilon = \varepsilon^2 L = -\varepsilon^2 g^{ij} \nabla_i^{\mathcal{A}} \nabla_j^{\mathcal{A}} + \varepsilon^2 Q\,. \tag{5.21}$$

Then we have the commutation formula

$$\exp\left(\frac{1}{\varepsilon} S\right) \left(\varepsilon \partial_t + \varepsilon^2 L\right) \exp\left(-\frac{1}{\varepsilon} S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 L\,, \tag{5.22}$$

where

$$T_0 = -\dot{S} - g^{ij} S_i S_j\,, \tag{5.23}$$

$$T_1 = \partial_t + 2 g^{ij} S_j (\nabla_i + \mathcal{A}_i) + g^{ij} S_{ij}\,,\,, \tag{5.24}$$

and $S_i = \nabla_i S$, $S_{ij} = \nabla_i \nabla_j S$. Similarly, the same commutation formula holds for the adjoint operator L^*, that is,

$$\exp\left(\frac{1}{\varepsilon} S\right) \left(\varepsilon \partial_t + \varepsilon^2 L^*\right) \exp\left(-\frac{1}{\varepsilon} S\right) = T_0^* + \varepsilon T_1^* + \varepsilon^2 L^*\,, \tag{5.25}$$

where

$$T_0^* = -\dot{S} - g^{i'j'} S_{i'} S_{j'} \,, \tag{5.26}$$

$$T_1^* = \partial_t + 2g^{i'j'} S_{j'} (\nabla_{i'} - \bar{\mathcal{A}}_{i'}) + g^{i'j'} S_{i'j'} \,, \,, \tag{5.27}$$

and $S_{i'} = \nabla_{i'} S$, $S_{i'j'} = \nabla_{i'} \nabla_{j'} S$.

Now, we look for a solution of the heat equations (5.10) and (5.11) in the asymptotic form (5.17). Then to cancel the leading terms we require $T_0 = T_0^* = 0$, that is, the function S (the action) to satisfy the following Hamilton-Jacobi equation

$$\partial_t S + g^{ij} (\nabla_i S)(\nabla_j S) = 0 \,, \tag{5.28}$$

$$\partial_t S + g^{i'j'} (\nabla_{i'} S)(\nabla_{j'} S) = 0 \,. \tag{5.29}$$

We can separate the time variable by assuming

$$S(t; x, x') = \frac{1}{2t} \sigma(x, x') \,. \tag{5.30}$$

Then the function σ satisfies the equations

$$\sigma = \frac{1}{2} g^{ij} (\nabla_i \sigma)(\nabla_j \sigma) \,, \tag{5.31}$$

$$\sigma = \frac{1}{2} g^{i'j'} (\nabla_{i'} \sigma)(\nabla_{j'} \sigma) \,. \tag{5.32}$$

This is nothing but the equations (3.222) and (3.223) that define the Synge function. This gives the exact form of the action S.

Therefore, our asymptotic ansatz (5.20) takes the form

$$U(t; x, x') \sim \varepsilon^{-n/2} (4\pi t)^{-n/2} \Delta^{1/2}(x, x') \exp\left\{ -\frac{1}{2\varepsilon t} \sigma(x, x') \right\} \sum_{k=0}^{\infty} \varepsilon^k t^k c_k(x, x') \,, \tag{5.33}$$

where $\Delta(x, x')$ is the Van Vleck-Morette determinant defined by (3.273). Also, the transport operators become

$$T_1 = \partial_t + \frac{1}{t} \left(D + \sigma^i \mathcal{A}_i + \frac{1}{2} \sigma^i{}_i \right) \,, \tag{5.34}$$

$$T_1^* = \partial_t + \frac{1}{t} \left(D' - \sigma^{i'} \bar{\mathcal{A}}_{i'} + \frac{1}{2} \sigma^i{}_i \right) \,, \tag{5.35}$$

where

$$D = \sigma^i \nabla_i, \qquad D' = \sigma^{i'} \nabla_{i'} \,. \tag{5.36}$$

Now, by using the eq. (3.283) we can rewrite the transport operators as

$$T_1 = t^{-n/2}\Delta^{1/2}\left\{\partial_t + \frac{1}{t}\left(D + \sigma^i \mathcal{A}_i\right)\right\} t^{n/2}\Delta^{-1/2}\,, \tag{5.37}$$

$$T_1^* = t^{-n/2}\Delta^{1/2}\left\{\partial_t + \frac{1}{t}\left(D' - \sigma^{i'} \bar{\mathcal{A}}_{i'}\right)\right\} t^{n/2}\Delta^{-1/2}\,, \tag{5.38}$$

and, further by using the generalized operator of parallel transport $\mathcal{P}(x, x')$ defined by (3.311) and the eq. (3.309) these operators take the form

$$T_1 = t^{-n/2}\mathcal{P}\Delta^{1/2}\left(\partial_t + \frac{1}{t}D\right) t^{n/2}\mathcal{P}^{-1}\Delta^{-1/2}\,, \tag{5.39}$$

$$T_1^* = t^{-n/2}\mathcal{P}\Delta^{1/2}\left(\partial_t + \frac{1}{t}D'\right) t^{n/2}\mathcal{P}^{-1}\Delta^{-1/2}\,. \tag{5.40}$$

Therefore, we define our asymptotic ansatz as

$$U(t; x, x') = (4\pi t)^{-n/2}\mathcal{P}(x, x')\Delta^{1/2}(x, x')\exp\left(-\frac{\sigma(x, x')}{2t}\right)\Omega(t; x, x')\,. \tag{5.41}$$

We will consider the case when the points x and x' are sufficiently close to each other so that all two-point functions are single-valued and well-defined.

Now, by using the commutation formulas (5.22) and (5.39) we find that the function $\Omega(t; x, x')$ satisfies a so called *transport equation*

$$\left(\partial_t + \frac{1}{t}D + \hat{L}\right)\Omega(t; x, x') = 0\,, \tag{5.42}$$

where

$$\hat{L} = \mathcal{P}^{-1}\Delta^{-1/2}L\Delta^{1/2}\mathcal{P}\,, \tag{5.43}$$

and the initial conditions

$$\Omega(0; x, x') = 1\,. \tag{5.44}$$

5.2 Minackshisundaram-Pleijel Expansion

We will assume the function $Q(x)$ to be bounded below by a sufficiently large positive parameter m^2, that is, for any x

$$Q(x) \geq m^2\,. \tag{5.45}$$

Then the operator L is *positive* and the heat kernel $U(t; x, x')$ as well as the function $\Omega(t; x, x')$ decreases at the infinity $t \to \infty$ more rapidly than any power of t. It is well known that as $t \to 0$ there is an asymptotic expansion of the function $\Omega(t; x, x')$ in positive integer powers of t. Thus, the function

Ω satisfies the following asymptotic conditions: for any $\alpha > 0$ and any $N \geq 0$

$$\lim_{t\to\infty,0} t^{\alpha} \left(\frac{\partial}{\partial t}\right)^{N} \Omega(t; x, x') = 0\,. \tag{5.46}$$

Now, motivated by the discussion in Sect. 1.6 (see eq. (1.89)) we consider the Mellin transformation of the transport function $\Omega(t)$,

$$b_q(x, x') = \frac{1}{\Gamma(-q)} \int_0^{\infty} dt\; t^{-q-1} \Omega(t; x, x')\,, \tag{5.47}$$

where $\Gamma(-q)$ is introduced for convenience. Under the above assumptions this integral converges in the region $\mathrm{Re}\, q < 0$. For $\mathrm{Re}\, q \geq 0$ the function b_q should be defined by analytic continuation. Integration by parts leads then to an entire function which is analytic on the whole complex plane of q. For example, for $\mathrm{Re}\, q < N$ we have

$$b_q(x, x') = \frac{1}{\Gamma(-q+N)} \int_0^{\infty} dt\; t^{-q-1+N} \left(-\frac{\partial}{\partial t}\right)^{N} \Omega(t; x, x')\,, \tag{5.48}$$

where N is an arbitrary positive integer.

Moreover, by integrating by parts and making use of the asymptotic properties (5.46) of the function $\Omega(t; x, x')$ it is not difficult to obtain the values of $b_q(x, x')$ at the positive integer points $q = k$, $(k = 0, 1, 2, ...)$,

$$b_k(x, x') = \left(-\frac{\partial}{\partial t}\right)^{k} \Omega(t; x, x')\Big|_{t=0}\,. \tag{5.49}$$

It is also not difficult to establish the crucial asymptotic property of b_q, namely, for any $N > 0$

$$\lim_{|q|\to\infty\,,\mathrm{Re}\, q<N} \Gamma(-q+N) b_q(x, x') = 0\,. \tag{5.50}$$

Thus, the function b_q can be viewed as an analytical continuation of the coefficients b_k on the whole complex plane of q from positive integer values with the asymptotic condition (5.50).

Now we can invert the Mellin transform and write down

$$\Omega(t; x, x') = \int_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i}\; t^{q} \Gamma(-q) b_q(x, x')\,, \tag{5.51}$$

where c is a negative constant. In particular, this gives the heat kernel diagonal as an integral of the coincidence limit of the function b_q,

$$U(t;x,x) = (4\pi t)^{-n/2} \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i}\, t^q \Gamma(-q) b_q(x,x)\,. \tag{5.52}$$

Deforming the contour of integration in (5.51) and taking into account the properties (5.49) and (5.50) we obtain

$$\Omega(t;x,x') = +R_N(t;x,x')\,, \tag{5.53}$$

where

$$R_N(t;x,x') = \int\limits_{c_N-i\infty}^{c_N+i\infty} \frac{dq}{2\pi i}\, t^q \Gamma(-q) b_q(x,x')\,, \tag{5.54}$$

with $N-1 < c_N < N$.

Here $R_N(t;x,x')$ is of order $O(t^N)$ as $t \to 0$ and is smaller than the last term of the sum in this limit. Therefore, eq. (5.53) gives the asymptotic expansion of $\Omega(t;x,x')$ as $t \to 0$

$$\Omega(t;x,x') \sim \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} b_k(x,x')\,. \tag{5.55}$$

Of course, this immediately gives the asymptotic expansion of the heat kernel diagonal

$$U(t;x,x) \sim (4\pi t)^{-n/2} \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} b_k(x,x)\,. \tag{5.56}$$

The coefficients $b_k(x,x')$ are some smooth functions that are usually called *Hadamard-Minakshisundaram-De Witt-Seeley (HMDS) coefficients* (or just *heat kernel coefficients*) and the asymptotic expansion itself is called the *Minackshisundaram-Pleijel expansion*. Our normalization differs by the factor $(-1)^k/k!$ from the usual one. We use this normalization since it appears naturally from the point of view of Mellin transform.

It is worth pointing out that the asymptotic expansion (5.55) is convergent only in the case when the remainder term $R_N(t;x,x')$ (5.54) vanishes as $N \to \infty$ in a neighborhood of the point $t = 0$. In this case the function $\Omega(t;x,x')$ is analytic in a neighborhood of $t = 0$. However, in general, $\Omega(t;x,x')$ is not analytic at the point $t = 0$. Therefore, in general, for any fixed $t > 0$ the remainder $R_N(t;x,x')$ does not vanish as $N \to \infty$ and the asymptotic expansion (5.55) diverges for any finite $t > 0$. Thus the asymptotic ansatz (5.55) makes sense only in cases when its lowest-order terms are essential. The correct ansatz for the function $\Omega(t;x,x')$ is given rather by the inverse Mellin transform (5.51).

5.3 Recurrence Relations

By substituting the ansatz (5.51) into the transport equation (5.42) we obtain a functional equation for the function $b_q(x, x')$

$$\left(1 + \frac{1}{q}D\right) b_q(x, x') = \hat{L} b_{q-1}(x, x') \,. \tag{5.57}$$

Recall that q is a complex variable. For positive integer values $q = 1, 2, \ldots$ this equation gives a differential recursive system for the heat kernel coefficients b_k. For $q = 0$ it gives

$$D b_0 = 0 \,. \tag{5.58}$$

From the initial condition (5.44) by taking into account eq. (5.49) we get the initial condition of the recursion

$$b_0(x, x') = 1 \,. \tag{5.59}$$

Thus instead of the differential equation (5.42) for the function $\Omega(t; x, x')$ with the initial condition (5.44) we obtained the functional equation (5.57) for the function $b_q(x, x')$ with the initial condition (5.59). One also has the asymptotic property (5.50) of the function $b_q(x, x')$ which reflects the property (5.48) for the function $\Omega(t; x, x')$.

5.4 Green Function

Let us introduce a complex degree L^{-p} of the operator L. The integral kernel of this operator can be defined via the heat kernel by

$$G^p(x, x') = \frac{1}{\Gamma(p)} \int\limits_0^\infty dt \; t^{p-1} U(t; x, x') \,. \tag{5.60}$$

Then by using our ansatz (5.41) for the heat kernel we get

$$G^p(x, x') = (4\pi)^{-n/2} \mathcal{P} \Delta^{1/2} \tag{5.61}$$
$$\times \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i} \frac{\Gamma(-q)}{\Gamma(p)} b_q \int\limits_0^\infty dt \; t^{p+q-n/2-1} \exp\left(-\frac{\sigma}{2t}\right) ,$$

where c is a sufficiently large negative constant satisfying the condition $c < \frac{n}{2} - \operatorname{Re} p$; next, by integrating over t we obtain

$$G^p(x,x') = (4\pi)^{-n/2}\mathcal{P}\Delta^{1/2} \times \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i}\frac{\Gamma(-q)\Gamma\left(-p-q+n/2\right)}{\Gamma(p)}\left(\frac{\sigma}{2}\right)^{p+q-n/2} b_q\,. \tag{5.62}$$

This representation of the kernel of the operator L^{-p} is especially useful for studying the short-distance behavior when the points x and x' are close to each other, that is, as $\sigma(x,x') \to 0$. In particular, for $p > n/2$ there is a well-defined diagonal value

$$G^p(x,x) = (4\pi)^{-n/2}\frac{\Gamma\left(p-n/2\right)}{\Gamma(p)} b_{n/2-p}(x,x)\,. \tag{5.63}$$

Further, by setting $p = 1$ we obtain the Green function of the operator L,

$$G(x,x') = (4\pi)^{-n/2}\mathcal{P}\Delta^{1/2} \times \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i}\Gamma(-q)\Gamma\left(\frac{n}{2}-q-1\right)\left(\frac{\sigma}{2}\right)^{1+q-n/2} b_q\,, \tag{5.64}$$

where $c < -1/2$.

This representation is well suited for studying the singularities of the Green function, or even more generally, for constructing the Green function as a power series in σ. The integrand in (5.64) is a meromorphic function with poles at the points $q = k$ and $q = k - 1 + \frac{n}{2}$, $(k = 0, 1, 2, \dots)$. In odd dimensions, the poles are at the points $q = k$ and $q = k + \left[\frac{n}{2}\right] - 1/2$ and are *simple*, whereas in even dimension there are simple poles at $q = 0, 1, 2, \dots, \frac{n}{2} - 2$ and *double* poles at the points $q = k + \frac{n}{2} - 1$.

Moving the contour of integration in (5.64) to the right to the infinity one can obtain an expansion of the Green function in powers of σ (*Hadamard series*). We obtain

$$G = G^{\rm sing} + G^{\rm non-anal} + G^{\rm reg}. \tag{5.65}$$

Here $G^{\rm sing}$ is the *singular part* which is polynomial in the inverse powers of $\sqrt{\sigma}$

$$G^{\rm sing} = (4\pi)^{-n/2}\mathcal{P}\Delta^{1/2}\sum_{k=0}^{[(n-3)/2]}\frac{(-1)^k}{k!}\Gamma\left(\frac{n}{2}-k-1\right)\left(\frac{2}{\sigma}\right)^{n/2-k-1} b_k\,, \tag{5.66}$$

where the square brackets denote the integer part of a real number, that is, $[x]$ is the largest integer smaller or equal x.

Further, in odd dimension $n = 1, 3, \dots$ we have

$$G^{\rm non-anal} \sim (-1)^{(n-1)/2}(4\pi)^{-n/2}\mathcal{P}\Delta^{1/2} \tag{5.67}$$
$$\times \sum_{k=0}^{\infty} \frac{\pi}{\Gamma\left[k+(n+1)/2\right]\Gamma\left[k+3/2\right]} \left(\frac{\sigma}{2}\right)^{k+1/2} b_{k+(n-1)/2}\,,$$

$$G^{\rm reg} \sim (-1)^{(n+1)/2}(4\pi)^{-n/2}\mathcal{P}\Delta^{\frac{1}{2}} \sum_{k=0}^{\infty} \frac{\pi}{k!\Gamma\left(k+n/2\right)} \left(\frac{\sigma}{2}\right)^{k} b_{k-1+n/2}\,. \tag{5.68}$$

And in even dimension $n = 2, 4, \dots$ we have

$$G^{\rm non-anal} \sim (-1)^{n/2-1}(4\pi)^{-n/2}\mathcal{P}\Delta^{1/2} \log\left(\frac{\sigma}{2}\right)$$
$$\times \sum_{k=0}^{\infty} \frac{1}{k!\Gamma\left(k+n/2\right)} \left(\frac{\sigma}{2}\right)^{k} b_{k-1+n/2}\,, \tag{5.69}$$

$$G^{\rm reg} \sim (-1)^{n/2-1}(4\pi)^{-n/2}\mathcal{P}\Delta^{1/2} \sum_{k=0}^{\infty} \frac{1}{k!\Gamma\left(k+n/2\right)} \left(\frac{\sigma}{2}\right)^{k} \tag{5.70}$$
$$\times \left\{ b'_{k-1+n/2} - \left[\Psi(k+1) + \Psi\left(k+\frac{n}{2}\right)\right] b_{k-1+n/2} \right\},$$

where $\Psi(z) = \Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the gamma-function and

$$b'_q = \frac{\partial b_q}{\partial q}\,. \tag{5.71}$$

Note that the singular part $G^{\rm sing}$ and the non-analytical part $G^{\rm non-anal}$ are expressed only in terms of the local HMDS-coefficients, that is, the values b_k of he function b_q at positive integer $q = k$, whereas the regular part $G^{\rm reg}$ contains the values of the function $b_{k+1/2}$ at half-integer positive points $q = k + \frac{1}{2}$ and the derivatives b'_k at integer positive points, which are *not* expressible in terms of the local information. These objects are global and cannot be expressed further in terms of the local HMDS-coefficients.

The regular part of the Green function has a well defined diagonal value. It reads in odd dimensions ($n = 1, 3, \dots$):

$$G^{\rm reg}(x,x) = (-1)^{(n+1)/2}(4\pi)^{-n/2} \frac{\pi}{\Gamma\left(n/2\right)} b_{n/2-1}(x,x)\,, \tag{5.72}$$

and in even dimensions ($n = 2, 4, \dots$)

$$G^{\rm reg}(x,x) = (-1)^{n/2-1} \frac{(4\pi)^{-n/2}}{\Gamma\left(n/2\right)} \left\{ b'_{n/2-1}(x,x) - \left[\Psi\left(\frac{n}{2}\right) - \mathbb{C}\right] b_{n/2-1}(x,x) \right\}, \tag{5.73}$$

where $\mathbb{C} = -\Psi(1) = 0.577\dots$ is the Euler's constant.

5.5 Non-recursive Solution of Recurrence Relations

Let us apply the method of covariant expansions described in a previous chapter to calculation of heat kernel coefficients b_k. We already know that $b_0 = 1$. Then we can write down the formal operator solution of the recursive system (5.57)

$$b_k = \left(1 + \frac{1}{k}D\right)^{-1} \hat{L} \left(1 + \frac{1}{k-1}D\right)^{-1} \hat{L} \cdots (1+D)^{-1} \hat{L} \cdot 1 \,. \tag{5.74}$$

Now, by expanding the coefficients b_k in covariant Taylor series

$$\begin{aligned} b_k &= \sum_{n=0}^{\infty} |n\rangle\langle n|b_k\rangle \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sigma^{i'_1} \cdots \sigma^{i'_n} \left[\nabla_{(i_1} \cdots \nabla_{i_n)} b_k\right](x') \end{aligned} \tag{5.75}$$

(recall that square brackets mean the coincidence limit of a two-point function $[f(x,x')] = f(x,x)$ and parenthesis denote the symmetrization over all included indices) and defining the inverse operator $\left(1 + \frac{1}{k}D\right)^{-1}$ by

$$\left(1 + \frac{1}{k}D\right)^{-1} = \sum_{n=0}^{\infty} \left(1 + \frac{n}{k}\right)^{-1} |n\rangle\langle n| \tag{5.76}$$

we obtain from (5.74)

$$\begin{aligned} \langle n|b_k\rangle = &\sum_{n_1,\cdots,n_{k-1}\geq 0} N(n,k;n_1,\ldots,n_k) \\ &\times \langle n|\hat{L}|n_{k-1}\rangle\langle n_{k-1}|\hat{L}|n_{k-2}\rangle \cdots \langle n_1|\hat{L}|0\rangle \,, \end{aligned} \tag{5.77}$$

where

$$N(n,k;n_1,\ldots,n_k) = \frac{k}{(k+n)} \cdot \frac{(k-1)}{(k-1+n_{k-1})} \cdots \frac{2}{(2+n_2)} \cdot \frac{1}{(1+n_1)} \,, \tag{5.78}$$

and $\langle m|\hat{L}|n\rangle$ are the *matrix elements* of the operator $\hat{L}$ defined by

$$\begin{aligned} \langle m|\hat{L}|n\rangle &= \langle i_1 \cdots i_m|\hat{L}|j_1 \cdots j_n\rangle \\ &= \left[\nabla_{(i_1} \cdots \nabla_{i_m)} \hat{L} \frac{(-1)^n}{n!} \sigma^{j'_1} \cdots \sigma^{j'_n}\right]_{x=x'} . \end{aligned} \tag{5.79}$$

Note that $\langle n|b_k\rangle$ is a symmetric tensor of type $(0,n)$, that is,

$$\langle n|b_k\rangle = b_{(k)i_1\dots i_n}\,, \tag{5.80}$$

and the matrix elements $\langle m|\hat{L}|n\rangle$ are tensors of type (n,m) which are symmetric in all upper indices and all lower indices separately, that is,

$$\langle m|\hat{L}|n\rangle = L^{j_1\dots j_n}_{i_1\dots i_m}\,. \tag{5.81}$$

Of course, the matrix element $\langle m|\hat{L}|0\rangle$ is just a symmetric tensor of type $(0,m)$:

$$\langle m|\hat{L}|0\rangle = L_{i_1\dots i_m}\,. \tag{5.82}$$

The product of matrix elements is defined then as an inner product in the space of symmetric tensors, that is,

$$\langle m|\hat{L}|n\rangle\langle n|\hat{L}|p\rangle = L^{j_1\dots j_n}_{i_1\dots i_m} L^{l_1\dots l_p}_{j_1\dots j_n}\,, \tag{5.83}$$

where the contraction over all indices $j_1,\dots j_n$ is understood. This notation is very convenient and should not cause any confusion. For example, with all indices written down our solution takes the form

$$\begin{aligned} b_{(k)i_1\dots i_n} = &\sum_{n_1,\cdots,n_{k-1}\geq 0} N(n,k;n_1,\dots,n_k) \\ &\times L^{j_1\dots j_{n_{k-1}}}_{i_1\dots i_n} L^{l_1\dots l_{n_{k-2}}}_{j_1\dots j_{n_{k-1}}} \cdots L^{p_1\dots p_{n_1}}_{m_1\dots m_{n_2}} L_{p_1\dots p_{n_1}}\,. \end{aligned} \tag{5.84}$$

Thus, we reduced the problem of calculation of heat kernel coefficients to the problem of computing the matrix elements of the operator $\hat{L}$. Note that the matrix elements are defined as coincidence limits of derivatives of the functions σ, Δ and $\mathcal{P}$. Because the vectors $\sigma^{i'}$ without derivatives vanish in the coincidence limit, that is, $[\sigma^{i'}] = 0$, and taking into account that $\hat{L}$ is a second-order differential operator we see that the matrix elements $\langle m|\hat{L}|n\rangle$ are non-zero only if $n \leq m+2$. Therefore, the summation over $n_1,\dots,n_{k-1}$ in eq. (5.77) is limited from above, that is, $n_1 \geq 0$ and

$$n_i \leq n_{i+1} + 2\,, \qquad i = 1,2,\dots,k-1\,, \tag{5.85}$$

where $n_k = n$. Thus the sum for the coefficient $\langle n|b_k\rangle$ contains only a finite number of terms.

5.6 Matrix Elements

For evaluation of matrix elements (5.79) we proceed as follows. We recall the definition of the matrices $\eta^{i'}{}_j$ and $\gamma^i{}_{j'}$, namely $\eta^{i'}{}_j = \nabla_j \sigma^{i'}$ and $\gamma^i{}_{j'}$ is the inverse of the matrix $\eta^{i'}{}_j$. Let us define the differential operators

$$\mathcal{D}_{i'} = \gamma^{j}{}_{i'}\nabla_j \,. \tag{5.86}$$

These operators have a nice property that

$$\mathcal{D}_{i'}\sigma^{j'} = \delta^{j'}{}_{i'} \,. \tag{5.87}$$

That is why, it is convenient to express the operator $\hat{L}$ in terms of these operators. By using the equations (3.263) and (3.287) we obtain

$$\hat{L} = -(\mathcal{D}_{i'} - \zeta_{i'} + \hat{\mathcal{A}}_{i'})X^{i'j'}(\mathcal{D}_{j'} + \zeta_{j'} + \hat{\mathcal{A}}_{j'}) + Q \,, \tag{5.88}$$

where

$$X^{i'j'} = \eta^{i'}{}_{k}\eta^{j'k} \,. \tag{5.89}$$

Recall also that

$$\zeta_{i'} = \mathcal{D}_{i'}\zeta \,, \tag{5.90}$$

$$\zeta = \log \Delta^{1/2} \,, \tag{5.91}$$

$$\hat{\mathcal{A}}_{i'} = \gamma^{j}{}_{i'}\mathcal{P}^{-1}\nabla^{\mathcal{A}}_{j}\mathcal{P} \,. \tag{5.92}$$

This can be further written in the form

$$\hat{L} = -X^{i'j'}\mathcal{D}_{i'}\mathcal{D}_{j'} - Y^{i'}\mathcal{D}_{i'} + Z \,, \tag{5.93}$$

where

$$Y^{i'} = \mathcal{D}_{j'}X^{i'j'} + 2X^{i'j'}\hat{\mathcal{A}}_{j'} \,, \tag{5.94}$$

$$Z = X^{i'j'}(\zeta_{i'}\zeta_{j'} - \hat{\mathcal{A}}_{i'}\hat{\mathcal{A}}_{j'}) - \mathcal{D}_{j'}\left[X^{i'j'}\left(\zeta_{i'} + \hat{\mathcal{A}}_{i'}\right)\right] + Q \,. \tag{5.95}$$

Inserting the operator $\hat{L}$ in the form (5.93) into the definition of the matrix elements (5.79) we obtain

$$\langle i_1 \cdots i_m|\hat{L}|j_1 \cdots j_n\rangle \tag{5.96}$$
$$= \frac{(-1)^n}{n!}\left[\nabla_{(i_1}\cdots\nabla_{i_m)}\left(-X^{i'j'}\mathcal{D}_{i'}\mathcal{D}_{j'} - Y^{i'}\mathcal{D}_{i'} + Z\right)\sigma^{j'_1}\cdots\sigma^{j'_n}\right]_{x=x'} \,.$$

Now by using the coincidence limits (5.106) and eqs. (5.87), (3.342) we obtain the matrix elements: for $n > m+2$ and $n = m+1$,

$$\langle m|\hat{L}|n\rangle = 0 \,, \tag{5.97}$$

for $n = m+2$,

$$\langle i_1 \cdots i_m|\hat{L}|j_1 \cdots j_{m+2}\rangle = -\delta^{(j_1\cdots j_m}_{i_1\cdots i_m}g^{j_{m+1}j_{m+2})} \,, \tag{5.98}$$

and for $n \leq m$,

$$\langle i_1 \cdots i_m | \hat{L} | j_1 \cdots j_n \rangle = \binom{m}{n} \delta^{j_1 \cdots j_n}_{(i_1 \cdots i_n} Z_{i_{n+1} \cdots i_m)} \tag{5.99}$$

$$+ \binom{m}{n-1} \delta^{(j_1 \cdots j_{n-1}} Y^{j_n)}{}_{i_n \cdots i_m)} - \binom{m}{n-2} \delta^{(j_1 \cdots j_{n-2}} X^{j_{n-1} j_n)}{}_{i_{n-1} \cdots i_m)} ,$$

where

$$X^{ij}{}_{l_1 \cdots l_n} = \left[\nabla_{(l_1} \cdots \nabla_{l_n)} X^{i'j'} \right] , \tag{5.100}$$

$$Y^{j}{}_{l_1 \cdots l_n} = \left[\nabla_{(l_1} \cdots \nabla_{l_n)} Y^{j'} \right] , \tag{5.101}$$

$$Z_{l_1 \cdots l_n} = \left[\nabla_{(l_1} \cdots \nabla_{l_n)} Z \right] . \tag{5.102}$$

Here it is meant that the binomial coefficients $\binom{n}{k}$ is equal to zero when k or $(n-k)$ are negative. Thus, we see that the summation over $n_1, \ldots n_{k-1}$ in (5.77) is limited from above

$$0 \leq n_1 \leq n_2 + 2 \leq \cdots \leq n_{k-1} + 2(k-2) \leq n + 2(k-1) , \tag{5.103}$$

and, therefore,this sum contains a finite number of terms.

Finally, by using the explicit expressions (5.89)–(5.95) we obtain from (5.100)–(5.102)

$$X^{ij}{}_{l_1 \cdots l_n} = \sum_{k=0}^{n} \binom{n}{k} \eta^{(i}{}_{m(l_1 \cdots l_k} \eta^{j)m}{}_{l_{k+1} \cdots l_n)} , \tag{5.104}$$

$$Y^{j}{}_{l_1 \cdots l_n} = -X^{ji}{}_{il_1 \cdots l_n} + 2 \sum_{k=0}^{n} \binom{n}{k} X^{j}{}_{m(l_1 \cdots l_k} \mathcal{A}^{m}{}_{l_{k+1} \cdots l_n)} , \tag{5.105}$$

$$\begin{aligned} Z_{l_1 \cdots l_n} = Q_{l_1 \cdots l_n} + \sum_{k=0}^{n} \binom{n}{k} \Big\{ & X_{ij(l_1 \cdots l_k} \left[-\zeta^{ij}{}_{l_{k+1} \cdots l_n)} + \mathcal{A}^{ij}{}_{l_{k+1} \cdots l_n)} \right] \\ & + X^{i}{}_{ji(l_1 \cdots l_k} \left[-\zeta^{j}{}_{l_{k+1} \cdots l_n)} + \mathcal{A}^{j}{}_{l_{k+1} \cdots l_n)} \right] \Big\} \\ & + \sum_{k=0}^{n} \sum_{m=0}^{n-k} \frac{n!}{k! m! (n-k-m)!} X_{ij(l_1 \cdots l_k} \Big[\zeta^{i}{}_{l_{k+1} \cdots l_{k+m}} \zeta^{j}{}_{l_{k+m+1} \cdots l_n)} \\ & - \mathcal{A}^{i}{}_{l_{k+1} \cdots l_{k+m}} \mathcal{A}^{j}{}_{l_{k+m+1} \cdots l_n)} \Big] , \end{aligned} \tag{5.106}$$

where

$$Q_{l_1 \cdots l_n} = \nabla_{(l_1} \cdots \nabla_{l_n)} Q \tag{5.107}$$

and $\eta^{i}{}_{jl_1\cdots l_n}$, $\zeta_{l_1\cdots l_n}$ and $\mathcal{A}_{jl_1\cdots l_n}$ are given explicitly by (3.385), (3.404) and (3.427). We correct here a misprint (a sign) in eq. (3.79) of [4].

So, by using the coincidence limits of symmetrized derivatives of two-point quantities from Chap. 3 one can calculate the matrix elements (5.79) of the operator $\hat{L}$ and, therefore, Taylor coefficients of the heat kernel coefficients b_k (5.77).

From the dimensional arguments it is obvious that for $m = n$ the matrix elements $\langle m|\hat{L}|n\rangle$ given by eq. (5.99) are expressed in terms of the curvature tensors $R^{i}{}_{jkl}$, $\mathcal{R}_{ij}$ and the potential term Q; for $m = n + 1$ — in terms of the quantities ∇R, $\nabla\mathcal{R}$ and ∇Q; for $m = n + 2$ — in terms of the quantities of the form R^2, $\nabla\nabla R$ etc.

5.7 Diagrammatic Technique

In the computation of the heat kernel coefficients by means of the matrix algorithm a "diagrammatic" technique, i.e., a graphic method for enumerating the different terms of the sum (5.77), turns out to be very convenient.

The matrix elements $\langle m|\hat{L}|n\rangle$ are presented by some blocks with m lines coming in from the left and n lines going out to the right (5.1),

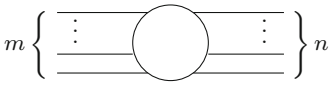


Fig. 5.1

and the product of the matrix elements $\langle m|\hat{L}|k\rangle\langle k|\hat{L}|n\rangle$ — by two blocks connected by k intermediate lines (5.2),

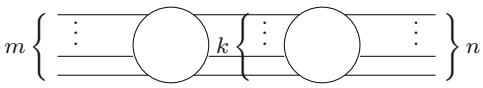


Fig. 5.2

that represents the contractions of the corresponding tensor indices (the inner product).

To obtain the coefficient $\langle n|b_k\rangle$ one should draw, first, all possible diagrams which have n lines incoming from the left and which are constructed from k blocks connected in all possible ways by any number of intermediate lines. When doing this, one should keep in mind that the number of lines, going out

of any block, cannot be greater than the number of lines, coming in, by more than two and by exactly one. Then one should sum up all diagrams with the weight determined for each diagram by the number of intermediate lines from eq. (5.78). Drawing such diagrams is very easy. This helps to keep under control the whole variety of different terms. Therefore, the main problem is reduced to the computation of some standard blocks, which can be computed once and for all.

For example, the diagrams for the diagonal values of the first two derivatives $\langle 1|b_1\rangle$ and $\langle 2|b_1\rangle$ of the coefficient b_1 have the form

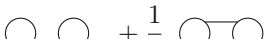
$$\langle 1|b_1\rangle = \frac{1}{2}$$ (5.108)

$$\langle 2|b_1\rangle = \frac{1}{3}$$ (5.109)

More interestingly, the diagrams for the diagonal values of the heat kernel coefficients $[b_k] = \langle 0|b_k\rangle$ for $k = 1, 2, 3$ have the form,

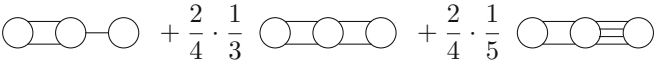
$[b_1] =$ (5.110)

$[b_2] =$ $+\frac{1}{3}$ (5.111)



$[b_3] =$ $+\frac{1}{3}$ $+\frac{2}{4}$ (5.112)

$+\frac{2}{4}\cdot\frac{1}{2}$ $+\frac{2}{4}\cdot\frac{1}{3}$ $+\frac{2}{4}\cdot\frac{1}{5}$

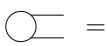


As an illustration let us compute the coefficients $[b_1]$, $\langle 1|b_1\rangle$, $\langle 2|b_1\rangle$ and $[b_2]$. We have

$$= \langle 0|L|0\rangle = [Z]\,,$$ (5.113)

$$= \langle i|L|0\rangle = Z_i\,,$$ (5.114)

$$= \langle ij|L|0\rangle = Z_{ij}\,,$$ (5.115)



$$= \langle 0|L|ij\rangle = -g^{ij}\,,$$ (5.116)

$$= \langle 0|L|2\rangle\langle 2|L|0\rangle = -g^{ij}Z_{ij}\,,$$ (5.117)

where the tensors $[Z]$, Z_i and Z_{ij} are defined by (5.106). By using eqs (5.104)-(5.107) and the equations (3.385), (3.404) and (3.427) we obtain

$$[Z] = Q - \frac{1}{6}R\,, \tag{5.118}$$

$$Z_i = \nabla_i Q - \frac{1}{6}\nabla_i R + \frac{1}{3}\nabla_j \mathcal{R}^j{}_i\,, \tag{5.119}$$

$$Z_{ij} = \nabla_i\nabla_j Q - \mathcal{R}_{ki}\mathcal{R}^k{}_j + \frac{1}{2}\nabla_{(i}\nabla_{|k|}\mathcal{R}^k{}_{j)} - \frac{3}{20}\nabla_i\nabla_j R \tag{5.120}$$
$$-\frac{1}{20}\Delta R_{ij} + \frac{1}{15}R_{il}R^l{}_j - \frac{1}{30}R_{iklm}R_j{}^{klm} - \frac{1}{30}R_{kl}R^k{}_i{}^l{}_j\,.$$

Here the symbol Δ denotes the Laplacian $\Delta = g^{ij}\nabla_i\nabla_j$ and not the Van Vleck determinant. This immediately gives

$$[b_1] = Q - \frac{1}{6}R\,, \tag{5.121}$$

$$[\nabla_i b_1] = \frac{1}{2}\nabla_i Q - \frac{1}{12}\nabla_i R + \frac{1}{6}\nabla_j \mathcal{R}^j{}_j\,, \tag{5.122}$$

$$[\nabla_i\nabla_j b_1] = \frac{1}{3}\nabla_i\nabla_j Q - \frac{1}{3}\mathcal{R}_{ki}\mathcal{R}^k{}_j + \frac{1}{6}\nabla_{(i}\nabla_{|k|}\mathcal{R}^k{}_{j)} - \frac{1}{20}\nabla_i\nabla_j R \tag{5.123}$$
$$-\frac{1}{60}\Delta R_{ij} + \frac{1}{45}R_{il}R^l{}_j - \frac{1}{90}R_{iklm}R_j{}^{klm} - \frac{1}{90}R_{kl}R^k{}_i{}^l{}_j\,,$$

$$[b_2] = \left(Q - \frac{1}{6}R\right)^2 - \frac{1}{3}\Delta Q + \frac{1}{6}\mathcal{R}_{ij}\mathcal{R}^{ij} + \frac{1}{15}\Delta R$$
$$-\frac{1}{90}R_{ij}R^{ij} + \frac{1}{90}R_{ijkl}R^{ijkl}\,. \tag{5.124}$$

Explicit expression for the heat kernel coefficients $[b_k]$ are known up to $[b_4]$ [42, 4, 10], but they become increasingly complicated with k; in fact, the number of terms grows exponentially, or, rather, as $k!$, which makes these expressions not very useful for practical calculations.

Let us write down the asymptotic form of the heat kernel at short times near the diagonal. Say, we introduce the small parameter ε and rescale the time t and the tangent vector $\sigma^{i'}(x, x')$ to the geodesic (which plays the role of $-(x - x')$ in flat space) by

$$t \mapsto \varepsilon^2 t, \qquad \sigma^{i'} \mapsto \varepsilon\sigma^{i'}\,. \tag{5.125}$$

Then by expanding Van Vleck determinant $\Delta^{1/2}$ and the coefficient b_1 in the covariant Taylor series and using the explicit results (3.413) and (5.121) we obtain the asymptotic expansion of the heat kernel as $\varepsilon \to 0$

$$U(t;x,x') = \varepsilon^{-n/2}(4\pi t)^{-n/2}\mathcal{P}\exp\left(-\frac{\sigma}{2t}\right)\Big\{1+\varepsilon^2 U_2(t)+\varepsilon^3 U_3(t) \\ +\varepsilon^4 U_4(t)+O(\varepsilon^5)\Big\}\,, \tag{5.126}$$

where

$$U_2(t) = -t[b_1] + \frac{1}{12}R_{i'j'}\sigma^{i'}\sigma^{j'}\,, \tag{5.127}$$

$$U_3(t) = \frac{t}{2}Z_{i'}\sigma^{i'} - \frac{1}{24}\nabla_{i'}R_{j'k'}\sigma^{i'}\sigma^{j'}\sigma^{k'}\,, \tag{5.128}$$

$$U_4(t) = \frac{t^2}{2}[b_2] - \frac{t}{12}[b_1]R_{i'j'}\sigma^{i'}\sigma^{j'} - \frac{t}{6}Z_{i'j'}\sigma^{i'}\sigma^{j'} + W_{i'j'k'l'}\sigma^{i'}\sigma^{j'}\sigma^{k'}\sigma^{l'}\,, \tag{5.129}$$

where Z_i and Z_{ij} are given by eqs. (5.119) and (5.120) and

$$W_{ijkl} = \frac{1}{80}\nabla_{(i}\nabla_j R_{kl)} + \frac{1}{360}R^p{}_{(i|m|j}R^m{}_{k|p|l)} + \frac{1}{288}R_{(ij}R_{kl)}\,. \tag{5.130}$$

Here all the coefficients (the curvatures) are evaluated at the point x'. As usual, the vertical lines denote the indices excluded from symmetrization, in this case, indices m and p.

5.8 Heat Kernel Coefficients for Constant Curvature

The method described above enables one to compute the heat kernel coefficients $b_k(x,x')$ for arbitrary manifolds. However, it is restricted mainly to the case when x is close to x' since we expand everything in covariant Taylor series.

It turns out that the high symmetry of manifolds with constant curvature, like spheres S^n and hyperbolic spaces H^n, with the curvature tensor

$$R^i{}_{jkl} = \Lambda(\delta^i{}_k g_{jl} - \delta^i{}_l g_{jk})\,, \tag{5.131}$$

enables one to compute the heat kernel coefficients in closed form simply by integrating the recursion relation along geodesics. We will need also the Ricci tensor and the scalar curvature

$$R_{ij} = (n-1)\Lambda g_{ij}\,, \tag{5.132}$$

$$R = n(n-1)\Lambda\,. \tag{5.133}$$

Let us restrict ourselves for simplicity to pure Laplacian

$$L = -g^{ij}\nabla_i\nabla_j\,. \tag{5.134}$$

Van Vleck determinant as well as all other two-point functions are known explicitly as functions of σ (see Sec. 3.8.5) and the Laplacian acting on functions of σ only becomes a second-order *ordinary* differential operator, (3.474). Then the heat kernel as well as the heat kernel coefficients depend only on the geodesic distance, that is, on the function σ. Let r be the geodesic distance so that

$$\sigma = \frac{1}{2}r^2\,. \tag{5.135}$$

Let also restrict ourselves to hyperbolic space H^n, when the curvature is negative,

$$\Lambda = -\varkappa^2\,. \tag{5.136}$$

Then by using the equations (3.470), (3.474) and (3.476) one can show that the operator D and the Laplacian when applied to radial functions are

$$Df(r) = r\partial_r f(r)\,, \tag{5.137}$$

$$Lf(r) = -\left[\partial_r^2 + (n-1)\varkappa\coth(\varkappa r)\partial_r\right] f(r)\,. \tag{5.138}$$

We recall also that, (3.467),

$$\Delta^{1/2} = \left(\frac{\sinh(\varkappa r)}{\varkappa r}\right)^{-(n-1)/2}\,. \tag{5.139}$$

Therefore the recursion relations (5.57) can be written now as

$$\left(1 + \frac{1}{k}r\partial_r\right) b_k = \hat{L}b_{k-1}\,, \tag{5.140}$$

where

$$\hat{L} = \Delta^{-1/2}L\Delta^{1/2}\,. \tag{5.141}$$

with the initial condition $b_0 = 1$. These relations can be easily integrated to get

$$b_k(r) = k\frac{1}{r^k}\int_0^r dr'\; r'^{k-1}\hat{L}_{r'}b_{k-1}(r')\,, \tag{5.142}$$

where the operator $\hat{L}_{r'}$, of course, acts on the variable r'.

It is not difficult to show that the operator $\hat{L}$ has the form (by using, in particular, eq. (3.477))

$$\hat{L} = -\partial_r^2 - \frac{n-1}{r}\partial_r + \frac{1}{4}(n-1)(n-3)\left[\varkappa^2\coth^2(\varkappa r) - \frac{1}{r^2}\right] + \frac{n-1}{2}\varkappa^2\,. \tag{5.143}$$

A remarkable fact is that in three dimensions, $n = 3$, this operator simplifies significantly

$$\hat{L} = -\partial_r^2 - \frac{2}{r}\partial_r + \varkappa^2 \,. \tag{5.144}$$

It is easy to see that in this case the solution of the recursion system (5.140) is trivial; all coefficients b_k are constant

$$b_k = \varkappa^{2k} \,. \tag{5.145}$$

This means that for $n = 3$ the heat kernel is known to all orders in t exactly

$$U_{H^3}(t; x, x') = (4\pi t)^{-3/2} \frac{\varkappa r}{\sinh(\varkappa r)} \exp\left(-\frac{r^2}{4t} - \varkappa^2 t\right) . \tag{5.146}$$

We will see later in Chap. 6, eq. (6.290), that this formula does indeed coincide with the exact heat kernel on the hyperbolic space H^3. This provides a good independent check that our method does indeed work correctly.

Let us compute the coefficients b_1 and b_2 in the general case. Since the first coefficient is known exactly, $b_0 = 1$, we can compute the coefficient b_1 simply by

$$b_1(r) = \frac{1}{r}\int_0^r dr' \, \left\{\frac{1}{4}(n-1)(n-3)\left[\varkappa^2 \coth^2(\varkappa r') - \frac{1}{r'^2}\right] + \frac{n-1}{2}\varkappa^2\right\} . \tag{5.147}$$

This integral can be computed exactly,

$$b_1(r) = \frac{(n-1)}{4}\left\{(n-1)\varkappa^2 - \frac{(n-3)}{r^2}\left[\varkappa r \coth(\varkappa r) - 1\right]\right\} . \tag{5.148}$$

Notice that when $r = 0$ this gives the coincidence limit

$$[b_1] = \frac{n(n-1)}{6}\varkappa^2 \,. \tag{5.149}$$

This coincides with the coincidence limit (5.121) obtained above for the general case.

Now, it is not very difficult to compute the next coefficient b_2. Omitting the straightforward but lengthy calculations we obtain (for details, see [19])

$$b_2(r) = \frac{n-1}{16}\Bigg\{(n-1)^3\varkappa^4 - 2(n-1)^2(n-3)\frac{\varkappa^3}{r}\coth(\varkappa r)$$
$$+(n+1)(n-3)(n-5)\frac{\varkappa^2}{r^2}\coth^2(\varkappa r) + \frac{2}{3}(n-3)(3n^2-10n+23)\frac{\varkappa^2}{r^2}$$
$$-2(n-3)^2(n-5)\frac{\varkappa}{r^3}\coth(\varkappa r) + (n-3)(n-5)(n-7)\frac{1}{r^4}\Bigg\}. \quad (5.150)$$

For $r = 0$ this gives the coincidence limit

$$[b_2] = \frac{1}{180}n(n-1)(5n^2-7n+6)\varkappa^4\,. \quad (5.151)$$

Since

$$R_{ij}R^{ij} = n(n-1)^2\varkappa^4\,, \quad (5.152)$$
$$R_{ijkl}R^{ijkl} = 2n(n-1)\varkappa^4\,, \quad (5.153)$$

this coincides, as it should, with (5.124) computed with $Q = \mathcal{R}_{ij} = 0$.

Thus the heat kernel on spaces of constant negative curvature, that is, hyperbolic spaces H^n, is approximated by

$$U_{H^n}(t;x,x') = (4\pi t)^{-n/2}\left(\frac{\sinh(\rho r)}{\rho r}\right)^{-(n-1)/2}\exp\left(-\frac{r^2}{4t}\right)$$
$$\times\left\{1 - tb_1(r) + \frac{t^2}{2}b_2(r) + O(t^3)\right\}, \quad (5.154)$$

where the functions $b_1(r)$ and $b_2(r)$ are given by eqs. (5.148) and (5.150).

Finally, we evaluate this result for two dimensions, $n = 2$,

$$U_{H^2}(t;x,x') = \frac{1}{4\pi t}\sqrt{\frac{\varkappa r}{\sinh(\varkappa r)}}\exp\left(-\frac{r^2}{4t}\right) \quad (5.155)$$
$$\times\left\{1 - tb_1(r) + \frac{t^2}{2}b_2(r) + O(t^3)\right\},$$

where

$$b_1(r) = \frac{1}{4}\left[\varkappa^2 + \frac{\varkappa}{r}\coth(\varkappa r) - \frac{1}{r^2}\right], \tag{5.156}$$

$$b_2(r) = \frac{1}{16}\Bigg\{\varkappa^4 + 2\frac{\varkappa^3}{r}\coth(\varkappa r) + \frac{\varkappa^2}{r^2}\left[9\coth^2(\varkappa r) - 10\right] + 6\frac{\varkappa}{r^3}\coth(\varkappa r) - \frac{15}{r^4}\Bigg\}. \tag{5.157}$$

5.9 Heat Kernel Coefficients in One Dimension

Let us illustrate the application of this technique to one-dimensional operators. Let us consider an operator acting on functions of one real variable, say in $\mathbb{R}$, of the form

$$L = -\partial_x^2 + Q\,, \tag{5.158}$$

where $Q = Q(x)$ is a smooth function. Let $U(t; x, x')$ be the heat kernel of this operator. Then there is an asymptotic expansion as $t \to 0$

$$U(t; x, x') \sim (4\pi t)^{-1/2}\exp\left[-\frac{1}{4t}(x - x')^2\right]\sum_{k=0}^{\infty}\frac{(-t)^k}{k!}b_k(x, x'). \tag{5.159}$$

By substituting this into the heat equation we get the recursion system

$$b_0(x, x') = 1, \tag{5.160}$$

$$\left[1 + \frac{1}{k}(x - x')\frac{\partial}{\partial x}\right]b_k = La_{k-1}\,. \tag{5.161}$$

We look for solution of this recursion system in form of a Taylor series

$$b_k(x, x') = \sum_{n=0}^{\infty}\frac{1}{n!}(x - x')^n b_k^{(n)}(x')\,. \tag{5.162}$$

Then the solution is

$$b_k^{(n)} = \sum_{n_1,\cdots,n_{k-1}\geq 0}\frac{k}{k+n}\cdot\frac{k-1}{k-1+n_{k-1}}\cdots\frac{1}{1+n_1} \times L_{nn_{k-1}}L_{n_{k-1}n_{k-2}}\cdots L_{n_1 0}\,. \tag{5.163}$$

Here L_{mn} are the matrix elements of the operator L $(m, n \geq 0)$

$$L_{mn} = -\delta_{n,(m+2)} + \binom{m}{n}Q^{(m-n)}\,, \tag{5.164}$$

where $Q^{(n)} = \partial_x^n Q$, and the summation is restricted to non-negative integers $n_1, \ldots, n_{k-1}$ satisfying the constraints

$$0 \le n_1 \le n_2 + 2 \le \cdots \le n_{k-1} + 2(k-1) \le n + 2(k-1)\,. \tag{5.165}$$

Because of the simplicity of the matrix elements in this case one can get an explicit expression for the heat kernel coefficients of *all orders* [14]. It has the form

$$b_k^{(n)} = \sum_{d=1}^{k} \sum_{|\mathbf{m}|=n+2k-2d} c(\mathbf{m}) Q^{(m_d)} \cdots Q^{(m_2)} Q^{(m_1)}\,, \tag{5.166}$$

where the second sum goes over multi-indices $\mathbf{m} = (m_1, m_2, \ldots, m_d)$ with non-negative integer components such that

$$|\mathbf{m}| = m_1 + m_2 + \cdots + m_d = n + 2k - 2d\,, \tag{5.167}$$

and $c(\mathbf{m})$ is a numerical factor. In order to describe it let us introduce the following notation. Let $|\mathbf{m}|_p$ denote the sum of the first p components of the multi-index $\mathbf{m}$, that is,

$$|\mathbf{m}|_p = m_1 + m_2 + \cdots + m_p\,. \tag{5.168}$$

Then, after some combinatorial gymnastics, one can obtain

$$c(\mathbf{m}) = \sum_{i_1, \cdots, i_{d-1}} \prod_{p=1}^{d} \binom{i_p}{i_{p-1}} \frac{\binom{|\mathbf{m}|_p - 2i_{p-1} + 2p}{m_p}}{\binom{|\mathbf{m}|_p - i_{p-1} + 2p + 1}{i_p - i_{p-1}}}\,, \tag{5.169}$$

where the summation goes now over all non-negative $i_1, \ldots, i_{d-1}$ such that

$$0 \equiv i_0 < i_1 < i_2 < \cdots < i_{d-1} < i_d \equiv k, \tag{5.170}$$

and

$$2i_p \le |\mathbf{m}|_{p+1} + 2p\,. \tag{5.171}$$

Without going into the details, we list some low-order coefficients

$$[b_1] = Q\,, \tag{5.172}$$

$$[b_2] = Q^2 - \frac{1}{3} Q''\,, \tag{5.173}$$

$$[b_3] = Q^3 - QQ'' - \frac{1}{2} Q'Q' + \frac{1}{10} Q^{(4)}\,. \tag{5.174}$$

5.10 Heat Kernel Asymptotics of Time-dependent Operators

We now generalize the singular perturbation method described in this chapter to a time-dependent operator

$$L = -\alpha^{ij}(t,x)\partial_i\partial_j + \beta^i(t,x)\partial_i + \gamma(t,x)\,, \tag{5.175}$$

where now all coefficients are functions of both t and x. As we saw in Chap. 3 such an operator can be expressed in the covariant form (3.622)

$$\begin{aligned} L &= -g^{-1/2}(\partial_i + \mathcal{A}_i)g^{1/2}g^{ij}(\partial_j + \mathcal{A}_j) + Q \\ &= -g^{ij}(\nabla_i + \mathcal{A}_i)(\nabla_j + \mathcal{A}_j) + Q\,, \end{aligned} \tag{5.176}$$

where

$$g^{ij} = \alpha^{ij}\,, \tag{5.177}$$

$$\mathcal{A}_i = -\frac{1}{2}g_{ij}\beta^j - \frac{1}{2}g^{-1/2}g_{ij}\partial_k\left(g^{1/2}g^{kj}\right)\,, \tag{5.178}$$

$$Q = \gamma + g^{ij}\mathcal{A}_i\mathcal{A}_j + g^{ij}\nabla_i\mathcal{A}_j\,. \tag{5.179}$$

Here, as usual, (g_{ij}) is the inverse matrix of (g^{ij}), $g = \det g_{ij}$, and ∇_i is the covariant derivative.

Let $\varepsilon > 0$ be a small parameter and let us introduce the following singularly perturbed operator

$$L_\varepsilon = \varepsilon^2 L = -\varepsilon^2 g^{ij}(\nabla_i + \mathcal{A}_i)(\nabla_j + \mathcal{A}_j) + \varepsilon^2 Q\,. \tag{5.180}$$

Note that we introduce the small parameter ε for the whole operator L rather than the partial derivatives ∂_i. This is done to simplify the method and to establish a connection with the method for time-independent operators described in this chapter. Since we deal with covariant derivatives rather than partial derivatives, this makes the whole method manifestly covariant. Of course, this is equivalent to having extra factors ε and ε^2 in the coefficients β^i and γ. We consider the singularly perturbed heat equation

$$(\varepsilon\partial_t + L_\varepsilon)\,U(t,x|t',x') = 0\,, \tag{5.181}$$

with the initial condition

$$U(t',x|t',x') = \delta(x,x')\,. \tag{5.182}$$

Then we look for a solution in form of an asymptotic series as $\varepsilon \to 0$

$$U(t,x|t',x') \sim \varepsilon^{-n/2} \exp\left\{-\frac{1}{\varepsilon} S(t,x|t',x')\right\} \sum_{k=0}^{\infty} \varepsilon^k b_k(t,x|t',x')\,. \tag{5.183}$$

The leading asymptotics of the heat kernel is

$$U(t,x|t',x') \sim \varepsilon^{-n/2} \exp\left[-\frac{1}{\varepsilon} S(t,x|t',x')\right] b_0(t,x|t',x')\,. \tag{5.184}$$

The functions S and b_0 as $t \to t'$ are normalized as follows. To satisfy the initial condition we require that as $t \to t'$

$$S(t,x|t',x') = \frac{1}{2(t-t')} \Phi(x,x') + O(1)\,, \tag{5.185}$$

$$b_0(t,x|t',x') = [4\pi(t-t')]^{-n/2} \det\left[-\partial_i \partial_{j'} \Phi(x,x')\right]^{1/2} + O\left[(t-t')^{-n/2+1}\right]\,, \tag{5.186}$$

where $\Phi(x,x')$ is a non-negative function that has a non-degenerate absolute minimum equal to zero at $x = x'$.

We have the commutation formula

$$\exp\left(\frac{1}{\varepsilon} S\right) (\varepsilon \partial_t + L_\varepsilon) \exp\left(-\frac{1}{\varepsilon} S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 T_2\,, \tag{5.187}$$

where T_0 is a function,

$$T_0 = -\dot{S} - g^{ij} S_i S_j\,, \tag{5.188}$$

$$T_1 = \partial_t + 2 g^{ij} S_j (\nabla_i + \mathcal{A}_i) + g^{ij} S_{ij}\,, \tag{5.189}$$

$$T_2 = L\,. \tag{5.190}$$

Here, $\dot{S} = \partial_t S$, $S_i = \nabla_i S$ and $S_{ij} = \nabla_i \nabla_j S$. Note that, contrary to the previous setup, the indices on S denote *covariant derivatives* rather than partial derivatives. Although, $\partial_i S = \nabla_i S$, the second derivatives are different $\partial_i \partial_j S \neq \nabla_i \nabla_j S$.

By substituting the asymptotic ansatz into the heat equation and using the above commutation formula we see that the function T_0 must be equal to zero. Thus, we obtain the equation (*Hamilton-Jacobi equation*)

$$\partial_t S + g^{ij}(t,x) (\nabla_i S)(\nabla_j S) = 0\,, \tag{5.191}$$

for the function S, that we call the *action*, and the recurrence relations (*transport equations*) for the coefficients b_k for $k = 0, 1, \ldots,$

$$T_1 b_0 = 0, \tag{5.192}$$

$$T_1 b_{k+1} = -T_2 b_k\,, \qquad k = 1, 2, \ldots\,. \tag{5.193}$$

First of all, we note that in the case when the metric $g^{ij}(x)$ does not depend on time the solution of the Hamilton-Jacobi equation is determined by the Synge function

$$S(t,x|,t',x') = \frac{1}{2(t-t')}\sigma(x,x')\,. \tag{5.194}$$

Recall that $\sigma(x,x')$ is equal to one half the square of the geodesic distance between x and x' and satisfies the equation

$$\sigma = \frac{1}{2}g^{ij}\sigma_i\sigma_j\,; \tag{5.195}$$

(recall that $\sigma_i = \nabla_i\sigma$). Indeed, by using this equation we see that the function S defined by (5.194) solves the Hamilton-Jacobi equation. That is, S is nothing but a generalization of the Synge function for the *time-dependent metric*.

The solution of Hamilton-Jacobi equation can be obtained as follows. We introduce the corresponding Hamiltonian,

$$H(t,x,p) = g^{ij}(t,x)p_ip_j\,, \tag{5.196}$$

and the corresponding Hamiltonian system,

$$\frac{dx^i}{d\tau} = 2g^{ij}(\tau,x)p_j\,, \tag{5.197}$$

$$\frac{dp_k}{d\tau} = -\partial_k g^{ij}(\tau,x)p_ip_j\,. \tag{5.198}$$

Note that in the case of time-independent metric this is nothing but the equation of geodesics. So, the solution of this system is a generalization of the geodesic flow to the time-dependent metrics. Notice that in this more general case the Hamiltonian depends on time and, therefore, there is no corresponding invariant, that is, the norm of the tangent vector $||\dot{x}||$ is not conserved.

Let $(x(\tau),p(\tau))$ be the solution of this system with the following boundary conditions

$$x(t') = x'\,, \qquad x(t) = x\,. \tag{5.199}$$

Note that the functions $x(\tau)$ and $p(\tau)$ depend on t,t',x, and x' as parameters. This boundary value problem has a unique solution, at least when the points x and x' are close to each other. Let us define

$$S(t,x|t',x') = \int_{t'}^{t} d\tau\ \frac{1}{4}g_{ij}(\tau,x(\tau))\frac{dx^i(\tau)}{d\tau}\frac{dx^j(\tau)}{d\tau}\,, \tag{5.200}$$

where the integral is taken along the phase trajectory. This is the action of a particle moving in a curved manifold with a time-dependent metric. Then one can show that

$$\frac{\partial}{\partial x^i} S(t, x|t', x') = p_i(t)\,, \tag{5.201}$$

$$\frac{\partial}{\partial x'^i} S(t, x|t', x') = -p_i(t')\,, \tag{5.202}$$

and that $S(t, x|t', x')$ satisfies Hamilton-Jacobi equation.

Next, we define the total time derivative d/dt (along the trajectories of the Hamiltonian system) of a function that depends on t and x, that is,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{dx^i}{dt}\frac{\partial}{\partial x^i}\,. \tag{5.203}$$

Then, it should be clear that the differential operator T_1 has the form

$$T_1 = \frac{d}{dt} + 2g^{ij} S_i \mathcal{A}_j + g^{ij} S_{ij}\,. \tag{5.204}$$

The action S has another important property. Let us define the determinant

$$Z(t, x|t', x') = g^{-1/2}(t, x) \det\left[-\partial_i \partial_{j'} S(t, x|t', x')\right] g^{-1/2}(t', x')\,. \tag{5.205}$$

Then one can show that the function Z satisfies the equation

$$\left(\partial_t + 2g^{ij} S_j \nabla_i + g^{ij} S_{ij}\right) Z^{1/2} = 0\,, \tag{5.206}$$

or

$$\left(\frac{d}{dt} + g^{ij} S_{ij}\right) Z^{1/2} = 0\,. \tag{5.207}$$

Notice that for time-independent metric the function Z is determined by the Van-Vleck determinant

$$Z(t, x|t', x') = \frac{1}{[2(t - t')]^n} \Delta(x, x') \tag{5.208}$$

and the above equation follows from the equation for Van Vleck determinant

$$\sigma^i \nabla_i \Delta^{1/2} = \frac{1}{2}\left(n - g^{ij}\sigma_{ij}\right) \Delta^{1/2}\,. \tag{5.209}$$

Therefore, the operator T_1 can be written as

$$T_1 = Z^{1/2}\left(\frac{d}{dt} + 2g^{ij} S_i \mathcal{A}_j\right) Z^{-1/2}\,. \tag{5.210}$$

Thus, by integrating the transport equation we get the coefficient b_0

$$b_0(t,x|t',x') = (2\pi)^{-n/2}\mathcal{W}(t,x|t',x')Z^{1/2}(t,x|t',x')\,, \tag{5.211}$$

where

$$\mathcal{W}(t,x|t',x') = \exp\left\{-\int\limits_{t'}^{t} d\tau\ \frac{dx^i(\tau)}{d\tau}\mathcal{A}_i(\tau,x(\tau))\right\}. \tag{5.212}$$

The normalization factor is chosen here in such a way to satisfy the initial condition. Notice that in case of time-independent metric the function $\mathcal{W}$ is nothing but the generalized operator of parallel transport, $\mathcal{P}(x,x')$, introduced in Sec. 3.7.3. Thus, the function $\mathcal{W}$ is the generalization of the operator of parallel transport for a time-dependent connection $\mathcal{A}_i(t,x)$ along geodesics of a time-dependent metric $g_{ij}(t,x)$.

Finally, the leading asymptotics of the singularly perturbed heat kernel as $\varepsilon \to 0$ has the form

$$U(t,x|t',x') \sim (2\pi)^{-n/2}Z^{1/2}(t,x|t',x')\mathcal{W}(t,x|t',x')\exp\left\{-\frac{1}{\varepsilon}S(t,x,x')\right\}. \tag{5.213}$$

By solving the differential recursion system we can get, in principle, as many coefficients b_k as needed. In the case, when the operator L does not depend on time this method gives precisely the asymptotic expansion of the heat kernel developed in a previous chapter.

There is a slightly more general setup of the problem. Namely we could have taken the potential term Q into account from the very beginning and not treat it as a perturbation. Even if the method described above is easier to handle, the approach that we are going to describe is more precise (and more complicated) since it catches more information of the problem even in the leading order approximation.

Let $\varepsilon > 0$ be a small parameter and let us consider a singularly perturbed operator

$$L_\varepsilon = -\varepsilon^2 g^{ij}(\nabla_i + \mathcal{A}_i)(\nabla_j + \mathcal{A}_j) + Q\,. \tag{5.214}$$

Note contrary to (5.180) we do not introduce the small parameter ε for the potential term Q. We consider the singularly perturbed heat equation

$$(\varepsilon\partial_t + L_\varepsilon)\,U(t,x|t',x') = 0\,, \tag{5.215}$$

with the initial condition

$$U(t',x|t',x') = \delta(x,x')\,, \tag{5.216}$$

and look for a solution in the form of an asymptotic series

$$U(t,x|t',x') \sim \varepsilon^{-n/2} \exp\left[-\frac{1}{\varepsilon} S(t,x|t',x')\right] \sum_{k=0}^{\infty} \varepsilon^k b_k(t,x|t',x')\,. \tag{5.217}$$

Since the initial condition is the same, the functions S and b_0 as $t \to t'$ are normalized exactly as before by (5.185) and (5.186).

Again, we have a commutation formula

$$\exp\left(\frac{1}{\varepsilon} S\right) (\varepsilon\partial_t + L_\varepsilon) \exp\left(-\frac{1}{\varepsilon} S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 T_2\,, \tag{5.218}$$

where now

$$T_0 = -\partial_t S - g^{ij} S_i S_j + Q\,, \tag{5.219}$$

$$T_1 = \partial_t + 2g^{ij} S_j (\nabla_i + \mathcal{A}_i) + g^{ij} S_{ij}\,, \tag{5.220}$$

$$T_2 = -g^{ij} (\nabla_i + \mathcal{A}_i)(\nabla_j + \mathcal{A}_j)\,. \tag{5.221}$$

Note that the potential form Q moved from T_2 to T_0.

Now, the Hamilton-Jacobi equation for the action has the form

$$\partial_t S + g^{ij}(t,x)(\nabla_i S)(\nabla_j S) - Q = 0\,, \tag{5.222}$$

and the recurrence relations (transport equations) for the coefficients b_k for $k = 0, 1, \ldots$, are formally the same,

$$T_1 b_0 = 0, \tag{5.223}$$

$$T_1 b_{k+1} = -T_2 b_k\,, \qquad k = 1, 2, \ldots\,. \tag{5.224}$$

The corresponding Hamiltonian system reads now

$$\frac{dx^i}{d\tau} = 2g^{ij}(\tau,x) p_j\,, \tag{5.225}$$

$$\frac{dp_k}{d\tau} = -\partial_k g^{ij}(\tau,x) p_i p_j + \partial_k Q(\tau,x)\,. \tag{5.226}$$

This system describes a particle on a curved manifold in a time-dependent metric and in a time-dependent potential $Q = Q(\tau,x)$.

Let $(x(\tau), p(\tau))$ be the solution of this system with the following boundary conditions

$$x(t') = x'\,, \qquad x(t) = x\,. \tag{5.227}$$

Let

$$S(t,x|t',x') = \int_{t'}^{t} d\tau \, \left\{ \frac{1}{4} g_{ij}(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} \frac{dx^j(\tau)}{d\tau} + Q(\tau, x(\tau)) \right\}, \tag{5.228}$$

and the integral is along the phase trajectory. This is the action of a particle moving in a curved manifold with a time-dependent metric in a time-dependent potential Q. Then one can show that $S(t, x|t', x')$ satisfies Hamilton-Jacobi equation.

After the Hamiltonian system has been solved and the action S has been found, the rest goes exactly as before. The function $Z(t, x|t', x')$ satisfies the same equation, and the transport operator T_1 has the same form. Therefore, the first coefficient b_0 and the heat kernel in the leading approximation is given by the same formulas. The only difference is now that the operator T_2 does not contain the potential Q any more. So, when solving the recursion system the coefficients b_k are not polynomial in Q but depend on Q in a rather complicated way through the action S.

5.11 Boundary Value Problems

In this section we briefly describe the construction of the heat kernel asymptotics on manifolds with boundary. We consider a Laplace type operator acting on real-valued scalar functions on a manifold M with a boundary ∂M of the form

$$L(x, \partial_x) = -\Delta + Q\,, \tag{5.229}$$

where Δ is the Laplacian and Q is a smooth function. Then the heat kernel $U(t; x, x')$ is defined as usual by requiring it to satisfy the equation

$$(\partial_t + L)U(t; x, x') = 0 \tag{5.230}$$

with the initial condition

$$U(0; x, x') = \delta(x, x')\,. \tag{5.231}$$

In this case it is also required to be symmetric

$$U(t; x, x') = U(t; x', x) \tag{5.232}$$

and to satisfy some additional boundary conditions at the boundary, which will be described below.

5.11.1 Geometry of the Boundary

Let M be a n-dimensional Riemannian manifold with a Riemannian metric g_{ij} and with boundary ∂M. We will restrict ourselves to the case when the boundary ∂M is a smooth $(n-1)$-dimensional manifold without boundary.

For simplicity one can assume that M is just a domain in the Euclidean space $\mathbb{R}^n$ with a smooth boundary.

We will denote the local coordinates on the manifold M by x^i, $i = 1, \dots, n$, and the local coordinates on the boundary ∂M by $\hat{x}^\mu$, $\mu = 1, \dots, (n-1)$. With our notation Latin indices will label the components of tensors on the manifold M and Greek indices will label the components of tensors on the boundary ∂M. In a sufficiently narrow strip near the boundary one can connect each point x inside M with a point $\hat{x}$ on the boundary ∂M by a unique geodesic. The length of this geodesic determines the normal geodesic distance r from the point x to the boundary. Therefore, there exists a local diffeomorphism

$$r = r(x) \qquad \hat{x}^\mu = \hat{x}^\mu(x)\,, \tag{5.233}$$

and the inverse diffeomorphism

$$x^i = x^i(r, \hat{x})\,, \tag{5.234}$$

such that for any point on the boundary

$$r(x) = 0\,, \tag{5.235}$$

and for any point in the interior $r(x) > 0$. The Jacobian of the above diffeomorphism is

$$J = \frac{\partial(x^1, x^2, \dots, x^n)}{\partial(r, \hat{x}^1, \dots, \hat{x}^{n-1})}\,. \tag{5.236}$$

We fix the orientation of the boundary by requiring the Jacobian J to be positive, that is, $J > 0$.

This diffeomorphism satisfies the obvious relations

$$\frac{\partial x^i}{\partial r}\frac{\partial r}{\partial x^j} + \frac{\partial x^i}{\partial \hat{x}^\mu}\frac{\partial \hat{x}^\mu}{\partial x^j} = \delta^i{}_j\,, \tag{5.237}$$

and

$$\frac{\partial r}{\partial x^i}\frac{\partial x^i}{\partial r} = 1\,, \tag{5.238}$$

$$\frac{\partial r}{\partial x^i}\frac{\partial x^i}{\partial \hat{x}^\mu} = 0\,, \tag{5.239}$$

$$\frac{\partial \hat{x}^\mu}{\partial x^i}\frac{\partial x^i}{\partial \hat{x}^\nu} = \delta^\mu{}_\nu\,. \tag{5.240}$$

Let us define the vectors

$$e_\mu{}^i = \frac{\partial x^i}{\partial \hat{x}^\mu}, \tag{5.241}$$

$$N^i = \frac{\partial x^i}{\partial r}\,. \tag{5.242}$$

On the boundary the vectors $e_\mu{}^i$ are tangent to the boundary and form a basis in the tangent space on the boundary and the vector N^i is an *inward pointing unit normal* to the boundary. These vectors satisfy the equations

$$g_{ij}N^iN^j = 1\,, \tag{5.243}$$

$$g_{ij}e_\mu{}^iN^j = 0\,. \tag{5.244}$$

By using the relations (5.238)-(5.240) one can also show that

$$N_i = g_{ij}N^j = \frac{\partial r}{\partial x^i}\,. \tag{5.245}$$

Moreover, it can also be written in the form

$$N_i = \varepsilon_{j_1\dots j_{n-1}i}e_1{}^{j_1}\cdots e_{n-1}{}^{j_{n-1}}\,, \tag{5.246}$$

where $\varepsilon_{j_1\dots j_n}$ is the Levi-Civita symbol defined by (3.58).

The metric in these coordinates has the form

$$ds^2 = dr^2 + \hat{g}_{\mu\nu}d\hat{x}^\mu d\hat{x}^\nu, \tag{5.247}$$

where $\hat{g}_{\mu\nu}$ is the *induced Riemannian metric* on hypersurfaces $r = \text{const}$ (also on the boundary) defined by

$$\hat{g}_{\mu\nu} = g_{ij}e_\mu{}^ie_\nu{}^j\,. \tag{5.248}$$

Of course, in these coordinates

$$g = \det g_{ij} = \hat{g} = \det \hat{g}_{\mu\nu}\,. \tag{5.249}$$

The induced metric defines the *extrinsic curvature* of the boundary

$$K_{\mu\nu} = -\frac{1}{2}\frac{\partial}{\partial r}\hat{g}_{\mu\nu}\,, \tag{5.250}$$

and the scalar extrinsic curvature

$$K = \hat{g}^{\mu\nu}K_{\mu\nu}\,. \tag{5.251}$$

The normal derivative of a scalar function f in these coordinates is simply the derivative with respect to r,

$$\nabla_N f = \frac{\partial}{\partial r} f \,. \tag{5.252}$$

The induced metric allows one to define the induced tangential covariant derivatives $\hat{\nabla}_\mu$ on the boundary as well.

Now by using the formula (3.89) for the divergence of a vector field V^i and the Gauss theorem (or more general Stokes' theorem) (2.46) we get

$$\int\limits_M dx g^{1/2} \nabla_i V^i = \int\limits_{\partial M} d\hat{x} \hat{g}^{1/2} N_i V^i \,. \tag{5.253}$$

This enables one to integrate by parts; for a vector field V^i and a scalar field φ we have

$$\int\limits_M dx\ g^{1/2} \varphi \nabla_i V^i = -\int\limits_M dx\ g^{1/2} (\nabla_i \varphi) V^i + \int\limits_{\partial M} d\hat{x}\ \hat{g}^{1/2} \varphi N_i V^i \,. \tag{5.254}$$

5.11.2 Boundary Conditions

The operator L (5.229) is *formally self-adjoint* (with the standard Riemannian measure $g^{1/2}$). Indeed, for any two smooth functions, φ and ψ, with compact support in the interior of the manifold by integrating by parts twice we see that

$$\int\limits_M dx\ g^{1/2} \varphi L \psi = \int\limits_M dx\ g^{1/2} (L\varphi) \psi \,. \tag{5.255}$$

We need to consider more general functions that do not vanish close to the boundary. Then the above condition is not necessarily true because of the boundary terms in the integration by parts formula (5.254). In order to make the operator L self-adjoint (and elliptic) we have to impose some boundary conditions, so that, in particular, the boundary terms in the integration by parts vanish and the above equation holds for any two functions satisfying the boundary conditions. We call such boundary conditions *admissible*.

Let f be a function on M. The *boundary data* are the values of the function $f\big|_{\partial M}$ and its normal derivative $\partial_r f\big|_{\partial M}$ at the boundary. The boundary conditions are some conditions on the boundary data, that is,

$$Bf\big|_{\partial M} = (B_1 \partial_r + B_2)\, f\big|_{\partial M} = 0 \,, \tag{5.256}$$

where B is the *boundary operator*, usually a first-order (or zero-order) differential operator. The classical boundary conditions are the *Dirichlet boundary conditions*

$$f\big|_{\partial M} = 0 \,, \tag{5.257}$$

and the *Neumann boundary conditions*

$$\partial_r f\big|_{\partial M} = 0\,. \tag{5.258}$$

There is also a slight modification of Neumann boundary conditions called *Robin boundary conditions*,

$$(\partial_r + h)\, f\big|_{\partial M} = 0 \tag{5.259}$$

where $h = h(\hat{x})$ is some function on the boundary.

The boundary ∂M could be, in general, a *disconnected* manifold consisting of a finite number of disjoint connected parts. In such case one can impose *different* boundary conditions on different connected parts of the boundary. More generally, one can impose different boundary conditions on connected parts of the boundary. In this case, usually called *Zaremba boundary value problem* [11], the boundary operator becomes discontinuous and the analysis becomes much harder. We will restrict ourselves for simplicity to Dirichlet or Neumann boundary conditions. Then, by integrating by parts one can easily show that for both Dirichlet and Neumann boundary conditions the operator L is self-adjoint.

Roughly speaking *ellipticity* means *local invertibility*. It has two components: i) in the interior of the manifold and ii) at the boundary. The operator L is called *elliptic in the interior* if its leading symbol $\sigma_L(x,p)$ is positive for any $p \neq 0$ at any interior point x in M. At the boundary yet another condition, so-called *strong ellipticity condition* (or Lopatinsky-Shapiro condition), has to be satisfied. This condition requires that the solution far away from the boundary 'forgets' about the boundary conditions and approaches the solution for the case without boundary, in other words, the boundary effects localize at a narrow strip close to the boundary. Without going into details let us just say that both Dirichlet and Neumann boundary conditions are elliptic [11].

For the sake of simplicity we will restrict ourselves in this section to Dirichlet boundary conditions. The case of Neumann boundary conditions can be treated similarly.

5.11.3 Interior Heat Kernel

We split the whole manifold in two disjoint parts, a narrow strip along the boundary $M_{\rm bnd}$, that we call the *boundary part*, and the remaining part $M_{\rm int}$, that we call the *interior part*. We will treat these two parts differently and construct the heat kernel in the boundary part and in the interior part separately. It turns out that the heat kernel in the interior part can be approximated by the heat kernel on manifolds without boundary, but the heat kernel in the boundary part behaves rather differently.

In the interior of the manifold we approximate the heat kernel by its value in the case of manifolds without boundary. We try to find the fundamental solution $U^{\rm int}(t;x,x')$ of the heat equation near diagonal for small t, i.e. $x \to x'$ and $t \to 0^+$, that, instead of the boundary conditions satisfies asymptotic condition at infinity. This means that effectively one introduces a small expansion parameter $\varepsilon > 0$ reflecting the fact that the points x and x' are close to each other and the parameter t is small. This can be done by fixing a point x' in the interior part $M^{\rm int}$, choosing the normal coordinates at this point (with $g_{ij}(x') = \delta_{ij}$), scaling

$$x \mapsto x' + \varepsilon(x - x'), \qquad t \mapsto \varepsilon^2 t, \tag{5.260}$$

and expanding in a power series in ε. Of course, the derivatives are scaled by

$$\partial_i \mapsto \frac{1}{\varepsilon}\partial_i\,, \qquad \partial_t \mapsto \frac{1}{\varepsilon^2}\partial_t\,. \tag{5.261}$$

We will label the scaled objects by ε, e.g. L_ε, U_ε, etc. The scaling parameter ε will be considered as a formal small parameter in the theory and we will use it to expand everything in (asymptotic) power series in ε. At the very end of calculations we set $\varepsilon = 1$. The non-scaled objects, i.e. those with $\varepsilon = 1$, will not have the label ε. Another way of doing this is by saying that we will expand all quantities in the homogeneous functions of $(x - x')$ and $\sqrt{t}$.

The expansion of the operator L has the form

$$L_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^{k-2} L_k\,, \tag{5.262}$$

where L_k are some second-order differential operators. By expanding the interior heat kernel in the power series in ε

$$U_\varepsilon^{\rm int} \sim \sum_{k=0}^{\infty} \varepsilon^{k-n} U_k\,, \tag{5.263}$$

and substituting these expansions in the heat equation (5.230) we get the following recursion

$$(\partial_t + L_0)U_0 = 0\,, \tag{5.264}$$

and for $k \geq 1$

$$(\partial_t + L_0)U_k = -\sum_{m=1}^{k} L_m U_{k-m}\,. \tag{5.265}$$

The initial condition for the coefficient U_0 is

$$U_0(t;x,x') = \delta(x,x')\,, \tag{5.266}$$

and the initial conditions for higher order coefficients, with $k \geq 1$, are

$$U_k(0;x,x') = 0\,. \tag{5.267}$$

Note that the leading order operator,

$$L_0 = -\delta^{ij}\partial_i\partial_j\,, \tag{5.268}$$

has constant coefficients, and, therefore, is easy to handle. The leading order interior heat kernel is nothing but the heat kernel for the Euclidean space,

$$U_0^{\rm int}(t;x,x') = (4\pi t)^{-n/2}\exp\left(-\frac{|x-x'|^2}{4t}\right)\,, \tag{5.269}$$

where $|x-x'|^2 = \delta_{ij}(x-x')^i(x-x')^j$. This enables one to solve the recursion system (5.265).

Of course, for the interior heat kernel there is a much better covariant approach described in previous sections of this chapter.

5.11.4 Heat Kernel Near Boundary

For an elliptic boundary-value problem the diagonal of the heat kernel $U^{\rm bnd}(t;x,x)$ in $M^{\rm bnd}$ has *exponentially small* terms, i.e. of order $\sim \exp(-r^2/t)$, (recall that r is the normal geodesic distance to the boundary) as $t \to 0^+$ and $r > 0$. These terms do not contribute to the asymptotic expansion of the heat-kernel diagonal outside the boundary as $t \to 0^+$. However, they behave like *delta-functions* near the boundary, and, therefore, lead to non-vanishing boundary contribution in the integral formulas.

The heat kernel $U^{\rm bnd}(t;x,x')$ in the boundary part of the manifold $M^{\rm bnd}$ is constructed as follows. Now we want to find the fundamental solution of the heat equation near diagonal, i.e. for $x \to x'$ and for small $t \to 0$ in the region $M^{\rm bnd}$ *close to the boundary*, i.e. for small r and r', that satisfies Dirichlet boundary conditions on the boundary and asymptotic condition at infinity. We fix a point on the boundary, $\hat{x}_0 \in \partial M$, and choose normal coordinates $\hat{x}^\mu$ on the boundary ∂M at this point (with $\hat{g}_{\mu\nu}(0,\hat{x}_0) = \delta_{\mu\nu}$).

To construct the heat kernel, we again scale the coordinates. But now we include the coordinates r and r' in the scaling

$$\hat{x} \mapsto \hat{x}_0 + \varepsilon(\hat{x}-\hat{x}_0), \qquad \hat{x}' \mapsto \hat{x}_0 + \varepsilon(\hat{x}'-\hat{x}_0), \tag{5.270}$$

$$r \mapsto \varepsilon r, \qquad r' \mapsto \varepsilon r', \qquad t \mapsto \varepsilon^2 t\,. \tag{5.271}$$

The corresponding differential operators are scaled by

$$\hat{\partial}_\mu \mapsto \frac{1}{\varepsilon}\hat{\partial}_\mu, \qquad \partial_r \mapsto \frac{1}{\varepsilon}\partial_r, \qquad \partial_t \mapsto \frac{1}{\varepsilon^2}\partial_t\,. \tag{5.272}$$

Then, we expand the scaled operator L_ε in the power series in ε, i.e.

$$L_\varepsilon = \sum_{k=0}^{\infty} \varepsilon^{k-2} L_k, \tag{5.273}$$

where L_k are second-order differential operators with homogeneous symbols. Since the Dirichlet boundary operator does not contain any derivatives and has constant coefficients it does not scale at all.

The subsequent strategy is rather simple. We expand the scaled heat kernel in ε

$$U_\varepsilon^{\mathrm{bnd}} \sim \sum_{k=0}^{\infty} \varepsilon^{k-n} U_k^{\mathrm{bnd}}, \tag{5.274}$$

and substitute into the scaled version of the heat equation (5.230) and the Dirichlet boundary condition (5.257). Then, by collecting the terms with the same power of ε one gets an infinite set of recursive differential equations

$$(\partial_t + L_0) U_0^{\mathrm{bnd}} = 0\,, \tag{5.275}$$

and for $k \geq 1$,

$$(\partial_t + L_0) U_k^{\mathrm{bnd}} = -\sum_{n=1}^{k} L_n U_{k-n}^{\mathrm{bnd}}\,. \tag{5.276}$$

The initial condition for U_0^{bnd} is

$$U_0^{\mathrm{bnd}}(0; r, \hat{x}; r', \hat{x}') = \delta(r - r')\delta(\hat{x}, \hat{x}')\,, \tag{5.277}$$

and the initial conditions for higher order terms with $k \geq 1$ are

$$U_k^{\mathrm{bnd}}(0; r, \hat{x}; r', \hat{x}') = 0\,. \tag{5.278}$$

The boundary conditions for Dirichlet boundary value problem take the following form

$$U_k^{\mathrm{bnd}}(t; 0, \hat{x}; r', \hat{x}') = U_k^{\mathrm{bnd}}(t; r, \hat{x}; 0, \hat{x}') = 0. \tag{5.279}$$

Moreover, we should impose asymptotic conditions (that guarantee strong ellipticity)

$$\lim_{r\to\infty} U_k^{\mathrm{bnd}}(t; r, \hat{x}; r', \hat{x}') = \lim_{r'\to\infty} U_k^{\mathrm{bnd}}(t; r, \hat{x}; r', \hat{x}') = 0\,. \tag{5.280}$$

These conditions fix a unique solution of the recursion system.

The basic case here (when the coefficients of the operator L are frozen at the point $\hat{x}_0$) is *one-dimensional*. The operator L in the leading order reads now

$$L_0 = -\partial_r^2 - \delta^{\mu\nu}\hat{\partial}_\mu\hat{\partial}_\nu\,, \tag{5.281}$$

with $\hat{\partial}_\mu = \partial/\partial\hat{x}^\mu$, and the appropriate initial, boundary and asymptotic conditions. The operator L_0 is a partial differential operator with *constant coefficients*. By using the Fourier transform in the boundary coordinates $(\hat{x} - \hat{x}')$ it reduces to an *ordinary* differential operator of second order in the radial variable r. Clearly, the boundary part factorizes and the solution to the remaining one-dimensional problem can be easily obtained by using the Laplace transform, for example. Thus, we obtain, the leading order heat kernel

$$U_0^{\rm bnd}(t; r, \hat{x}; r', \hat{x}') = (4\pi t)^{-n/2} \exp\left(-\frac{|\hat{x} - \hat{x}'|^2}{4t}\right) K(t; r, r')\,, \qquad (5.282)$$

where $|\hat{x}-\hat{x}'|^2 = \delta_{\mu\nu}(\hat{x}-\hat{x}')^\mu(\hat{x}-\hat{x}')^\nu$ and the function $K(t; r, r')$ (for Dirichlet problem) has the form

$$K(t; r, r') = \exp\left(-\frac{(r - r')^2}{4t}\right) - \exp\left(-\frac{(r + r')^2}{4t}\right) \qquad (5.283)$$

This enables one, in principle, to solve the recursion system (5.276).

5.11.5 Method of Geodesics Reflected from the Boundary

Let us describe briefly another, more geometric, method for calculation of the heat kernel $U(t; x, x')$ near boundary for small t and x close to x' following [5] . Let us consider the Dirichlet boundary conditions, for simplicity.

This method is based on the following semi-classical ansatz (discussed in detail in the previous sections of this chapter)

$$U(t; x, x') = (4\pi t)^{-n/2} \Delta^{1/2}(x, x') \exp\left[-\frac{\sigma(x, x')}{2t}\right] \Omega(t; x, x'), \qquad (5.284)$$

where σ is the Synge function defined as one half the square of the geodesic distance between the points x and x' and Δ is the corresponding Val Vleck-Morette determinant. This ansatz works well when there is a unique geodesic connecting the points x and x'. However in general there are more than one geodesic between the points x and x'. Therefore the semi-classical ansatz, in general case, should have a form of a sum of analogous contributions from all geodesics connecting the points x and x'. When the points x and x' are close to each other there is always one leading contribution determined by the shortest geodesic. Multiple geodesics are caused by two factors. First of all, many compact manifolds (like spheres, for example) have closed geodesics. In such case in addition to the shortest geodesic there are always geodesics that emanate from point x', pass through the whole manifold one or several

times and return to the point x. Second, geodesics could be reflected from the boundary of the manifold one or more times.

We want to construct an asymptotic expansion of the heat kernel as $t \to 0$. We can order all geodesics according to their length. It is obvious that the larger the length of the geodesic the smaller its contribution to the heat kernel. As $t \to 0$, if the length of the geodesics is non-zero, then the contribution to the heat kernel is exponential small. This is so for all global geodesics that pass through the whole manifold. However, there is one geodesic whose length could vanish. This is the geodesics with only one reflection from the boundary. The contribution of such a geodesic to the semi-classical ansatz has the factor $\exp(-r^2/t)$, where r is the distance to the boundary, and, therefore, such a term behaves like a delta-function $\delta(r)$ near the boundary as $t \to 0$. Such geodesic is the only local geodesic in the sense that it does not leave the boundary part of the manifold if two points x and x' are near the boundary (and close to each other). That is why, as $t \to 0$ it is sufficient to restrict ourselves to the direct (shortest) geodesic and the geodesic with one reflection from the boundary.

This motivates a new semi-classical ansatz

$$U(t;x,x') = (4\pi t)^{-n/2}\Bigg\{\exp\left[-\frac{\sigma(x,x')}{2t}\right]\Delta^{1/2}(x,x')\Omega(t;x,x') + \exp\left[-\frac{\phi(x,x')}{2t}\right]\Psi(t;x,x')\Bigg\}, \tag{5.285}$$

where $\phi(x,x')$ is equal to one half the square of the length of the geodesic connecting the points x and x' with one reflection from the boundary and $\Psi(t;x,x')$ is the corresponding transport function.

The function ϕ is nothing but Synge function for the geodesic between the points x and x' with one reflection from the boundary. It satisfies equations similar to the equations (3.222), (3.223), for the function σ,

$$\phi = \frac{1}{2}g^{ij}(\nabla_i\phi)(\nabla_j\phi), \tag{5.286}$$

$$\phi = \frac{1}{2}g^{i'j'}(\nabla_{i'}\phi)(\nabla_{j'}\phi)\,, \tag{5.287}$$

with the same initial conditions (3.221).

Now, the part due to the direct geodesic, that is, the function Ω, was analyzed in detail in previous sections of this chapter. It has exactly the same form here. What we need to do now is to compute the function Ψ. The function Ψ satisfies an equation similar to the transport equation (5.42) for the function Ω,

$$F\Psi = 0, \tag{5.288}$$

where

$$F = \partial_t + \frac{1}{t}\left(\phi^i\nabla_i + \frac{1}{2}\left(\phi^i{}_i - n\right)\right) - L\,, \tag{5.289}$$

where $\phi_i = \nabla_i\phi$ and $\phi^i{}_i = \nabla^i\nabla_i\phi$.

Now, we choose the coordinate system $(r, \hat{x}^\mu)$ introduced above, where r is the geodesic distance to the boundary and $\hat{x}^\mu$ are coordinates on the boundary and expand all quantities in covariant Taylor series in the neighborhood of the boundary, that is, at $r = 0$.

Recall that the purpose of introducing the function Ψ was to satisfy the boundary conditions. The part with only one direct geodesics obviously does not satisfy the boundary conditions. That is why the function $\Psi(t; r, \hat{x}, r', \hat{x}')$ has to satisfy some boundary condition that (for the Dirichlet boundary value problem) has the form

$$\begin{aligned}\Delta^{1/2}(0, \hat{x}, r', \hat{x}')\Omega(t; 0, \hat{x}, r', \hat{x}') + \Psi(t; 0, \hat{x}, r', \hat{x}') = 0\,,\\ \Delta^{1/2}(r, \hat{x}, 0, \hat{x}')\Omega(t; r, \hat{x}, 0, \hat{x}') + \Psi(t; r, \hat{x}, 0, \hat{x}') = 0\,.\end{aligned} \tag{5.290}$$

Here we used the fact that if one of the points x or x' is on the boundary, that is, $r = 0$ or $r' = 0$, then $\sigma(x, x') = \phi(x, x')$.

The further strategy is rather simple. We scale the coordinates as described above (5.270)-(5.272). We expand the transport operator F and the transport function Ψ in formal series in the small parameter ε

$$F_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^{k-2} F_k, \tag{5.291}$$

$$\Psi \sim \sum_{k=0}^{\infty} \varepsilon^k \Psi_k\,, \tag{5.292}$$

and obtain the following differential recursion relations

$$F_0\Psi_0 = 0\,, \tag{5.293}$$

$$F_0\Psi_k = -\sum_{m=1}^{k} F_k\Psi_{k-m}\,. \tag{5.294}$$

The leading order coefficient is easy to find. It is just

$$\Psi_0(t; x, x') = -1. \tag{5.295}$$

The calculation of the next orders is considerably more difficult (for details, see [5]). We present here the result just for the coincidence limit $\Psi(t; x, x)$. Let $h(z)$ be a function defined by

$$h(z) = \int_0^\infty dx \exp(-x^2 - 2zx) = \exp(z^2)\mathrm{Erfc}\,(z), \tag{5.296}$$

where $\mathrm{Erfc}\,(z)$ is the complimentary error function. Let $f_1(z)$ and $f_2(z)$ be the functions defined by

$$f_1(z) = \frac{1}{6} + \frac{z^2}{6}\left(2 + \frac{1}{2}z^2 - z(z^2+6)h(z)\right), \tag{5.297}$$

$$f_2(z) = -\frac{1}{6} + \frac{1}{12}z^2\left(-4 + \frac{1}{2}z^2 - 4z^3 h(z)\right). \tag{5.298}$$

Then the coincidence limit of the first two correction terms is

$$\Psi_1(t;x,x) = -\frac{r^2}{\sqrt{t}} h\left(\frac{r}{\sqrt{t}}\right) K, \tag{5.299}$$

$$\begin{aligned}\Psi_2(t;x,x) = t\Bigg\{&\left(Q - \frac{1}{6}\hat{R}\right) - \frac{1}{3}\left(1 + \frac{r^2}{t}\right) N^i N^j R_{ij} \\ &+ f_1\left(\frac{r}{\sqrt{t}}\right) K^2 + f_2\left(\frac{r}{\sqrt{t}}\right) K_{\mu\nu}K^{\mu\nu}\Bigg\},\end{aligned} \tag{5.300}$$

where R_{ij} is the Ricci tensor, $\hat{R}$ is the scalar curvature of the boundary, $K_{\mu\nu}$ is the extrinsic curvature of the boundary (5.250) and K is the scalar extrinsic curvature (5.251). Here all tensor quantities are calculated on the boundary.

5.12 Notes

This is the main chapter of the book. We have developed in detail a systematic effective method for the calculation of the asymptotic expansion of the heat kernel for second-order elliptic partial differential operators. We followed mainly our own papers and books [4, 14, 13, 14, 9, 5, 11]. There are, of course, many other books on the heat kernel from the classic one [76] to more advanced works [42, 46, 22, 18, 20].

Chapter 6
Advanced Topics

Abstract This chapter is devoted to some advanced methods for calculation of the heat kernel. Most of these methods are algebraic rather than analytic in nature, that is, instead of solving the heat equation directly we compute the heat semigroup; then the heat kernel is just the integral kernel of the heat semigroup. We also discuss basic concepts of path integrals.

6.1 Various Approximation Schemes

We saw that the heat kernel is an effective and powerful tool. However, generically, in most cases, it is impossible to find it exactly. Therefore, one should try to develop various approximate calculational schemes that are well suited in some particular cases. All of them are based on some kind of a perturbation theory whereas one tries to model the case under study by an exactly solvable one and then to identify a small parameter that would describe the difference of the original problem from the model problem and, assuming that this difference is small, develop an expansion in this parameter. This chapter will be devoted to such methods. One of the most important properties of the perturbation theory is that it should be *covariant*, which means that the diffeomorphism invariance should be preserved at each order of the approximation. Otherwise, applying the perturbation theory in different coordinates one would get different results, which is, of course, unacceptable.

We consider the scalar Laplace type operator

$$\begin{aligned} L &= -g^{ij}\nabla_j^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q \\ &= -g^{-1/2}(\partial_i + \mathcal{A}_i)g^{1/2}g^{ij}(\partial_j + \mathcal{A}_j) + Q\,. \end{aligned} \tag{6.1}$$

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_6

In this section we are going to investigate the general structure of the heat kernel coefficients b_k introduced in Sect. 5.2. Since locally one can always expand the metric and the potential term Q in the covariant Taylor series, they are completely characterized by their Taylor coefficients, which are polynomials in the covariant derivatives of the curvature. Let us call the Riemann curvature tensor R_{ijkl}, the generalized curvature $\mathcal{R}_{ij}$ and the potential Q the *background fields* and denote them by

$$\mathfrak{R} = \{R_{ijkl}, \mathcal{R}_{ij}, Q\}\,. \tag{6.2}$$

Let us introduce, in addition, the set of all covariant derivatives of the curvatures, so-called *covariant jets*,

$$\mathfrak{R}_{(i)} = \nabla_{(j_1} \cdots \nabla_{j_i)} \mathfrak{R}\,, \tag{6.3}$$

the number i will be called the order of a jet $\mathfrak{R}_{(i)}$. It is worth noting that the jets are defined by symmetrized covariant derivatives. This makes them well defined as the order of the covariant derivatives becomes not important—it is only the number of derivatives that plays a role.

Let us make a deformation of the background fields by introducing some deformation parameters α and ε,

$$g_{ij} \mapsto g_{ij}(\alpha, \varepsilon), \qquad \mathcal{A}_i \mapsto \mathcal{A}_i(\alpha, \varepsilon)\,, \qquad Q \mapsto Q(\alpha, \varepsilon)\,, \tag{6.4}$$

in such a way that the jets transform uniformly,

$$\mathfrak{R}_{(i)} \mapsto \alpha\varepsilon^i \mathfrak{R}_{(i)}. \tag{6.5}$$

This means that the parameter α counts the number of curvatures and the parameter ε counts the number of covariant derivatives. Such deformation of the background fields leads to the corresponding deformation of the operator L,

$$L \mapsto L(\alpha, \varepsilon) \tag{6.6}$$

and the heat kernel

$$U(t) \mapsto U(t; \alpha, \varepsilon). \tag{6.7}$$

Let us note that this deformation is manifestly covariant. Therefore, it gives a natural framework to develop various approximation schemes based on asymptotic expansions of the heat kernel in the deformation parameters. It is obvious that the limit $\alpha \to 0$ corresponds to the case of small curvatures, $\mathfrak{R} \to 0$, while the limit $\varepsilon \to 0$ corresponds to small covariant derivatives of the curvatures, $\nabla\mathfrak{R} \to 0$.

More precisely, we recognize two cases: i) the *short-wave approximation*,

$$\nabla\nabla\mathfrak{R} \gg \mathfrak{R}\mathfrak{R} \qquad \text{or} \qquad \varepsilon^2 \gg \alpha, \tag{6.8}$$

which correspond to the situation when the curvatures are small but rapidly varying, and ii) the *long-wave approximation*,

$$\nabla\nabla\Re \ll \Re\Re \qquad \text{or} \qquad \varepsilon^2 \ll \alpha\,, \tag{6.9}$$

which corresponds to the case when the curvatures are strong but slowly varying, that is, this is the case of homogeneous manifolds (symmetric spaces, Lie groups, etc.)

For simplicity we restrict here to the heat kernel diagonal. As we have seen in Chap. 5 there is an asymptotic expansion of the heat kernel diagonal $[U(t)] = U(t; x, x)$ as $t \to 0$

$$[U(t)] \sim (4\pi t)^{-n/2} \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} [b_k], \tag{6.10}$$

where $[b_k] = b_k(x, x)$ are the coincidence limits of the heat kernel coefficients $b_k(x, x')$.

At this point, it is worth to discuss the dimensions of various quantities. Let L denote the unit of length (do not confuse with the operator L!). Then the dimension of time t is L^2. Then the derivatives ∇ and $\nabla^{\mathcal{A}}$ have dimension L^{-1} and the curvatures R, $\mathcal{R}$ and the potential term Q have the dimension L^{-2}. Therefore, the jets $\Re_{(i)}$ have the dimension L^{-2-i}. Since the quantity $t^k b_k$ is dimensionless, the dimension of the heat kernel coefficients b_k is L^{-2k}.

The coefficients $[b_k]$ are polynomial in the jets. The first two coefficients are given by (5.59) and (5.121)

$$[b_0] = 1\,, \tag{6.11}$$

$$[b_1] = Q - \frac{1}{6} R\,. \tag{6.12}$$

For $k \geq 2$ one can classify the terms in $[b_k]$ according to the number of curvatures and the number of the derivatives. First, there are terms linear in the curvature, then it follows the class of terms quadratic in the curvature, etc.. The last class of terms does not contain any covariant derivatives at all but only the powers of the curvatures. This general structure emerges by the expansion of $[b_k]$ in the deformation parameters

$$[b_k] = \sum_{n=1}^{k} \alpha^n \varepsilon^{2k-2n} b_{k,n}. \tag{6.13}$$

Here $b_{k,n}$ are the homogeneous parts of $[b_k]$ of order n in the curvatures. Note that the dimension of the coefficients $b_{k,n}$ is L^{-2k}. Since it already has n curvatures, it must have then $(2k - 2n)$ derivatives. Therefore, they can be symbolically written in the form

$$b_{k,n} = \sum_{\substack{i_1,\dots,i_n \geq 0 \\ i_1+\dots+i_n=2k-2n}} \sum \Re_{(i_1)} \cdots \Re_{(i_n)}, \tag{6.14}$$

where the second summation is over different invariant structures.

By using the invariance theory one can show that there are only very few terms with highest derivatives that can appear in the heat kernel coefficients. Therefore, the general structure of the homogeneous parts of the higher order coefficients $[b_k]$, $k \geq 2$, can be found in our papers [10, 4]

$$b_{k,1} = \alpha_k^{(1)} \Delta^{k-1} Q + \alpha_k^{(2)} \Delta^{k-1} R, \tag{6.15}$$

$$\begin{aligned} b_{k,2} &= \beta_k^{(1)} Q \Delta^{k-2} Q + 2\beta_k^{(2)} \mathcal{R}^i{}_j \nabla_i \Delta^{k-3} \nabla_m \mathcal{R}^{mj} - 2\beta_k^{(3)} Q \Delta^{k-2} R \\ &\quad + \beta_k^{(4)} R_{ij} \Delta^{k-2} R^{ij} + \beta_k^{(5)} R \Delta^{k-2} R + O(\nabla(\Re^2)), \end{aligned} \tag{6.16}$$

$$\dots$$

$$b_{k,k} = \sum \Re^k, \tag{6.17}$$

where $\alpha_k^{(i)}$ and $\beta_k^{(i)}$ are some universal numerical constants and $O(\nabla(\Re^2))$ denotes the terms the total derivatives of terms of order 2 in curvatures. Note that here $\Delta = \nabla^i \nabla_i$ is the Laplacian and not the Van Vleck determinant. Note also that there are only five quadratic invariant structures (up to the total derivatives) but very many structures of the type $\Re^k$. For the exact values of these universal constants see Sec. 6.2 below.

Thus we have the asymptotic expansion

$$[U(t)] \sim (4\pi t)^{-n/2} \left(1 + \sum_{k=1}^{\infty} \sum_{n=1}^{k} \frac{(-t)^k}{k!} \alpha^n \varepsilon^{2k-2n} b_{k,n} \right). \tag{6.18}$$

Let us consider now the asymptotic expansion of the heat kernel diagonal in the limit $\alpha \to 0$ of the perturbation theory (short-wave approximation). It can be obtained by reordering the sum in (6.18) and summing up all leading derivatives (that is, the powers of ε),

$$[U(t)] \sim (4\pi t)^{-n/2} \left(1 + \sum_{n=1}^{\infty} (\alpha t)^n h_n(t) \right), \tag{6.19}$$

where $h_n(t)$ are some *nonlocal* functionals that have the following asymptotic expansion as $t \to 0$

$$h_n(t) \sim \sum_{l=0}^{\infty} \frac{(-1)^{n+l}}{(n+l)!} (\varepsilon^2 t)^l b_{n+l,n}. \tag{6.20}$$

For explicit form of the first two functionals h_n see Sec. 6.2 below.

Let us consider now the asymptotic expansion of the heat kernel diagonal in the limit $\varepsilon \to 0$ of the perturbation theory (long-wave approximation). It can be obtained by reordering the sum in (6.18) and summing up the powers of curvatures (that is, the powers of α),

$$[U(t)] \sim (4\pi t)^{-n/2} \sum_{l=0}^{\infty} (\varepsilon^2 t)^l u_l(t)\,, \tag{6.21}$$

where the coefficients $u_l(t)$ are *essentially non-perturbative* functionals that have the following perturbative asymptotic expansion as $t \to 0$

$$u_l(t) \sim \sum_{n=0}^{\infty} \frac{(-1)^{n+l}}{(n+l)!} (\alpha t)^n b_{l+n,n}. \tag{6.22}$$

The leading term of this asymptotic expansion,

$$[U(t)] \sim (4\pi t)^{-n/2} u_0(t), \tag{6.23}$$

corresponds to covariantly constant background fields

$$\Re_{(i)} = 0 \qquad \text{for } i \geq 1, \tag{6.24}$$

or, more explicitly,

$$\nabla_m R_{ijkl} = 0, \qquad \nabla_m \mathcal{R}_{ij} = 0\,, \qquad \nabla_m Q = 0. \tag{6.25}$$

This defines the so-called *symmetric spaces* in differential geometry.

The zeroth order functional $u_0(t)$ has the following perturbative asymptotic expansion

$$u_0(t) \sim \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (\alpha t)^n b_{n,n}, \tag{6.26}$$

or, symbolically,

$$u_0(t) \sim \sum_{n=0}^{\infty} \sum (\alpha t \Re)^n, \tag{6.27}$$

and can be viewed on as the *generating function* for the part of the heat kernel coefficients, $b_{k,k}$, that does not contain any covariant derivatives.

6.2 Leading Derivatives in Heat Kernel Diagonal

In this section we show how the leading derivatives in the heat kernel coefficients, (6.15) and (6.16) can be computed by the technique developed in

Chap. 5 following [10, 4]. We also give a formal non-local expression for the heat kernel that might be of interest in mathematical physics.

To organize such an expansion one should slightly modify the diagrammatic technique developed in the previous chapters. Let us consider all diagrams for calculation of a heat kernel coefficient, say, $\langle n|b_k\rangle$. They all have k blocks $\langle m|\hat{L}|n\rangle$ but, as a matter of fact, they are of different order in background fields. As we have seen the blocks that have m incoming lines and $m+2$ outgoing ones are dimensionless

$$\langle m|\hat{L}|m+2\rangle = -\delta^{(i_1\cdots i_m}_{j_1\cdots j_m} g^{i_{m+1}i_{m+2})} \,. \tag{6.28}$$

Therefore one can order all diagrams in the following way. The first diagram contains only one dimensional block, all other being dimensionless. The second class of diagrams contains two dimensional blocks, the third one — three etc. The last class of diagrams does not contain any dimensionless blocks. To obtain the heat kernel coefficients in the first order in background fields it is enough to restrict oneself to the first diagram. To get the second order terms one has to consider in addition the second class of diagrams with two dimensional blocks, etc..

After such modification of the sum (5.77) (and some heavy combinatorics) one obtains

$$\begin{aligned}\langle n|b_k\rangle = \sum_{N=1}^{k}(-1)^{N-k} & \sum_{1\le i_1<i_2<\cdots<i_{N-1}\le k-1} \quad \sum_{n_1,\cdots,n_{N-1}\ge 0} \\ & \times N(i_1,n_1,\cdots i_{N-1},n_{N-1},k,n) \\ & \times\langle n;k-i_{N-1}-1|\hat{L}|n_{N-1}\rangle\langle n_{N-1};i_{N-1}-i_{N-2}-1|\hat{L}|n_{N-2}\rangle\cdots \\ & \times\langle n_2;i_2-i_1-1|\hat{L}|n_1\rangle\langle n_1;i_1-1|\hat{L}|0\rangle\,,\end{aligned} \tag{6.29}$$

where

$$\langle n;k|\hat{L}|m\rangle = g^{i_1i_2}\cdots g^{i_{2k-1}i_{2k}}\langle i_1\cdots i_{2k}i_{2k+1}\cdots i_{n+2k}|\hat{L}|j_1\cdots j_m\rangle\,, \tag{6.30}$$

$$\begin{aligned}& N(i_1,n_1\cdots i_{N-1},n_{N-1},k,n) \\ & \quad = \frac{1}{\binom{2k+n-1}{k}}\frac{\binom{2i_2+n_2-1}{i_1}}{\binom{2i_1+n_1-1}{i_1}}\cdots\frac{\binom{2i_{N-1}+n_{N-1}-1}{i_{N-2}}}{\binom{2i_{N-2}+n_{N-2}-1}{i_{N-2}}}\frac{\binom{2k+n-1}{i_{N-1}}}{\binom{2i_{N-1}+n_{N-1}-1}{i_{N-1}}}\end{aligned} \tag{6.31}$$

and the summation over n_1, …, n_{N-1} should be carried out in such limits that all matrix elements should be dimensional, i.e. for each factor $\langle n;k|\hat{L}|m\rangle$ it should be $n+2k\ge m$, that is,

$$n_1 + 2(i_1 - 1) \geq 0, \quad n_2 + 2(i_2 - i_1 - 1) \geq n_1, \qquad \cdots \qquad ,$$
$$n + 2(k - i_{N-1} - 1) \geq n_{N-1}\,. \tag{6.32}$$

In present section we are going to calculate the linear and quadratic terms in the background fields. Therefore we shall always neglect the terms of the third order in background fields denoting them $O(\Re^3)$. We have from (6.29) for the coincidence limit of heat kernel coefficients

$$[b_k] = \frac{(-1)^{k-1}}{\binom{2k-1}{k}}\langle 0; k-1|\hat{L}|0\rangle$$
$$+(-1)^k \sum_{i=1}^{k-1} \sum_{n_i=0}^{2(k-i-1)} \frac{\binom{2k-1}{i}}{\binom{2k-1}{k}\binom{2i+n_i-1}{i}} \langle 0; k-i-1|\hat{L}|n_i\rangle\langle n_i; i-1|\hat{L}|0\rangle$$
$$+O(\Re^3)\,. \tag{6.33}$$

Here we have taken into account in (6.29) the first diagram ($N = 1$) and the second class of diagrams ($N = 2$).

Now we should make use of the formulas (5.99)-(5.106) of Chap. 5 and Sec. 3.8.4 to calculate the matrix elements $\langle n; k|\hat{L}|m\rangle$ within the same accuracy $O(\Re^3)$, substitute them in eq. (6.33) and carry out the summation. Omitting these very cumbersome calculations we write down the result (for $k \geq 2$), which can be found in our papers [10, 4],

$$[b_k] = b_{k,1} + b_{k,2} + O(\Re^3)\,, \tag{6.34}$$

where

$$b_{k,1} = \frac{2}{k+1}\left(F_{k+1}^{(1)}(\Delta)Q - F_{k+1}^{(3)}(\Delta)R\right)\,, \tag{6.35}$$
$$b_{k,2} = QF_k^{(1)}(\Delta)Q + 2\mathcal{R}^i{}_j\nabla_i\Delta^{-1}F_k^{(2)}(\Delta)\nabla_m\mathcal{R}^{mj} - 2QF_k^{(3)}(\Delta)R$$
$$+R_{ij}F_k^{(4)}(\Delta)R^{ij} + RF_k^{(5)}(\Delta)R + O(\nabla(\Re^2))\,,$$

where the total derivatives and terms of order higher than two are omitted. Here Δ is the Laplacian and $F_k^{(i)}(\Delta)$ are differential operators of order $(2k-4)$

$$F_k^{(i)}(\Delta) = \frac{1}{2}\frac{k!(k-2)!}{(2k-3)!}f_k^{(i)}(-\Delta)^{k-2}\,, \tag{6.36}$$

where $f_k^{(i)}$ are numerical coefficients defined by

$$f_k^{(1)} = 1\,, \tag{6.37}$$

$$f_k^{(2)} = \frac{1}{2(2k-1)}\,, \tag{6.38}$$

$$f_k^{(3)} = \frac{k-1}{2(2k-1)}\,, \tag{6.39}$$

$$f_k^{(4)} = \frac{1}{2(4k^2-1)}\,, \tag{6.40}$$

$$f_k^{(5)} = \frac{k^2-k-1}{4(4k^2-1)}\,. \tag{6.41}$$

It is not difficult to show that $F_k^{(i)}(\Delta)$ (6.36) can be represented in an integral form which will be very useful for further consideration

$$F_k^{(i)}(\Delta) = \frac{1}{2}k(k-1)\int\limits_0^1 d\xi\, f^{(i)}(\xi)(1-\xi^2)^{k-2}\left(-\frac{\Delta}{4}\right)^{k-2}\,, \tag{6.42}$$

where

$$f^{(1)}(\xi) = 1\,, \tag{6.43}$$

$$f^{(2)}(\xi) = \frac{1}{2}\xi^2\,, \tag{6.44}$$

$$f^{(3)}(\xi) = \frac{1}{4}(1-\xi^2)\,, \tag{6.45}$$

$$f^{(4)}(\xi) = \frac{1}{6}\xi^4\,, \tag{6.46}$$

$$f^{(5)}(\xi) = \frac{1}{48}(3-6\xi^2-\xi^4)\,. \tag{6.47}$$

Now, as was noted in Sec. 5.2 we can compute the function b_q, (5.48), by making the analytical continuation of the heat kernel coefficients b_k, (6.35), to the whole complex plane of their order. The result of such an analytical continuation has the form (6.35) where one should substitute k for q . The differential operators $F_k^{(i)}(\Delta)$ become then nonlocal formfactors $F_q^{(i)}(\Delta)$ of the form (6.42), with k being replaced by q. This can also be written by using the gamma-function

$$F_q^{(i)}(\Delta) = \frac{1}{2}\frac{\Gamma(q+1)\Gamma(q-1)}{\Gamma(2q-2)} f_q^{(i)}(-\Delta)^{q-2}\,. \tag{6.48}$$

Making use of the obtained function b_q one can easily calculate the coincidence limit of heat kernel either by direct summation of the power series

(5.56) or by computing the integral (5.52)

$$[U(t)] = (4\pi t)^{-n/2} \left\{1 + th_1(t) + t^2 h_2(t) + O(\Re^3)\right\} , \tag{6.49}$$

where

$$h_1(t) = -\gamma^{(1)}(t\Delta)Q + \gamma^{(3)}(t\Delta)R\,, \tag{6.50}$$

$$\begin{aligned} h_2(t) = \frac{1}{2}\Big[& Q\gamma^{(1)}(t\Delta)Q + 2\mathcal{R}^i{}_j \nabla_i \Delta^{-1}\gamma^{(2)}(t\Delta)\nabla_m \mathcal{R}^{mj} \\ & -2Q\gamma^{(3)}(t\Delta)R + R_{ij}\gamma^{(4)}(t\Delta)R^{ij} + R\gamma^{(5)}(t\Delta)R\Big] \\ & +O(\nabla(\Re^2))\,, \end{aligned} \tag{6.51}$$

and $\gamma^{(i)}(t\Delta)$ are some non-local (pseudo-differential) operators defined by

$$\gamma^{(i)}(t\Delta) = \int\limits_0^1 d\xi\, f^{(i)}(\xi) \exp\left(\frac{1-\xi^2}{4} t\Delta\right) \tag{6.52}$$

with $f^{(i)}(\xi)$ given by (6.47).

By integrating the heat kernel diagonal over the whole manifold and omitting the total derivatives (since there is no boundary) we obtain the heat trace (1.166)

$$\begin{aligned} \mathrm{Tr}\, \exp(-tL) &= \int\limits_M dx g^{1/2} [U(t)] \\ &= (4\pi t)^{-n/2} \int\limits_M dx g^{1/2} \Big\{ 1 + t\left(Q - \frac{1}{6}R\right) \\ &\quad + \frac{t^2}{2}\Big[Q\gamma^{(1)}(t\Delta)Q + 2\mathcal{R}^i{}_j \nabla_i \Delta^{-1}\gamma^{(2)}(t\Delta)\nabla_m \mathcal{R}^{mj} \\ &\quad -2Q\gamma^{(3)}(t\Delta)R + R_{ij}\gamma^{(4)}(t\Delta)R^{ij} + R\gamma^{(5)}(t\Delta)R\Big] + O(\Re^3)\Big\}. \end{aligned} \tag{6.53}$$

This formula is very useful in studying the spectral functions of the operator L, such as, the trace of the heat kernel, the zeta-function, the determinant etc, which describe the propagators and the effective action in quantum field theory.

6.3 Fourier Transform Method

6.3.1 Non-covariant Fourier Transform

Here we derive a very simple alternative derivation of the asymptotic expansion of the heat kernel by using the semi-group perturbation theory. Let L be an elliptic second-order partial differential operator acting on smooth real functions on $\mathbb{R}^n$ of the form

$$L(x,\partial) = -\alpha^{ij}(x)\partial_i\partial_j + \beta^i(x)\partial_i + \gamma(x)\,. \tag{6.54}$$

The heat kernel of the operator L is given by

$$U(t;x,x') = \exp(-tL)\delta(x,x')\,, \tag{6.55}$$

where $\delta(x,x') = g^{-1/2}\delta(x-x')$ and $g = [\det(\alpha^{ij})]^{-1}$. By using Fourier representation for the delta-function we obtain

$$\begin{aligned} U(t;x,x') &= g^{-1/2}\int\limits_{\mathbb{R}^n}\frac{dp}{(2\pi)^n}e^{-i\langle p,x'\rangle}\exp[-tL(x,\partial)]e^{i\langle p,x\rangle} \\ &= g^{-1/2}\int\limits_{\mathbb{R}^n}\frac{dp}{(2\pi)^n}e^{i\langle p,(x-x')\rangle}\exp[-tL(x,\partial+ip)]\cdot 1\,, \\ &= g^{-1/2}\int\limits_{\mathbb{R}^n}\frac{dp}{(2\pi)^n}e^{i\langle p,(x-x')\rangle}\exp[-t(H+K+L)]\cdot 1\,, \end{aligned} \tag{6.56}$$

where H is the leading symbol of the operator L

$$H(x,p) = \alpha^{ij}(x)p_ip_j\,, \tag{6.57}$$

and K is a first-order differential operator defined by

$$K = ip_j\left[\beta^j(x) - 2i\alpha^{jk}(x)\partial_k\right]\,. \tag{6.58}$$

Here the operators in the exponent act on 1 from the left. Now, by rescaling $p \to t^{-1/2}p$ we obtain

$$\begin{aligned} U(t;x,x') = (4\pi t)^{-n/2}g^{-1/2}\int\limits_{\mathbb{R}^n}\frac{dp}{\pi^{n/2}}\exp\left[it^{-1/2}\,\langle p,(x-x')\rangle\right] \\ \times\exp\left(-H-\sqrt{t}\,K-tL\right)\cdot 1\,. \end{aligned} \tag{6.59}$$

Of course, in the case of operators with constant coefficients the operators H, K and L commute, also, the action of the differential operator ∂_i on 1 is

zero. Therefore,

$$U(t;x,x') = (4\pi t)^{-n/2} g^{-1/2} \int\limits_{\mathbb{R}^n} \frac{dp}{\pi^{n/2}} \exp\left[it^{-1/2} \langle p, (x-x') \rangle \right] \times \exp\left\{ - \langle p, Ap \rangle - i\sqrt{t}\ \langle p, \beta \rangle - t\gamma \right\}, \tag{6.60}$$

where $A = (\alpha^{ij})$ and by computing the Gaussian integral over p we obtain the same well known result (2.196). The only difference is the absence of the factor $g^{1/2} = (\det A)^{-1/2}$ since we took the heat kernel in the invariant form here, not the density form as in (2.196). This difference comes from the difference of the initial condition, instead of the coordinate delta function $\delta(x-x')$ we took the covariant delta function $\delta(x,x')$.

However, by using the heat semigroup perturbation theory of Sec. 1.17 one can compute this integral even in the general case. Namely, by expanding the exponential $\exp[-H - \sqrt{t}\ K - tL)]$ in a power series in t we can get the asymptotic expansion of the heat kernel. Since $H(x,p)$ is quadratic in the momenta p, all integrals over p are standard Gaussian integrals and are easily computed. Of course, one should keep in mind that the operators H, K and L in the exponent do not commute. So, one should use Volterra series (1.214) to get the expansion.

6.3.2 Covariant Fourier Transform

In this section we use extensively the machinery developed in Chap. 3 and in Sec. 3.8.3, in particular. We refer to that chapter for notation and definition of various differential-geometric objects. We remind the definition of some objects that we will need (for more details see Chap. 3 on differential geometry). As usual, $\sigma(x,x')$ denotes the Synge function, $\sigma_{i'} = \nabla_{i'}\sigma$, $\eta^{i'}{}_{j} = \nabla_j \sigma^{i'}$ and $\gamma = (\gamma^{i}{}_{j'})$ is the inverse of the matrix $\eta = (\eta^{i'}{}_{j})$. We will use the operators $\mathcal{D}_{i'}$ (5.86)

$$\mathcal{D}_{i'} = \gamma^{j}{}_{i'} \nabla_j \,, \tag{6.61}$$

These operators are very convenient in curved space since they satisfy the following commutation relations

$$[\mathcal{D}_{i'}, \mathcal{D}_{j'}] = 0\,, \qquad \left[\mathcal{D}_{i'}, \sigma^{j'}\right] = \delta^{j'}{}_{i'}\,. \tag{6.62}$$

Thus, the operators $\mathcal{D}_{i'}$ and the vectors $\sigma^{j'}$ play the role of usual derivatives and coordinates in flat space. Further, let $\Delta(x,x')$ denote the Van Vleck determinant, $\zeta = \log \Delta^{1/2}$, and $\mathcal{P}(x,x')$ be the generalized operator of parallel transport. Then we also define

$$\hat{\mathcal{A}}_{i'} = \mathcal{P}^{-1}\mathcal{D}^{\mathcal{A}}_{i'}\mathcal{P} = \mathcal{P}^{-1}\mathcal{D}_{i'}\mathcal{P} + \mathcal{A}_i\,, \tag{6.63}$$

$$\zeta_{i'} = \mathcal{D}_{i'}\zeta = \Delta^{-1/2}\mathcal{D}_{i'}\Delta^{1/2}\,. \tag{6.64}$$

Let L be a Laplace type differential operator acting on scalar functions on a Riemannian manifold of the form

$$L = -g^{ij}\nabla^{\mathcal{A}}_i\nabla^{\mathcal{A}}_i + Q\,. \tag{6.65}$$

The covariant Fourier transform method is based on the formal representation of the heat kernel in the form

$$U(t;x,x') = \exp(-tL)\delta(x,x'). \tag{6.66}$$

Using the representation of the δ-function in form of a covariant Fourier integral (3.358)

$$\delta(x,x') = \mathcal{P}(x,x')\Delta^{1/2}(x,x')\int\limits_{\mathbb{R}^n}\frac{dk}{(2\pi)^n}g^{-1/2}(x')e^{ik(x)}\,, \tag{6.67}$$

with $k(x) = k_{j'}\sigma^{j'}(x,x')$, we get

$$U(t;x,x') = \mathcal{P}(x,x')\Delta^{1/2}(x,x')\int\limits_{\mathbb{R}^n}\frac{dk}{(2\pi)^n}g^{-1/2}(x')e^{ik(x)}\exp(-tA)\cdot 1\,, \tag{6.68}$$

where A is an operator defined by

$$A = e^{-ik(x)}\hat{L}e^{k(x)}\,, \tag{6.69}$$

and the operator $\hat{L}$ is defined by (5.43)

$$\hat{L} = \mathcal{P}^{-1}\Delta^{-1/2}L\Delta^{1/2}\mathcal{P}\,. \tag{6.70}$$

We can express the operator $\hat{L}$ in terms of the operators $\mathcal{D}_{i'}$, (5.93)

$$\hat{L} = -X^{i'j'}\mathcal{D}_{i'}\mathcal{D}_{j'} - Y^{i'}\mathcal{D}_{i'} + Z\,, \tag{6.71}$$

where the functions $X^{i'j'}$, $Y^{i'}$ and Z are defined by (5.90), (5.94) and (5.95)

$$X^{i'j'} = \eta^{i'}{}_k\eta^{j'k}\,, \tag{6.72}$$

$$Y^{i'} = \mathcal{D}_{j'}X^{i'j'} + 2X^{i'j'}\hat{\mathcal{A}}_{j'}\,, \tag{6.73}$$

$$Z = X^{i'j'}(\zeta_{i'}\zeta_{j'} - \hat{\mathcal{A}}_{i'}\hat{\mathcal{A}}_{j'}) - \mathcal{D}_{j'}\left[X^{i'j'}\left(\zeta_{i'} + \hat{\mathcal{A}}_{i'}\right)\right] + Q\,. \tag{6.74}$$

Therefore, the operator A can be written in the form

$$A = \hat{L} - ik_{i'}T^{i'} + k_{j'}k_{l'}X^{j'l'}\,, \tag{6.75}$$

where $T^{i'}$ is a first-order differential operator defined by

$$T^{i'} = 2X^{i'j'}\mathcal{D}_{j'} + Y^{i'}\,. \tag{6.76}$$

Now by rescaling the integration variable $k \to k/\sqrt{t}$ one can rewrite the heat kernel in a form that is convenient to get the asymptotic expansion as $t \to 0$ and $x \to x'$

$$U(t;x,x') = (4\pi t)^{-n/2}\mathcal{P}(x,x')\Delta^{1/2}(x,x')\int\limits_{\mathbb{R}^n}\frac{dk}{\pi^{n/2}}g^{-1/2}(x')\exp\left[it^{-1/2}k(x)\right]$$
$$\times\exp\left\{-k_{i'}k_{j'}X^{i'j'} + ik_{j'}\sqrt{t}\,T^{j'} - t\hat{L}\right\}\cdot 1\,. \tag{6.77}$$

Assuming that t and $\sigma^{i'}$ are small (that is, the points x and x' are close to each other) one can simply expand this expression in an asymptotic series in powers of t. The coefficients of this expansion are represented as the result of the action of some differential operators on the identity. Moving the derivatives to the right until they act on the identity and give zero the final result will be expressed in terms of derivatives of the two-point functions $X^{i'j'}$, $Y^{i'}$ and Z. These functions can be expanded in covariant Taylor series; the Taylor coefficients of these functions are expressed in terms of covariant quantities $R^{i}{}_{jkl}$, $\mathcal{R}_{ij}$ and Q and their derivatives.

To be specific, let us consider the coincidence limit (the diagonal) of the heat kernel. Then the above formula for the heat kernel simplifies to

$$[U(t)] = (4\pi t)^{-n/2} \tag{6.78}$$
$$\times\lim_{x\to x'}\int\limits_{\mathbb{R}^n}\frac{dk}{\pi^{n/2}}g^{-1/2}(x')\exp\left\{-k_{i'}k_{j'}X^{i'j'} + ik_{j'}\sqrt{t}T^{j'} - t\hat{L}\right\}\cdot 1\,.$$

Let us separate the value of the function $X^{i'j'}$ at x', that is,

$$X^{i'j'} = g^{i'j'}(x') + \tilde{X}^{i'j'}\,. \tag{6.79}$$

Then the above formula can be written in terms of Gaussian average over the momenta $k_{i'}$.

We define the Gaussian average of a two-point function $f(k,x,x')$ over momenta k by

$$\langle f(k)\rangle = \lim_{x\to x'}\int\frac{dk}{\pi^{n/2}}g^{-1/2}\exp\left[-g^{i'j'}(x')k_{i'}k_{j'}\right]f(k)\,, \tag{6.80}$$

so that

$$\langle k_{i_1} \cdots k_{i_{2n+1}} \rangle = 0\,, \tag{6.81}$$

$$\langle k_{i_1} \cdots k_{i_{2n}} \rangle = \frac{(2n)!}{2^{2n} n!} g_{(i_1 i_2} \cdots g_{i_{2n-1} i_{2n})}\,. \tag{6.82}$$

Here the parenthesis indicate the complete symmetrization over all indices included. Further, let

$$A_0 = \hat{L}\,, \tag{6.83}$$

$$A_1 = -ik_{j'}\, T^{j'}\,, \tag{6.84}$$

$$A_2 = k_{i'} k_{j'} \tilde{X}^{i'j'}\,. \tag{6.85}$$

Then the heat kernel diagonal takes the form

$$[U(t)] = (4\pi t)^{-n/2} [\Omega(t)]\,, \tag{6.86}$$

where

$$[\Omega(t)] = \lim_{x \to x'} \left\langle \exp\left(-A_2 - \sqrt{t} A_1 - t A_0\right) \cdot 1 \right\rangle\,. \tag{6.87}$$

By expanding it in the asymptotic series as $t \to 0$

$$[\Omega(t)] \sim \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} [b_k]\,, \tag{6.88}$$

we obtain the heat kernel coefficients in the form

$$[b_k] = \lim_{x \to x'} \sum_{N=0}^{\infty} \frac{k!}{N!} \sum_{\substack{0 \le k_1, \ldots, k_N \le 2 \\ k_1 + \cdots + k_N = k}} \langle A_{k_1} \cdots A_{k_N} \cdot 1 \rangle\,. \tag{6.89}$$

Here the summation goes over all integers $k_1, \ldots, k_N$ taking the values 0, 1 and 2 and such that their sum is equal to k. Taking this into account one can show that the sum over N is, in fact, always finite. The reason why this works is that the function A_2 is vanishing in the coincidence limit as $x \to x'$.

6.4 Long Time Behavior of the Heat Kernel

Let L be a Laplace type operator,

$$L = -g^{ij} \nabla_i^A \nabla_j^A + Q \tag{6.90}$$

acting on functions on some compact manifold M. As we already stressed above if $\mathcal{R}_{ij} = \partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i \neq 0$, then the operator L is not self-adjoint. It would be self-adjoint if $\mathcal{A}_i$ is purely imaginary, however, since we consider only

real functions, we exclude that possibility. Let us restrict to the case $\mathcal{R}_{ij} = 0$. Then L is similar to a self-adjoint operator. Then the spectrum $(\lambda_k)_{k=1}^{\infty}$ of the operator L is real, discrete, with finite multiplicities, and bounded from below. We can order the eigenvalues in an increasing order,

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots , \tag{6.91}$$

where each eigenvalue is taken with its multiplicity. Then there is an orthonormal basis $(\varphi_k)_{k=1}^{\infty}$ in the Hilbert space $L^2(M)$ consisting of eigenvectors of the operator L. Of course, in this basis, the operator L acts just by multiplication.

In particular, the heat kernel of the operator L can be written in form of a spectral sum

$$U(t; x, x') = \sum_{k=1}^{\infty} \exp(-t\lambda_k)\varphi_k(x)\varphi_k(x') . \tag{6.92}$$

This expansion is not very good for small t, in fact, it diverges for $t = 0$. However, this series gives an excellent approximation for large t. Since all eigenvalues are ordered, then the leading asymptotics as $t \to \infty$ is determined by the smallest eigenvalue,

$$U(t; x, x') = \exp(-t\lambda_1)P_1(x, x'), + \cdots , \tag{6.93}$$

where

$$P_1(x, x') = \sum_{i=1}^{d_1} \varphi_i(x)\varphi_i(x') \tag{6.94}$$

is the projection to the first eigenspace and d_1 is the multiplicity of the first eigenvalue. In particular, if the bottom eigenvalue is positive, $\lambda_1 > 0$, then the heat kernel decreases exponentially as $t \to \infty$. If $\lambda_1 = 0$ then the heat kernel approaches a constant (that depends on x and x'), and if $\lambda_1 < 0$, then the heat kernel grows exponentially as $t \to \infty$. Thus, the negative eigenvalues signal instability.

However, generically, in most cases it is impossible to find the spectrum or even the smallest eigenvalue. Only in some exceptional cases, for operators with high level of symmetry, like homogeneous spaces, symmetric spaces, Lie groups, etc, one can apply powerful algebraic methods to obtain the spectrum of the operator. There is a huge literature on 'exactly solvable' operators, in particular, in quantum mechanics (see, for example, [2]). There exist even an encyclopedia of exactly solvable problems [61]. In all such cases the spectrum is known exactly, which gives the long-time behavior of the heat kernel.

We should also stress that for non-compact manifolds the spectra of differential operators are not discrete. In this case the leading asymptotics as $t \to \infty$ is not given by the lowest eigenvalue. It is a much more complicated

issue then. Roughly speaking it depends on the behavior of the coefficients of the operator at infinity.

6.5 Quantum Operator Method

6.5.1 General Framework

This is a rather formal approach pioneered by Schwinger and generalized to curved manifolds by De Witt [26]. We will modify it accordingly.

Let us consider a partial differential operator (more generally, a pseudo-differential operator) acting on smooth functions, say, on $\mathbb{R}^n$, of the form

$$L(x,\partial) = \sum_{k=0}^{\infty} L^{i_1\dots i_k}(x)\partial_{i_1}\cdots\partial_{i_k}\,. \tag{6.95}$$

We treat the coordinates x^i as the operators of multiplication of smooth functions by x^i. Of course, they do not commute with the operators of derivatives ∂_j; their commutators are

$$[x^i, x^j] = 0\,, \tag{6.96}$$

$$[\partial_i, \partial_j] = 0\,, \tag{6.97}$$

$$[\partial_i, x^j] = \delta^j{}_i\,. \tag{6.98}$$

That is why we order the coordinates x^i and the operators ∂_j in the operator L so that all coordinates are on the left and all derivatives are on the right. Of course, the operator acts on functions of x from the left, as usual.

Now, let us define time-dependent operators

$$\hat{x}^i(t) = \exp[tL(x,\partial)]\hat{x}^i \exp[-tL(x,\partial)]\,, \tag{6.99}$$

$$\hat{p}_j(t) = \exp[tL(x,\partial)]\partial_j \exp[-tL(x,\partial)]\,. \tag{6.100}$$

Obviously, they satisfy the initial conditions

$$\hat{x}^i(0) = x^i\,, \qquad \hat{p}_j(0) = \partial_j\,, \tag{6.101}$$

and the operator equations

$$\frac{d\hat{x}^i}{dt} = [L(\hat{x},\hat{p}), \hat{x}^i]\,, \tag{6.102}$$

$$\frac{d\hat{p}_j}{dt} = [L(\hat{x},\hat{p}), \hat{p}_j]\,. \tag{6.103}$$

Because of the similarity with quantum dynamics these equations are called *Heisenberg equations*. These equations can be solved in form of a Taylor series in t. By using the formula for the commutators (1.211) we have

$$\hat{x}^i(t) = \exp(tAd_L)x^i = x^i + \sum_{k=1}^{\infty} \frac{t^k}{k!} \underbrace{[L,[L,\cdots,[L,x^i]\cdots]]}_{k}, \quad (6.104)$$

$$\hat{p}_j(t) = \exp(tAd_L)\partial_j = \partial_j + \sum_{k=1}^{\infty} \frac{t^k}{k!} \underbrace{[L,[L,\cdots,[L,\partial_j]\cdots]]}_{k}, \quad (6.105)$$

where, as usual, Ad_L is the operator defined by

$$Ad_L B = [L,B]\,. \quad (6.106)$$

The operators $\hat{x}(t)$ and $\hat{p}(t)$ are some pseudo-differential operators of the form

$$\hat{x}^i(t) = \hat{x}^i(t;x,\partial) = \sum_{k=0}^{\infty} X^{ii_1\cdots i_k}(t,x)\partial_{i_1}\cdots\partial_{i_k}\,. \quad (6.107)$$

$$\hat{p}_i(t) = \hat{p}_i(t;x,\partial) = \sum_{k=0}^{\infty} P_i^{\,i_1\cdots i_k}(t,x)\partial_{i_1}\cdots\partial_{i_k}\,. \quad (6.108)$$

Notice that the commutation relations (6.98) and the operator $L(x,\partial)$ are invariant under the quantum dynamics, that is,

$$[\hat{x}^i(t),\hat{x}^j(t)] = 0\,, \quad (6.109)$$

$$[\hat{p}_i(t),\hat{p}_j(t)] = 0\,, \quad (6.110)$$

$$[\hat{p}_i(t),\hat{x}^j(t)] = \delta^j{}_i\,, \quad (6.111)$$

and

$$L(\hat{x}(t),\hat{p}(t)) = L(x,\partial)\,. \quad (6.112)$$

The operators $\hat{x}(t)$ and x intertwine the heat semigroup, that is,

$$e^{-tL}\hat{x}^i(t) = x^i e^{-tL}\,, \quad (6.113)$$

more generally,

$$e^{-tL}\hat{x}^{i_1}(t)\cdots\hat{x}^{i_k}(t) = x^{i_1}\cdots x^{i_k}e^{-tL}\,, \quad (6.114)$$

The main idea of this approach is to solve the operator equations (6.102), (6.103) and use the commutation relations to compute the heat kernel. Now, suppose that we could integrate the operator equations, that is, find the functions $\hat{x}(t;x,\partial)$ and $\hat{p}(t;x,\partial)$, (6.107), (6.108), and one can express the

derivatives in terms of coordinate operators from the equation (6.107) and express them in the form

$$\partial_i = q_i(t;\hat{x}(t),x) = \sum_{k=0}^{\infty} \hat{x}^{i_1}(t)\cdots\hat{x}^{i_k}(t)Q_{ii_1\ldots i_k}(x)\,. \tag{6.115}$$

Notice that the operators are ordered so that all $\hat{x}(t)$ are on the left and all x are on the right. Next, one could substitute the derivatives ∂ given by (6.115) into $L(x,\partial)$ to get

$$L(x,\partial) = H(t;\hat{x}(t),x) = \sum_{k=0}^{\infty} \hat{x}^{i_1}(t)\cdots\hat{x}^{i_k}(t)H_{i_1\ldots i_k}(x)\,, \tag{6.116}$$

where $H(t;x,x')$ is some function and the operators $\hat{x}(t)$ are placed to the left and all x to the right.

Now, the heat kernel is given by

$$U(t;x,x') = \exp[-tL(x,\partial_x)]\delta(x,x')\,. \tag{6.117}$$

By using the representation (6.116) and eq. (6.114) we obtain

$$\begin{aligned} Le^{-tL} &= e^{-tL}L = e^{-tL}H(t;\hat{x}(t),x) \\ &= \sum_{k=0}^{\infty} x^{i_1}\cdots x^{i_k}e^{-tL}H_{i_1\ldots i_k}(x)\,. \end{aligned} \tag{6.118}$$

Therefore, by acting on the delta-function $\delta(x-x')$ we get

$$\begin{aligned} LU(t;x,x') &= \sum_{k=0}^{\infty} x^{i_1}\cdots x^{i_k}e^{-tL}H_{i_1\ldots i_k}(x)\delta(x,x') \\ &= \sum_{k=0}^{\infty} x^{i_1}\cdots x^{i_k}H_{i_1\ldots i_k}(x')e^{-tL}\delta(x,x') \\ &= H(t;x,x')U(t;x,x')\,. \end{aligned} \tag{6.119}$$

Thus, the heat kernel satisfies the equation

$$[\partial_t + H(t;x,x')]\,U(t;x,x') = 0\,. \tag{6.120}$$

The beauty of this equation is that it is not an operator equation, here $H(t;x,x')$ is just a function. That is why, it can be easily integrated to give

$$U(t;x,x') = \mathcal{P}(x,x')\exp\{-S(t;x,x')\}\,, \tag{6.121}$$

where

$$S(t;x,x') = \int dt\, H(t;x,x') \tag{6.122}$$

is nothing but the action, and $\mathcal{P}(x,x')$ is a function that should be determined from the initial condition

$$U(0;x,x') = \delta(x,x')\,. \tag{6.123}$$

Thus, the essence of the method is in the integrating the Heisenberg equations and calculating the function $H(t;x,x')$.

6.5.2 Linear Connection

We illustrate this method on a simple example. Let us consider the operator

$$\begin{aligned} L(x,\partial) &= -g^{jk}\nabla_j\nabla_k \\ &= -g^{jk}\left[\partial_j + \mathcal{A}_j(x)\right]\left[\partial_k + \mathcal{A}_k(x)\right]\,, \end{aligned} \tag{6.124}$$

where g^{ij} is a constant symmetric positive definite matrix, the vector $\mathcal{A}_i$ is a linear function,

$$\mathcal{A}_i(x) = -\frac{1}{2}\mathcal{R}_{ij}x^j\,, \tag{6.125}$$

$\mathcal{R}_{jk}$ is an anti-symmetric constant 2-tensor, and ∇_i are the covariant derivatives

$$\nabla_i = \partial_i + \mathcal{A}_i\,. \tag{6.126}$$

The operators of covariant derivatives satisfy the commutation relations

$$[\nabla_i, x^j] = \delta_i^j\,, \tag{6.127}$$

$$[\nabla_i, \nabla_j] = \mathcal{R}_{ij}\,. \tag{6.128}$$

To simplify the exposition we will use the matrix notation, $\mathcal{R} = (\mathcal{R}_{ij})$. As usual, we interpret the inverse of the matrix $g^{-1} = (g^{ij})$ as a metric $g = (g_{ij})$. We use this metric to raise and lower tensor indices. It is easy to see that

$$L = -g^{jk}\partial_j\partial_k + C^i{}_j x^j\partial_i + D_{ij}x^i x^j\,, \tag{6.129}$$

where the matrices $C = (C^i{}_j)$ and $D = (D_{ij})$ are defined by

$$C = g^{-1}\mathcal{R}\,, \tag{6.130}$$

$$D = \frac{1}{4}\mathcal{R}g^{-1}\mathcal{R} = \frac{1}{4}gC^2. \tag{6.131}$$

Therefore, this is a degenerate case in which the matrix $C^2 - 4g^{-1}D$ is exactly equal to zero (compare with Sec. 4.3.6).

We define the operators

$$\begin{aligned}\hat{\Pi}_i(t) &= \hat{p}_i(t) + \mathcal{A}_i(\hat{x}(t)) \\ &= \hat{p}_i(t) - \frac{1}{2}\mathcal{R}_{ij}\hat{x}^j(t)\,. \end{aligned} \tag{6.132}$$

so that

$$\hat{\Pi}_i(0) = \nabla_i\,. \tag{6.133}$$

Then the Heisenberg equations take the form

$$\frac{d\hat{x}^j}{dt} = -2g^{jk}\hat{\Pi}_k\,, \tag{6.134}$$

$$\frac{d\hat{\Pi}_j}{dt} = 2\mathcal{R}_{jm}g^{mk}\hat{\Pi}_k\,. \tag{6.135}$$

These equations are linear and can be easily solved. We will write the solution in the matrix form. By introducing the vectors $\hat{x} = (\hat{x}^i)$ and $\hat{\Pi} = (\hat{\Pi}_i)$ we have

$$\hat{\Pi}(t) = g\exp(2tC)g^{-1}\nabla\,, \tag{6.136}$$

$$\hat{x}(t) = \hat{x} - \frac{\exp(2tC) - 1}{C}g^{-1}\nabla\,. \tag{6.137}$$

Thus, we can express the operators of covariant derivatives in terms of the coordinate operators,

$$\begin{aligned}\nabla &= -g\frac{C}{\exp(2tC) - 1}[\hat{x}(t) - \hat{x}] \\ &= -\frac{1}{2}g\exp(-tC)\frac{C}{\sinh(tC)}[\hat{x}(t) - \hat{x}]\,. \end{aligned} \tag{6.138}$$

Now, by using the anti-symmetry of the matrix $\mathcal{R}$ we can rewrite the operator L in the form

$$L = -\frac{1}{4}\left\langle [\hat{x}(t) - \hat{x}], g\frac{C^2}{\sinh^2(tC)}[\hat{x}(t) - \hat{x}]\right\rangle\,, \tag{6.139}$$

where, as usual, the brackets $\langle\ ,\ \rangle$ mean the usual $\mathbb{R}^n$ pairing, $\langle x, Ax\rangle = x^i A_{ij}x^j$.

Finally, we compute the commutator

$$[\hat{x}^j(t), \hat{x}^k] = -\left[\frac{\exp(2tC) - 1}{C}g^{-1}\right]^{jk}\,. \tag{6.140}$$

By using this commutator we can reorder the operators $\hat{x}(t)$ and $\hat{x}$ in the operator L to bring all x to the right and $\hat{x}(t)$ to the left. This gives the function H, (6.116),

$$H(t;x,x') = -\frac{1}{4}\left\langle (x-x'), g\frac{C^2}{\sinh^2(tC)}(x-x')\right\rangle + \frac{1}{2}\mathrm{tr}\left[C\coth(tC)\right], \tag{6.141}$$

where tr is the matrix trace.

Now, by integrating the function $H(t;x,x')$ over t and using the eq. (1.95), the heat kernel (6.121) takes the form

$$U(t;x,x') = (4\pi t)^{-n/2}\mathcal{P}(x,x')\det\left(\frac{\sinh(tC)}{tC}\right)^{-1/2} \times \exp\left\{-\frac{1}{4}\langle (x-x'), gC\coth(tC)(x-x')\rangle\right\}, \tag{6.142}$$

where, as usual, $g = \det g_{ij}$ and $\mathcal{P}(x,x')$ is a function determined from the initial conditions and the transformation properties of the heat kernel. It satisfies the equation

$$(x-x')^j\left(\partial_j - \frac{1}{2}\mathcal{R}_{jm}x^m\right)\mathcal{P}(x,x') = 0 \tag{6.143}$$

and the initial condition

$$\mathcal{P}(x,x) = 1\,. \tag{6.144}$$

Therefore,

$$\mathcal{P}(x,x') = \exp\left(\frac{1}{2}\langle x, \mathcal{R}x'\rangle\right). \tag{6.145}$$

We did not include here the factor $g^{1/2} = (\det g_{ij})^{1/2}$ since we take the heat kernel in the invariant form, not the density form. The formula (6.143) should be compared with eqs. (4.208) and (4.192) obtained by a completely different method.

6.5.3 Harmonic Oscillator

The case of a harmonic oscillator

$$L(x,\partial) = -g^{ij}\partial_i\partial_j + D_{ij}x^ix^j\,, \tag{6.146}$$

where g^{ij} and D_{ij} are constant symmetric positive definite tensors, can be treated similarly. Both these cases are solvable because the operator equations are linear. The Heisenberg equations take the form

$$\frac{d\hat{x}^j}{dt} = -2g^{jk}\hat{p}_k\,, \tag{6.147}$$

$$\frac{d\hat{p}_j}{dt} = -2D_{jk}x^k\,, \tag{6.148}$$

with the initial conditions

$$\hat{x}^i(0) = x^i, \qquad \hat{p}_i(0) = \partial_i\,, \tag{6.149}$$

These equations are linear and can be easily solved. Let $\rho = (\rho^i{}_j)$ be a matrix defined by

$$\rho = 2\sqrt{g^{-1}D}, \tag{6.150}$$

so that the matrix $g\rho$ is symmetric. Then we obtain (in matrix notation)

$$\hat{x}(t) = \cosh(t\rho)x - 2\frac{\sinh(t\rho)}{\rho}g^{-1}\partial\,, \tag{6.151}$$

$$\hat{p}(t) = \frac{1}{2}g\sinh(t\rho)\rho x + g\cosh(t\rho)g^{-1}\partial\,. \tag{6.152}$$

Thus we can express the operators of derivatives in terms of the coordinate operators,

$$\partial = \frac{1}{2}g\frac{\rho}{\sinh(t\rho)}\hat{x}(t) - \frac{1}{2}g\rho\coth(t\rho)x\,. \tag{6.153}$$

Now, the operator L takes the form

$$\begin{aligned} L = &-\frac{1}{4}\left\langle \hat{x}(t), g\frac{\rho^2}{\sinh^2(t\rho)}\hat{x}(t)\right\rangle + \frac{1}{4}\left\langle \hat{x}(t), g\frac{\rho^2\cosh(t\rho)}{\sinh^2(t\rho)}x\right\rangle \\ &+\frac{1}{4}\left\langle x, g\frac{\rho^2\cosh(t\rho)}{\sinh^2(t\rho)}\hat{x}(t)\right\rangle - \frac{1}{4}\left\langle x, g\frac{\rho^2}{\sinh^2(t\rho)}x\right\rangle\,. \end{aligned} \tag{6.154}$$

Finally, we compute the commutator

$$[\hat{x}^j(t), x^k] = -2\left[\frac{\sinh(t\rho)}{\rho}g^{-1}\right]^{jk}\,. \tag{6.155}$$

By using this commutator we can reorder the operators $\hat{x}(t)$ and x in the operator L putting all x to the right and all $\hat{x}(t)$ to the left to obtain

$$\begin{aligned} H(t;x,x') = &-\frac{1}{4}\left\langle x, g\frac{\rho^2}{\sinh^2(t\rho)}x\right\rangle + \frac{1}{2}\left\langle x, g\frac{\rho^2\cosh(t\rho)}{\sinh^2(t\rho)}x'\right\rangle \\ &-\frac{1}{4}\left\langle x', g\frac{\rho^2}{\sinh^2(t\rho)}x'\right\rangle + \frac{1}{2}\,\mathrm{tr}\,[\rho\coth(t\rho)]\,. \end{aligned} \tag{6.156}$$

This can be written in an alternative form

$$H(t;x,x') = \frac{1}{2}\,\mathrm{tr}\,[\rho\coth(t\rho)] + \frac{1}{4}\left\langle x, g\frac{\rho^2}{\cosh^2\left(\frac{t\rho}{2}\right)}x'\right\rangle \qquad (6.157)$$

$$-\frac{1}{4}\left\langle (x-x'), g\frac{\rho^2}{\sinh^2(t\rho)}(x-x')\right\rangle .$$

Now, we compute the integral of $H(t;x,x')$ over t to get

$$S(t;x,x') = \frac{1}{2}\,\mathrm{tr}\,\log\frac{\sinh(t\rho)}{\rho} + \frac{1}{2}\left\langle x, g\rho\tanh\left(\frac{t\rho}{2}\right)x'\right\rangle$$

$$+\frac{1}{4}\left\langle (x-x'), g\rho\coth(t\rho)(x-x')\right\rangle . \qquad (6.158)$$

Finally, we use the eqs. (6.121) and (1.95) to obtain the solution of the heat equation with the correct initial condition

$$U(t;x,x') = (4\pi t)^{-n/2}\det\left[\frac{\sinh(t\rho)}{t\rho}\right]^{-1/2} \qquad (6.159)$$

$$\times\exp\left\{-\frac{1}{2}\left\langle x, g\rho\tanh\left(\frac{t\rho}{2}\right)x'\right\rangle\right\}$$

$$\times\exp\left\{-\frac{1}{4}\left\langle (x-x'), g\rho\coth(t\rho)(x-x')\right\rangle\right\} .$$

We remind the reader once again that this is an invariant heat kernel; that is why it does not contain the factor $g^{1/2} = (\det g_{ij})^{1/2}$. It is instructive to compare this result with the result (4.192) and (4.193) obtained by the method of singular asymptotics considered in Chapter 4.

6.5.4 General Systems with Linear Heisenberg Equations

The quantum operator method can be applied to any differential operator that is quadratic in derivatives and coordinates when the corresponding Heisenberg equations are linear. This is the class of operators considered in Sec. 4.3.6 which have the form

$$L(x,\partial) = -A^{ij}\partial_i\partial_j + (B^i + C^i{}_j x^j)\partial_i + G + E_i x^i + D_{ij}x^i x^j , \qquad (6.160)$$

where the matrices A and D are symmetric and positive. Recall that by a similarity transformation $L \mapsto e^{-\omega}Le^{\omega}$ with a quadratic function ω it is always possible to cancel the vector B and to make the matrix CA antisymmetric (see Sec. 4.3.6). We will assume that this has already been done so that the

operator has the form

$$L(x,\partial) = -A^{ij}\partial_i\partial_j + C^i{}_j x^j \partial_i + G + E_i x^i + D_{ij} x^i x^j \,, \tag{6.161}$$

where the matrix C satisfies

$$C^T = -A^{-1} C A. \tag{6.162}$$

It is easy to see that both problems considered above are obtained as special cases from this operator. In the case,

$$A^{ij} = g^{ij}, \qquad B^i = C^i{}_j = G = E_i = 0, \tag{6.163}$$

it reduces to the harmonic oscillator, and in the case

$$A^{ij} = g^{ij}, \qquad C^i{}_j = g^{ik}\mathcal{R}_{kj}, \qquad D_{ij} = -\frac{1}{4}\mathcal{R}_{ik} g^{km} \mathcal{R}_{jm}, \tag{6.164}$$

$$B^i = G = E^i = 0, \tag{6.165}$$

it reduces to the case of linear connection.

Let us define the vectors $\hat{x} = (\hat{x}^i)$ and $\hat{p} = (\hat{p}_i)$. The the corresponding Heisenberg equations (6.102) and (6.103) have the following matrix form

$$\frac{d\hat{x}}{dt} = C\hat{x} - 2A\hat{p} \,, \tag{6.166}$$

$$\frac{d\hat{p}}{dt} = -E - 2D\hat{x} + A^{-1} C A \hat{p} \,. \tag{6.167}$$

As in Sec. 4.3.6 we will assume for simplicity that the matrices C and AD commute, that is,

$$CAD = ADC. \tag{6.168}$$

Let ρ be a matrix defined by

$$\rho = 2\sqrt{AD} \,. \tag{6.169}$$

Then, of course, the matrices C and ρ commute. Note that in the case of the linear connection (6.164) we have the relation

$$C^2 = \rho^2 \,. \tag{6.170}$$

Thus, we will exclude this possibility and assume that $C^2 \neq \rho^2$. Moreover, we assume that the matrix

$$J = C^2 - \rho^2 \tag{6.171}$$

is invertible. Then the Heisenberg system has a constant solution

$$x_0 = 2J^{-1}AE, \tag{6.172}$$

$$p_0 = A^{-1}CJ^{-1}AE. \tag{6.173}$$

Now, we make the change of variables

$$\hat{x}(t) = x_0 + \hat{y}(t)\,, \tag{6.174}$$

$$\hat{p}(t) = p_0 + A^{-1}\hat{q}(t)\,, \tag{6.175}$$

This kills the linear terms in the operator L, that is,

$$L = -\left\langle \hat{q}, A^{-1}\hat{q}\right\rangle + \left\langle \hat{q}, A^{-1}Cy\right\rangle + \frac{1}{4}\left\langle y, A^{-1}\rho^2 y\right\rangle + L_0\,, \tag{6.176}$$

where $\hat{q} = \hat{q}(0) = A(\partial - p_0)$, $y = x - x_0$ and

$$L_0 = G + \left\langle E, A^{-1}J^{-1}AE\right\rangle\,. \tag{6.177}$$

We note that this Heisenberg system is the same system as the Hamiltonian system (4.143), (4.144) with the only change $p \mapsto -p$. Since it is linear the operators can be treated just as real variables. Therefore, we can solve this system by the same method as in Sec. 4.3.6. The solution with the initial conditions $\hat{x}(0) = x$ and $\hat{p}(0) = \partial$ is given by (see eqs. (4.168), (4.169))

$$\hat{y}(t) = e^{tC}\cosh(t\rho)y - 2e^{tC}\frac{\sinh\,(t\rho)}{\rho}\hat{q}\,, \tag{6.178}$$

$$\hat{q}(t) = -\frac{1}{2}e^{tC}\rho\sinh\,(t\rho)\,y + e^{tC}\cosh(t\rho)\hat{q}\,, \tag{6.179}$$

where $y = x - x_0$ and $\hat{q} = \hat{q}(0) = A(\partial - p_0)$. This allows one to compute the initial value of the momentum $\hat{q}$ in terms of the coordinate operators

$$\hat{q} = -e^{-tC}\frac{\rho}{2\sinh(t\rho)}\hat{y}(t) + \frac{1}{2}\rho\coth(t\rho)y\,, \tag{6.180}$$

Now, the operator L takes the form

$$\begin{aligned} L = &-\frac{1}{4}\left\langle \hat{y}(t), A^{-1}\frac{\rho^2}{\sinh^2(t\rho)}\hat{y}(t)\right\rangle - \frac{1}{4}\left\langle y, A^{-1}\frac{\rho^2}{\sinh^2(t\rho)}y\right\rangle \\ &+\frac{1}{4}\left\langle \hat{y}(t), A^{-1}e^{tC}\left[\rho^2\frac{\cosh(t\rho)}{\sinh^2(t\rho)} - 2C\frac{\rho}{\sinh(t\rho)}\right]y\right\rangle \\ &+\frac{1}{4}\left\langle y, A^{-1}e^{-tC}\rho^2\frac{\cosh(t\rho)}{\sinh^2(t\rho)}\hat{y}(t)\right\rangle + L_0\,. \end{aligned} \tag{6.181}$$

Next, by using the commutator

$$[\hat{y}^j(t), y^k] = -2\left[e^{tC}\frac{\sinh(t\rho)}{\rho}A\right]^{jk} \tag{6.182}$$

we can reorder the operators $\hat{y}(t)$ and y to put all operators $\hat{y}(t)$ to the left of all y to obtain the function $H(t;x,x')$

$$\begin{aligned} H(t;x,x') = &-\frac{1}{4}\left\langle y, A^{-1}\frac{\rho^2}{\sinh^2(t\rho)}y\right\rangle - \frac{1}{4}\left\langle y', A^{-1}\frac{\rho^2}{\sinh^2(t\rho)}y'\right\rangle \\ &+\frac{1}{2}\left\langle y, A^{-1}\left[e^{tC}\rho^2\frac{\cosh(t\rho)}{\sinh^2(t\rho)} - Ce^{tC}\frac{\rho}{\sinh(t\rho)}\right]y'\right\rangle \\ &+\frac{1}{2}\,\mathrm{tr}\,[\rho\coth(t\rho)] + L_0\,, \end{aligned} \tag{6.183}$$

where $y = x - x_0$ and $y' = x' - x_0$. This can be written in an alternative form

$$\begin{aligned} H(t;x,x') = &-\frac{1}{4}\left\langle (y-y'), A^{-1}\frac{\rho^2}{\sinh^2(t\rho)}(y-y')\right\rangle \\ &+\frac{1}{2}\left\langle y, A^{-1}\left[-\frac{\rho^2}{\sinh^2(t\rho)} + e^{tC}\rho^2\frac{\cosh(t\rho)}{\sinh^2(t\rho)} - Ce^{tC}\frac{\rho}{\sinh(t\rho)}\right]y'\right\rangle \\ &+\frac{1}{2}\,\mathrm{tr}\,[\rho\coth(t\rho)] + L_0\,. \end{aligned} \tag{6.184}$$

Now, we compute the integral of the function $H(t;x,x')$ over t to get

$$S(t;x,x') = \tilde{S}(t;x,x') + \frac{1}{2}\,\mathrm{tr}\,\log\frac{\sinh(t\rho)}{\rho} + tL_0\,, \tag{6.185}$$

where

$$\begin{aligned} \tilde{S}(t;x,x') = &\frac{1}{4}\left\langle (x-x'), A^{-1}\rho\coth(t\rho)(x-x')\right\rangle \\ &+\frac{1}{2}\left\langle (x-x_0), A^{-1}\left[\rho\coth(t\rho) - e^{tC}\frac{\rho}{\sinh(t\rho)}\right](x'-x_0)\right\rangle\,. \end{aligned} \tag{6.186}$$

Here we used the fact that $y = x - x_0$ and $y' = x' - x_0$. Finally, we use eqs. (6.121) and (1.95) to obtain the heat kernel

$$\begin{aligned} U(t;x,x') = &(4\pi t)^{-n/2}\mathcal{P}(x,x')\det\left(\frac{\sinh(t\rho)}{t\rho}\right)^{-1/2} e^{-tL_0} \\ &\times\exp\left\{-\tilde{S}(t;x,x')\right\}\,, \end{aligned} \tag{6.187}$$

where

$$\mathcal{P}(x,x') = \exp\left(\frac{1}{2}\left\langle x, A^{-1}Cx'\right\rangle\right). \tag{6.188}$$

The formula (6.187) should be compared with eqs. (4.184) and (4.192) obtained by a completely different method. The only difference is the absence of the factor $g^{1/2} = (\det A)^{-1/2}$ since we took the heat kernel in the invariant form here, not the density form.

It is instructive to compare these results with the method of singular perturbations applied to operators with quadratic Hamiltonians considered in Sec. 4.3.6. Notice that while the method of singular perturbations gives only an asymptotic expansion, the quantum operator, when it is solvable, gives the exact heat kernel.

6.6 Algebraic Methods

The long-wave approximation corresponds to slowly changing background fields. In the zero order of this approximation the fields are assumed to be just covariantly constant. It is worth stressing here the point that it is the *covariantly constant* background and not just constant background that should be considered. The condition that a tensor is covariantly constant is diffeomorphism invariant, it does not depend on the local coordinate system. If we just assume that say the metric is constant then it just means that the curvature is zero and the manifold is flat. This is a very restrictive condition. What we have instead is an idea of *covariantly constant curvature* (and the potential term), which is not necessarily zero but rather can be arbitrarily large. An example of such situation is the sphere S^n or a hyperbolic space H^n. Thus, in this section we consider only the covariantly constant background (and slight modifications thereof).

There exist a very elegant indirect possibility to construct the heat kernel without solving the heat equation but using only the commutation relations of some first order differential operators. The main idea is in a generalization of the usual Fourier transform to the case of operators and consists in the following. Let us consider a second-order partial differential operator of Laplace type,

$$\begin{aligned} L &= -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q \\ &= |g|^{-1/2}(\partial_i + \mathcal{A}_i)|g|^{1/2}g^{ij}(\partial_j + \mathcal{A}_j) + Q\,, \end{aligned} \tag{6.189}$$

where $\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i$, ∇_i are the covariant derivatives, g_{ij} is a Riemannian metric, $\mathcal{A}_i$ is a connection and Q is a potential function. We denote the determinant of the metric here by

$$|g| = \det g_{ij} \tag{6.190}$$

to avoid confusion with the matrix $g = (g_{ij})$. The heat kernel of the operator L is defined as usual by

$$U(t; x, x') = \exp(-tL)\delta(x, x')\,, \tag{6.191}$$

where

$$\delta(x, x') = \mathcal{P}(x, x')|g|^{-1/2}(x)\delta(x - x'), \tag{6.192}$$

where $\mathcal{P}(x, x')$ is the generalized operator of parallel transport defined by (3.311). The factors $g^{-1/2}$ and $\mathcal{P}$ are introduced to maintain the transformation properties of the heat kernel. Now, the idea is to express the heat semigroup of a second-order differential operator L in terms of the heat semigroup of some *first-order* differential operators. It turns out that it is much easier to compute the action of the exponential of a first-order operator than the action of the exponential of a second-order operator.

To illustrate this idea let us consider for a moment a trivial case of vanishing curvature, $R^i{}_{jkl} = \mathcal{R}_{ij} = 0$, and constant potential term $Q = \text{const}$ in $\mathbb{R}^n$; in this case $\mathcal{A}_i = 0$ and $\mathcal{P} = 1$. In this case (in a particular coordinate system) the operators of covariant derivatives are just partial derivatives, $\nabla_i = \partial_i$; they obviously commute and form together with the potential term and the metric an Abelian algebra

$$[\nabla_i, \nabla_j] = 0, \qquad [\nabla_i, Q] = 0\,, \qquad [\nabla_i, g_{jk}] = 0\,. \tag{6.193}$$

As a result, the operators ∇_i can be treated as usual commuting variables. Therefore, by using (1.25) one can easily compute the standard Gaussian integral

$$\int\limits_{\mathbb{R}^n} dk\, \exp\left(-\frac{1}{4t}\,\langle k, gk\rangle\right) \exp\langle k, \nabla\rangle = (4\pi t)^{n/2}|g|^{-1/2} \exp\left(-t\left\langle \nabla, g^{-1}\nabla\right\rangle\right), \tag{6.194}$$

where $\langle k, \nabla\rangle = k^i\nabla_i$ and $\left\langle \nabla, g^{-1}\nabla\right\rangle = g^{ij}\nabla_i\nabla_j$. Here, as usual, $g = (g_{ij})$ and $g^{-1} = (g^{ij})$ are the matrices formed from the metric and its inverse.

This equation can be used to express the heat-semigroup of the operator L in form of a Gaussian integral

$$\exp(-tL) = (4\pi t)^{-n/2} \exp(-tQ) \int\limits_{\mathbb{R}^n} dk\, |g|^{1/2} \exp\left(-\frac{1}{4t}\,\langle k, gk\rangle\right) \exp\langle k, \nabla\rangle\,. \tag{6.195}$$

Acting with this operator on the delta-function $\delta(x, x') = |g|^{-1/2}\delta(x - x')$ and using the obvious relation

$$\exp\langle k, \nabla\rangle\, \delta(x, x') = |g|^{-1/2}\delta(x - x' + k) \tag{6.196}$$

one can simply integrate over k to obtain the heat kernel in coordinate representation

$$U(t;x,x') = (4\pi t)^{-n/2} \exp\left[-\frac{1}{4t}\,\langle (x-x'), g(x-x')\rangle - tQ\right]. \qquad (6.197)$$

For non-Euclidean flat manifolds, say a torus T^n, one needs to add a corresponding summation over a lattice to make the heat kernel periodic. The heat kernel diagonal is obtained by taking the coincidence limit $x \to x'$

$$[U(t)] = (4\pi t)^{-n/2} \exp\left(-tQ\right). \qquad (6.198)$$

Of course, for non-zero curvature the covariant differential operators $\nabla_i^{\mathcal{A}}$ do not commute and the commutators of them are proportional to the curvatures, the Riemann curvature R_{ijkl}, and the curvature $\mathcal{R}_{ij}$ of the connection $\mathcal{A}_i$, that we collectively denote by $\Re$ defined by (6.2). The commutators of covariant derivatives with the curvatures give the first derivatives of the curvatures, i.e. the jets $\Re_{(1)}$ defined by (6.3), the commutators of covariant derivatives with $\Re_{(1)}$ give the second jets $\Re_{(2)}$ etc.

$$\begin{aligned} [\nabla^{\mathcal{A}}, \nabla^{\mathcal{A}}] &= \Re, \\ [\nabla^{\mathcal{A}}, \Re] &= \Re_{(1)}, \\ &\cdots \\ [\nabla^{\mathcal{A}}, \Re_{(i)}] &= \Re_{(i+1)}, \\ &\cdots \end{aligned} \qquad (6.199)$$

For scalar operators the commutators of jets with themselves vanish

$$[\Re_{(i)}, \Re_{(k)}] = 0\,. \qquad (6.200)$$

Thus the operators of covariant derivatives, $\nabla^{\mathcal{A}}$, together with the whole set of all jets form an *infinite dimensional* Lie algebra $\{\nabla^{\mathcal{A}}, \Re_{(i)}\}$. In the long-wave approximation the derivatives of the fields are small. Therefore, the higher the order of a jet the smaller it is. Thus, one can take into account a *finite* number of low-order jets, i.e. the low-order covariant derivatives of the background fields, and neglect all the higher order jets, i.e. the covariant derivatives of higher orders. Then one can show that there exist a set of covariant differential operators that together with the background fields and their low-order derivatives generate a *finite dimensional* Lie algebra. This procedure is very similar to the polynomial approximation of functions of real variables. The difference is that we are dealing, in general, with the *covariant* derivatives and the curvatures.

Thus one can try to generalize the above idea in such a way that (6.195) would be the zeroth order approximation in the commutators of the covariant derivatives, i.e. in the curvatures. Roughly speaking, we would like to find a representation of the heat semi-group in the form

$$\exp(-tL) = \int dk\, \Psi(t,k) \exp\left\{-\frac{1}{4t}\,\langle k, \Phi(t) k\rangle\right\} \exp\langle k, \xi\rangle\,, \tag{6.201}$$

where $k = (k^A)$, $\xi = (\xi_A) = (X_a, Y_\mu)$, $X_a = X_a{}^i \nabla_i$ are some first order differential operators and Y_μ are some functions. Here $a = 1, \ldots, p$, $i = 1, \ldots, n$, $\mu = 1, \ldots, q$ and $A, B = 1, \ldots, N$ with $N = p + q$. The functions $\Phi(t)$ and $\Psi(t,k)$ are expressed in terms of the commutators of these operators, i.e. in terms of the curvatures.

In general, the operators ξ_A do not form a closed finite dimensional Lie algebra because at each stage taking more commutators there appear more and more derivatives of the curvatures. If one restricts oneself to the low-order jets of some fixed order, this algebra closes and becomes finite dimensional.

Using this representation one could, as above, act with $\exp\langle k, \xi\rangle$ on the delta-function to get the heat kernel. The main point of this idea is that it is much easier to calculate the action of the exponential of the *first-order* operator $\langle k, \xi\rangle$ on the delta-function than that of the exponential of the second order operator L.

6.6.1 Linear Connection in Flat Space

In this section we follow our paper [6]. We consider a slightly more complicated case of a Euclidean space $\mathbb{R}^n$ when the metric g_{ij} is still flat, that is, $R^i{}_{jkl} = 0$, but the covariant derivatives $\nabla_j^{\mathcal{A}}$ have a linear connection, which simply means that

$$\nabla_j^{\mathcal{A}} = \partial_j + \mathcal{A}_j\,, \tag{6.202}$$

where

$$\mathcal{A}_j = -\frac{1}{2}\mathcal{R}_{jk} x^k\,, \tag{6.203}$$

with $\mathcal{R}_{jk}$ being a *constant* tensor. That is, we consider an operator L that acts on scalar functions in $\mathbb{R}^n$ of the form

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q\,, \tag{6.204}$$

with the Euclidean metric and the covariant derivatives defined above. First, we consider the case of *constant potential term* Q. In this case the covariant derivatives form a *nilpotent* Lie algebra

$$[\nabla_j^{\mathcal{A}}, \nabla_k^{\mathcal{A}}] = \mathcal{R}_{jk}, \tag{6.205}$$

$$[\nabla_j^{\mathcal{A}}, \mathcal{R}_{kl}] = [\nabla_j^{\mathcal{A}}, Q] = [\nabla_j^{\mathcal{A}}, g_{kl}] = 0. \tag{6.206}$$

For this algebra one can prove a theorem expressing the heat semi-group in terms of an average over some Lie group [6]

$$\exp(-tL) = (4\pi t)^{-n/2} \det\left(\frac{\sinh(tC)}{tC}\right)^{-1/2} \exp(-tQ) \tag{6.207}$$
$$\times \int_{\mathbb{R}^n} dk \exp\left\{-\frac{1}{4t}\langle k, gtC\coth(tC)k\rangle\right\} \exp\langle k, \nabla^{\mathcal{A}}\rangle ,$$

where C denotes the matrix $C = (C^i{}_j)$ with $C^i{}_j = g^{ik}\mathcal{R}_{kj}$ and $g = (g_{ij})$.

This equation can be proved by checking directly that the integral on the right-hand side satisfies the heat equation and the correct initial condition. Indeed, let $\Phi(t)$ be the right-hand side of the eq. (6.207). Then by rescaling the integration variable $k \mapsto \sqrt{t}k$ and taking the limit $t \to 0$ we get

$$\Phi(0) = I . \tag{6.208}$$

Further, we need to compute the derivative of $\Phi(t)$ with respect to t. By using the formula for the derivative of the determinant (1.101) we compute

$$\partial_t \det\left(\frac{\sinh(tC)}{tC}\right)^{-1/2} = \frac{1}{2t}\{n - \operatorname{tr}[tC\coth(tC)]\} \det\left(\frac{\sinh(tC)}{tC}\right)^{-1/2} . \tag{6.209}$$

Therefore,

$$(\partial_t + L)\Phi(t) = (4\pi t)^{-n/2} \det\left(\frac{tC}{\sinh(tC)}\right)^{1/2} \exp(-tQ) \tag{6.210}$$
$$\times \int_{\mathbb{R}^n} dk \exp\left\{-\frac{1}{4t}\langle k, gtC\coth(tC)k\rangle\right\}$$
$$\times \left\{-g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} - \frac{1}{2}\operatorname{tr} C\coth(tC) + \frac{1}{4}\left\langle k, g\frac{C^2}{\sinh^2(tC)}k\right\rangle\right\} \exp\langle k, \nabla^{\mathcal{A}}\rangle ,$$

Further, one can show that

$$\frac{\partial}{\partial k^i} \exp\langle k, \nabla^{\mathcal{A}}\rangle = \left(\nabla_i^{\mathcal{A}} - \frac{1}{2}\mathcal{R}_{im}k^m\right) \exp\langle k, \nabla^{\mathcal{A}}\rangle . \tag{6.211}$$

Therefore,

$$\nabla_i^{\mathcal{A}} \exp\langle k, \nabla^{\mathcal{A}}\rangle = \left(\frac{\partial}{\partial k^i} + \frac{1}{2}\mathcal{R}_{im}k^m\right) \exp\langle k, \nabla^{\mathcal{A}}\rangle \tag{6.212}$$

and

$$g^{ij}\nabla_j^{\mathcal{A}}\nabla_i^{\mathcal{A}} \exp\langle k, \nabla^{\mathcal{A}}\rangle \tag{6.213}$$
$$= g^{ij}\left(\frac{\partial}{\partial k^i} + \frac{1}{2}\mathcal{R}_{im}k^m\right)\left(\frac{\partial}{\partial k^j} + \frac{1}{2}\mathcal{R}_{jl}k^l\right) \exp\langle k, \nabla^{\mathcal{A}}\rangle .$$

Next, by using this equation we can integrate over k^i by parts twice to obtain

$$\int\limits_{\mathbb{R}^n} dk \exp\left\{-\frac{1}{4t}\left\langle k, gtC\coth(tC)k\right\rangle\right\} g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} \exp\left\langle k, \nabla^{\mathcal{A}}\right\rangle$$
$$= \int\limits_{\mathbb{R}^n} dk \exp\left\{-\frac{1}{4t}\left\langle k, gtC\coth(tC)k\right\rangle\right\} \exp\left\langle k, \nabla^{\mathcal{A}}\right\rangle$$
$$\times\left\{-\frac{1}{2}\operatorname{tr} C\coth(tC) + \frac{1}{4}\left\langle k, g\frac{C^2}{\sinh^2(tC)}k\right\rangle\right\}. \tag{6.214}$$

Finally, by substituting this equation in (6.210) we see that $\Phi(t)$ satisfies the heat equation

$$(\partial_t + L)\Phi(t) = 0 \tag{6.215}$$

and, therefore, $\Phi(t) = \exp(-tL)$. This proves the equation (6.207).

Further, one can show that

$$\exp\left\langle k, \nabla^{\mathcal{A}}\right\rangle \delta(x, x') = \mathcal{P}(x, x')\delta(x - x' + k), \tag{6.216}$$

where the function $\mathcal{P}(x, x')$ is defined by (6.145). Subsequently, the integral over k^j becomes trivial and we immediately obtain the heat kernel

$$U(t; x, x') = (4\pi t)^{-n/2}\det\left(\frac{tC}{\sinh(tC)}\right)^{1/2}\exp(-tQ) \tag{6.217}$$
$$\times\mathcal{P}(x, x')\exp\left\{-\frac{1}{4t}\left\langle (x - x'), gtC\coth(tC)(x - x')\right\rangle\right\}.$$

Of course, this is the same result that was obtained before by the operator method. Expanding it in a power series in t one can find *all* heat kernel coefficients b_k.

As we have seen the contribution of the matrix $\mathcal{R}$ is not as trivial as that of the potential term. However, the algebraic approach does work in this case too. It is a good example of how one can get the heat kernel without solving any differential equations but using only the algebraic properties of the covariant derivatives.

6.6.2 Linear Connection with Quadratic Potential

In this section we follow our paper [7]. We consider the operator

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q \tag{6.218}$$

where $\nabla_i^{\mathcal{A}} = \partial_i + \mathcal{A}_i$, the connection $\mathcal{A}_i$ is a linear function

$$\mathcal{A}_i = -\frac{1}{2}\mathcal{R}_{ij}x^j\,, \tag{6.219}$$

and the potential Q is a quadratic function. To parametrize the potential function we introduce some linear functions

$$L_\mu = E_{i\mu}x^i + K_\mu\,, \tag{6.220}$$

where $\mu = 1, \ldots, p$. Here Greek indices range over $(\mu = 1, \ldots, p)$, with some $p \leq n$. Then the potential has the form

$$Q = M - \beta^{\mu\nu}L_\mu L_\nu\,, \tag{6.221}$$

where M is a constant and $\beta^{\mu\nu}$ is a constant symmetric non-degenerate $p \times p$ matrix. The derivatives of the potential are

$$\nabla_i Q = -2\beta^{\mu\nu}E_{i\mu}L_\nu, \tag{6.222}$$

$$\nabla_i\nabla_j Q = Q_{;ij} = -2\beta^{\mu\nu}E_{i\mu}E_{j\nu}\,. \tag{6.223}$$

Thus we have a nilpotent Lie algebra $\{\nabla_j^{\mathcal{A}}, \mathcal{R}_{jk}, Q, Q_{;j}, Q_{;jk}\}$ whose non-zero commutators are

$$[\nabla_j^{\mathcal{A}}, \nabla_k^{\mathcal{A}}] = \mathcal{R}_{jk}, \tag{6.224}$$

$$[\nabla_i^{\mathcal{A}}, Q] = Q_{;i}, \tag{6.225}$$

$$[\nabla_i^{\mathcal{A}}, Q_{;j}] = Q_{;ij}, \tag{6.226}$$

where $Q_{;i} = \nabla_i Q$.

Notice that the double commutators of the functions L_μ with the derivatives vanish,

$$[\nabla_i^{\mathcal{A}}, [\nabla_j^{\mathcal{A}}, L_\mu]] = 0\,. \tag{6.227}$$

This defines another nilpotent Lie algebra, $\{\nabla_i^{\mathcal{A}}, \mathcal{R}_{ij}, M, L_\mu, L_{\mu;j}\}$, with the following nontrivial commutators

$$[\nabla_i^{\mathcal{A}}, \nabla_j^{\mathcal{A}}] = \mathcal{R}_{ij}, \tag{6.228}$$

$$[\nabla_i^{\mathcal{A}}, L_\mu] = E_{i\mu}\,. \tag{6.229}$$

Now, let us introduce the generators $(\xi_A) = (\nabla_i^{\mathcal{A}}, L_\mu)$, where the capital Latin indices range over $(A = 1, \ldots, N)$, with $N = n+p$. Then we can rewrite the above commutation relations in a more compact form

$$[\xi_A, \xi_B] = \mathcal{F}_{AB}, \tag{6.230}$$

$$[\xi_A, \mathcal{F}_{CD}] = 0, \tag{6.231}$$

where $\mathcal{F} = (\mathcal{F}_{AB})$ is a $N \times N$ matrix defined by

$$(\mathcal{F}_{AB}) = \begin{pmatrix} \mathcal{R}_{kj} & E_{k\mu} \\ -E^T_{\mu j} & 0 \end{pmatrix} . \tag{6.232}$$

The operator L can now be written in the form

$$L = -\gamma^{AB}\xi_A\xi_B + M, \tag{6.233}$$

where

$$(\gamma^{AB}) = \begin{pmatrix} g^{jk} & 0 \\ 0 & \beta^{\mu\nu} \end{pmatrix}. \tag{6.234}$$

The matrices $\beta^{\mu\nu}$ and γ^{AB} (and their inverses $\beta_{\mu\nu}$ and γ_{AB}) play the role of metrics and can be used to raise and to lower the Greek indices and the capital Latin indices respectively. We will denote these matrices by $\beta = (\beta_{\mu\nu})$ and $\gamma = (\gamma_{AB})$.

Note that the Lie algebra (6.230) is a nilpotent algebra of the same type as (6.205). As was shown in the previous section for algebras of this kind the heat semi-group is given by the integral over the corresponding Lie group [6]

$$\begin{aligned} \exp(-tL) = (4\pi t)^{-N/2} \det \left(\frac{\sinh(t\tilde{\mathcal{F}})}{t\tilde{\mathcal{F}}} \right)^{-1/2} \exp(-tM) \\ \times \int\limits_{\mathbb{R}^N} dk\ |\gamma|^{1/2} \exp\left\{ -\frac{1}{4t} \left\langle k, t\gamma\tilde{\mathcal{F}} \coth(t\tilde{\mathcal{F}})k \right\rangle \right\} \exp\langle k, \xi\rangle\ , \end{aligned} \tag{6.235}$$

where $\tilde{\mathcal{F}} = \gamma^{-1}\mathcal{F}$, $|\gamma| = |g|\ |\beta|$, $|g| = \det g_{ij}$, $|\beta| = \det \beta_{\mu\nu}$ and $\langle k, \xi\rangle = k^A\xi_A$. Thus we have expressed the heat semi-group in terms of the operator $\exp\langle k, \xi\rangle$.

Now, we need to compute analytic functions of the matrix $\tilde{\mathcal{F}}$. We have

$$\tilde{\mathcal{F}} = \begin{pmatrix} C & \tilde{E} \\ -\bar{E} & 0 \end{pmatrix}, \tag{6.236}$$

where $C = g^{-1}\mathcal{R}$ is the $n \times n$ matrix defined by $C^i{}_j = g^{ik}\mathcal{R}_{kj}$, $\tilde{E} = g^{-1}E$ is a $n \times p$ matrix and $\bar{E} = \beta^{-1}E^T$ is a $p \times n$ matrix defined by

$$\tilde{E}^i{}_\mu = g^{ij}E_{j\mu}, \qquad \bar{E}^\mu{}_j = \beta^{\mu\nu}E_{j\mu}\,. \tag{6.237}$$

First, we compute the powers of the matrix $\tilde{\mathcal{F}}$, [7]

$$\left(\tilde{\mathcal{F}}\right)^k = \begin{pmatrix} J_k & J_{k-1}\tilde{E} \\ -\bar{E}J_{k-1} & -\bar{E}J_{k-2}\tilde{E} \end{pmatrix}, \tag{6.238}$$

where J_k are $n \times n$ matrices defined by the recursion

$$J_{k+1} = CJ_k + PJ_{k-1}, \tag{6.239}$$

where $P = (P^i{}_j) = -\tilde{E}\bar{E}$ is the matrix defined by the second derivatives of the potential

$$P^i{}_j = \frac{1}{2} g^{ik} \nabla_k \nabla_j Q\,, \tag{6.240}$$

with the initial conditions

$$J_{-1} = 0, \qquad J_0 = I\,. \tag{6.241}$$

It should be clear that the matrices J_k are polynomials in two noncommuting variables C and P. These polynomials can be calculated in terms of a generating function

$$G(z) = [I - zC - z^2 P]^{-1} = \sum_{k=0}^{\infty} z^k J_k\,, \tag{6.242}$$

via a contour integral

$$J_k = \frac{1}{2\pi i} \oint_C dz z^{-k-1} G(z)\,, \tag{6.243}$$

where C is a sufficiently small circle oriented counterclockwise so that $G(z)$ is analytic inside the circle.

By using these properties we can compute [7]

$$\frac{\sinh(t\tilde{\mathcal{F}})}{t\tilde{\mathcal{F}}} = \begin{pmatrix} K(t) & tS(t)\tilde{E} \\ -t\bar{E}S(t) & \left[I - t^2 \bar{E} N(t) \tilde{E}\right] \end{pmatrix}, \tag{6.244}$$

where

$$K(t) = \oint_C \frac{dz}{2\pi i} \frac{1}{z^2} \sinh(z^{-1}) G(tz), \tag{6.245}$$

$$S(t) = \oint_C \frac{dz}{2\pi i} \frac{1}{z} \sinh(z^{-1}) G(tz), \tag{6.246}$$

$$N(t) = \oint_C \frac{dz}{2\pi i} \sinh(z^{-1}) G(tz). \tag{6.247}$$

This enables us to compute the determinant [7]

$$\begin{aligned} \det\left(\frac{\sinh(t\tilde{\mathcal{F}})}{t\tilde{\mathcal{F}}}\right) = {} & \det\left[I + t^2 N(t) P\right] \\ & \times \det\left[K(t) - t^2 S(t) P (I + t^2 N(t) P)^{-1} S(t)\right]\,. \end{aligned} \tag{6.248}$$

Now, we split the integration variables $(k^A) = (q^i, \omega^\mu)$ and use the Campbell-Hausdorff formula to single out the non-commutative part,

$$\exp\langle k, \xi\rangle = \exp\left(q^i \nabla_i^{\mathcal{A}} + \omega^\mu L_\mu\right) = \exp\left[\langle \omega, L\rangle + \frac{1}{2}\langle q, E\omega\rangle\right] \exp\left\langle q, \nabla^{\mathcal{A}}\right\rangle . \tag{6.249}$$

Next, we compute the matrix

$$t\tilde{\mathcal{F}} \coth\left(t\tilde{\mathcal{F}}\right) = \begin{pmatrix} B(t) & tA(t)\tilde{E} \\ -t\bar{E}A(t) & \left[I - t^2\bar{E}N(t)\tilde{E}\right] \end{pmatrix}, \tag{6.250}$$

where

$$B(t) = \oint_C \frac{dz}{2\pi i}\frac{1}{z^2}\coth\left(z^{-1}\right)G(tz), \tag{6.251}$$

$$A(t) = \oint_C \frac{dz}{2\pi i}\frac{1}{z}\coth\left(z^{-1}\right)G(tz), \tag{6.252}$$

$$R(t) = \oint_C \frac{dz}{2\pi i}\coth\left(z^{-1}\right)G(tz). \tag{6.253}$$

Then the integral over ω^μ is Gaussian and can be easily computed. After some long but straightforward calculation (for details, see [7]) we obtain the heat semi-group

$$\begin{aligned}\exp(-tL) = {} & (4\pi t)^{-n/2}\left[\Phi(t)\right]^{-1/2}\exp\left\{-tQ + \frac{1}{4}t^3\left\langle \nabla Q, \Psi(t)g^{-1}\nabla Q\right\rangle\right\} \\ & \times \int_{\mathbb{R}^n} dq\, \exp\left\{-\frac{1}{4t}\langle q, gD(t)q\rangle - \frac{t}{2}\left\langle \nabla Q, \left[I + A(t)\right]q\right\rangle\right\}\exp\left\langle q, \nabla^{\mathcal{A}}\right\rangle,\end{aligned} \tag{6.254}$$

where $\Phi(t)$ is a scalar function defined by

$$\begin{aligned}\Phi(t) = {} & \det\left[I + t^2 N(t)P\right]\det\left[I + t^2 R(t)P\right] \\ & \times \det\left\{K(t) - t^2 S(t)P[I + t^2 N(t)P]^{-1}S(t)\right\},\end{aligned} \tag{6.255}$$

and $D(t)$ and $\Psi(t)$ are matrix-valued functions defined by

$$D(t) = B(t) + t^2[I - A(t)]P[I + t^2 R(t)P]^{-1}[I + A(t)], \tag{6.256}$$

$$\Psi(t) = [I + t^2 R(t)P]^{-1}R(t)\,. \tag{6.257}$$

We corrected here a misprint in the formulas defining the functions $A(t), R(t)$, $S(t)$ and $N(t)$ in [7].

To obtain the heat kernel in coordinate representation we have just to act with the heat semi-group $\exp(-tL)$, on the coordinate delta-function. By using eq. (6.216) the integration over q in (6.254) becomes trivial and we obtain the heat kernel

$$U(t;x,x') = (4\pi t)^{-n/2}\mathcal{P}(x,x')\left[\Phi(t)\right]^{-1/2}\exp\left[-tQ(x)\right]$$
$$\times\exp\left\{\frac{1}{4}t^3\left\langle\nabla Q(x),\Psi(t)g^{-1}\nabla Q(x)\right\rangle+\frac{t}{2}\left\langle\nabla Q(x),[I+A(t)](x-x')\right\rangle\right\}$$
$$\times\exp\left\{-\frac{1}{4t}\left\langle(x-x'),gD(t)(x-x')\right\rangle\right\}. \tag{6.258}$$

Expanding this expression in a power series in $(x-x')$ one can easily get *all* off-diagonal heat kernel coefficients.

Recall that we considered a similar problem but by a different method in earlier section. In particular, the eq. (6.187) was obtained under an additional assumption that the matrices $C = g^{-1}\mathcal{R}$ and P commute, i.e.

$$C^i{}_jP^j{}_k = P^i{}_jC^j{}_k\,. \tag{6.259}$$

Thus, one should be able to obtain eq. (6.187) from the more general result (6.258) of this section. In the case when the matrices C and P commute the generating function $G(z)$ is simply

$$G(z) = \frac{1}{\rho}\left(\frac{G_+}{I-zG_+}-\frac{G_-}{I-zG_-}\right), \tag{6.260}$$

where

$$G_\pm = \frac{1}{2}\left(C\pm\rho\right) \tag{6.261}$$

and

$$\rho = \left(4P+C^2\right)^{1/2}. \tag{6.262}$$

Therefore, the polynomials J_k are given by simple formulas

$$J_k = \frac{1}{\rho}\left(G_+^{k+1}-G_-^{k+1}\right). \tag{6.263}$$

and, consequently, the formulas for the functions A, B, R, K, S, N simplify significantly

$$B(t) = \frac{t}{\rho}\left(G_+^2 \coth(tG_+) - G_-^2 \coth(tG_-)\right), \tag{6.264}$$

$$A(t) = \frac{1}{\rho}\left(G_+ \coth(tG_+) - G_- \coth(tG_-)\right), \tag{6.265}$$

$$R(t) = \frac{1}{t\rho}\left(\coth(tG_+) - \coth(tG_-)\right), \tag{6.266}$$

$$K(t) = \frac{1}{t\rho}\left(\sinh(tG_+) - \sinh(tG_-)\right), \tag{6.267}$$

$$S(t) = \frac{1}{t^2\rho}\left(\frac{\sinh(tG_+)}{G_+} - \frac{\sinh(tG_-)}{G_+}\right), \tag{6.268}$$

$$N(t) = \frac{1}{t^3\rho}\left(\frac{\sinh(tG_+)}{G_+^2} - \frac{\sinh(tG_-)}{G_-^2}\right). \tag{6.269}$$

One can show that in this special case the function $\Phi(t)$ and the matrix $\Psi(t)$ read

$$\Phi(t) = \det\left(\frac{\sinh(t\rho)}{t\rho}\right), \tag{6.270}$$

$$\Psi(t) = \frac{1}{t^2 P}\left(\frac{\rho}{\sinh(t\rho)}\frac{\cosh(tC) - \cosh(t\rho)}{2tP} + I\right). \tag{6.271}$$

If the second derivatives of the potential vanish, $\frac{1}{2}\nabla_i\nabla_j Q = 0$, then these functions simplifies even further

$$\Phi(t) = \det\left(\frac{\sinh(tC)}{tC}\right), \tag{6.272}$$

$$\Psi(t) = \frac{tC\coth(tC) - I}{t^2C^2}. \tag{6.273}$$

In the case when the curvature vanishes, $\mathcal{R}_{ij} = 0$, these functions have the form

$$\Phi(t) = \det\left(\frac{\sinh\left(2t\sqrt{P}\right)}{2t\sqrt{P}}\right), \tag{6.274}$$

$$\Psi(t) = \frac{t\sqrt{P} - \tanh\left(t\sqrt{P}\right)}{t^3 P^{3/2}}. \tag{6.275}$$

This is the case of a harmonic oscillator (with a quadratic potential).

The heat kernel diagonal has a very simple form

$$[U(t)] = (4\pi t)^{-n/2} [\Phi(t)]^{-1/2} \exp\left\{-tQ + \frac{1}{4}t^3 \left\langle \nabla Q, \Psi(t) g^{-1} \nabla Q \right\rangle\right\}. \quad (6.276)$$

This formula exhibits the general structure of the heat kernel diagonal. Namely, one sees immediately how the potential term and its first derivatives enter the result. The complete nontrivial information is contained only in a scalar, $\Phi(t)$, and a tensor, $\Psi_{ij}(t)$, which are constructed purely from the curvature tensor $\mathcal{R}_{ij}$ and the second derivatives of the potential term, $P_{ij} = \frac{1}{2}\nabla_i \nabla_j Q$.

6.7 Heat Kernel on Semi-Simple Lie Groups

As was discussed in Chap. 3 semi-simple Lie groups with a bi-invariant metric are symmetric spaces. The heat kernel on such manifolds can be evaluated exactly.

Let G be a semi-simple Lie group of dimension n with the structure constants $C^i{}_{jk}$. Let C_i be the generators of the adjoint representation defined by $(C_i)^j{}_k = C^j{}_{ik}$. Let $\gamma = (\gamma_{ij})$ be the matrix satisfying the relation

$$C_i^T = -\gamma C_i \gamma^{-1}. \quad (6.277)$$

Let g_{ij} be the bi-invariant metric on the group G with the scalar curvature

$$R = -\frac{1}{4}\gamma^{ij} C^k{}_{im} C^m{}_{jk}. \quad (6.278)$$

For such Lie groups for any two points x and x' there is only one geodesic connecting these points and the Synge function $\sigma(x, x')$ and the Van Vleck-Morette determinant $\Delta(x, x')$ are given in canonical coordinates with the origin at x' by

$$\sigma(x, x') = \frac{1}{2}\langle x, \gamma x \rangle = \frac{1}{2}\gamma_{ij} x^i x^j, \quad (6.279)$$

$$\Delta(x, x') = \det\left(\frac{C(x)/2}{\sinh[C(x)/2]}\right). \quad (6.280)$$

Then the heat kernel of the scalar Laplacian on the group G is given by

$$U(t; x, x') = (4\pi t)^{-n/2} \Delta^{1/2}(x, x') \exp\left\{-\frac{\sigma(x, x')}{2t} + \frac{1}{6}Rt\right\}. \quad (6.281)$$

It is instructive to compare this with the asymptotic ansatz (5.41). We see that for the non-compact semi-simple Lie groups the transport function is known exactly,

$$\Omega(t;x,x') = \exp\left(\frac{1}{6}Rt\right) . \tag{6.282}$$

By using the eq. (3.566) one can show directly that the function (6.281) satisfies the heat equation

$$(\partial_t - \Delta)U(t;x,x') = 0 \tag{6.283}$$

and the initial condition

$$U(0;x,x') = \delta(x,x') = |\gamma|^{-1/2}\delta(x-x') , \tag{6.284}$$

where $|\gamma| = \det \gamma_{ij}$, and is, therefore, the heat kernel.

For compact semi-simple groups one has to take into account infinitely many geodesics connecting the points x and x'. Then the heat kernel is obtained as an infinite sum of terms like (6.281) over all geodesics connecting the points x and x'.

6.7.1 Heat Kernel on H^3 and S^3

As an example, we compute the heat kernel on the three-dimensional spaces of constant curvature, the hyperbolic space H^3 and the sphere S^3. It turns out that the theory of these symmetric spaces is significantly simpler than the theory of two-dimensional symmetric spaces, the hyperbolic plane H^2 and S^2. The reason is that these three-dimensional spaces are, in fact, Lie groups, that is, the three sphere S^3 is nothing else but the group $SU(2)$ and the hyperbolic space H^3 is the group $SO(1,3)$.

The curvature tensor is equal to

$$R^a{}_{bcd} = \Lambda(\delta^a{}_c g_{bd} - \delta^a{}_d g_{bc}) \tag{6.285}$$

with $\Lambda = \frac{1}{a^2} > 0$ for S^3 and $\Lambda = -\frac{1}{a^2} < 0$ for H^3. The Ricci curvature tensor and the scalar curvature are

$$R_{ab} = \Lambda\delta_{ab} , \qquad R = 6\Lambda . \tag{6.286}$$

Therefore, $R = \frac{6}{a^2}$ for S^3 and $R = -\frac{6}{a^2}$ for H^3.

The key observation is that because of the invariance properties the heat kernel $U(t;x,x')$ can only depend on the geodesic distance r between the points x and x'. Then by the definition of the Synge function

$$\sigma(x,x') = \frac{1}{2}r^2 . \tag{6.287}$$

Now, the Van Vleck-Morette determinant is given by (3.467)

$$\Delta(x,x') = \left(\frac{r/a}{\sin[r/a]}\right)^2 \tag{6.288}$$

for S^3 and

$$\Delta(x,x') = \left(\frac{r/a}{\sinh[r/a]}\right)^2 \tag{6.289}$$

for H^3.

Then by using the eq. (6.281) we obtain

$$U_{H^3}(t;x,x') = (4\pi t)^{-3/2}\frac{r/a}{\sinh[r/a]}\exp\left(-\frac{t}{a^2}-\frac{r^2}{4t}\right). \tag{6.290}$$

As to S^3 we recall that it is a compact simple Lie group $SU(2)$. Therefore, in addition to the direct geodesic connecting the points x and x' there are infinitely many additional geodesics that wrap around the whole space. By adding the contribution of such geodesics we obtain the correct formula for the heat kernel on S^3

$$U_{S^3}(t;x,x') = \sum_{n=-\infty}^{\infty}(4\pi t)^{-3/2}\frac{r/a+2\pi n}{\sin[r/a]}\exp\left[\frac{t}{a^2}-\frac{(r+2\pi na)^2}{4t}\right]. \tag{6.291}$$

It is not difficult to verify directly that these functions satisfy the heat equation. By using the eq. (3.474) we see that the Laplacian, when acting on a function that depends only on the geodesic distance r, has the form

$$\nabla_i\nabla^i = \partial_r^2 + \frac{2}{a}\coth[r/a]\,\partial_r\,, \tag{6.292}$$

for H^3 and

$$\nabla_i\nabla^i = \partial_r^2 + \frac{2}{a}\cot[r/a]\,\partial_r\,, \tag{6.293}$$

for S^3. By using this form one can check that the functions (6.290) and (6.291) satisfy the heat equation and the initial condition.

Notice that all formulas for S^3 can be obtained from the formulas for H^3 by replacing $a \mapsto ia$ (and adding a summation over multiple geodesics).

6.7.2 Heat Kernel on the Hyperbolic Space H^n

We study the heat kernel of the Laplacian on the symmetric spaces of negative constant curvature, the hyperbolic space H^n for a general $n \neq 3$ (for more details, see [47]). The curvature tensor is equal to

$$R^a{}_{bcd} = -\varkappa^2(\delta^a{}_c g_{bd} - \delta^a{}_d g_{bc}) \tag{6.294}$$

The key observation is that because of the invariance properties the heat kernel $U(t;x,x') = U(t;r)$ can only depend on the geodesic distance r between the points x and x'. Therefore, the Laplacian simplifies and becomes an ordinary differential operator, (3.476),

$$\Delta = \partial_r^2 + (n-1)\varkappa \coth(\varkappa r)\partial_r \,. \tag{6.295}$$

This operator simplifies further by introducing new variables

$$z = \cosh(\varkappa r)\,, \tag{6.296}$$

$$\tau = \varkappa^2 t\,; \tag{6.297}$$

then

$$\Delta = \varkappa^2 \left[(z^2-1)\partial_z^2 + nz\partial_z\right]\,, \tag{6.298}$$

and, therefore, the heat equation simplifies to

$$\left[\partial_\tau - (z^2-1)\partial_z^2 - nz\partial_z\right] U(\tau;z) = 0\,. \tag{6.299}$$

Now, we observe the following intertwining property

$$\partial_z\left[(z^2-1)\partial_z^2 + nz\partial_z\right] = \left[(z^2-1)\partial_z^2 + (n+2)z\partial_z + n\right]\partial_z\,, \tag{6.300}$$

which further means

$$e^{-n\tau}\partial_z\left[\partial_\tau - (z^2-1)\partial_z^2 - nz\partial_z\right] = \left[\partial_\tau - (z^2-1)\partial_z^2 - (n+2)z\partial_z\right] e^{-n\tau}\partial_z\,. \tag{6.301}$$

This equation means that if $U_{H^n}(\tau;z)$ is the heat kernel on the space H^n, then

$$U_{H^{n+2}}(\tau;z) = -\frac{\varkappa^2}{2\pi} e^{-n\tau}\partial_z U_{H^n}(\tau;z) \tag{6.302}$$

is the heat kernel on the space H^{n+2}. The normalization constant is chosen to satisfy the initial asymptotic condition, as $\tau \to 0$,

$$U_{H^n}(\tau;z) \sim (4\pi\tau)^{-n/2}\varkappa^n \exp\left(-\frac{z-1}{2\tau}\right)\,. \tag{6.303}$$

This reduces the calculation of the heat kernel for higher dimensions to the calculation of the heat kernel $n = 1$ and $n = 2$ (see [47, 21, 45]). Similar results also hold for the sphere S^n as shown in [45, 21].

Note that for $n = 1$ the Laplacian is simply $\Delta = \partial_r^2$. Therefore, the corresponding heat kernel is simply the one-dimensional Euclidean one

$$U_{\mathbb{R}}(t;r) = (4\pi t)^{-1/2}\exp\left(-\frac{r^2}{4t}\right)\,. \tag{6.304}$$

Namely, for odd $n = 2m+1$

$$U_{H^n}(\tau;z)=\left(\frac{\varkappa^2}{2\pi}\right)^{(n-1)/2}\exp\left[-\frac{1}{4}(n-1)^2t\right](-\partial_z)^{(n-1)/2}U_{\mathbb{R}}(\tau;z) \quad (6.305)$$

and for even $n=2m$

$$U_{H^n}(\tau;z)=\left(\frac{\varkappa^2}{2\pi}\right)^{(n-2)/2}\exp\left[-\frac{1}{4}n(n-2)t\right](-\partial_z)^{(n-2)/2}U_{H^2}(\tau;z)\,. \quad (6.306)$$

In particular, this immediately gives the heat kernel on H^3 already computed in a previous section. Indeed, by using

$$\partial_z=\frac{1}{\varkappa\sinh(\varkappa r)}\partial_r \quad (6.307)$$

and applying this to $U_{\mathbb{R}}(t;r)$, (6.304), we get the explicit form (6.290) for $U_{H^3}(t;r)$.

Thus, we only need to compute the heat kernel on H^2. The easiest way to solve the heat equation for $n=2$ is to use the so-called *Mehler-Fock transform*

$$U(\tau;z)=\int_0^\infty d\mu\;\mu\,\tanh(\pi\mu)P_{i\mu-1/2}(z)F(\tau;\mu)\,, \quad (6.308)$$

$$F(\tau;\mu)=\int_1^\infty dz\;\sqrt{z^2-1}\,P_{i\mu-1/2}(z)U(\tau;z)\,, \quad (6.309)$$

where $P_\nu(z)$ is the Legendre function [29]. The Legendre function satisfies the equation

$$\left[(z^2-1)\partial_z^2+2z\partial_z+\frac{1}{4}+\mu^2\right]P_{i\mu-1/2}(z)=0\,. \quad (6.310)$$

Therefore, the function $F(t;\mu)$ satisfies the equation

$$\left(\partial_\tau+\frac{1}{4}+\mu^2\right)F(\tau;\mu)=0\,, \quad (6.311)$$

which is easily solved

$$F(\tau;\mu)=\frac{1}{2\pi}\exp\left[-\left(\frac{1}{4}+\mu^2\right)\tau\right]\,. \quad (6.312)$$

The normalization constant is chosen here in such a way to ensure the initial condition for the heat kernel $U(0;x,x')=\delta(x,x')$.

Thus, the heat kernel takes the form

$$U(\tau;z)=\frac{1}{2\pi}\int\limits_0^\infty d\mu\;\mu\,\tanh(\pi\mu)P_{i\mu-1/2}(z)\exp\left[-\left(\frac{1}{4}+\mu^2\right)\tau\right] \quad (6.313)$$

Finally, by using an integral representation for the Legendre function one can transform this expression to a more simple form [47]

$$U_{H^2}(t;r)=\int\limits_r^\infty ds\;\frac{\sqrt{2}\,s}{\sqrt{\cosh(\varkappa s)-\cosh(\varkappa r)}}(4\pi t)^{-3/2}\exp\left(-\frac{1}{4}\varkappa^2 t-\frac{s^2}{4t}\right). \quad (6.314)$$

This formula can be interpreted as a fractional derivative of $U_{\mathbb{R}}(t;r)$ by applying the eq. (6.305) [21].

6.7.3 Covariantly Constant Fields

We follow in this section our papers [8, 12]. We are considering the operator

$$\begin{aligned} L&=-g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}}+Q\\ &=-|g|^{-1/2}(\partial_i+\mathcal{A}_i)|g|^{1/2}g^{ij}(\partial_j+\mathcal{A}_j)+Q\,, \end{aligned} \quad (6.315)$$

where g_{ij} is a metric, $\mathcal{A}_i$ is a connection and Q is a function. Now we come to the most interesting and, of course, at the same time the most difficult case. We want to obtain an approximate solution for the heat kernel in the situation when these fields vary slowly. This does not mean that the metric g_{ij} and the vector $\mathcal{A}_i$ are almost constant. This means rather that the curvatures $R^i{}_{jkl}$ and $\mathcal{R}_{ij}$ (and Q) are almost *covariantly constant*, that is, their covariant derivatives are small. What we want is to develop a perturbation series in the powers of the covariant derivatives of the curvatures. In the zero order of such perturbation theory we have to consider *covariantly constant* background fields, $R^i{}_{jkl}$ and $\mathcal{R}_{ij}$ and Q,

$$\nabla_i R^j{}_{klm}=\nabla_i\mathcal{R}_{jk}=\nabla_i Q=0\,. \quad (6.316)$$

As far as the potential term Q is concerned this just means that Q is constant. Since the addition of a constant to an operator has a trivial effect on the heat kernel, that is, the factor $\exp(-tQ)$, without loss of generality it can be omitted.

However, since $R^i{}_{jkl}$ and $\mathcal{R}_{ij}$ are tensors they cannot be simply constant; the value of the components of a tensor depends on the coordinate system. The condition of covariant constancy imposes rather strict constraints on the possible algebraic structure of these tensors. By taking the commutator of

second covariant derivatives of these tensors we get

$$R^{ij}{}_{km}R^{k}{}_{nlp} - R^{ij}{}_{kn}R^{k}{}_{mlp} + R^{ij}{}_{kl}R^{k}{}_{pmn} - R^{ij}{}_{kp}R^{k}{}_{lmn} = 0\,, \quad (6.317)$$

$$\mathcal{R}_{km}R^{k}{}_{lij} - \mathcal{R}_{kl}R^{k}{}_{mij} = 0\,. \quad (6.318)$$

The condition on the Riemann curvature tensor $R^{i}{}_{jkl}$ determines the geometry of so-called *symmetric spaces* discussed in chapter 3. The condition on the tensor $\mathcal{R}_{ij}$ (if it is non-zero) significantly restricts possible symmetric spaces which allow the existence of covariantly constant anti-symmetric 2-tensors. For example, the n-sphere, S^n and the hyperbolic space H^n are symmetric spaces with the curvature tensor given by

$$R^{i}{}_{jkl} = \Lambda(\delta^{i}{}_{k}g_{jl} - \delta^{i}{}_{l}g_{jk})\,, \quad (6.319)$$

with some constant Λ ($\Lambda > 0$ for the sphere and $\Lambda < 0$ for the hyperbolic space). Substituting this curvature tensor in eq. (6.318) and contracting the indices l and i we obtain

$$(n-2)\mathcal{R}_{jm} = 0\,. \quad (6.320)$$

This means that such covariantly constant tensor can exists only in two dimensions, either S^2 or H^2. In higher dimensions these constraints can be satisfied only if $\mathcal{R}_{ij} = 0$.

That is why we will restrict ourselves below to a particular case of scalar Laplacian

$$L = -\Delta\,. \quad (6.321)$$

The case of scalar Laplacian is considered in [8] and the much more general case of arbitrary matrix-valued operators of Laplace type is studied in [12]. The two-dimensional case is rather special and we will discuss it separately.

Because of the importance of the non-compact symmetric spaces in finance we will restrict ourselves below, for simplicity, to semi-simple non-compact symmetric space which does not have a Euclidean factor. The heat kernel has a very important factorization property, which means that on product manifolds it factorizes. That is, without loss of generality one can study the heat kernel on irreducible symmetric spaces. In particular, the Euclidean part adds just a trivial factor to the heat kernel. That is why, below we assume that M is semi-simple and noncompact. Then M is topologically homeomorphic to $\mathbb{R}^n$. Another simplification is the fact that for noncompact symmetric spaces the geodesics do not intersect and, therefore, the normal coordinates cover the whole manifold. Thus, we will use the normal coordinates for the whole manifold.

We have to warn the reader that this material is rather advanced; it requires some background in differential geometry, Lie groups and geometric analysis that goes beyond the primary scope of this book. So, our exposition will be necessarily sketchy, in particular, we omit most of the proofs and just try to describe the general ideas and results.

6.7.4 Heat Semi-group

Let M be a semi-simple irreducible non-compact symmetric space. Let G be the isometry group of M and H be its isotropy subgroup. Both these groups have compact Lie algebras. The isotropy group is always compact and the isometry group of a semi-simple symmetric space is semi-simple. Thus, in our case G is a non-compact group and H is a maximal compact subgroup of G. Let the dimension of the manifold M be n, the dimension of the isometry group be N and the dimension of the isotropy group be $p = N - n$. We use below the notation introduced in Sec. 3.14.

Let $(\xi_A{}^i) = (P_a{}^i, L_\mu{}^i)$ be the Killing vectors (3.595), (3.596) on M and

$$\mathcal{L}_A = \xi_A{}^i \partial_i \tag{6.322}$$

be the corresponding Lie derivatives (3.599), (3.600). Here the indices range as follows $A = 1, \dots, N$, $a = 1, \dots, n$, and $\mu = 1, \dots, p$. Let $\gamma = (\gamma_{AB})$ be the matrix defined by (3.585). Then the Laplacian on the symmetric space M has the form

$$\Delta = \gamma^{AB} \mathcal{L}_A \mathcal{L}_B \,. \tag{6.323}$$

Let ω^μ be the canonical coordinates on the isotropy group H and $(k^A) = (p^a, \omega^\mu)$ be the canonical coordinates on the isometry group G. Let X_A be the right-invariant vector fields on the isometry group G defined by (3.544), (3.553). Then the Laplacian on the isometry group is

$$\Delta_G = \gamma^{AB} X_A X_B \,. \tag{6.324}$$

Let $\mathcal{L}(k)$ be a differential operator defined by

$$\mathcal{L}(k) = k^A \mathcal{L}_A \,. \tag{6.325}$$

Then one can show that

$$X_A \exp[\mathcal{L}(k)] = \exp[\mathcal{L}(k)] \mathcal{L}_A \,, \tag{6.326}$$

$$\Delta_G \exp[\mathcal{L}(k)] = \exp[\mathcal{L}(k)] \Delta \,. \tag{6.327}$$

Let us clarify, to avoid confusion, that here X_A and Δ_G are differential operators on the isometry group G (in the variables k^A), while the operators $\mathcal{L}_A$, $\mathcal{L}(k)$ and Δ are the differential operators on the symmetric space M (in the variables x^i).

Let $U_G(t; k, 0)$ be the heat kernel on the isometry group G (6.281) with one point fixed at the origin. It can be analytically continued to the whole complex plane of the canonical variables k^A. In particular, it is analytic when all coordinates k^A are rotated counterclockwise by $\pi/4$. We will treat them as complex variables below.

By using these properties and the heat kernel on the isometry group one can show that the heat semigroup $\exp(t\Delta)$ can be represented in form of the integral [8, 12]

$$\exp(t\Delta) = \int\limits_{\mathbb{R}^N} dk\ |G(k)|^{1/2} U_G(t;k,0) \exp[\mathcal{L}(k)]\,, \tag{6.328}$$

where $|G(k)| = \det G_{AB}(k)$ and $G_{AB}(k)$ is the metric on the isometry group G defined by (3.557). Even though the matrix γ is not positive definite, this formula is valid for complex values of k^A, more precisely, for k^A on the real line rotated by $\pi/4$ in the counterclockwise direction.

The heat kernel can be obtained now by acting by the heat semigroup $\exp(t\Delta)$ on the delta-function,

$$\begin{aligned} U(t;x,x') &= \exp(t\Delta)\delta(x,x') \\ &= \int\limits_{\mathbb{R}^N} dk\ |G(k)|^{1/2} U_G(t;k,0) \exp[\mathcal{L}(k)]\delta(x,x')\,. \end{aligned} \tag{6.329}$$

In particular, the heat kernel diagonal $U(t;x,x)$ is given by

$$U(t;x,x) = \int\limits_{\mathbb{R}^N} dk\ |G(k)|^{1/2} U_G(t;k,0) \exp[\mathcal{L}(k)]\delta(x,x')\Big|_{x=x'}\,. \tag{6.330}$$

To be able to use this integral representation we need to compute the action of the isometries $\exp[\mathcal{L}(k)]$ on the delta-function.

6.7.5 Isometries

The heat kernel diagonal on a symmetric space is constant. So, it can be computed at any point. We fix a point x' in M such that Killing vectors satisfy the initial conditions described above and are given by the explicit formulas (3.599)-(3.600) and compute the heat kernel diagonal at the point x'.

Let $f = f(x)$ be a scalar function on M and let $\varphi = \varphi(\tau, p, \omega; x, x')$ be a new scalar function that depends on a new real parameter τ and the canonical coordinates $k^A = (p^a, \omega^\mu)$ on the isometry group defined by

$$\varphi(\tau, p, \omega; x, x') = \exp[\tau\mathcal{L}(k)] f(x)\,, \tag{6.331}$$

where, as usual, $\mathcal{L}(k) = k^A \xi_A{}^i(x)\partial_i$. It also depends on the coordinates of the point x' as a parameter where the initial conditions for the Killing vectors are imposed. This function satisfies the first-order differential equation

$$\partial_\tau \varphi = \mathcal{L}(k)\varphi \tag{6.332}$$

with the initial condition

$$\varphi\Big|_{\tau=0} = f\,. \tag{6.333}$$

The operator $\mathcal{L}(k)$ generates a *flow* ψ_τ on the manifold M so that the curve $\hat{x}(\tau) = \psi_\tau(x)$ satisfies the equation

$$\frac{d\hat{x}^i}{d\tau} = k^A \xi_A{}^i(\hat{x}) \tag{6.334}$$

with the initial condition

$$\hat{x}^i\Big|_{\tau=0} = x^i\,. \tag{6.335}$$

The solution of this equation depends on the parameters τ, p, ω, x and x', that is,

$$\hat{x} = \hat{x}(\tau, p, \omega, x, x')\,. \tag{6.336}$$

We will be interested mainly in the case when the points x and x' are close to each other. In fact, at the end of our calculations we will take the limit $x = x'$. In this case, the Jacobian

$$\det\left(\frac{\partial \hat{x}^i}{\partial p^a}\right) \neq 0 \tag{6.337}$$

is not equal to zero, and, therefore, the coordinates p can be used to parametrize the point $\hat{x}$, that is, the eq. (6.336) defines the function

$$p = p(\tau, \omega, \hat{x}, x, x')\,. \tag{6.338}$$

It is not difficult to prove (see Sec. 2.1) that

$$\varphi(\tau, p, \omega, x, x') = f(\hat{x}(\tau, p, \omega, x, x'))\,. \tag{6.339}$$

Therefore,

$$\exp[\mathcal{L}(k)]f(x) = f(\hat{x}(1, p, \omega, x, x'))\,, \tag{6.340}$$

in particular,

$$\exp[\mathcal{L}(k)]\delta(x, x') = \delta(\hat{x}(1, p, \omega, x, x'), x')\,. \tag{6.341}$$

This delta-function picks those trajectories that reach the point x' at the time $\tau = 1$. So, we look at the values $\hat{x}(1, p, \omega, x, x')$ when the parameters p are varied. Then there is always a value of the parameters p, that we call $\bar{p}$, such that

$$\hat{x}(1, \bar{p}, \omega, x, x') = x'\,. \tag{6.342}$$

Thus, eq. (6.342) defines a function $\bar{p} = \bar{p}(\omega, x, x')$. Therefore, the parameters $\bar{p}$ can be used to parameterize the point x. In other words,

$$\bar{p}(\omega, x, x') = p(1, \omega, \hat{x}, x, x')\Big|_{\hat{x}=x'} . \tag{6.343}$$

Then by making the change of variables $\hat{x} \mapsto p$ we obtain

$$\exp[\mathcal{L}(k)]\delta(x, x') = J(\omega, x, x')\delta[p - \bar{p}(\omega, x, x')] , \tag{6.344}$$

where

$$J(\omega, x, x') = g^{-1/2}(x') \det \left(\frac{\partial \hat{x}^i}{\partial p^a}\right)^{-1} \Big|_{p=\bar{p},\tau=1} . \tag{6.345}$$

Thus, we see that the integration over the variables p^a becomes trivial and we are left with an integral over the variables ω^μ only, that is, over the holonomy algebra.

Now we need to compute the Jacobian $J(\omega, x, x')$. We choose normal coordinates y^a of the point x defined above and the normal coordinates $\hat{y}^a$ of the point $\hat{x}$ with the origin at x', so that the normal coordinates y' of the point x' are equal to zero, $y'^a = 0$. Then by taking into account eqs. (3.599) and (3.600) the equation (6.334) becomes

$$\frac{d\hat{y}^a}{d\tau} = T^a{}_b(y)p^b - \omega^\mu D^a{}_{\mu b}\hat{y}^b , \tag{6.346}$$

where

$$T = \sqrt{-K(\hat{y})} \coth \sqrt{-K(\hat{y})}, \tag{6.347}$$

with the initial condition

$$\hat{y}^a\big|_{\tau=0} = y^a . \tag{6.348}$$

Here, as usual,

$$K^{ab}(\hat{y}) = R^a{}_c{}^b{}_d \hat{y}^c \hat{y}^d = \beta^{\mu\nu} D^a{}_{\mu c} D^b{}_{\nu d} \hat{y}^c \hat{y}^d . \tag{6.349}$$

The solution of this equation defines a function $\hat{y} = \hat{y}(\tau, p, \omega, y)$, which implicitly defines the function

$$p = p(\tau, \omega, \hat{y}, y) . \tag{6.350}$$

The function $\bar{p} = \bar{p}(\omega, y)$ is now defined by the equation

$$\hat{y}(1, \bar{p}, \omega, y) = 0 , \tag{6.351}$$

or

$$\bar{p}(\omega, y) = p(1, \omega, 0, y) , \tag{6.352}$$

and the Jacobian $J(\omega, x, x')$ is now determined by

$$J(\omega, x, x') = \det \left(\frac{\partial \hat{y}^a}{\partial p^b}\right)^{-1} \Big|_{p=\bar{p},\tau=1} . \tag{6.353}$$

Next, we define the matrix $D(\omega)$ by

$$D(\omega) = \omega^\mu D_\mu \,. \tag{6.354}$$

Then the Taylor expansion of the function $\hat{y} = \hat{y}(\tau, p, \omega, y)$ in p and y reads (in the matrix notation)

$$\hat{y} = \exp[-\tau D(\omega)]y + \left(\frac{1 - \exp[-\tau D(\omega)]}{D(\omega)}\right) p + O(y^2, p^2, py) \,. \tag{6.355}$$

Therefore, we find with the same accuracy the Taylor expansion of the function $\bar{p}(\omega, y)$ in y

$$\bar{p} = -\left(D(\omega)\frac{\exp[-D(\omega)]}{1 - \exp[-D(\omega)]}\right) y + O(y^2) \,. \tag{6.356}$$

By using these equations we finally obtain the Jacobian

$$J(\omega, x, x') = \det\left(\frac{\sinh[\,D(\omega)/2]}{D(\omega)/2}\right)^{-1} + O(y) \,. \tag{6.357}$$

This should be enough to compute the heat kernel for small y (or x close to x'), in particular, the heat kernel diagonal when $x = x'$.

6.7.6 Heat Kernel

We define the matrix $F(\omega)$ by

$$F(\omega) = \omega^\mu F_\mu \,, \tag{6.358}$$

a scalar R_H by

$$R_H = \frac{1}{4}\beta^{\alpha\beta} F^\mu{}_{\alpha\gamma} F^\gamma{}_{\beta\mu} \,, \tag{6.359}$$

and a matrix $B(\omega)$ by

$$B(\omega) = \left(\frac{\sin[\,D(\omega)/2]}{D(\omega)/2}\right)^{-2} \,. \tag{6.360}$$

Then by using the above results one can compute the heat kernel of the scalar Laplacian Δ for x close to x'. Recall that the canonical coordinates $(k^a) = (p^a, \omega^\mu)$ are rotated by $\pi/4$ in the complex plane countercloskwise. By rotating the canonical coordinates ω^j further by $\pi/4$ so that they are now purely imaginary we obtain [8, 12]

$$U(t;x,x') = (4\pi t)^{-n/2} \exp\left\{\left(\frac{1}{8}R + \frac{1}{6}R_H\right)t\right\} \tag{6.361}$$
$$\times \int\limits_{\mathbb{R}^p} \frac{d\omega}{(4\pi t)^{p/2}}\ |\beta|^{1/2} \exp\left\{-\frac{1}{4t}\left[\langle\omega,\beta\omega\rangle + \langle y, B(\omega)y\rangle\right]\right\}$$
$$\times \det\left(\frac{\sin\left[F(\omega)/2\right]}{F(\omega)/2}\right)^{1/2} \det\left(\frac{\sin\left[D(\omega)/2\right]}{D(\omega)/2}\right)^{-1/2} + O(y)\,,$$

where $|\beta| = \det \beta_{\mu\nu}$, $\langle\omega,\beta\omega\rangle = \beta_{\mu\nu}\omega^\mu\omega^\nu$ and $\langle y, B(\omega)y\rangle = y^a B_{ab}(\omega) y^b$.

In particular, by setting $x = x'$, that is, $y = 0$, we obtain the heat kernel diagonal

$$U(t;x,x) = (4\pi t)^{-n/2} \exp\left\{\left(\frac{1}{8}R + \frac{1}{6}R_H\right)t\right\} \tag{6.362}$$
$$\times \int\limits_{\mathbb{R}^p} \frac{d\omega}{(4\pi t)^{p/2}}\ |\beta|^{1/2} \exp\left\{-\frac{1}{4t}\,\langle\omega,\beta\omega\rangle\right\}$$
$$\times \det\left(\frac{\sin\left[F(\omega)/2\right]}{F(\omega)/2}\right)^{1/2} \det\left(\frac{\sin\left[D(\omega)/2\right]}{D(\omega)/2}\right)^{-1/2}.$$

This formula can be written as a Gaussian average over the canonical variables ω^μ of the holonomy group. We introduce a Gaussian average over the holonomy algebra by

$$\langle f(\omega)\rangle = \int\limits_{\mathbb{R}^p} \frac{d\omega}{(4\pi)^{p/2}}\ |\beta|^{1/2} \exp\left(-\frac{1}{4}\,\langle\omega,\beta\omega\rangle\right) f(\omega). \tag{6.363}$$

Then we can write

$$U(t;x,x) = (4\pi t)^{-n/2} \exp\left\{\left(\frac{1}{8}R + \frac{1}{6}R_H\right)t\right\} \tag{6.364}$$
$$\times\left\langle \det\left(\frac{\sin\left[\sqrt{t}\,F(\omega)/2\right]}{\sqrt{t}\,F(\omega)/2}\right)^{1/2} \det\left(\frac{\sin\left[\sqrt{t}\,D(\omega)/2\right]}{\sqrt{t}\,D(\omega)/2}\right)^{-1/2}\right\rangle.$$

This equation can be used now to generate all heat kernel coefficients $[b_k]$ for any locally symmetric space simply by expanding it in a power series in t. By using the standard Gaussian averages

$$\langle\omega_1^\mu \cdots \omega^{\mu_{2k+1}}\rangle = 0\,, \tag{6.365}$$

$$\langle\omega^{\mu_1} \cdots \omega^{\mu_{2k}}\rangle = \frac{(2k)!}{k!}\beta^{(\mu_1\mu_2} \cdots \beta^{\mu_{2k-1}\mu_{2k})}\,, \tag{6.366}$$

one can obtain now all heat kernel coefficients in terms of traces of various contractions of the matrices $D^a{}_{\mu b}$ and $F^\alpha{}_{\mu\beta}$ with the matrix $\beta^{\mu\nu}$. All these quantities are curvature invariants and can be expressed directly in terms of the Riemann tensor.

There is an alternative representation of the Gaussian average in purely algebraic terms. Let a^j and a^*_k be operators, called *creation* and *annihilation operators*, acting on a Hilbert space, that satisfy the following commutation relations

$$[a^\mu, a^*_\nu] = \delta^\mu{}_\nu\,, \tag{6.367}$$

$$[a^\mu, a^\nu] = [a^*_\mu, a^*_\nu] = 0\,. \tag{6.368}$$

Let $|0\rangle$ be a unit vector in the Hilbert space, called the *vacuum vector*, that satisfies the equations

$$\langle 0|0\rangle = 1\,, \tag{6.369}$$

$$a^\mu|0\rangle = \langle 0|a^*_\nu = 0\,. \tag{6.370}$$

Then the Gaussian average is nothing but the vacuum expectation value

$$\langle f(\omega)\rangle = \langle 0|f(a)\exp\langle a^*, \beta a^*\rangle|0\rangle\,, \tag{6.371}$$

where $\langle a^*, \beta a^*\rangle = \beta^{\mu\nu}a^*_\mu a^*_\nu$. This should be computed by the so-called *normal ordering*, that is, by simply commuting the operators a^μ through the operators a^*_ν until they hit the vacuum vector giving zero. The remaining non-zero commutation terms precisely reproduce the eqs. (6.365), (6.366).

6.7.7 Hyperbolic Plane H^2

For the hyperbolic plane H^2 the isometry group is $SO(1,2)$ and the isotropy group is $SO(2)$. Let y^a be the normal coordinates defined above. On H^2 they range over $-\infty \le y^a \le \infty$. We define the polar coordinates u and φ by

$$y^1 = u\cos\varphi, \qquad y^2 = u\sin\varphi\,, \tag{6.372}$$

so that $0 \le u \le \infty$ and $0 \le \varphi \le 2\pi$.

The metric and the orthonormal frame of 1-forms in these coordinates are

$$ds^2 = du^2 + a^2\sinh^2\left(\frac{u}{a}\right)d^2\varphi\,, \tag{6.373}$$

$$e^1 = du\,, \qquad e^2 = a\sinh\left(\frac{u}{a}\right)d\varphi\,, \tag{6.374}$$

where a is a real parameter (pseudo-radius), which gives the curvature

$$R_{abcd} = -\frac{1}{a^2}\varepsilon_{ab}\varepsilon_{cd} = -\frac{1}{a^2}(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})\,, \tag{6.375}$$

$$R_{ab} = -\frac{1}{a^2}\delta_{ab}\,, \tag{6.376}$$

$$R = -\frac{2}{a^2}\,. \tag{6.377}$$

Since the holonomy group $SO(2)$ is one-dimensional, it is obviously Abelian, so all structure constants $F^{\alpha}{}_{\mu\beta}$ are equal to zero, and therefore, the curvature of the holonomy group vanishes, $R_H = 0$. The metric of the isotropy group $\beta_{\mu\nu}$ is just a constant,

$$\beta = \frac{1}{a^2}, \tag{6.378}$$

and the only generator of the isotropy group in the vector representation is given by

$$D_{ab} = \frac{1}{a^2}E_{ab} = \frac{1}{a^2}\varepsilon_{ab}\,. \tag{6.379}$$

The Lie derivatives $\mathcal{L}_A$ are now

$$\mathcal{L}_1 = \cos\varphi\partial_u - \frac{\sin\varphi}{a}\coth\left(\frac{u}{a}\right)\partial_\varphi\,, \tag{6.380}$$

$$\mathcal{L}_2 = \sin\varphi\partial_u + \frac{\cos\varphi}{a}\coth\left(\frac{u}{a}\right)\partial_\varphi\,, \tag{6.381}$$

$$\mathcal{L}_3 = -\frac{1}{a^2}\partial_\varphi\,, \tag{6.382}$$

and form a representation of the $SO(1,2)$ algebra

$$[\mathcal{L}_1, \mathcal{L}_2] = -\mathcal{L}_3\,, \tag{6.383}$$

$$[\mathcal{L}_3, \mathcal{L}_1] = \frac{1}{a^2}\mathcal{L}_2, \tag{6.384}$$

$$[\mathcal{L}_3, \mathcal{L}_2] = -\frac{1}{a^2}\mathcal{L}_1\,. \tag{6.385}$$

The Laplacian is given by

$$\begin{aligned}\Delta &= \mathcal{L}_1^2 + \mathcal{L}_2^2 + a^2\mathcal{L}_3^2 \\ &= \partial_u^2 + \frac{1}{a}\coth\left(\frac{u}{a}\right)\partial_u + \frac{1}{a^2\sinh^2(u/a)}\partial_\varphi^2\,.\end{aligned} \tag{6.386}$$

The contour of integration over ω in (6.362) for the heat kernel should be the real axis rotated counterclockwise by $\pi/4$. Since H^2 is non-compact, we rotate it back to the real axis and rescale ω for $t > 0$ by $\omega \to a\sqrt{t}\,\omega$ to obtain the heat kernel diagonal for the Laplacian on H^2

$$U_{H^2}(t;x,x) = \frac{1}{4\pi t}\exp\left(-\frac{t}{4a^2}\right) \times \int\limits_{-\infty}^{\infty} \frac{d\omega}{\sqrt{4\pi}}\exp\left(-\frac{\omega^2}{4}\right)\frac{\omega\sqrt{t}/(2a)}{\sinh\left[\omega\sqrt{t}/(2a)\right]}\,. \tag{6.387}$$

6.7.8 Sphere S^2

Next, we apply our result to the special case of a two-sphere S^2 of radius a, which is a compact symmetric space with the isometry group $SO(3)$ and the isotropy group $SO(2)$.

Let y^a be the normal coordinates defined above. On the 2-sphere of radius a they range over $-a\pi \le y^a \le a\pi$. We define the polar coordinates ρ and φ by

$$y^1 = \rho\cos\varphi, \qquad y^2 = \rho\sin\varphi\,, \tag{6.388}$$

so that $0 \le \rho \le a\pi$ and $0 \le \varphi \le 2\pi$.

The orthonormal frame of 1-forms is

$$e^1 = d\rho\,, \qquad e^2 = r\sin\left(\frac{\rho}{r}\right)d\varphi\,, \tag{6.389}$$

which gives the curvature

$$R_{abcd} = \frac{1}{a^2}\varepsilon_{ab}\varepsilon_{cd} = \frac{1}{a^2}(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})\,, \tag{6.390}$$

with ε_{ab} being the antisymmetric Levi-Civita tensor, that is, $\varepsilon_{12} = -\varepsilon_{21} = 1$, the Ricci tensor

$$R_{ab} = \frac{1}{a^2}\delta_{ab}\,, \tag{6.391}$$

and the scalar curvature

$$R = \frac{2}{a^2}\,. \tag{6.392}$$

The metric of the holonomy group $\beta_{\mu\nu}$ is now just a constant, $\beta = -1/a^2$. The only generator of the holonomy group in the vector representation is

$$D_{ab} = -\frac{1}{a^2}E_{ab} = -\frac{1}{a^2}\varepsilon_{ab}\,. \tag{6.393}$$

The Lie derivatives $\mathcal{L}_A$ are given by

$$\mathcal{L}_1 = \cos\varphi\partial_\rho - \frac{\sin\varphi}{a}\cot\left(\frac{\rho}{a}\right)\partial_\varphi\,, \tag{6.394}$$

$$\mathcal{L}_2 = \sin\varphi\partial_\rho + \frac{\cos\varphi}{a}\cot\left(\frac{\rho}{a}\right)\partial_\varphi\,, \tag{6.395}$$

$$\mathcal{L}_3 = \frac{1}{a^2}\partial_\varphi\,, \tag{6.396}$$

and form a representation of the $SO(3)$ algebra

$$[\mathcal{L}_1, \mathcal{L}_2] = -\mathcal{L}_3\,, \tag{6.397}$$

$$[\mathcal{L}_3, \mathcal{L}_1] = -\frac{1}{a^2}\mathcal{L}_2 \tag{6.398}$$

$$[\mathcal{L}_3, \mathcal{L}_2] = \frac{1}{a^2}\mathcal{L}_1\,. \tag{6.399}$$

The Laplacian is given by

$$\Delta = \partial_\rho^2 + \frac{1}{a}\cot\left(\frac{\rho}{a}\right)\partial_\rho + \frac{1}{a^2\sin^2(\rho/a)}\partial_\varphi^2\,. \tag{6.400}$$

The contour of integration over ω in (6.362) should be the real axis rotated counterclockwise by $\pi/4$. Since S^2 is compact, we rotate it further to the imaginary axis and rescale ω for $t<0$ by $\omega \to a\sqrt{-t}\,\omega$ to obtain an analytic function of t

$$U_{S^2}(t;x,x) = \frac{1}{4\pi t}\exp\left(\frac{t}{4a^2}\right) \times \int\limits_{-\infty}^{\infty}\frac{d\omega}{\sqrt{4\pi}}\exp\left(-\frac{\omega^2}{4}\right)\frac{\omega\sqrt{-t}/(2a)}{\sinh\left[\omega\sqrt{-t}/(2a)\right]}\,. \tag{6.401}$$

If we would have rotated the contour to the real axis instead then we would have obtained after rescaling $\omega \to a\sqrt{t}\,\omega$ for $t>0$,

$$U_{S^2}(t;x,x) = \frac{1}{4\pi t}\exp\left(\frac{t}{4a^2}\right) \times P\int\limits_{-\infty}^{\infty}\frac{d\omega}{\sqrt{4\pi}}\exp\left(-\frac{\omega^2}{4}\right)\frac{\omega\sqrt{t}/(2a)}{\sin\left[\omega\sqrt{t}/(2a)\right]}\,, \tag{6.402}$$

where $P\int$ denotes the Cauchy principal value of the integral. This can also be written as

$$U_{S^2}(t;x,x) = \frac{1}{4\pi t}\exp\left(\frac{t}{4a^2}\right) \tag{6.403}$$

$$\times \sum_{k=-\infty}^{\infty}(-1)^k \int_0^{2\pi r/\sqrt{t}} \frac{d\omega}{\sqrt{4\pi}}\exp\left[-\frac{1}{4}\left(\omega+\frac{2\pi a}{\sqrt{t}}k\right)^2\right]\frac{\left[\omega\sqrt{t}/(2a)+\pi k\right]}{\sin\left[\omega\sqrt{t}/(2a)\right]}\,.$$

This is nothing but the sum over the closed geodesics of S^2.

6.7.9 Duality of H^2 and S^2

There is a remarkable duality between compact and non-compact symmetric spaces. One can show that the exact results for compact symmetric spaces can be obtained by an analytic continuation from the dual noncompact case.

We see that the heat kernel in the compact case of the two-sphere, S^2, is related with the heat kernel in the non-compact case of the hyperboloid, H^2, by the analytical continuation, $a \mapsto ia$ or, alternatively, by replacing $t \to -t$ (and keeping a unchanged). One can go even further and compute so-called Plancherel (or Harish-Chandra) measure $\mu(\nu)$ in the case of H^2 and the spectrum in the case of S^2 (for details, see [12]).

For H^2 we rescale the integration variable in (6.387) by $\omega \to \omega a/\sqrt{t}$, substitute

$$\frac{a}{\sqrt{4\pi t}}\exp\left(-\frac{a^2}{4t}\omega^2\right) = \int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\exp\left(-\frac{t}{a^2}\nu^2+i\omega\nu\right)\,, \tag{6.404}$$

integrate by parts over ν, and use

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\,\frac{e^{i\omega\nu}}{\sinh\,(\omega/2)} = \tanh\,(\pi\nu) \tag{6.405}$$

to represent the heat kernel diagonal for H^2 in the form

$$U_{H^2}(t;x,x) = \frac{1}{4\pi a^2}\int_{-\infty}^{\infty} d\nu\;\mu(\nu)\exp\left\{-\left(\frac{1}{4}+\nu^2\right)\frac{t}{a^2}\right\}\,, \tag{6.406}$$

where

$$\mu(\nu) = \nu\tanh\nu\,. \tag{6.407}$$

For S^2 we proceed as follows. We cannot just substitute $a \mapsto ia$ in (6.406). Instead, first, we deform the contour of integration in (6.406) to the V-shaped contour that consists of two segments of straight lines, one going from $e^{i3\pi/4}\infty$

to 0, and another going from 0 to $e^{i\pi/4}\infty$. Then, after we replace $a \mapsto ia$, we can deform the contour further to go counterclockwise around the positive imaginary axis.

Then we notice that the function $\mu(\nu)$ is a meromorphic function with simple poles on the imaginary axis at $\nu_k = id_k$, where

$$d_k = k + \frac{1}{2}, \qquad k = 0, \pm 1 \pm 2, \dots , \tag{6.408}$$

Therefore, we can compute the integral by residue theory to get

$$U_{S^2}(t; x, x) = \frac{1}{4\pi a^2} \sum_{k=0}^{\infty} d_k \exp\left(-\lambda_k t\right) , \tag{6.409}$$

where

$$\lambda_k = \frac{1}{a^2} k(k+1) . \tag{6.410}$$

Thus, the analytic continuation from the hyperbolic plane allowed us to compute the spectrum for the sphere.

6.8 Heat Kernel of Non-Selfadjoint Operators

As we have discussed in Sec. 2.3 an elliptic partial differential operator of the form

$$L = -\alpha^{ij}\partial_i\partial_j + \beta^i\partial_i + \gamma \tag{6.411}$$

can be decomposed as follows

$$L = -\Delta + \mathcal{L} + \gamma , \tag{6.412}$$

where Δ is the Laplacian corresponding to the metric $g^{ij} = \alpha^{ij}$ and $\mathcal{L}$ is a first-order partial differential operator of the form

$$\mathcal{L} = \xi^i\partial_i , \tag{6.413}$$

where

$$\xi^i = \beta^i + \Gamma^i \tag{6.414}$$

and

$$\Gamma^i = g^{-1/2}\partial_i(g^{1/2}g^{ij}) . \tag{6.415}$$

Notice that this operator is not self-adjoint. However, in some cases one can compute its heat kernel exactly. Now, suppose that the function γ is constant and the operator $\mathcal{L}$ is equal to the Lie derivative along a Killing vector of the metric g_{ij}. Then it commutes with the Laplacian (see Sec. 3.5) and, therefore, the heat semi-group factorizes

$$\exp(-tL) = e^{-t\gamma} \exp(-t\mathcal{L}) \exp(t\Delta) \,. \tag{6.416}$$

Then by acting on the delta function we obtain the heat kernel of the operator L

$$\begin{aligned} U_L(t; x, x') &= e^{-t\gamma} \exp(-t\mathcal{L}) \exp(t\Delta) \delta(x, x') \\ &= e^{-t\gamma} \exp(-t\mathcal{L}) U_\Delta(t; x, x') \,, \end{aligned} \tag{6.417}$$

where $U_\Delta(t; x, x')$ is the heat kernel of the Laplacian.

Next, since the Lie derivative $\mathcal{L}$ is a first-order operator the action of the exponential $\exp(-t\mathcal{L})$ can be computed exactly (see Sec. 2.1). Namely,

$$U_L(t; x, x') = e^{-t\gamma} U_\Delta(t; \hat{x}(t, x), x') \,, \tag{6.418}$$

where $\hat{x}(t, x)$ is the solution of the system

$$\frac{d\hat{x}^i}{dt} = \xi^i(\hat{x}) \tag{6.419}$$

with the initial condition

$$\hat{x}(0) = x \,. \tag{6.420}$$

This formula can be used in cases when the heat kernel of the Laplacian is known exactly, like on semi-simple groups and symmetric spaces, in particular, hyperbolic space H^n.

6.9 Path Integrals

6.9.1 Discretization

Let us consider a (time-dependent, in general) elliptic second-order partial differential operator L of the form

$$L(t) = -\alpha^{ij}(t, x)\partial_i\partial_j + \beta^j(t, x)\partial_j + \gamma(t, x) \,. \tag{6.421}$$

Finding the heat semi-group $U(t, t')$ of the operator L for finite t is equivalent to solving the heat equation. However, for small t it can be obtained by perturbation theory. For a time-independent operator L we have

$$U(t) = \exp(-tL) = I - tL + O(t^2) \,. \tag{6.422}$$

By using the semi-group property we can represent the heat semi-group for finite t as a limit the product of short-time semi-groups

$$U(t) = \lim_{N\to\infty} \left[U\left(\frac{t}{N}\right)\right]^N . \tag{6.423}$$

A similar representation exists even in the case when the operator $L = L(t)$ is time-dependent. As we have seen in Sec. 1.17.5 the heat semi-group $U(t,t')$ for t close to t' is given by (1.234)

$$\begin{aligned} U(t,t') &= I - \int_{t'}^{t} d\tau\ L(\tau) + O[(t-t')^2] \\ &= \exp\left[- \int_{t'}^{t} d\tau\ L(\tau)\right] + O[(t-t')^2]\,. \end{aligned} \tag{6.424}$$

Let us partition the interval (t',t), (we assume that $t > t'$) in N equal subintervals of length $(t-t')/N$ and let

$$t_k = t' + k\frac{(t-t')}{N}\,, \qquad k = 0,1,\dots,N,. \tag{6.425}$$

Also, let τ_k be some arbitrary points in the subintervals $[t_{k-1}, t_k]$. Then by using the semi-group property we have

$$U(t,t') = U(t,t_{N-1})U(t_{N-1},t_{N-2})\cdots U(t_2,t_1)U(t_1,t')\,. \tag{6.426}$$

By taking the limit as $N\to\infty$ we can replace each heat semi-group by the approximate exponential form to get

$$U(t,t') = \lim_{N\to\infty} \exp\left[- \int_{t_{N-1}}^{t} d\tau_N L(\tau_N)\right] \cdots \exp\left[- \int_{t'}^{t_1} d\tau_1 L(\tau_1)\right]\,. \tag{6.427}$$

Such representation of the heat semi-group is the basis for the *Feynmann path integral* representation of the heat kernel. By using the above formulas we obtain for the heat kernel of the operator L

$$\begin{aligned} U(t,x|t',x') &= \lim_{N\to\infty} \int_{\mathbb{R}^{Nn}} dx_1 \dots dx_N\ U(t,x|t_{N-1},x_{N-1}) \\ &\times U(t_{N-1},x_{N-1}|t_{N-2},x_{N-2})\cdots U(t_2,x_2|t_1,x_1)U(t_1,x_1|t',x')\,. \end{aligned} \tag{6.428}$$

6.9.2 Formal Expression

We know that as $t\to t'$ the heat kernel (in the density form) looks like

$$U(t,x|t',x') \sim [4\pi(t-t')]^{-n/2}[\det A]^{-1/2} \tag{6.429}$$
$$\times \exp\left\{-\frac{1}{4(t-t')}\left\langle (x-x'), A^{-1}(x-x')\right\rangle\right\}$$
$$\times \exp\left\{\frac{1}{2}\left\langle (x-x'), A^{-1}\beta\right\rangle - (t-t')\left[\gamma + \frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle\right]\right\},$$

where A is the matrix $A = (\alpha^{ij})$. The coefficients A, β and γ are computed here at some point between t and t' and some point between x and x' (recall that this approximation is valid for t close to t' and x close to x'). Substituting this form of the heat kernel in the above formula we obtain the following *formal* formula

$$U(t,x|t',x') = \int_{\mathcal{M}} \mathcal{D}x(\tau)\exp[-S(t,x|t',x')]\,. \tag{6.430}$$

Here the formal symbols $\mathcal{D}x(\tau)$ and $\mathcal{M}$ mean that the integral is taken over all continuous paths $x(\tau)$ starting at x' at $\tau = t'$ and ending at x at $\tau = t$, that is,

$$x(t') = x'\,, \qquad x(t) = x\,, \tag{6.431}$$

and $S(t,x|t',x')$ is the following function called the *action functional*

$$S(t,x|t',x') = \int_{t'}^{t} d\tau \left\{\frac{1}{4}\left\langle \frac{dx(\tau)}{d\tau}, A^{-1}(\tau,x(\tau))\frac{dx(\tau)}{d\tau}\right\rangle \right. \tag{6.432}$$
$$-\frac{1}{2}\left\langle \frac{dx(\tau)}{d\tau}, A^{-1}(\tau,x(\tau))\beta(\tau,x(\tau))\right\rangle$$
$$\left. +\frac{1}{4}\left\langle \beta(\tau,x(\tau)), A^{-1}(\tau,x(\tau))\beta(\tau,x(\tau))\right\rangle + \gamma(\tau,x(\tau))\right\}.$$

This formal integral originated in quantum mechanics and is known as *Feynmann path integral*. We should warn the reader that our derivation of this formula was rather formal. One should be more careful in replacing the heat kernel by its short-time asymptotic form and justify taking the limit $N \to \infty$.

Of course, we could have started with the operator L in geometric terms

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{A} + Q\,, \tag{6.433}$$

where $\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i$, $g^{ij} = \alpha^{ij}$, and $\mathcal{A}_i$ and Q are related to β^i and γ by the relations (5.2)-(5.5). Then the short time heat kernel is given by (5.213), which can be written in a slightly modified form (by including the function $\mathcal{W}$, (5.212), in the function S, (5.228)) as follows

$$U(t,x|t',x') \sim (2\pi)^{-n/2} Z^{1/2}(t,x|t',x') \exp\left[-S(t,x|t',x')\right] , \tag{6.434}$$

where

$$S(t,x|t',x') = \int_{t'}^{t} d\tau \left\{ \frac{1}{4} \left\langle \frac{dx(\tau)}{d\tau}, g(\tau,x(\tau)) \frac{dx(\tau)}{d\tau} \right\rangle \right.$$
$$\left. + \left\langle \mathcal{A}(\tau,x(\tau)), \frac{dx(\tau)}{d\tau} \right\rangle + Q(\tau,x(\tau)) \right\} . \tag{6.435}$$

and the function Z is defined by (5.205),

$$Z(t,x|t',x') = g^{-1/2}(t,x) \det\left[-\partial_i \partial_{j'} S(t,x|t',x')\right] g^{-1/2}(t',x') . \tag{6.436}$$

Recall that the coincidence limit of the function Z is equal to one, $Z(t,x|t,x) = 1$. Moreover, for a time-independent metric we have (5.208)

$$Z^{1/2}(t,x|t',x') = [2(t-t')]^{-n/2} \Delta^{1/2}(x,x') , \tag{6.437}$$

where $\Delta(x,x')$ is the Van Vleck determinant. Now, by substituting $\Delta = e^{\zeta}$ and using the Taylor expansion of ζ for x close to x', (3.403)-(3.406), we get

$$Z^{1/2}(t,x|t',x') \sim [2(t-t')]^{-n/2} \exp\left\{ \frac{1}{12} R_{i'j'} \sigma^{i'} \sigma^{j'} \right\} . \tag{6.438}$$

More generally, one can show that for a time-dependent operator for t close to t' and x close to x' it has the following form

$$Z^{1/2}(t,x|t',x') \sim [2(t-t')]^{-n/2} \tag{6.439}$$
$$\times \exp\left\{ \frac{1}{12}(t-t') \int_{t'}^{t} d\tau \; R_{ij}(\tau,x(\tau)) \frac{dx^i(\tau)}{d\tau} \frac{dx^j(\tau)}{d\tau} \right\} .$$

Because of the extra factor $(t-t')$ in the exponent this term does not contribute to the action and should be absorbed in the path integral measure $\mathcal{D}x(\tau)$. By substituting this form in the discretized heat kernel we obtain the path integral (6.430). A more careful treatment shows that there could also appear a term proportional to the scalar curvature R of the metric g_{ij}. The exact coefficient of this term depends on the regularization scheme. This shows, in particular, that the path integrals are defined only with a prescribed discretization/regularization procedure. Without a precise algorithm for computation of the path integral it is ill-defined.

6.9.3 Perturbation Theory

It is worth mentioning that since there are no systematic rigorous mathematical methods for computing such integrals, the only practical method remains the perturbation theory. For small times, as $t \to t'$, one can get an asymptotic expansion of this integral by applying the general methods for computing the asymptotic expansions of integrals with a small (or a large parameter). Essentially, one looks for critical points of the action, which represent classical trajectories and expands the action in a functional Taylor series near these trajectories. Then one leaves in the exponent quadratic terms and expands the rest in a power series. Then the only path integrals that appear are *Gaussian path integrals* for which very similar techniques are available as for finite-dimensional Gaussian integrals (see Sec. 1.2). In this way, one obtains finally a perturbative expansion of the heat kernel, which should be equivalent to the one obtained by other more established methods, for example, the method of semi-classical approximation (or singular perturbations) discussed in Chap. 4.

The classical trajectories are given by the critical points of the action functional determined by the variational (functional) derivative

$$\frac{\delta S}{\delta x(\tau)} = 0\,. \tag{6.440}$$

By varying the action functional (6.433) with respect to the path $x(\tau)$ with fixed endpoints, $x(t') = x'$ and $x(t) = x$, we get the equations for classical trajectories

$$\frac{d^2x^m}{dt^2} + B^m{}_{jk}(t,x)\frac{dx^j}{dt}\frac{dx^k}{dt} + C^m{}_j(t,x)\frac{dx^j}{dt} + D^m(t,x) = 0\,, \tag{6.441}$$

where $B^m{}_{jk}(x,t)$, $C^m{}_j(x,t)$ and $D(x,t)$ are some functions defined as follows. As usual, here and everywhere below the summation over repeated indices is understood. Let α_{ij} be the entries of the matrix $A^{-1} = (\alpha_{ij})$ inverse to the matrix $A = (\alpha^{ij})$. Then

$$B^m{}_{jk} = \frac{1}{2}\alpha^{im}\left(\partial_k\alpha_{ij} + \partial_j\alpha_{ik} - \partial_i\alpha_{kj}\right)\,, \tag{6.442}$$

$$C^m{}_j = \partial_j\beta^m + \beta^k\alpha^{im}\partial_j\alpha_{ik} - \alpha^{im}\partial_i(\alpha_{kj}\beta^k) + \alpha^{im}\partial_t\alpha_{ij}\,, \tag{6.443}$$

$$D^m = -2\alpha^{im}\partial_i\gamma - \frac{1}{2}\alpha^{im}\partial_i(\alpha_{kj}\beta^k\beta^j) + \partial_t\beta^m + \alpha^{im}\beta^j\partial_t\alpha_{ij}\,. \tag{6.444}$$

These are pretty complicated equations. However, they simplify a lot if one uses the machinery of differential geometry. In particular, the matrix α_{ij} should be identified with the Riemannian metric. Then, for example, in the

case when α^{ij} does not depend on time and $\beta = \gamma = 0$, these equations describe nothing but the geodesics in a Riemannian manifold.

In the geometric language the critical points of the action functional S are determined by

$$\frac{d^2x^m}{d\tau^2} + \Gamma^m{}_{kj}\frac{dx^k}{d\tau}\frac{dx^j}{d\tau} + \left[g^{im}(\partial_t g_{ik}) - 2g^{im}\mathcal{R}_{ik}\right]\frac{dx^k}{d\tau} + 2g^{im}\partial_t\mathcal{A}_i - 2g^{im}\partial_i Q = 0\,, \tag{6.445}$$

where $\Gamma^m{}_{kj}$ are Christoffel symbols of the metric g_{ij} and $\mathcal{R}_{ij} = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i$.

Suppose that there is a unique solution $x_0(\tau)$ of these equations with the boundary conditions $x(t') = x'$ and $x(t) = x$. At least for t close to t' and x close to x' this is indeed so. The classical trajectory gives the main contribution to the path integral. In the neighborhood of the classical trajectory we write

$$x(\tau) = x_0(\tau) + y(\tau)\,, \tag{6.446}$$

where $y(\tau)$ is a continuous path with zero boundary conditions, that is,

$$y(t') = y(t) = 0\,, \tag{6.447}$$

expand the action in a functional Taylor series in powers of y and separate the quadratic terms

$$S(x(\tau)) = S(x_0(\tau)) + \frac{1}{2}\int_{t'}^{t} d\tau\ \langle y(\tau), H(\tau)y(\tau)\rangle + V(y(\tau))\,, \tag{6.448}$$

where H is a second-order ordinary differential operator acting on vectors determined by the second variational derivative of the action at the critical point

$$H_{ij} = \left.\frac{\delta^2 S(x(\tau))}{\delta x^i(\tau)\delta x^j(\tau')}\right|_{x(\tau)=x_0(\tau)}, \tag{6.449}$$

and $V(y(\tau))$ is a functional of $y(\tau)$ whose expansion in y begins with the terms of order y^3. Note that the operator H is nothing but the functional Hessian. It has the form

$$H = -\frac{1}{4}\frac{d}{d\tau}A^{-1}(\tau)\frac{d}{d\tau} + E(\tau)\frac{d}{d\tau} - \frac{d}{d\tau}E^T(\tau) + F(\tau)\,, \tag{6.450}$$

where $A^{-1}(\tau) = (\alpha_{ij}(\tau, x_0(\tau)))$, and the matrices $E = (E_{ij})$ and $F = (F_{ij})$ are defined by

$$E_{ij} = \frac{1}{4}\left[\dot{x}_0^k \partial_i \alpha_{kj} - \beta^k \partial_i \alpha_{kj} - \alpha_{kj}\partial_i \beta^k\right] , \tag{6.451}$$

$$F_{ij} = \partial_i\partial_j\gamma + \frac{1}{4}\Big[\beta^k\beta^l\partial_i\partial_j\alpha_{kl} + 2\beta^l(\partial_j\beta^k)\partial_i\alpha_{kl} + 2\beta^l(\partial_i\beta^k)\partial_j\alpha_{kl}$$

$$+2\alpha_{kl}\beta^k\partial_i\partial_j\beta^l + 2\alpha_{kl}(\partial_i\beta^k)(\partial_j\beta^l)\Big] \tag{6.452}$$

$$-\frac{1}{2}x_0^l\left[\beta^k\partial_i\partial_j\alpha_{kl} + \alpha_{kl}\partial_i\partial_j\beta^k + (\partial_i\alpha_{kl})(\partial_j\beta^k) + (\partial_j\alpha_{kl})(\partial_i\beta^k)\right]$$

$$+\frac{1}{4}\dot{x}_0^k\dot{x}_0^l\partial_i\partial_j\alpha_{kl}\,. \tag{6.453}$$

Here, as usual, T denotes the transposition of matrices and all matrices are evaluated at the classical trajectory $x_0(\tau)$.

Then we obtain

$$\int_{\mathcal{M}} \mathcal{D}x(\tau)\exp\left[-S(t,x|t',x')\right] = \exp\left[-S(x_0(\tau))\right] \tag{6.454}$$

$$\times \int_{\mathcal{M}} \mathcal{D}y(\tau)\exp\left[-\frac{1}{2}\int_{t'}^{t} d\tau\ \langle y(\tau), H(\tau)y(\tau)\rangle\right]\exp[-V(y(\tau))].$$

6.9.4 Gaussian Path Integrals

By expanding the $\exp(-V)$ in a powers series in V we get a perturbation theory with only *Gaussian path integrals*

$$\mathcal{G}^{i_1\ldots i_k}(\tau_1,\ldots,\tau_k) = \tag{6.455}$$

$$\times \int_{\mathcal{M}_y} \mathcal{D}y(\tau)\exp\left\{-\frac{1}{2}\int_{t'}^{t} d\tau\ \langle y(\tau), H(\tau)y(\tau)\rangle\right\} y^{i_1}(\tau_1)\cdots y^{i_k}(\tau_k)\,.$$

Such integrals can be evaluated exactly in the same way as Gaussian integrals in finite dimensions (see Sec. 1.2).

As far as the integrals of even monomials are concerned, they are computed as follows. Formally, we would like to take the limit $N \to \infty$ in eq. (1.25). However, there is a factor $\pi^{N/2}$ on the right-hand side of this equation, which, of course, does not have a limit as $N \to \infty$. However, such a factor can be absorbed in the measure. That is, if we replace dx by $dx\,\pi^{-N/2}$ in eq. (1.25), then the dimension does not appear on the right hand-side at all. All we need then is to define the inverse operator $G = H^{-1}$ and its determinant $\mathrm{Det}\,H$.

The inverse of the operator H is nothing but its Green function $G^{ij}(\tau,\tau')$ defined by

$$H_{ij}(\tau)G^{jk}(\tau,\tau') = \delta^k{}_i\delta(\tau-\tau')\,. \tag{6.456}$$

The determinant of the operator H is one of the spectral invariants of the operator H called the *functional determinant*. That is why we denote it by $\operatorname{Det} H$ instead of $\det H$. It can be defined in terms of the zeta function $\zeta(s)$ of the operator H introduced in Sec. 1.16 as follows (1.189)

$$\operatorname{Det} H = \exp\left[-\zeta'(0)\right]\,. \tag{6.457}$$

Moreover, the determinant $\operatorname{Det} H$ can also be absorbed in the definition of the measure $\mathcal{D}x(\tau)$ of the path integral. The normalization of the measure is a separate complicated issue. In any way the normalization should be obtained by comparing the path integral with the initial condition for the heat kernel and/or with known solvable cases.

With all this in mind we define the basic Gaussian path integral by (compare with (1.25))

$$\begin{aligned}&\int\limits_{\mathcal{M}_y}\mathcal{D}y(\tau)\exp\left\{\int\limits_{t'}^{t}d\tau\ \left[-\frac{1}{2}\left\langle y(\tau),H(\tau)y(\tau)\right\rangle+\left\langle J(\tau),y(\tau)\right\rangle\right]\right\}\\ &=(\operatorname{Det}H)^{-1/2}\exp\left\{\frac{1}{2}\int\limits_{t'}^{t}d\tau\int\limits_{t'}^{t}d\tau'\ \left\langle J(\tau),G(\tau,\tau')J(\tau')\right\rangle\right\}\,,\end{aligned} \tag{6.458}$$

where $J=(J_i)$ is an arbitrary vector.

Now, by expanding both sides of this integral in a functional powers series in the powers of J we obtain all Gaussian integrals (6.455). The integrals of odd monomials vanish, as usual,

$$\mathcal{G}^{i_1\cdots i_{2k+1}}(\tau_1,\dots,\tau_{2k+1}) = 0\,, \tag{6.459}$$

and the integrals of even monomials are (compare with (1.29))

$$\begin{aligned}\mathcal{G}^{i_1\cdots i_{2k}}(\tau_1,\dots,\tau_{2k}) &= \frac{(2k)!}{2^k k!}\,(\operatorname{Det}H)^{-1/2}\\ &\quad\times\operatorname{Sym}G^{i_1\,i_2}(\tau_1,\tau_2)\cdots G^{i_{2k-1}\,i_{2k}}(\tau_{2k-1},\tau_{2k})\,.\end{aligned}$$

Here the operator Sym denotes the complete symmetrization over the arguments of the Green function including the discrete indices. For example,

$$\begin{aligned}\operatorname{Sym}G^{i_1\,i_2}(\tau_1,\tau_2)G^{i_3\,i_4}(\tau_3,\tau_4) &= \frac{1}{3}\Big\{G^{i_1\,i_2}(\tau_1,\tau_2)G^{i_3\,i_4}(\tau_3,\tau_4)\\ &\quad+G^{i_1\,i_3}(\tau_1,\tau_3)G^{i_2\,i_4}(\tau_2,\tau_4)+G^{i_1\,i_4}(\tau_1,\tau_4)G^{i_2\,i_3}(\tau_2,\tau_3)\Big\}\,.\end{aligned} \tag{6.460}$$

Let us consider the (trivial) case of operators with constant coefficients (compare with Sec. 4.3.5). In this case the classical trajectories are the straight lines

$$x_0^i(\tau) = \frac{(x^i - x'^i)}{t - t'}(\tau - t') + x'^i\,, \tag{6.461}$$

and therefore, the classical action is

$$S(x_0(\tau)) = \frac{1}{4(t-t')}\left\langle (x-x'), A^{-1}(x-x')\right\rangle - \frac{1}{2}\left\langle \beta, A^{-1}(x-x')\right\rangle + \left[\frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle + \gamma\right](t-t')\,. \tag{6.462}$$

The operator H has the form

$$H_{ij} = -\frac{1}{4}\alpha_{ij}\frac{d^2}{d\tau^2}\,, \tag{6.463}$$

and all higher order terms, $V(y) = 0$. Therefore, the path integral (6.430) gives the correct heat kernel provided we normalize the Gaussian path integral measure by

$$\int\limits_{\mathcal{M}_y} \mathcal{D}y(\tau) \exp\left[-\frac{1}{2}\int\limits_{t'}^{t} d\tau\ \langle y(\tau), H(\tau)y(\tau)\rangle\right] = [4\pi(t-t')]^{-n/2}(\det A)^{-1/2}\,. \tag{6.464}$$

6.10 Notes

In this chapter we presented briefly some advanced methods for the calculation of the heat kernel following our papers [6, 7, 8, 12]. For the most part these are some algebraic methods that exploit some symmetries of the model; these symmetries lead to the existence of some finite-dimensional Lie algebra that enables one to calculate the heat semigroup and then the heat kernel. Therefore, some background in Lie groups and differential geometry is required to take advantage of these methods. Good references on Lie groups and symmetric spaces are [15, 33, 43, 44, 50, 51]. We followed mainly our papers [6, 7, 8, 12, 13]. Some other useful references on this subject are [21, 45, 47]. Exact solvable models of quantum mechanics are treated in [2, 39, 61]. The classic references on path integrals are [38, 70]; the book [70] contains an extensive bibliography on path integrals for further study.

Part IV
Applications

Chapter 7
Stochastic Processes

Abstract In this chapter we introduce the basic concepts of probability and stochastic processes such as Wiener process and Poisson process. Next, we present some basic concepts of stochastic calculus and discuss stochastic differential equations, in particular, such fundamental topics as Itô's Lemma and forward and backward Kolmogorov equations.

7.1 Stochastic Processes

7.1.1 Basic Concepts of Probability

It is an empirical fact that the prices of financial assets are random. The mathematical model of a random quantity is a random variable. To define it we first review some basic probability concepts following [80, 66, 32].

The basic model of probability theory is a repeatable *experiment*, which consists of a *procedure* and *observations*. The mother of all probability theory is dice which have been used by people since ancient times. Classical dice is a pair of cubes marked on each of their six faces with different number of dots, from 1 to 6. An example of an experiment could be: roll dice (procedure) and observe the number of dots, that is, two integers (observation).

An *outcome* ω of an experiment is any possible observation of that experiment. In the dice experiment an outcome is an (unordered) pair of integers (from 1 to 6) such as $\{2, 3\}$.

The *sample space* Ω of an experiment is the set of all possible outcomes. The sample space in the dice experiment is the set

$$\Omega = \{\{n, m\} \mid n, m = 1, 2, 3, 4, 5, 6\}\,. \tag{7.1}$$

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_7

It is not difficult to see that there are 21 different outcomes, so that in this example Ω is a finite set. In general, Ω can be an infinite set, countable or uncountable.

In the dice experiment an *event* A could be characterized by a condition like this: "in the outcome $\{n, m\}$ both n and m are greater than or equal to 4". Then the event can be identified with the collection of outcomes which satisfy this condition, that is,

$$A = \{\{4,4\},\{4,5\},\{4,6\},\{5,5\},\{5,6\},\{6,6\}\}\ . \tag{7.2}$$

From that point of view, an *event* A is an arbitrary set of outcomes of an experiment. Of course, every outcome ω defines an event by itself, $B_\omega = \{\omega\}$. Such events contain just one outcome. Then the total *event space* $\mathcal{F}$ is the set of all possible events containing all possible combinations of outcomes. This is nothing but the power set of the sample space Ω.

These definitions work for a finite sample space and even for a countable sample space. However, for an uncountable sample space Ω one encounters the following difficulty. The primary focus of probability theory is an attempt to assign to every event A a *probability* $P(A)$ (a non-negative number less than or equal to 1). A subset $A \subset \Omega$ of the sample space Ω for which this is possible is called *measurable*. In the case of an uncountable sample space Ω there are subsets which are not measurable. Therefore, such subsets cannot be interpreted as events, since such 'events' would not have a well-defined probability. Thus one should include in the event space $\mathcal{F}$ only measurable subsets. Such collection $\mathcal{F}$ of subsets of Ω must contain the empty set $\emptyset$, the whole set Ω, and it must be closed under taking complements and countable unions of sets. Such a family of subsets of the set Ω is called a *σ-algebra* on Ω and the pair $(\Omega, \mathcal{F})$ is called a *measurable space*.

Notice that a σ algebra is by no means unique. We may be not interested in the whole σ-algebra $\mathcal{F}$, but only in its subset containing a collection $\mathcal{A}$ of events, which is not necessarily a σ-algebra. Then there is the smallest σ-algebra $\mathcal{H}$ that contains $\mathcal{A}$, that is, $\mathcal{A} \subset \mathcal{H}$. Then the σ-algebra $\mathcal{H}$ is said to be *generated* by the collection of events $\mathcal{A}$. For example, the σ-algebra generated by a single event A is

$$\mathcal{H}_A = \{\emptyset, A, A^c, \Omega\}, \tag{7.3}$$

where $A^c = \Omega - A$ is the complement of A.

The *probability* $P(A)$ of an event A is defined by specifying an additive real-valued non-negative function $P : \mathcal{F} \to [0,1]$ on the σ-algebra $\mathcal{F}$, called a *probability measure*, that satisfies the natural conditions:

$$0 \le P(A) \le 1 \qquad \text{for any} \qquad A \in \mathcal{F}, \tag{7.4}$$

$$P(\emptyset) = 0\,, \qquad P(\Omega) = 1, \tag{7.5}$$

and for any countable collection of mutually disjoint sets (mutually exclusive events) $\{A_i\}_{i=1}^{\infty}$

$$P\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} P(A_i)\,. \tag{7.6}$$

Then the triple $(\Omega, \mathcal{F}, P)$ is called a *probability space*.

For example, if our dice is perfect, we could assign equal probabilities to each outcome, then for any outcome ω, $P(\omega) = 1/21$, and the probability of the event A given by (7.2) is $P(A) = 6/21 = 2/7$ since the event A contains 6 outcomes of equal probability.

Given a probability measure P and an event B we define the *conditional probability* $P(A|B)$ of an event A given B by

$$P(A|B)P(B) = P(A \cap B)\,. \tag{7.7}$$

This defines a new probability measure called the *conditional probability measure* given the occurrence of the event B. Two events A and B are *independent* if

$$P(A \cap B) = P(A)P(B)\,, \tag{7.8}$$

or if

$$P(A|B) = P(A), \qquad P(B|A) = P(B)\,. \tag{7.9}$$

It is useful to generalize the concept of independence of events to independence of σ-algebras. We say that two σ-algebras are *independent* if any pair of events from each of the σ-algebras are independent, that is, the σ-algebras $\mathcal{F}$ and $\mathcal{H}$ are independent if for any $A \in \mathcal{F}$ and any $B \in \mathcal{H}$, the events A and B are independent.

An important example of a measurable space is $(\mathbb{R}, \mathcal{B})$, where $\mathcal{B}$ is the so-called *Borel σ-algebra* on $\mathbb{R}$ containing all open sets, all closed sets, all countable unions of closed sets, etc. The elements of the Borel σ-algebra are called *Borel sets*. An example of a probability space $(\mathbb{R}, \mathcal{B}, P)$ can be obtained as follows. Let us define the *characteristic function* $\chi_B : \mathbb{R} \to \{0, 1\}$ of a Borel set B by

$$\chi_B(x) = \begin{cases} 1, & \text{if} \quad x \in B, \\ 0, & \text{if} \quad x \notin B. \end{cases} \tag{7.10}$$

In many probability books this function is called the *indicator function* and denoted by $1_{x \in B}$. Let dx be the usual Lebesgue measure on $\mathbb{R}$ and $f : \mathbb{R} \to [0, 1]$ be a continuous non-negative function on $\mathbb{R}$, called a *probability density*, such that

$$\int_{-\infty}^{\infty} f(x)dx = 1\,. \tag{7.11}$$

Then a probability measure on the Borel σ-algebra $\mathcal{B}$ can be defined by

$$P(B) = \int_{-\infty}^{\infty} \chi_B(x) f(x) dx = \int_B f(x) dx \,. \tag{7.12}$$

A generalization to $\mathbb{R}^n$ is obvious.

Another important example is a discrete distribution constructed as follows. Let $y \in \mathbb{R}$ be a given point on the real line. Then we can define a probability measure P_y on $\mathcal{B}$ which is not continuous but rather concentrated at a single point $y \in \mathbb{R}$,

$$P_y(B) = \chi_B(y) \,. \tag{7.13}$$

This defines the *Dirac distribution* δ_y by

$$\int_B \delta_y(x) dx = \chi_B(y) \,, \tag{7.14}$$

or, formally,

$$\delta_y(x) = \delta(x - y) \,, \tag{7.15}$$

where $\delta(x)$ is the Dirac delta-function.

More generally, a discrete distribution can be defined by

$$f(x) = \sum_{i=1}^{\infty} c_i \delta(y_i - x) \,, \tag{7.16}$$

where $c_i \geq 0$ are non-negative real constants such that $\sum_{i=1}^{\infty} c_i = 1$. This defines the probability measure

$$P(B) = \sum_{i=1}^{\infty} c_i \chi_B(y_i) \,. \tag{7.17}$$

Of course, in general, we could have a combination of a continuous distribution and a discrete distribution.

A random quantity can take different values. The mathematical model of such a quantity is a real-valued *random variable* $X : \Omega \to \mathbb{R}$. Let us go back to our dice experiment. An example of a random variable would be a function that assigns to each outcome the sum of the number of dots on the dice, that is, for any outcome $\omega = \{n, m\}$ we assign

$$X(\{n, m\}) = n + m \,. \tag{7.18}$$

A random variable X is called *finite* if the function X has a finite range $X(\Omega)$ and *discrete* if the range $X(\Omega)$ is countable. The random variable X defined above can take all positive integers from 2 to 12, that is, the range of this random variable is

$$X(\Omega) = \{n \in \mathbb{Z}_+ \mid 2 \leq n \leq 12\} \,, \tag{7.19}$$

so X is a finite random variable.

Given a real-valued random variable X there is the smallest σ-algebra containing the inverse images of all open sets in $\mathbb{R}$. One can show that this σ-algebra is equal to the σ-algebra of inverse images of all Borel sets

$$\mathcal{H}_X = \{X^{-1}(B) \mid B \in \mathcal{B}\}\,, \tag{7.20}$$

where $X^{-1}(B)$ is the inverse image of the set B, that is, the set of all elements $\omega \in \Omega$ such that $X(\omega) \in B$ and $\mathcal{B}$ is the Borel σ-algebra on $\mathbb{R}$. The σ-algebra $\mathcal{H}_X$ is said to be *generated* by the random variable X.

A random variable X induces a probability measure $\mu_X : \mathcal{B} \to [0,1]$, called the *distribution* of X, on $(\mathbb{R}, \mathcal{B})$, by

$$\mu_X(B) = P(X^{-1}(B))\,, \tag{7.21}$$

in other words,

$$\mu_X(B) = P(X \in B)\,. \tag{7.22}$$

For a real-valued random variable X this defines the *cumulative distribution function* $F_X : \mathbb{R} \to [0,1]$ by

$$F_X(x) = \mu_X((-\infty, x]) = P(X \leq x)\,. \tag{7.23}$$

A random variable X is called a *continuous random variable* if it has a continuous cumulative distribution function F_X.

If the random variable has a continuous *probability density function* $f_X : \mathbb{R} \to [0,1]$ (described above), then the cumulative distribution

$$F_X(x) = \int_{-\infty}^{x} f_X(y)dy \tag{7.24}$$

is not just continuous but also differentiable and

$$F'_X(x) = f_X(x)\,. \tag{7.25}$$

More gnerally, for any Borel set B

$$\mu_X(B) = \int_B f_X(x)dx\,, \tag{7.26}$$

which means

$$d\mu_X(x) = f_X(x)dx\,. \tag{7.27}$$

The same formulas formally hold for a discrete distribution but then the probability density is not a usual continuous function but is allowed to have Dirac δ-functions.

Two random variables X and Y are called *independent* if the σ-algebras they generate are independent. It is instructive to put it in another form.

Given two random variables X and Y we define the *joint probability distribution* $\mu_{X,Y} : \mathcal{B} \times \mathcal{B} \to [0,1]$ of X and Y by: for any $A, B \in \mathcal{B}$

$$\mu_{X,Y}(A,B) = P(X^{-1}(A) \cap Y^{-1}(B)) \,. \tag{7.28}$$

The random variables X and Y are *independent* if for any Borel sets A and B, the events $X \in A$ and $Y \in B$ are independent, that is,

$$\mu_{X,Y}(A,B) = \mu_X(A)\mu_Y(B) \,. \tag{7.29}$$

This defines the *joint cumulative distribution* $F_{X,Y}$ by

$$F_{X,Y}(x,y) = \mu_{X,Y}\big((-\infty,x],(-\infty,y]\big) \,, \tag{7.30}$$

and *joint probability density function* $f_{X,Y}$ by

$$F_{X,Y}(x,y) = \int_{-\infty}^{x} \int_{-\infty}^{y} f_{X,Y}(x,y)\, dx\, dy \,. \tag{7.31}$$

Then the random variables X and Y are independent if

$$F_{X,Y}(x,y) = F_X(x)F_Y(y) \,, \tag{7.32}$$

which also means

$$f_{X,Y}(x,y) = f_X(x)f_Y(y) \,. \tag{7.33}$$

The *expected value* of the random variable X with respect to the probability measure P is defined by

$$E(X) = \int_\Omega X(\omega) dP(\omega) = \int_{-\infty}^{\infty} x\, d\mu_X(x) \,. \tag{7.34}$$

Notice that if two real-valued random variables $X, Y : \Omega \to \mathbb{R}$ are independent then

$$E(XY) = E(X)E(Y) \,. \tag{7.35}$$

Similarly, for a real valued function $\varphi : \mathbb{R} \to \mathbb{R}$

$$E(\varphi(X)) = \int_{-\infty}^{\infty} \varphi(x)\, d\mu_X(x) \,. \tag{7.36}$$

This enables one to define the *variance*

$$\mathrm{Var}(X) = E\left[(X - m_X)^2\right] = E(X^2) - m_X^2 \,, \tag{7.37}$$

where

$$m_X = E(X) \tag{7.38}$$

is the expected value, and the *standard deviation*

$$\sigma(X) = \sqrt{\mathrm{Var}(X)}\,. \tag{7.39}$$

Notice that the variance is non-negative, so that the standard deviation is well defined.

A dual description of a random variable X is provided by its *characteristic function* defined for any $z \in \mathbb{R}$ by

$$\varphi_X(z) = E\left(e^{izX}\right)\,, \tag{7.40}$$

which is nothing but the Fourier transform of the probability density function

$$\varphi_X(z) = \int_{-\infty}^{\infty} e^{izx} f_X(x)\,dx\,. \tag{7.41}$$

This function should not be confused with the characteristic function χ_A of a set A defined above.

For a real valued random variable $X : \mathcal{B} \to \mathbb{R}$ the function

$$f_X(x) = (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{(x-m)^2}{2\sigma^2}\right]\,. \tag{7.42}$$

defines the *normal distribution*. A random variable with a normal distribution is called *normal* (or *Gaussian*). The nice property of Gaussian integrals is that they can be computed exactly (see Sec. 1.2). By using eqs. (1.19) and (1.20) we see that the parameter m is the expected value and the parameter σ^2 is the variance of the normal distribution. Also, by using eq. (1.18) it is not difficult to show that the characteristic function of the normal random variable is

$$\varphi_X(z) = \exp\left(-\frac{\sigma^2}{2}z^2 + izm\right)\,. \tag{7.43}$$

Another important example of a (one-dimensional) real-valued random variable $X : \mathcal{B} \to \mathbb{R}$ is so-called *Poisson random variable* defined by the discrete distribution

$$f_X(x) = e^{-m} \sum_{k=0}^{\infty} \frac{m^k}{k!}\delta(x-k)\,. \tag{7.44}$$

The presence of the delta function makes the evaluation of the integrals trivial. It is a straightforward calculation to see that the parameter m is the expected value of the Poisson random variable. Also, by summing the series one can show that the characteristic function of the Poisson random variable is

$$\varphi_X(z) = \exp\left[m\left(e^{iz} - 1\right)\right]\,. \tag{7.45}$$

The above concepts can be easily generalized to a *random vector* $X = (X^i) = (X^1, \cdots, X^n)$ with values in $\mathbb{R}^n$ as a function $X : \Omega \to \mathbb{R}^n$. A random vector is simply a collection of n random variables. For such an n-

dimensional random vector the *covariance matrix* $\mathrm{Cov}(X^i, X^j)$ is an $n \times n$ symmetric real matrix defined by

$$\mathrm{Cov}(X^i, X^j) = E\left[\left(X^i - m_X^i\right)\left(X^j - m_X^j\right)\right] = E(X^i X^j) - m_X^i m_X^j\,, \quad (7.46)$$

where $m_X^i = E(X^i)$ is the expected value of the random vector X. The *correlation matrix* $\rho(X^i, X^j)$ is defined by

$$\rho(X^i, X^j) = \frac{\mathrm{Cov}(X^i, X^j)}{\sigma(X^i)\sigma(X^j)}\,. \quad (7.47)$$

It is not difficult to see that the covariance matrix and, hence, the correlation matrix are positive-definite.

The random vector X is *normal* if it has the *n-dimensional normal distribution* given by

$$f_X(x) = (2\pi)^{-n/2}\sqrt{\det A}\,\exp\left[-\frac{1}{2}\,\langle (x-m), A(x-m)\rangle\right]\,, \quad (7.48)$$

where $m = (m^i)$ is a n-vector, $A = (A_{ij})$ is a symmetric real positive definite $n \times n$ matrix, and

$$\langle (x-m), A(x-m)\rangle = \sum_{i,j=1}^{n} (x^i - m^i) A_{ij} (x^j - m^j)\,. \quad (7.49)$$

You should have noticed that the indices on the variables x^i are upper indices, whereas on the matrix A_{ij} the indices are in low position. This is the first example of a general rule in linear algebra and, more generally, in differential geometry that an invariant, a number, is obtained only when multiplying objects of different kinds that are in a certain sense *dual* to each other; strictly speaking, they belong to different vector spaces, for example, vectors and covectors etc. That is why, to avoid confusion, it is customary to place vector indices in the upper position and covector indices in the low position. We will use this rule throughout this book (more on this later).

By using the multi-dimensional Gaussian integrals (1.26) and (1.27) one can show that the expected value of a normal random vector is equal to the vector m,

$$m^i = E(X^i) \quad (7.50)$$

and the covariance matrix is equal to the inverse of the matrix A, that is,

$$\mathrm{Cov}(X^i, X^j) = A^{ij}\,, \quad (7.51)$$

where A^{ij} are the enries of the inverse matrix $A^{-1} = (A^{ij})$.

An important concept is the *conditional expected value* of a random variable. Let $X : \Omega \to \mathbb{R}$ be a random variable on a probability space $(\Omega, \mathcal{F}, P)$.

Given an event $A \in \mathcal{F}$, the conditional expectation of X given A is defined by

$$E(X|A)P(A) = \int_A X(\omega)dP(\omega)\,. \tag{7.52}$$

More generally, given a sub-σ-algebra, $\mathcal{H} \subset \mathcal{F}$, of the σ-algebra $\mathcal{F}$, the conditional expected value of X given $\mathcal{H}$ is defined as the unique function $E(X|\mathcal{H}) : \Omega \to \mathbb{R}$ (that is, $E(X|\mathcal{H})$ is a random variable) such that for any event $A \in \mathcal{H}$

$$\int_A E(X|\mathcal{H})(\omega)dP(\omega) = E(X|A)P(A)\,, \tag{7.53}$$

in particular,

$$E(X) = \int_\Omega E(X|\mathcal{H})(\omega)dP(\omega)\,. \tag{7.54}$$

A time-dependent random quantity takes random values at each time. A mathematical model of such quantity is a *stochastic process*, which is a one-parameter family of random variables $\{X_t\}$, where $t \in [0, \infty)$ is a real-valued non-negative parameter called the time. Then for each fixed t this defines a random variable, $\omega \mapsto X_t(\omega)$, and for a fixed outcome $\omega \in \Omega$ this defines a function $t \mapsto X_t(\omega)$ called a *path* of X_t. The increments of the stochastic process, $X_t - X_s$, with $s < t$, are also random variables. We will be interested in the formal infinitesimal increments $dX_t = X_{t+dt} - X_t$, where dt stands for a infinitesimally small time step.

A stochastic process X_t is said to satisfy *Markov property*, or to be *Markov*, if the future behavior of the process, given what has happened up to the time t, is the same as the behavior obtained when starting the process at X_t. Roughly speaking, a Markov process does not have memory, it is local in time. The prices of financial assets as functions of time, for example, are believed to be Markov.

A *filtration* on the probability space $(\Omega, \mathcal{F}, P)$ is an increasing one-parameter family of sub-σ-algebras $\{\mathcal{F}_t\}$ of $\mathcal{F}$, with $t \geq 0$, that is, $\mathcal{F}_s \subset \mathcal{F}_t \subset \mathcal{F}$ for any $s < t$. Given a stochastic process X_t there is always a filtration $\mathcal{F}_t^X$ generated by the family of random variables $\{X_s; s \leq t\}$. A stochastic process X_t is a *martingale* with respect to a filtration $\mathcal{F}_t$ and a probability measure P if for all $s \leq t$

$$E(X_t|\mathcal{F}_s) = X_s\,. \tag{7.55}$$

7.1.2 Wiener Process

One of the most important stochastic processes is the Wiener process. The *Wiener process* is a real-valued (one-dimensional) stochastic process $W_t : \mathcal{B} \to \mathbb{R}$ characterized by the properties:

1. $W_0 = 0$,

2. W_t is almost surely continuous,
3. the increments $W_t - W_s$, for any non-overlapping time intervals are independent and normally distributed with the mean value 0 and the variance $|t-s|$.

The Wiener process has many nice properties. We mention just two most important ones for us:

1. W_t is Markov, and
2. W_t is a martingale with respect to the filtration $\{\mathcal{F}_t^W\}$ generated by $\{W_s; s \le t\}$.

Since the increments are normal with mean 0 and variance $(t-s)$ we have

$$E(W_t - W_s) = 0, \tag{7.56}$$

$$E\left[(W_t - W_s)^2\right] = |t-s|\,, \tag{7.57}$$

in particular, for $dW_t = W_{t+dt} - W_t$,

$$E(dW_t) = 0, \tag{7.58}$$

$$E\left[(dW_t)^2\right] = dt\,. \tag{7.59}$$

By setting $s = 0$ we see that the random variable W_t at a fixed t is normally distributed with the mean value 0 and the variance t, that is, it has the distribution density

$$p(t;x) = (2\pi t)^{-1/2} \exp\left(-\frac{x^2}{2t}\right). \tag{7.60}$$

We would like to observe right away that this function is the solution of the partial differential equation

$$\frac{\partial}{\partial t} p(t,x) = \frac{1}{2}\frac{\partial^2}{\partial x^2} p(t,x) \tag{7.61}$$

for any $t \ge 0$ and $x \in \mathbb{R}$ with the initial condition

$$p(0,x) = \delta(x)\,. \tag{7.62}$$

This equation is called the *heat equation* (or *diffusion equation*). Thus, $p(t,x)$ is the fundamental solution of the heat equation called the *heat kernel*. This is our first and simplest example of a heat kernel. This whole book is about the heat kernel for more general situations.

The heat equation is a particular form of the evolution equation of the form

$$\left(\frac{\partial}{\partial t} + L\right) u(t,x) = 0\,, \tag{7.63}$$

where L is some operator acting on a function of the space variable x that does not depend on t. The solution of such an evolution equation can be written in the form

$$u(t,x) = \exp(-tL)u_0(x)\,, \tag{7.64}$$

where $u_0(x) = u(0,x)$. Here $\exp(-tL)$ is an operator called the *heat semigroup* and the operator L is the generator of the semigroup. This means that the function $p(t,x)$ can be written in the form

$$p(t,x) = \exp\left(\frac{1}{2}t\partial_x^2\right)\delta(x)\,, \tag{7.65}$$

where $\partial_x = \frac{\partial}{\partial x}$. Indeed, by using the Fourier integral representation of the delta-function

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{i\omega x}\,, \tag{7.66}$$

we obtain

$$p(t,x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \exp\left(-\frac{1}{2}t\omega^2 + i\omega x\right)\,, \tag{7.67}$$

which gives back the result (7.60).

The Wiener process is a fundamental tool in describing many real-world random phenomena, such as diffusion, heat transfer, behavior of prices of financial assets etc. In particular, it is a mathematical model of the physical phenomenon of random movement of pollen particles suspended in a fluid (observed by Robert Brown in 1872 and called now *Brownian motion*). This phenomenon puzzled physicists for quite a while until Albert Einstein in 1905 finally explained the physical origin of this random behavior; it is caused by collisions of pollen particles with molecules of the fluid (the random behavior of the molecules is determined, in turn, by the temperature). Note that today many people just call the Wiener process itself Brownian motion. We will be using the Wiener process to model *continuous random fluctuations* of asset prices.

7.1.3 Poisson Process

Another important example of a stochastic process is the Poisson process. It is a so-called *counting process*, that is, the process starts at $t = 0$ and counts the occurrences of some incidents called *arrivals*. This means that for a fixed outcome ω the path $Q_t(\omega)$ is a piecewise constant non-negative non-decreasing function of time. Such paths are, in general, discontinuous with the jumps occurring exactly at the arrival times.

Let $\lambda > 0$ be a positive real number. The *Poisson process* of rate λ is an integer-valued stochastic process $Q_t : \mathcal{B} \to \mathbb{Z}$, characterized by the properties:

1. $Q_0 = 0$,
2. Q_t is integer-valued and non-decreasing,
3. the increments $Q_t - Q_s$, for non-overlapping intervals are independent and have the Poisson distribution with the expected value $\lambda|t-s|$.

The increments of the Poisson process satisfy, for $s < t$,

$$Q_t - Q_s \geq 0\,, \tag{7.68}$$

and

$$E(Q_t - Q_s) = \lambda(t-s)\,. \tag{7.69}$$

For the infinitesimal increments $dQ_t = Q_{t+dt} - Q_t$ this means that

$$dQ_t = \begin{cases} 1 & \text{with probability } \lambda dt\,, \\ 0 & \text{with probability } (1-\lambda dt)\,, \end{cases} \tag{7.70}$$

and, therefore,

$$E(dQ_t) = \lambda\, dt\,. \tag{7.71}$$

By setting $s = 0$ we see that the random variable Q_t for a fixed t is Poisson with the mean value λt, that is, it has the distribution density

$$q(t;x) = e^{-\lambda t} \sum_{k=0}^{\infty} \frac{\lambda^k t^k}{k!} \delta(x-k)\,. \tag{7.72}$$

This function satisfies the evolution equation

$$\frac{\partial}{\partial t} q(t,x) = -\lambda\left[q(t,x) - q(t,x-1)\right]\,, \tag{7.73}$$

with initial condition

$$q(0,x) = \delta(x)\,. \tag{7.74}$$

In contrast to the equation (7.61) this equation is not a partial differential equation, but rather a functional equation, which is non-local in x. However, if we introduce an operator J by

$$Jf(x) = f(x-1)\,, \tag{7.75}$$

then the eq. (7.73) can be written as the evolution equation

$$\left[\frac{\partial}{\partial t} + \lambda(1-J)\right] q(t,x) = 0\,, \tag{7.76}$$

with the solution

$$q(t,x) = \exp\left[\lambda t(J-1)\right]\delta(x)$$
$$= e^{-\lambda t}\exp\left(\lambda t J\right)\delta(x)\,. \tag{7.77}$$

Indeed, by expanding the exponent in powers of J, we obtain back the result (7.72).

The Poisson process also has Markov property (no memory). Many real-world phenomena are believed to be well-modeled by the Poisson processes: the number of customers in a queue, the number of insurance claims, the number of particles emitted via radioactive decay, the number of raindrops, the number of phone calls at a switchboard, the number of requests from a web server, etc. We will be using the Poisson process to model (rare but real) *random jumps* in the prices of financial assets.

7.2 Stochastic Calculus

7.2.1 Stochastic Differential Equations

A *stochastic differential equation* is a differential equation that depends on one or more given stochastic processes. Of course, a solution of a stochastic differential equation is also a stochastic process. We will only consider in this book (systems of) ordinary stochastic differential equations of first order. Since stochastic processes are usually not differentiable as functions of time, they are written, most of the time, in the differential form by specifying the infinitesimal increment dX_t of the unknown stochastic process X_t (which itself is a random variable) in terms of a given stochastic process.

For example, we may require that dX_t is a normally distributed random variable with expected value $a\,dt$ and variance b^2dt and is independent of the past behavior of the process, where a and b are two constants, that is,

$$dX_t = a\,dt + b\,dW_t\,, \tag{7.78}$$

where W_t is a Wiener stochastic process. The first term in this equation is deterministic and is called the *drift* term, and the second term in this equation is stochastic and is called the *diffusion term*. Such process is called the *drift-diffusion process*. The solution is, of course, the sum of a linear deterministic term and a stochastic term

$$X_t = X_0 + at + bW_t\,. \tag{7.79}$$

More generally, we may consider a stochastic differential equation

$$dX_t = \mu X_t\,dt + \sigma X_t\,dW_t\,, \tag{7.80}$$

where μ and σ are some constants. Such differential equation describes a so-called *log-normal process*. The parameter μ is called the *drift* and the parameter σ is the *volatility*.

You might think that by changing the variable according to $Y_t = \log X_t$, so that $X_t = \exp(Y_t)$, and applying the chain rule of the usual calculus we would get the previous equation

$$dY_t = \mu\, dt + \sigma\, dW_t\,, \tag{7.81}$$

so that the solution of the original equation is

$$X_t = X_0 \exp\left(\mu t + \sigma W_t\right)\,. \tag{7.82}$$

Well, it turns out that this is wrong! The correct solution is

$$X_t = X_0 \exp\left[\left(\mu - \frac{\sigma^2}{2}\right) t + \sigma W_t\right]\,, \tag{7.83}$$

which means that the stochastic term in the differential equation (volatility) affects the deterministic part of the solution. The natural question is: "What is the origin of the correction term $-\sigma^2/2$ in the drift? Have we done something wrong by applying the rules of the usual calculus?" The answer is: Yes! When dealing with stochastic processes the rules of the usual calculus do not apply. They should be modified in a very specific way resulting in so-called *stochastic calculus*. The most important rule of stochastic calculus is a modified chain rule called *Itô's Lemma*. We will explain what it means in the next section.

Now, in general, we may require that dX_t is a normally distributed random variable with expected value $a(t, X_t)dt$ and variance $b^2(t, X_t)dt$ and is independent of the past behavior of the process, where $a, b : [0, \infty) \times \mathbb{R} \to \mathbb{R}$ are two functions of two real variables. That is,

$$dX_t = a(t, X_t)dt + b(t, X_t)dW_t\,. \tag{7.84}$$

This is a classical example of a stochastic differential equation. There is a theorem that guarantees the existence and uniqueness of the solution of this equation under certain conditions on the functions a and b [66]. Such a solution is given by the so-called *Itô's stochastic integral*. A stochastic process that satisfies such a stochastic differential equation is called an *Itô process*, (or *Itô diffusion*).

The Itô process can be generalized to higher-dimensions. First, we can increase the number of diffusion terms. Let $W_t = (W_t^i)$ be an m-dimensional Wiener process, such that

$$E(dW_t^i\, dW_t^j) = \rho^{ij} dt\,, \tag{7.85}$$

where $\rho = (\rho^{ij})$ is a real symmetric $m \times m$ matrix, called the *correlation matrix*. Let $a : [0, \infty) \times \mathbb{R} \to \mathbb{R}$ be a real-valued function of two variables, and $b : [0, \infty) \times \mathbb{R} \to \mathbb{R}^m$ be a m-vector-valued function of two variables. Then the Itô process X_t is defined by

$$dX_t = a(t, X_t)dt + \sum_{j=1}^{m} b_j(t, X_t)dW_t^j \,. \tag{7.86}$$

Even more generally, one can consider a vector-valued Itô process. Let $a = (a^\mu) : [0, \infty) \times \mathbb{R}^n \to \mathbb{R}^n$ be a n-vector-valued function of $(n + 1)$ variables, and $b = (b^\mu{}_j) : [0, \infty) \times \mathbb{R}^n \to \mathbb{R}^{nm}$ be a $n \times m$-matrix-valued function of $(n + 1)$ variables. Then the Itô process $X_t = (X_t^\mu)$ is defined by

$$dX_t^\mu = a^\mu(t, X_t)dt + \sum_{j=1}^{m} b^\mu{}_j(t, X_t)dW_t^j \,. \tag{7.87}$$

One can consider more general stochastic differential equations that incorporate both diffusion and jumps. Let W_t be a Wiener process and Q_t be a Poisson process with rate λ. Then we can define a process X_t that satisfies the stochastic differential equation

$$dX_t = a(t, X_t)\, dt + b(t, X_t)\, dW_t + c(t, X_t)dQ_t \,. \tag{7.88}$$

This, of course, can also be generalized to higher dimensions by introducing several Poisson processes. Then we get a system of stochastic differential equations

$$dX_t^\mu = a^\mu(t, X_t)dt + \sum_{j=1}^{m} b^\mu{}_j(t, X_t)dW_t^j + \sum_{i=1}^{l} c^\mu{}_i(t, X_t)dQ_t^i \,. \tag{7.89}$$

7.2.2 Change of Variables and Itô's Lemma

One of the most important rules in stochastic calculus is the so-called *Itô's Lemma* which is a generalized rule for the change of variables. Let $F : [0, \infty) \times \mathbb{R} \to \mathbb{R}$ be a smooth function of two variables. Suppose that $x = x(t)$ is a function of t. Then the infinitesimal change $dF(t, x)$ in $F(t, x)$ when t changes from t to $t + dt$ is given by

$$\begin{aligned} dF(t, x(t)) &= \frac{\partial F(t, x)}{\partial t} dt + \frac{\partial F(t, x)}{\partial x} dx \\ &= \left[\frac{\partial F(t, x)}{\partial t} + \frac{\partial F(t, x)}{\partial x} \frac{dx}{dt} \right] dt \,, \end{aligned} \tag{7.90}$$

which is obtained by restricting oneself by linear terms in dt and dx in the Taylor series. This is justified if dx and dt are of the same infinitesimal order, which is indeed so for smooth functions when $\frac{dx}{dt}$ is well defined.

However, this is not so in stochastic calculus when X_t is a stochastic process satisfying the stochastic differential equation

$$dX_t = a(t, X_t)dt + b(t, X_t)dW_t\,, \tag{7.91}$$

where W_t is a Wiener process. The fundamental reason for this is that the infinitesimal increment of the Wiener process dW_t has the variance dt, that is, $E[(dW_t)^2] = dt$. This means that $(dW_t)^2 = dt + Z_t$, where $E(Z_t) = 0$ and $E(Z_t^2) = 2dt^2$. Therefore, in the infinitesimal limit we may neglect Z_t and Z_t^2 but not dW_t^2. We see that dW_t is not of order dt as it is for a smooth deterministic function of t but rather of order $(dt)^{1/2}$. That is why, we need to take into account terms of quadratic order in dx in the Taylor expansion of the function $F(t, x)$,

$$dF(t,x) = \frac{\partial F(t,x)}{\partial t}dt + \frac{\partial F(t,x)}{\partial x}dx + \frac{1}{2}\frac{\partial^2 F(t,x)}{\partial x^2}dx^2 + \cdots\,, \tag{7.92}$$

where we neglected terms of quadratic order in dt and of qubic order in dx. Then Itô's Lemma says that $Y_t = F(t, X_t)$ is an Itô process satisfying the equation

$$\begin{aligned} dY_t = &\left[\frac{\partial F(t,X_t)}{\partial t} + a(t,X_t)\frac{\partial F(t,X_t)}{\partial x} + \frac{1}{2}b^2(t,X_t)\frac{\partial^2 F(t,X_t)}{\partial x^2}\right]dt \\ &+ b(t,X_t)\frac{\partial F(t,X_t)}{\partial x}dW_t\,. \end{aligned} \tag{7.93}$$

This can be formally obtained by expanding the function F in a Taylor series, keeping the term $(dX_t)^2$, replacing dW_t^2 by dt and neglecting terms of higher order in dt. The most important observation that one should make here is that the *deterministic drift term for the process Y_t depends on the stochastic (diffusion) term of the process X_t.*

Itô's Lemma can be generalized to higher-dimensions. Let F be a smooth function of two variables, $F : [0, \infty) \times \mathbb{R} \to \mathbb{R}$ and X_t be a process satisfying the equation (7.86)

$$dX_t = a(t, X_t)dt + \sum_{j=1}^{m} b_j(t, X_t)dW_t^j\,. \tag{7.94}$$

Then $Y_t = F(t, X_t)$ is an Itô process satisfying

$$dY_t = \left[\frac{\partial F(t,X_t)}{\partial t} + a(t,X_t)\frac{\partial F(t,X_t)}{\partial x} \right.$$
$$\left. + \frac{1}{2}\sum_{k,l=1}^{m} \rho^{kl} b_l(t,X_t) b_k(t,X_t) \frac{\partial^2 F(t,X_t)}{\partial x^2} \right] dt$$
$$+ \sum_{k=1}^{m} b_k(t,X_t)\frac{\partial F(t,X_t)}{\partial x} dW_t^k \,. \tag{7.95}$$

This formula can be also obtained by expanding the function F in the Taylor series and replacing $dW_t^i dW_t^j$ by $\rho^{ij} dt$.

More generally, let F be a smooth p-vector-valued function of $(n+1)$ variables, $F : [0,\infty) \times \mathbb{R}^n \to \mathbb{R}^p$ and X_t be a process described by the equations (7.87)

$$dX_t^\mu = a^\mu(t,X_t)dt + \sum_{j=1}^{m} b^\mu{}_j(t,X_t) dW_t^j \,. \tag{7.96}$$

Then $Y_t = F(t,X_t)$ is an Itô process satisfying

$$dY_t^c = \left[\frac{\partial F^c(t,X_t)}{\partial t} + \sum_{\mu=1}^{n} a^\mu(t,X_t)\frac{\partial F^c(t,X_t)}{\partial x^\mu} \right.$$
$$\left. + \frac{1}{2}\sum_{k,l=1}^{m}\sum_{\mu,\nu=1}^{n} \rho^{kl} b^\mu{}_l(t,X_t) b^\nu{}_k(t,X_t) \frac{\partial^2 F^c(t,X_t)}{\partial x^\mu \partial x^\nu} \right] dt$$
$$+ \sum_{\mu=1}^{n}\sum_{k=1}^{m} b^\mu{}_k(t,X_t)\frac{\partial F^c(t,X_t)}{\partial x^\mu} dW_t^k \,. \tag{7.97}$$

One can consider more general stochastic differential equations that incorporate both diffusion and jumps. Let W_t be a Wiener process and Q_t be a Poisson process with rate λ. Let X_t be a process satisfying the equation

$$dX_t = c(X_t) dQ_t \,. \tag{7.98}$$

This simply means that in the time step from t to $t+dt$ the process stays constant, that is, $X_{t+dt} = X_t$, if there is no jump ($dQ_t = 0$), and instantaneously changes from X_t to $X_{t+dt} = X_t + c(X_t)$ if there is a jump ($dQ_t = 1$). This means that $Y_t = F(X_t)$ is a stochastic process satisfying the equation

$$dY_t = F(X_{t+dt}) - F(X_t)$$
$$= [F(X_t + c(X_t)) - F(X_t)]\, dQ_t \,. \tag{7.99}$$

This enables one to easily generalize Itô lemma to the jump-diffusion stochastic processes.

Let X_t be a jump-diffusion process satisfying the equation

$$dX_t = a(t, X_t)dt + b(t, X_t)dW_t + c(t, X_t)dQ_t\,, \tag{7.100}$$

where W_t is a Wiener process and Q_t is a Poisson process; we assume that they are not correlated. Then $Y_t = F(t, X_t)$ is also a jump-diffusion process satisfying the equation

$$dY_t = \left[\frac{\partial F(t,X_t)}{\partial t} + a(t,X_t)\frac{\partial F(t,X_t)}{\partial x} + \frac{1}{2}b^2(t,X_t)\frac{\partial^2 F(t,X_t)}{\partial x^2}\right]dt$$
$$+b(t,X_t)\frac{\partial F(t,X_t)}{\partial x}dW_t + \left[F(t,X_t + c(t,X_t)) - F(t,X_t)\right]dQ_t\,.$$

This, of course, can also be generalized to higher dimensions by introducing several Poisson processes. If X_t^μ is a vector-valued process satisfying the equations

$$dX_t^\mu = a^\mu(t,X_t)dt + \sum_{j=1}^{m} b^\mu{}_j(t,X_t)dW_t^j + \sum_{i=1}^{l} c^\mu{}_i(t,X_t)dQ_t^i\,, \tag{7.101}$$

then $Y_t = F(t, X_t)$ satisfies the equation

$$dY_t^c = \left[\frac{\partial F^c(t,X_t)}{\partial t} + \sum_{\mu=1}^{n} a^\mu(t,X_t)\frac{\partial F^c(t,X_t)}{\partial x^\mu}\right.$$
$$\left.+\frac{1}{2}\sum_{k,l=1}^{m}\sum_{\mu,\nu=1}^{n}\rho^{kl}b^\mu{}_l(t,X_t)b^\nu{}_k(t,X_t)\frac{\partial^2 F^c(t,X_t)}{\partial x^\mu \partial x^\nu}\right]dt$$
$$+\sum_{\mu=1}^{n}\sum_{k=1}^{m} b^\mu{}_k(t,X_t)\frac{\partial F^c(t,X_t)}{\partial x^\mu}dW_t^k$$
$$+\sum_{i=1}^{l}\left[F^c(t,X_t + c_i(t,X_t)) - F^c(t,X_t)\right]dQ_t^i\,. \tag{7.102}$$

7.2.3 Conditional Probability Density

Let X_t be a one-dimensional Îto process described by

$$dX_t = a(t,X_t)dt + b(t,X_t)dW_t\,, \tag{7.103}$$

Let t' be a time moment in the past so that $t' < t$. The *conditional probability density function* (*transitional distribution*) $p_X(t, x; t', x')$ is the probability density function of the random variable X_t at time t given that the stochastic process X_t started with value x' at time t'. In other words, the probability that the random variable X_t at time t lies between x_1 and x_2, with $x_1 < x_2$, given that $X_{t'} = x'$ is

$$P(x_1 \leq X_t \leq x_2 \mid X_{t'} = x') = \int_{x_1}^{x_2} p_X(t, x; t', x') dx \,. \tag{7.104}$$

Obviously, at equal times the conditional probability density degenerates to the delta-function

$$p_X(t', x; t', x') = \delta(x - x') \,. \tag{7.105}$$

There are many ways to show that the conditional probability density satisfies two partial differential equations, the *forward Kolmogorov equation* (also called *Fokker-Planck equation*) and the adjoint *backward Kolmogorov equation* The forward equation describes the future time evolution of the probability density with the initial condition set at the initial time $t = t'$. The backward equation describes the past time evolution of the probability density with a terminal condition set at a future time $t = T$. The forward equation describes probabilities of reaching various future states from a given current state. The backward equation describes probabilities of reaching a specified final state from various initial states.

These equations can be derived as follows. Let t' be the initial time and T be a terminal time so that $t' \leq t \leq T$. Let $F(t, x)$ be a smooth function of compact support (or decreasing fast at infinity as $x \to \pm\infty$) such that $F(t', x) = F(T, x) = 0$. Then by Îto formula

$$dF(t, X_t) = \left[\frac{\partial F(t, X_t)}{\partial t} + a(t, X_t) \frac{\partial F(t, X_t)}{\partial x} + \frac{1}{2} b^2(t, X_t) \frac{\partial^2 F(t, X_t)}{\partial x^2} \right] dt$$

$$+ b(t, X_t) \frac{\partial F(t, X_t)}{\partial x} dW_t \,. \tag{7.106}$$

Now, by noting that $E(dW_t) = 0$ and by integrating this equation over t from t' to T we obtain the expected value of this equation given $X_{t'} = x'$

$$
\begin{aligned}
&E(F(T,X_T)|X_{t'}=x') - E(F(t',x')|X_{t'}=x') \\
&\quad = \int_{t'}^{T} E(dF(t,X_t)|X_{t'}=x') \qquad (7.107)\\
&\quad = \int_{t'}^{T}\int_{-\infty}^{\infty}\Big[\frac{\partial F(t,x)}{\partial t} + a(t,x)\frac{\partial F(t,x)}{\partial x} \\
&\qquad\qquad + \frac{1}{2}b^2(t,x)\frac{\partial^2 F(t,x)}{\partial x^2}\Big] p_X(t,x;t',x')dx\,dt\,.
\end{aligned}
$$

Next, by recalling that $F(T,X_T) = F(t',x') = 0$ and integrating by parts in x and t we get

$$
\int_{t'}^{T}\int_{-\infty}^{\infty} F(t,x)\left[-\frac{\partial}{\partial t} - \frac{\partial}{\partial x}a(t,x) + \frac{1}{2}\frac{\partial^2}{\partial x^2}b^2(t,x)\right] p_X(t,x;t',x')dx\,dt = 0\,. \qquad (7.108)
$$

Since the function $F(t,x)$ is arbitrary we obtain the *forward Kolmogorov equation*

$$
\left(\frac{\partial}{\partial t} - L_{x,t}\right) p_X(t,x;t',x') = 0\,, \qquad (7.109)
$$

where

$$
L_{x,t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}b^2(t,x) - \frac{\partial}{\partial x}a(t,x)\,, \qquad (7.110)
$$

The backward Kolmogorov equation can be obtained similarly. Let

$$
F(t,x) = E(f(X_T)|X_t = x) = \int_{-\infty}^{\infty} p_X(T,y;t,x)f(y)dy \qquad (7.111)
$$

be the expected value of a function $f(X_T)$ at a future time T given $X_t = x$. Then for any $t' < T$

$$
F(T,X_T) - F(t',X_{t'}) = \int_{t'}^{T} dF(t,X_t)\,, \qquad (7.112)
$$

and, therefore,

$$
E(F(T,X_T)|X_{t'}=x') - E(F(t',X_{t'})|X_{t'}=x') = \int_{t'}^{T} E(dF(t,X_t)|X_{t'}=x')\,. \qquad (7.113)
$$

Further, it is easy to see that

$$
E(F(T,X_T)|X_{t'}=x') = E(f(X_T)|X_{t'}=x') = F(t',x')\,, \qquad (7.114)
$$

and

$$
E(F(t',X_{t'})|X_{t'}=x') = F(t',x')\,. \qquad (7.115)
$$

Therefore,

$$\int_{t'}^{T} E(dF(t, X_t)|X_{t'} = x') = 0\,, \tag{7.116}$$

and since t' is arbitrary

$$E(dF(t, X_t)|X_t = x) = 0\,. \tag{7.117}$$

Now, by applying Îto formula we obtain the backward Kolmogorov equation for the function $F(t, x)$

$$\frac{\partial F(t,x)}{\partial t} + a(t,x)\frac{\partial F(t,x)}{\partial x} + \frac{1}{2}b^2(t,x)\frac{\partial^2 F(t,x)}{\partial x^2} = 0\,, \tag{7.118}$$

and since the function f is arbitrary we finally get the *backward Kolmogorov equation* for the transition probability

$$\left(\frac{\partial}{\partial t'} + L^*_{x',t'}\right) p_X(t, x; t', x') = 0\,, \tag{7.119}$$

where

$$L^*_{x',t'} = \frac{1}{2}b^2(t', x')\frac{\partial^2}{\partial x'^2} + a(t', x')\frac{\partial}{\partial x'}\,. \tag{7.120}$$

This can be generalized to higher dimensions too. For a one-dimensional Îto process that depends on several Wiener processes

$$dX_t = a(t, X_t)dt + \sum_{j=1}^{m} b_j(t, X_t)dW_t^j\,. \tag{7.121}$$

the forward and the backward Kolmogorov equations take the same form as above with the operators L and L^* defined by

$$L_{x,t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}B(t,x) - \frac{\partial}{\partial x}a(t,x)\,, \tag{7.122}$$

$$L^*_{x',t'} = \frac{1}{2}B(t', x')\frac{\partial^2}{\partial x'^2} + a(t', x')\frac{\partial}{\partial x'}\,, \tag{7.123}$$

where

$$B(t,x) = \sum_{i,j=1}^{m} \rho^{ij} b_i(t,x) b_j(t,x)\,. \tag{7.124}$$

Finally, for a vector-valued Itô process defined by

$$dX_t^\mu = a^\mu(t, X_t)dt + \sum_{j=1}^{m} b^\mu{}_j(t, X_t)dW_t^j\,, \tag{7.125}$$

the forward and the backward Kolmogorov equations have the same form as above where the operators L and L^* are now higher-dimensional partial differential equations

$$L_{x,t} = \frac{1}{2}\sum_{\mu,\nu=1}^{n} \frac{\partial^2}{\partial x^\mu \partial x^\nu} B^{\mu\nu}(t,x) - \sum_{\mu=1}^{n} \frac{\partial}{\partial x^\mu} a^\mu(t,x)\,, \tag{7.126}$$

$$L^*_{x',t'} = \frac{1}{2}\sum_{\mu,\nu=1}^{n} B^{\mu\nu}(t',x') \frac{\partial^2}{\partial x'^\mu \partial x'^\nu} + \sum_{\mu=1}^{n} a^\mu(t',x') \frac{\partial}{\partial x'^\mu}\,, \tag{7.127}$$

where

$$B^{\mu\nu}(t,x) = \sum_{i,j=1}^{m} \rho^{ij} b^\mu{}_i(t,x) b^\nu{}_j(t,x)\,. \tag{7.128}$$

It is, of course, not a coincidence that these partial differential operators look very similar. This is because they are, in fact, *adjoints* of each other which is reflected in the notation (more on this later).

The conditional probability density function is one of the most important characterizations of the stochastic process. This whole book is devoted to the development of effective mathematical techniques for calculation of this function. The forward and the backward Kolmogorov equations are linear parabolic partial differential equations that, together with the initial condition (7.105), determine the conditional probability density function.

7.3 Notes

This chapter is a crash course on stochastic calculus. We introduced the basic concepts of probability and the most important stochastic processes such as the Wiener process and the Poisson process needed to describe the models in mathematical finance discussed in the next chapter. We introduced the stochastic differential equations and such important topics as the Itô Lemma. The material on the stochastic calculus and stochastic differential equations can be found in [80, 63, 32, 66].

Chapter 8
Applications in Mathematical Finance

Abstract This chapter presents an introduction to mathematical finance. After a short review of financial instruments we introduce various models, including, Black-Scholes model, stochastic volatility models and jump diffusion models, and apply the methods described in previous chapters to SABR model and Heston model.

8.1 Derivatives

8.1.1 Financial Instruments

In this section we briefly describe various financial assets and financial instruments. A reader interested in a more detailed description is referred to an excellent book [56, 53, 79] and references therein. Contrary to real assets that are necessary for producing goods and services for the society, the *financial assets* (also called *securities*) are legal documents that entitle its holder to a claim on a fraction of the real assets and to the income generated by these real assets. In other words, financial assets are economic resources that are capable of being owned to produce value, that is, financial assets represent ownership of value.

Financial instruments are specific forms of financial assets, that is, they are legal documents representing the ownership of some financial assets. There are three major groups of financial instruments: equities (or *stocks*, or shares), fixed income securities also called *bonds*, and *derivative securities*. Equities represent the ownership of a small piece (a share) of a company. The value of holding a stock comes from the *dividends* (which is a form of sharing the profits of the company) and a possible growth in the stock's value. Fixed income securities provide a return in the form of fixed periodic payments and the eventual return of principal at maturity.

I.G. Avramidi, *Heat Kernel Method and its Applications*,
DOI 10.1007/978-3-319-26266-6_8

Derivative securities are financial instruments that have a value determined by the price of some other assets (called the *underlying assets* or simply the underlying). An excellent resource on derivatives is the classic book [53]. One example of derivatives are forwards and futures. A *futures* contract is a contract between two parties to buy or sell a specified asset (usually raw products, such as oil, precious metals, etc. called *commodities*) of some quantity and quality at a specified future date at a price agreed today. Futures contracts are standardized by *clearinghouses* and are traded on an *exchange*. *Forward contracts* are similar to the futures contract but are not standardized.

Swaps are contracts to exchange cash on or before a specified future date based on the underlying value of currencies/exchange rates, bonds/interest rates, commodities, stocks or other assets. *Options* are contracts that give the owner the right, but not the obligation, to buy or sell (depending on the type of the option) an asset at (or any time before) a specified time in the future at an specified price agreed today.

8.1.2 Options

One of the most useful resources on options from the individual investor practical point of view is the book [62]. The present book will deal mostly with the theoretical side of options, similar to the books [79, 52]; an alternative approach is presented, for example, in [17]. As we already mentioned above options give the owner the right, but not the obligation, to buy or sell an asset at (or any time before) a specified time in the future at a specified price. The specified price K is called the *strike price* (or *exercise price*) and the specified date T is called the *expiry* (or the *expiration date*). The financial asset we agreed to buy (or to sell) is called the *underlying asset*. The price S of the asset at the current time is called the *spot price*. The amount paid for the option initially is called the *premium*. The value of the option at expiry is a function of the strike price called the *payoff function*. The *intrinsic value* of the option is the difference between the payoff function and the spot price. The *time value* of the option is any value that remains above the intrinsic value. An option is called *in the money* if the intrinsic value is positive, *out of the money* if the intrinsic value is negative and *at the money* if the intrinsic value is near zero.

A *call option* gives the purchaser of the option the right to *buy* the asset *at expiry* at the strike price, and the *put option* gives the right to *sell* the asset *at expiry* at the strike price. The person who promises to deliver the underlying asset and receives the premium is called the *writer* of the option. Such options are called *European options*. The *American options* give the right to buy (or sell) the asset *at any time before expiry*. The Bermudan options give the right to buy (or sell) the asset *on specified dates or time periods*. We will be dealing

mostly with European options, so when we say option we actually mean an European option.

The value $V(T, S)$ of an option at expiry T as a function of the underlying S is called the *payoff diagram*. Let us review the payoff diagrams of various options [62, 79]. It will be convenient to introduce the *Heaviside step function*

$$\theta(x) = \begin{cases} 1, & \text{if} \quad x > 0, \\ 0, & \text{if} \quad x \leq 0, \end{cases} \tag{8.1}$$

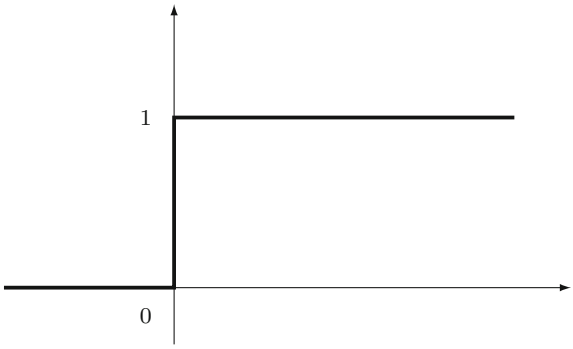


Fig. 8.1 Heaviside step function

and the function x_+ defined by

$$x_+ = x\theta(x) = \max(x, 0) = \begin{cases} x, & \text{if} \quad x > 0, \\ 0, & \text{if} \quad x \leq 0. \end{cases} \tag{8.2}$$

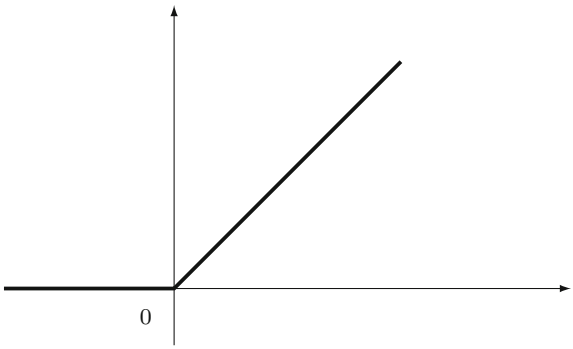


Fig. 8.2 Function x_+

It is easy to see that for any $x \neq 0$

$$\theta(x) = \frac{1}{2}\left(\frac{|x|}{x} + 1\right), \qquad \text{and} \qquad x_+ = \frac{1}{2}\left(|x| + x\right), \tag{8.3}$$

where $|x|$ is the absolute value of x, and, therefore, for any x

$$x_+ - (-x)_+ = x\,. \tag{8.4}$$

To avoid confusion let us note that the Heaviside step function is denoted differently by people coming from different areas: probabilists denote it by $1_{x>0}$ and applied mathematicians by $H(x)$; our notation $\theta(x)$ is used quite often in physics.

To distinguish between call options and put options let us denote the price of a call option by $C(t, S)$ and the price of a put option by $P(t, S)$. Let us look at the call option first. If the asset price at expiry is S and the strike price is K, then we would exercise the option only if $S > K$ and not exercise it at all if $S \leq K$. This means that the payoff of the call option is

$$C(T, S) = (S - K)_+\,. \tag{8.5}$$

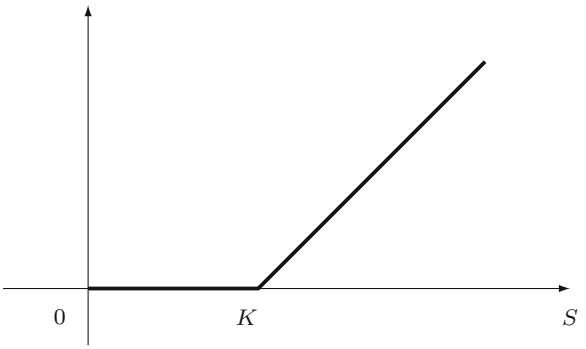


Fig. 8.3 Call option

Similarly, we would exercise a put option only if $S < K$ and not exercise it at all if $S \geq K$, which means that the payoff of the put option is

$$P(T, S) = (K - S)_+ . \tag{8.6}$$

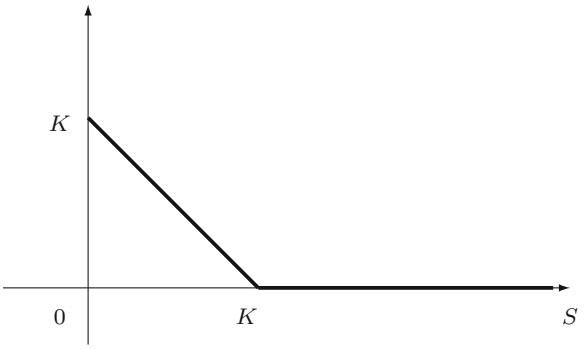


Fig. 8.4 Put option

By using the eq. (8.4) we see that there is the *duality* between the call and put payoffs

$$C(T, S) - P(T, S) = S - K . \tag{8.7}$$

A similar relation holds for the option prices at any time t, $0 \leq t \leq T$. The only difference is an exponential discount factor $e^{-r(T-t)}$, where r is the risk-free interest rate, which accounts for the *time value of money*, that is, 1\$ at the expiration time T is worth only $e^{-r(T-t)}$\$ at time t. Thus

$$C(t, S) - P(t, S) = S - Ke^{-r(T-t)} . \tag{8.8}$$

This means that if one knows the value of a call option one can easily find the value of a put option, and, therefore, one can restrict oneself only to the study of the call options.

The *binary options* have discontinuous payoff functions. The binary call pays a fixed amount B at expiry T if the asset price S is greater than the strike price K, that is,

$$C(T,S) = B\theta(S-K)\,. \tag{8.9}$$

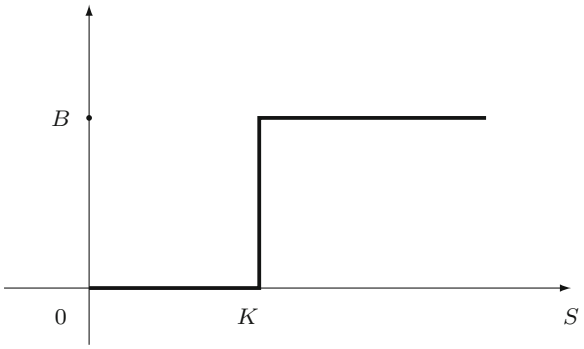


Fig. 8.5 Binary call option

The binary put pays a fixed amount B at expiry T if the asset price S is less than the strike price K, that is,

$$P(T,S) = B\theta(K-S)\,. \tag{8.10}$$

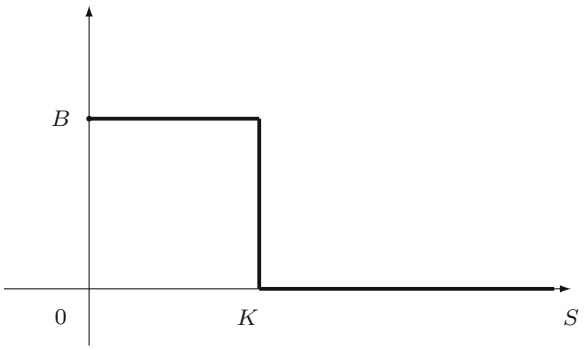


Fig. 8.6 Binary put option

One can achieve more complicated payoffs with a suitable *portfolio strategy*. In fact, any piece-wise linear payoff function can be represented as a linear combination of puts and calls.

A strategy involving options of the same type is called a *spread*. Let K_1 and K_2 be two strike prices such that $K_1 < K_2$. A *call spread* (or a *bull spread*) is an option with the payoff function

$$V(T,S) = (S-K_1)_+ - (S-K_2)_+$$

$$= \begin{cases} 0, & \text{if} \quad S \le K_1, \\ S-K_1, & \text{if} \quad K_1 < S < K_2, \\ K_2-K_1, & \text{if} \quad S \ge K_2. \end{cases} \tag{8.11}$$

This payoff can be achieved by buying a call with strike K_1 and writing a call with strike K_2 with the same expiration date.

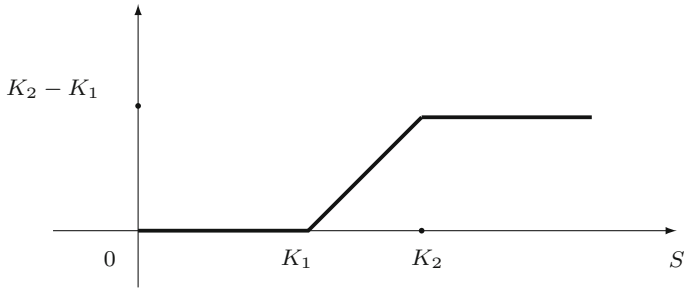


Fig. 8.7 Call spread option

A *put spread* (or a *bear spread*) is an option with the payoff function

$$V(T,S) = (K_2-S)_+ - (K_1-S)_+$$

$$= \begin{cases} K_2-K_1, & \text{if} \quad S \le K_1, \\ K_2-S, & \text{if} \quad K_1 < S < K_2, \\ 0, & \text{if} \quad S \ge K_2. \end{cases} \tag{8.12}$$

This payoff can be achieved by writing a put with a strike K_1 and buying a put with a strike K_2 with the same expiration date.

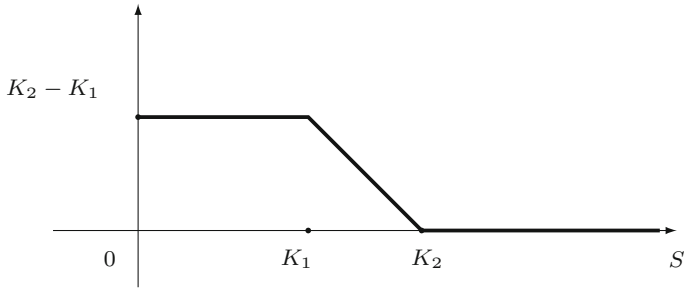


Fig. 8.8 Put spread option

A portfolio strategy involving options of different types is called a *combination*. A *straddle* is a combination of a call and a put with the same strike price K with the payoff

$$V(T,S) = (S-K)_+ + (K-S)_+ = |S-K|$$
$$= \begin{cases} K-S, & \text{if} \quad S \le K, \\ S-K, & \text{if} \quad S \ge K. \end{cases} \tag{8.13}$$

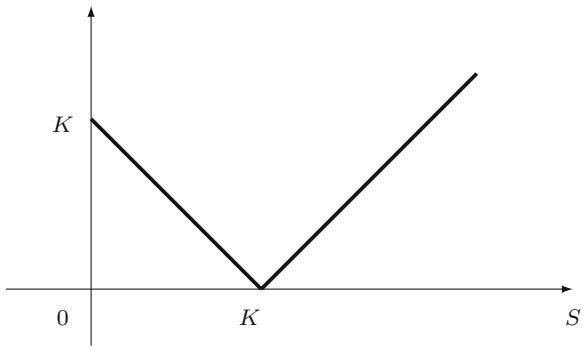


Fig. 8.9 Straddle option

A *strangle* is a combination of a call and a put with different strike prices K_1 and K_2 with the payoff

$$V(T,S) = (K_1 - S)_+ + (S-K_2)_+ . \tag{8.14}$$

If $K_1 > K_2$, then the option is called *in-the-money*. Its payoff function is

$$V(T,S) = \begin{cases} K_1 - S, & \text{if} \quad S \le K_2, \\ K_1 - K_2, & \text{if} \quad K_2 < S < K_1, \\ S - K_2, & \text{if} \quad S \ge K_1. \end{cases} \tag{8.15}$$

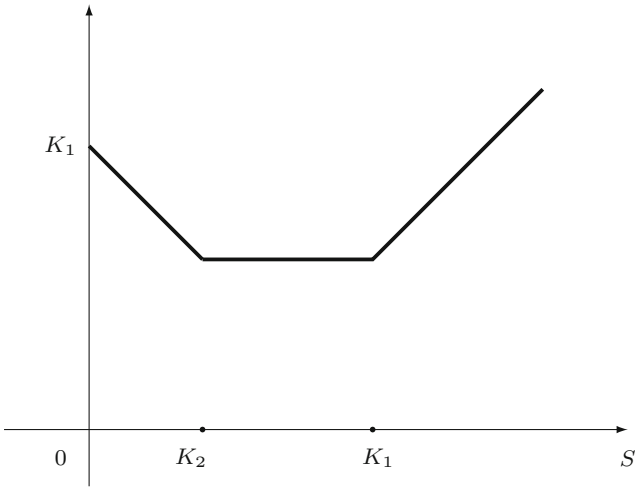


Fig. 8.10 In-the-money strangle option

If $K_1 < K_2$, then the option is called *out-of-the-money* with the payoff function

$$V(T,S) = \begin{cases} K_1 - S, & \text{if} \quad S \le K_1, \\ 0, & \text{if} \quad K_1 < S < K_2, \\ S - K_2, & \text{if} \quad S \ge K_2. \end{cases} \tag{8.16}$$

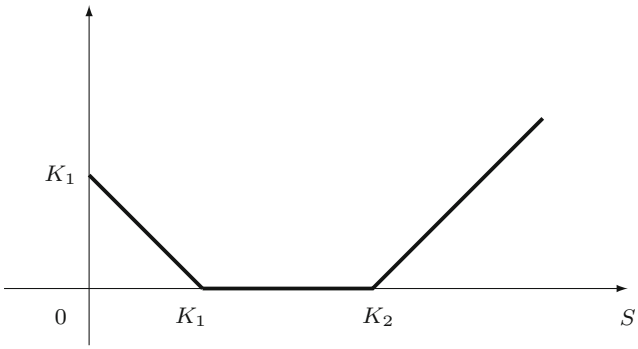


Fig. 8.11 Out-of-the-money strangle option

The *risk reversal* is a combination of a long call with strike above the spot price and a short put with a strike below the spot price with the same expiry. The payoff of the risk reversal is (with $K_1 < K_2$)

$$V(T,S) = (S-K_2)_+ - (K_1-S)_+$$

$$= \begin{cases} S-K_1, & \text{if} \quad S \le K_1, \\ 0, & \text{if} \quad K_1 < S < K_2, \\ S-K_2, & \text{if} \quad S \ge K_2. \end{cases} \tag{8.17}$$

This is the first payoff function that becomes negative, namely if $S < K_1$, reaching the minimum $(-K_1)$ if the stock price falls to zero, $S = 0$.

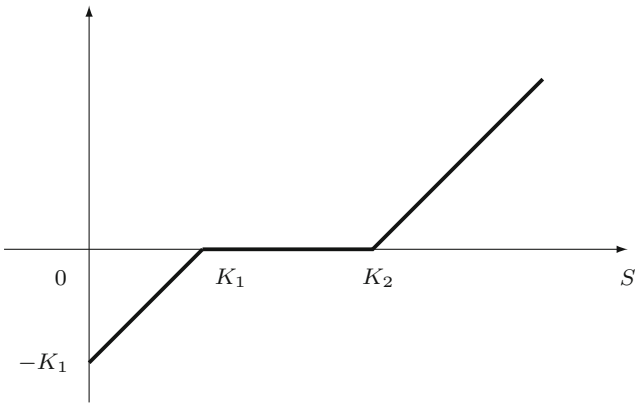


Fig. 8.12 Risk reversal option

Even more complicated strategy can be achieved by combining more than two options with different strikes and the same expiry. A *butterfly spread* is achieved by writing two calls with strikes K, buying a call with a strike $K-E$, and buying a call with a strike $K+E$; here, of course, $K, E > 0$. The payoff function of a butterfly spread is

$$V(T,S) = (S-K+E)_+ - 2(S-K)_+ + (S-K-E)_+ .$$

$$= \begin{cases} 0, & \text{if} \quad S \le K-E, \\ S-K+E, & \text{if} \quad K-E < S \le K, \\ K+E-S, & \text{if} \quad K < S \le K+E, \\ 0, & \text{if} \quad S \ge K+E. \end{cases} \tag{8.18}$$

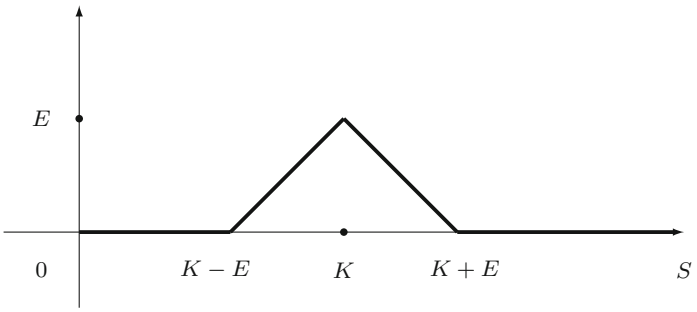


Fig. 8.13 Butterfly spread option

The payoff function of a *condor* strategy is achieved by using four call options

$$V(T,S) = (S-K_1+E)_+ - (S-K_1)_+ - (S-K_2)_+ + (S-K_2-E)_+ .$$

$$= \begin{cases} 0, & \text{if} \quad S \le K_1-E, \\ S-K_1+E, & \text{if} \quad K_1-E < S \le K_1, \\ E, & \text{if} \quad K_1 < S \le K_2, \\ K_2+E-S, & \text{if} \quad K_2 < S \le K_2+E, \\ 0, & \text{if} \quad S \ge K_2+E, \end{cases} \tag{8.19}$$

where $K_1, K_2, E > 0$ and $K_1 < K_2$.

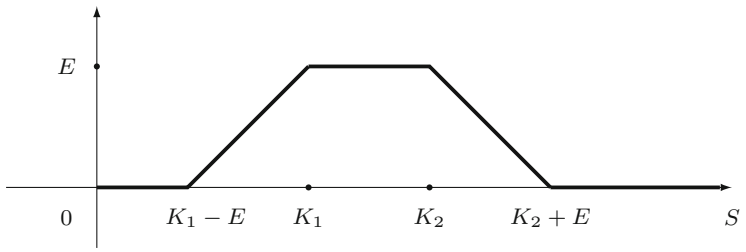


Fig. 8.14 Condor option

8.2 Models in Mathematical Finance

8.2.1 Quantitative Analysis

To correctly estimate the value of derivative securities, such as options, we need a working model of the underlying assets [17, 41, 52, 79]. An empirical fact is that most of the underlying assets exhibit random behavior. That is why, instead of trying to predict the prices of financial assets it makes a lot of sense to model them as stochastic processes. Then, as we shall see later, there is a way to construct a portfolio such that the value of the derivative product is not random but rather deterministic. Thus, quantitative analysis involves four major steps:

1. construct a stochastic model for random underlying assets,
2. derive a deterministic equation for the derivative security,
3. solve that deterministic equation, and
4. calibrate the model, that is, determine the parameters of the model from the empirical data.

Let us say from the beginning that most of this book is about the solution of the deterministic equation derived from continuous-time stochastic models for the underlying assets.

The fundamental foundation for modeling the behavior of financial assets is the so called *efficient market hypothesis*. Roughly speaking it states that the market is efficient (or in equilibrium). There are three major versions of the hypothesis: weak, semi-strong, and strong. The weak form claims that prices of assets already reflect all *past publicly available* information. The semi-strong form claims both that prices reflect all publicly available information

and that prices instantly change to reflect *new public* information. The strong form additionally claims that prices instantly reflect even *hidden or insider* information. We will simply assume that:

1. the securities have their fair prices,
2. the current market prices have only small and temporary deviations from their fair prices, and
3. changes in prices of securities are, up to a drift, random.

It may sound surprising that the value of a derivative is deterministic even though the underlying asset is random. This is achieved by constructing a very special risk-free (in theory!) portfolio by applying what is generally called *hedging* and *no arbitrage principle*. We will explain the basics of model building on a simple classical example, the *Black-Scholes model*.

8.2.2 Black-Scholes Model

Let us consider an asset whose price at time t is S_t. There are many reasons to believe that the asset price S_t follows a log-normal stochastic process with some drift μ and a volatility σ. In other words, we assume that the asset price S_t evolves according to the stochastic differential equation

$$dS_t = \mu S_t dt + \sigma S_t dW_t \,, \tag{8.20}$$

where W_t is a Wiener process. We see that the change of the asset price consists of two terms, the deterministic (risk-free) drift, proportional to dt, and the stochastic (random, risky) one, proportional to dW_t.

Let us consider a European call option with strike price K and the expiration time T. The price of the option is a function of two variables t and S. Let $V(t, S)$ be the price of the option at time t and the asset price $S = S_t$.

The main idea of *hedging* is as follows. We construct a portfolio strategy under which one holds a single long option position and continuously trades in the underlying asset to hold some short position of the underlying. Let $\Delta = \Delta(t, S)$ denote the size of the short underlying position. Note that Δ is not a constant but a function of t and S. Then the value $\Pi = \Pi(t, S)$ of the portfolio at time t is

$$\Pi = V - \Delta S \,. \tag{8.21}$$

The minus sign in front of the second term reflects the fact that the underlying position is short. Now we consider the change of the value of our portfolio from the time t to the time $t + dt$ by taking that the quantity $\Delta(t, S)$ is constant during this time step. Now, let $R = R(t, S)$ denote the *accumulated profit* (or loss) from following this strategy. Then over the time period from t to $t + dt$ the instantaneous profit is

$$dR = dV - \Delta dS, \tag{8.22}$$

Assuming the log-normal process (8.20) for the underlying and applying the Itô lemma we get

$$dR = \left(\frac{\partial}{\partial t}V + \frac{\sigma^2}{2}S^2\frac{\partial^2}{\partial S^2}V\right)dt + \left(\frac{\partial}{\partial S}V - \Delta\right)dS\,. \tag{8.23}$$

As we see the instantaneous profit consists of two terms, the risk-free deterministic one, proportional to dt, and the risky stochastic one, proportional to dS. The main idea of *hedging* is to reduce the risk. In this simple model we can completely eliminate risk by choosing the size of the short stock position in the portfolio according to

$$\Delta = \frac{\partial}{\partial S}V\,. \tag{8.24}$$

Then

$$dR = \left(\frac{\partial}{\partial t}V + \frac{\sigma^2}{2}2S^2\frac{\partial^2}{\partial S^2}V\right)dt\,. \tag{8.25}$$

This portfolio strategy is called *delta hedging*.

This equation contains no random dW_t term, that is, it is entirely risk-free. Then applying the *no-arbitrage principle* we conclude that the rate of return on this portfolio must be equal at all times to the rate of return on any other risk-free investment. Let r be the interest rate of a risk-free investment. Then over the time period from t to $t + dt$ we must have

$$dR = r\Pi\, dt \tag{8.26}$$

Then by using eqs. (8.24), (8.25) and (8.21) we see that the price of the option satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right)V = 0\,, \tag{8.27}$$

where L is a differential operator defined by

$$L = \frac{\sigma^2}{2}S^2\frac{\partial^2}{\partial S^2} + rS\frac{\partial}{\partial S} - r\,. \tag{8.28}$$

We will call such a deterministic equation of the evolution type (8.27) for the value of the option the *valuation equation*, and the operator L the *valuation operator*.

It is worth noting that the valuation equation, and, therefore, the price of the option, does not depend on the drift parameter μ but only on the volatility of the underlying asset.

The Black-Scholes valuation equation is a linear parabolic partial differential equation. Since we are only interested in the price of the option from the initial time to the expiration time and the price of the underlying asset cannot be negative the ranges of the variables t and S are

$$0 \le t \le T, \qquad 0 \le S < \infty\,. \tag{8.29}$$

The price of the option at expiry is equal to the payoff function of the call option which gives a *terminal condition*:

$$V(T,S) = (S-K)_+\,, \quad \text{for any} \quad S \ge 0\,. \tag{8.30}$$

More generally, the price of any European option with a payoff function $P(S)$ is described by the same equation and the terminal condition

$$V(T,S) = P(S)\,. \tag{8.31}$$

Recall that all payoff functions of interest are piecewise linear.

Strictly speaking for the existence of a unique solution to such a partial differential equation, we also need a boundary condition at the boundary of the domain, $S = 0$ and $S \to \infty$. This is a subtle issue since both the point $S = 0$ and the infinity are singular points of the Black-Scholes equation. This means that the whole boundary of the domain is singular, and one cannot impose an arbitrary boundary condition. Even though this is an interesting (for mathematicians) question we should not worry too much about things like this. Let me just say that such problem has a unique solution if the solution is not allowed to grow too fast at the boundary.

As we discussed above this is the simplest and the most important model in quantitative finance. Of course, it makes many simplifying assumptions about the real world that are not necessarily true. Later we will consider more complicated models, in particular, various models where the volatility is not constant but is stochastic as well, as well as models where the stochastic behavior of the underlying is not described by just a diffusion but also incorporates jumps.

Let us discuss some generalizations and particular cases of the Black-Scholes model. First of all, one can easily generalize the model to include stocks paying dividends. Let us assume, for simplicity that underlying stock receives a constant and continuous *dividend yield*, d, so that in time dt the instantaneous profit is

$$dR = dV - d\frac{\partial V}{\partial S} S dt\,. \tag{8.32}$$

Then, again, from the non-arbitrage principle, eq. (8.26), we get the same parabolic valuation equation (8.27) with a little more general valuation operator

$$L = \frac{\sigma^2}{2} S^2 \frac{\partial^2}{\partial S^2} + (r-d) S \frac{\partial}{\partial S} - r\,. \tag{8.33}$$

The *currency options* are very similar to stock options paying dividends since holding a foreign currency with a foreign rate of interest r_f is the same as receiving a continuous dividend $d = r_f$. Therefore, the valuation operator for currency options is

$$L = \frac{\sigma^2}{2} S^2 \frac{\partial^2}{\partial S^2} + (r - r_f) S \frac{\partial}{\partial S} - r \,. \tag{8.34}$$

The *commodity options* are exactly the opposite to stocks options paying dividends since commodities have *cost of carry* (storage cost), that is, holding a commodity is the same as receiving a negative dividend $d = -q$, where q is the fraction of the value of a commodity that pays for the cost of carry. Therefore, the valuation operator for commodity options is

$$L = \frac{\sigma^2}{2} S^2 \frac{\partial^2}{\partial S^2} + (r + q) S \frac{\partial}{\partial S} - r \,. \tag{8.35}$$

Finally, recall that the future price F of a (non-dividend paying) stock is related to the current price S by the discount factor

$$F = e^{r(T-t)} S \,. \tag{8.36}$$

By using this relation it is easy to see that the valuation operator for the *options on futures* is

$$L = \frac{\sigma^2}{2} F^2 \frac{\partial^2}{\partial F^2} - r \,. \tag{8.37}$$

8.2.3 Higher-Dimensional Black-Scholes Model

It is easy to generalize the classical Black-Scholes model to options with many underlying assets called *basket options* (or *rainbow options*). Let us consider n assets whose prices at time t are S_t^i, $i = 1, 2, \ldots, n$. Suppose that all assets S_t^i evolve according to log-normal processes with drifts μ_i and volatilities σ_i, that is,

$$dS_t^i = \mu_i S_t^i \, dt + \sigma_i S_t^i \, dW_t^i \,, \tag{8.38}$$

where W_t^i are n Wiener processes with a correlation matrix ρ^{ij}.

Let us consider an option, which is the right to buy, sell or exchange the underlying assets in the basket at the expiration time T. Let $V = V(t, S^1, \ldots, S^n)$ be the price of the option at time t and the stock prices $S^i = S_t^i$. Let r be the interest rate of a risk-free investment and d_i be the dividend rates for underlying assets S_i. Then, by using essentially the same delta-hedging method we construct a risk-free portfolio

$$\Pi = V - \sum_{i=1}^{n} \frac{\partial V}{\partial S^i} S^i \,, \tag{8.39}$$

and by no arbitrage principle we obtain the valuation equation

$$\left(\frac{\partial}{\partial t} + L \right) V = 0 \,, \tag{8.40}$$

where the valuation operator is

$$L = \frac{1}{2} \sum_{i,j=1}^{n} C_{ij} S^i S^j \frac{\partial^2}{\partial S^i \partial S^j} + \sum_{i=1}^{n} (r - d_i) S^i \frac{\partial}{\partial S^i} - r \,, \tag{8.41}$$

with the matrix C_{ij} defined by

$$C_{ij} = \rho^{ij} \sigma_i \sigma_j \,. \tag{8.42}$$

This valuation equation is also a parabolic partial differential equation. The terminal condition

$$V(T, S^1, \ldots, S^n) = P(S^1, \ldots, S^n) \,. \tag{8.43}$$

is specified by the payoff function $P(S^1, \ldots, S^n)$, which is determined by the type of the option (call, put, mixed). Assuming an admissible boundary condition this valuation equation will have a unique solution that determines the price of the option.

8.2.4 Beyond Black-Scholes

The Black-Scholes model was a remarkable achievement of quantitative finance. Due to its remarkable robustness it became a golden standard in finance that is widely used by both traders and quants. However, some of the assumptions of Black-Scholes model are not very realistic, which calls for improved more general models. A detailed analysis of the assumptions of the Black-Scholes model and their possible generalizations can be found in [79]. We just list some of them:

1. delta hedging can only be done discreetly,
2. there are transaction costs associated with the delta hedging,
3. volatility of the underlying is not constant but rather highly unpredictable,
4. interest rates and dividends are not constant,
5. the underlying asset paths are discontinuous,
6. the returns on underlying assets are not normally distributed.

8.2.5 Deterministic Volatility Models

One of the simplest generalizations of the Black-Scholes model is to replace the volatility σ and the drift of the underlying asset by deterministic functions of time, that is,

$$dS_t = \mu(t)S_t dt + \sigma(t)S_t dW_t \,. \tag{8.44}$$

One could even assume that the volatility is a deterministic function of both time t and the underlying S_t, that is,

$$dS_t = \mu(t)S_t dt + \sigma(t, S_t)S_t dW_t \,. \tag{8.45}$$

This is somewhat better than the original Black-Scholes model, however, it is still not very realistic. We need to find a function $\sigma(t, S)$ once and for all that would reproduce the real volatility of the underlying asset. The problem is that such a function does not exist.

That is why we will not consider deterministic volatility models. A much more appealing idea is that the volatility itself is stochastic or depends on some factors that are stochastic.

8.3 Stochastic Volatility Models

A general stochastic volatility model can be constructed as follows. Let S_t be the price of an underlying asset. We assume that the volatility of this asset is a function of n stochastic factors v_t^i, $i = 1, 2, \ldots, n$. More precisely, we consider $(n + 1)$ Wiener processes X_t, W_t^1, $\ldots$, W_t^n, with the constant correlation matrix $\rho^{\mu\nu}$, $\mu, \nu = 0, 1, \ldots, n$,

$$E(dX_t dW_t^i) = \rho^{0i} dt \,, \qquad E(dW_t^i dW_t^j) = \rho^{ij} dt \,. \tag{8.46}$$

Then the model is described by the following system of stochastic differential equations

$$dS_t = \mu S_t \, dt + \sigma(S_t, v_t) S_t \, dX_t \tag{8.47}$$

$$dv_t^i = a^i(S_t, v_t) \, dt + \sum_{j=1}^{n} b^i{}_j(S_t, v_t) \, dW_t^j \,, \qquad i = 1, \ldots, n \,, \tag{8.48}$$

where $a^i(S, v)$ are drift coefficients and $b^i{}_j(S, v)$ is a diffusion matrix.

Since volatility is not a traded asset it is not so easy to hedge away the randomness to get a risk-free portfolio. We set up a portfolio strategy under which one holds a single long option position with value $V = V(t, S, v)$ and continuously trades in the underlying asset and some other options $V^i = V^i(t, S, v)$ to hold a short position of the underlying and short positions in

other options. Let $\Delta = \Delta(t, S, v)$ denote the size of the short underlying position and $\Delta_i = \Delta_i(t, S, v)$ denote the size of the short positions in other options. Then the value of such portfolio at time t is

$$\Pi = V - \Delta S - \sum_{i=1}^{n} \Delta_i V^i \,. \tag{8.49}$$

Now, we consider the change of the value of our portfolio from time t to the time $t + dt$ by assuming the quantities Δ and Δ_i to be constant during this time step. Let $R = R(t, S, v)$ be the accumulated profit/loss from following this strategy. Then, over the time period from t to $t + dt$ the instantaneous profit is

$$dR = dV - \Delta dS - \sum_{i=1}^{n} \Delta_i dV^i \,. \tag{8.50}$$

Let us introduce a convenient notation

$$A^k = \sum_{j=1}^{n} b^k{}_j \rho^{j0} \,, \tag{8.51}$$

$$B^{kl} = \sum_{i,j=1}^{n} b^k{}_i \rho^{ij} b^l{}_j \,. \tag{8.52}$$

Then by the Îto lemma we have

$$dV = \left(\frac{\partial V}{\partial t} + \tilde{L} V \right) dt + \frac{\partial V}{\partial S} dS_t + \sum_{i=1}^{n} \frac{\partial V}{\partial v^i} dv_t^i \,, \tag{8.53}$$

where $\tilde{L}$ is a second-order linear partial differential operator defined by

$$\tilde{L} = \frac{1}{2}\sigma^2 S^2 \frac{\partial^2}{\partial S^2} + \sum_{i=1}^{n} \sigma S A^i \frac{\partial^2}{\partial S \partial v^i} + \frac{1}{2} \sum_{i,j=1}^{n} B^{ij} \frac{\partial^2}{\partial v^i \partial v^j} \,. \tag{8.54}$$

Therefore, the instantaneous profit/loss is

$$\begin{aligned} dR = & \left[\frac{\partial V}{\partial t} + \tilde{L} V - \sum_{i=1}^{n} \Delta_i \left(\frac{\partial V^i}{\partial t} + \tilde{L} V^i \right) \right] dt \\ & + \left[\frac{\partial V}{\partial S} - \Delta - \sum_{i=1}^{n} \Delta_i \frac{\partial V^i}{\partial S} \right] dS_t \\ & + \sum_{j=1}^{n} \left[\frac{\partial V}{\partial v^j} - \sum_{i=1}^{n} \Delta_i \frac{\partial V^i}{\partial v^j} \right] dv_t^i \,. \end{aligned} \tag{8.55}$$

To eliminate all randomness from the portfolio we need first to choose Δ_i so that

$$\sum_{i=1}^{n} \Delta_i \frac{\partial V^i}{\partial v^j} = \frac{\partial V}{\partial v^j}\,, \tag{8.56}$$

(which is a linear system of n equations for n variables) and then to choose Δ so that

$$\Delta = \frac{\partial V}{\partial S} - \sum_{i=1}^{n} \Delta_i \frac{\partial V^i}{\partial S}\,. \tag{8.57}$$

The above system has a unique solution if the matrix $\frac{\partial V^i}{\partial v^j}$, is non-degenerate. Let $D = (D^i{}_j)$ be the $n \times n$ matrix inverse to this matrix, that is,

$$\sum_{j=1}^{n} D^i{}_j \frac{\partial V^j}{\partial v^k} = \delta^i{}_k\,, \tag{8.58}$$

where $\delta^i{}_k$ is the Kronecker delta-symbol defined by

$$\delta^i{}_k = \begin{cases} 1, \text{ if } i = k\,, \\ 0, \text{ if } i \neq k\,. \end{cases} \tag{8.59}$$

Notice that the matrix D depends only on V^i but not on V. Let C^j be a vector defined by

$$C^j = \sum_{i=1}^{n} D^j{}_i \frac{\partial V^i}{\partial S}\,. \tag{8.60}$$

Then the solution can be written as

$$\Delta_i = \sum_{j=1}^{n} D^j{}_i \frac{\partial V}{\partial v^j}\,. \tag{8.61}$$

$$\Delta = \frac{\partial V}{\partial S} - \sum_{j=1}^{n} C^j \frac{\partial V}{\partial v^j}\,. \tag{8.62}$$

Then the change in portfolio is purely deterministic

$$\begin{aligned} dR &= \left[\frac{\partial V}{\partial t} + \tilde{L}V - \sum_{i=1}^{n} \Delta_i \left(\frac{\partial V^i}{\partial t} + \tilde{L}V^i\right)\right] dt \\ &= \left[\frac{\partial V}{\partial t} + \tilde{L}V - \sum_{i,j=1}^{n} D^j{}_i \left(\frac{\partial V^i}{\partial t} + \tilde{L}V^i\right) \frac{\partial V}{\partial v^j}\right] dt\,. \end{aligned} \tag{8.63}$$

Now, by applying the no-arbitrage principle the rate of return of this portfolio must be equal to the rate of return of a risk-free investment, that is,

$$dR = r\Pi dt\,, \tag{8.64}$$

where r is the interest rate of the risk-free investment. This gives the equation

$$\frac{\partial V}{\partial t} + \tilde{L}V + rS\frac{\partial V}{\partial S} - rV = \sum_{i=1}^{n} \Delta_i \left[\frac{\partial V^i}{\partial t} + \tilde{L}V^i + rS\frac{\partial V^i}{\partial S} - rV^i\right] \tag{8.65}$$

$$= \sum_{i,j=1}^{n} D^j{}_i \left[\frac{\partial V^i}{\partial t} + \tilde{L}V^i + rS\frac{\partial V^i}{\partial S} - rV^i\right] \frac{\partial V}{\partial v^j}\,.$$

This is one equation for $(n+1)$ unknown functions, V and V^i. We assume that all options (V and V^i) satisfy the same equation. It is easy to see that the equation (8.65) will be satisfied if all options satisfy the equation

$$\frac{\partial V}{\partial t} + \tilde{L}V + rS\frac{\partial V}{\partial S} - rV = -\sum_{i=1}^{n} \gamma^i \frac{\partial V}{\partial v^i}\,. \tag{8.66}$$

The vector $\gamma^i = \gamma^i(S, v)$ is called the *risk-neutral drift rate*. It is sometimes written in the form

$$\gamma^i = a^i - \sum_{j=1}^{n} b^i{}_j \varphi^j\,, \tag{8.67}$$

where the vector φ^j is called the *market price of volatility risk*. Notice that the functions γ^i remain undetermined from the model. They should be chosen based on the market conditions.

Thus the option price satisfies the parabolic second-order partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) V = 0\,, \tag{8.68}$$

where L is the second-order partial differential operator (called the valuation operator)

$$L = \frac{1}{2}\sigma^2 S^2 \frac{\partial^2}{\partial S^2} + \sum_{i=1}^{n} A^i \sigma S \frac{\partial^2}{\partial S \partial v^i}$$

$$+ \frac{1}{2}\sum_{i,j=1}^{n} B^{ij} \frac{\partial^2}{\partial v^i \partial v^j} + rS\frac{\partial}{\partial S} + \sum_{i=1}^{n} \gamma^i \frac{\partial}{\partial v^i} - r\,. \tag{8.69}$$

8.4 Two-dimensional Stochastic Volatility Models

Usually, one considers just one extra stochastic factor, that is, $n = 1$. Then we have just two Wiener processes X_t and W_t with correlation ρ, that is,

$$E(dX_t dW_t) = \rho dt\,. \tag{8.70}$$

Then the stochastic differential equations of the model read

$$dS_t = \mu S_t\, dt + \sigma(S_t, v_t) S_t\, dX_t\,, \tag{8.71}$$

$$dv_t = a(S_t, v_t)\, dt + b(S_t, v_t)\, dW_t\,. \tag{8.72}$$

The valuation operator L becomes now

$$L = \frac{1}{2}\sigma^2 S^2 \frac{\partial^2}{\partial S^2} + \rho b \sigma S \frac{\partial^2}{\partial S \partial v} + \frac{1}{2} b^2 \frac{\partial^2}{\partial v^2} + rS\frac{\partial}{\partial S} + \gamma \frac{\partial}{\partial v} - r\,, \tag{8.73}$$

where

$$\gamma(S, v) = a(S, v) - b(S, v)\varphi(S, v) \tag{8.74}$$

is the risk-neutral drift and $\varphi(S, v)$ is the market price of volatility risk.

8.4.1 Heston Model

A popular model proposed by Heston is described by the stochastic differential equations

$$dS_t = \mu\, S_t\, dt + \sqrt{v_t}\, S_t\, dX_t\,, \tag{8.75}$$

$$dv_t = \varkappa(\theta - v_t)\, dt + \eta \sqrt{v_t}\, dW_t\,, \tag{8.76}$$

where $\varkappa$, θ and η are constant parameters.

8.4.2 Hull-White Model

A wide class of models is described by the following stochastic differential equations

$$dS_t = \mu S_t\, dt + \sigma(v_t) S_t\, dX_t, \tag{8.77}$$

$$dv_t = \varkappa(\theta - v_t) dt + \tilde{\eta} v_t\, dW_t\,, \tag{8.78}$$

where $\mu, \varkappa, \theta$ and $\tilde{\eta}$ are some constant parameters and $\sigma(v)$ is a function. For example, one can consider a model with the function $\sigma(v) = v^\alpha$, where α is a real parameter, and rescale the parameter $\tilde{\eta}$ accordingly, $\tilde{\eta} = \eta/\alpha$ for convenience, that is,

$$dS_t = \mu S_t\, dt + v_t^{\alpha} S_t\, dX_t, \tag{8.79}$$

$$dv_t = \varkappa(\theta - v_t)dt + \frac{\eta}{\alpha} v_t\, dW_t\,. \tag{8.80}$$

The Hull-White model is a special case of the above model when $\alpha = 1/2$, that is, $\sigma(v) = \sqrt{v}$, and $\theta = \rho = 0$, that is,

$$dS_t = \mu S_t\, dt + \sqrt{v_t}\, S_t\, dX_t, \tag{8.81}$$

$$dv_t = -\varkappa v_t\, dt + 2\eta v_t\, dW_t\,. \tag{8.82}$$

8.4.3 GARCH Model

Another popular model is the so-called GARCH model, which in the continuous time limit becomes equivalent to the model described by the stochastic differential equations

$$dS_t = \mu\, S_t\, dt + \sqrt{v_t}\, S_t\, dX_t\,, \tag{8.83}$$

$$dv_t = \varkappa(\theta - v_t)\, dt + 2\eta\, v_t\, dW_t\,. \tag{8.84}$$

8.4.4 Ornstein-Uhlenbeck Model

This model is described by the stochastic differential equations

$$dS_t = \mu\, S_t\, dt + e^{v_t}\, S_t\, dX_t\,, \tag{8.85}$$

$$dv_t = \varkappa(\theta - v_t)\, dt + \eta\, dW_t\,. \tag{8.86}$$

8.4.5 SABR Model

The SABR model was developed for forward assets. Although, usually the price of a forward asset is denoted by F we will still denote it by S for the sake of uniformity of notation. The SABR model is described by the stochastic differential equations

$$dS_t = v_t f(S_t) S_t\, dX_t\,, \tag{8.87}$$

$$dv_t = \eta v_t\, dW_t\,, \tag{8.88}$$

where X_t and W_t are Wiener processes with the constant correlation ρ, η is a parameter and $f(S)$ is a positive monotone function. A popular choice is

$$f(S) = S^{-\alpha}\,, \tag{8.89}$$

where α is a constant parameter such that $0 \leq \alpha \leq 1$. There are two special cases of interest here. In the case $\alpha = 0$ one gets the log-normal model, which for $\eta = 0$ degenerates to the Black-Scholes model (with $r = 0$). In the case $\alpha = 1$ we get the normal model.

8.4.6 SABR Model with Mean-Reverting Volatility

One can generalize the standard SABR model by including a *mean-reverting drift* in the volatility process

$$dS_t = v_t S_t^{1-\alpha}\, dX_t\,, \tag{8.90}$$

$$dv_t = \varkappa(\theta - v_t)dt + \eta v_t\, dW_t\,, \tag{8.91}$$

where $\varkappa$ is the mean reverting rate and θ is the long-term volatility, which are assumed to be constant parameters. As before, X and W are Wiener processes with the correlation ρ.

8.5 Jump Diffusion Models

An even more general class of models could include the jumps in the underlying asset S. Let X_t and W_t be two Wiener processes with correlation ρ and Q_t be a Poisson process with constant intensity λ. We assume that there is no correlation between the Wiener processes X_t and W_t and the Poisson process Q. That is,

$$E(dQ_t) = \lambda dt\,, \tag{8.92}$$

$$E(dX_t dQ_t) = E(dW_t dQ_t) = 0\,. \tag{8.93}$$

8.5.1 Jumps Probability Density

Also, we assume that the jump of magnitude J in the logarithm of the asset S_t is a random variable with the probability density function $\omega(J)$ independent of the Wiener and Poisson processes above. The Fourier transform of the probability density defines the characteristic function

$$\hat{\omega}(z) = E(e^{izJ}) = \int_{-\infty}^{\infty} dJ e^{izJ} \omega(J)\,, \tag{8.94}$$

so that the average jump amplitude is

$$m = E\left(e^J - 1\right) = \hat{\omega}(-i) - 1 = \int_{-\infty}^{\infty} dJ\, \omega(J) e^J - 1\,. \tag{8.95}$$

One of the basic distributions is the normal one

$$\omega(J) = (4\pi\delta)^{-1/2} \exp\left[-\frac{(J-\nu)^2}{4\delta}\right], \tag{8.96}$$

where ν is the expected value of the jump and 2δ is the variance. The characteristic function and the average jump amplitude for this distribution are

$$\hat{\omega}(z) = e^{-\delta z^2 + i\nu z}\,, \tag{8.97}$$

$$m = e^{\nu+\delta} - 1\,. \tag{8.98}$$

Another popular choice is the double-exponential distribution

$$\begin{aligned}\omega(J) &= \theta(J)\frac{p_+}{\delta_+}\exp\left(-\frac{J}{\delta_+}\right) + \theta(-J)\frac{p_-}{\delta_-}\exp\left(\frac{J}{\delta_-}\right) \\ &= \begin{cases} \dfrac{p_+}{\delta_+}\exp\left(-\dfrac{J}{\delta_+}\right) & \text{if } J > 0, \\ \dfrac{p_-}{\delta_-}\exp\left(\dfrac{J}{\delta_-}\right) & \text{if } J < 0\,, \end{cases}\end{aligned} \tag{8.99}$$

where $p_\pm \geq 0$ are the probabilities of positive and negative jumps, so that $p_+ + p_- = 1$, and $\delta_\pm$ are the means of positive and negative jumps. It is assumed that $0 < \delta_+ < 1$ and $\delta_- > 0$. The characteristic function and the average jump amplitude are now

$$\hat{\omega}(z) = \frac{p_+}{1 - iz\delta_+} + \frac{p_-}{1 + iz\delta_-}\,, \tag{8.100}$$

$$m = \frac{p_+}{1-\delta_+} + \frac{p_-}{1+\delta_-} - 1\,. \tag{8.101}$$

Obviously, in the limit $\delta_+, \delta_- \to 0$ the probability density degenerates, that is,

$$\omega(J) \to \delta(J)\,, \qquad \hat{\omega}(z) \to 1\,, \tag{8.102}$$

so that the average jump amplitude vanishes

$$m \to 0\,. \tag{8.103}$$

Notice also, that as $z \to \infty$

$$\hat{\omega}(z) = \frac{1}{iz}\left(-\frac{p_+}{\delta_+} + \frac{p_-}{\delta_-}\right) + O\left(\frac{1}{z^2}\right)\,. \tag{8.104}$$

8.5.2 Stochastic Volatility Model with Jumps

Now, we can combine the stochastic volatility with jumps in the underlying. Then the stochastic differential equations of the model read

$$dS_t = \mu S_t\,dt + \sigma(S_t, v_t)S_t\,dX_t + (e^J - 1)S_t\,dQ_t\,, \tag{8.105}$$

$$dv_t = a(S_t, v_t)\,dt + b(S_t, v_t)\,dW_t\,. \tag{8.106}$$

Hedging in the presence of jumps is tricky since there are two sources of randomness, the diffusion and the jumps, and there is no way to hedge away both processes. We set up a portfolio strategy under which one holds a single long option position with value $V = V(t, S, v)$ and continuously trades in the underlying asset and some other option $V_1 = V_1(t, S, v)$ to hold a short position of the underlying and short positions in other options. Let $\Delta = \Delta(t, S, v)$ denote the size of the short underlying position and $\Delta_1 = \Delta_1(t, S, v)$ denote the size of the short positions in the other option. Then the value of such portfolio at time t is

$$\Pi = V - \Delta S - \Delta_1 V_1\,. \tag{8.107}$$

Now, we consider the change of the value of our portfolio from time t to the time $t + dt$ by considering the quantities Δ and Δ_1 constant during this time step. Let $R = R(t, S, v)$ be the accumulated profit/loss from following this strategy. Then, over the time period from t to $t + dt$ the instantaneous profit is

$$dR = dV - \Delta dS - \Delta_1 dV_1\,. \tag{8.108}$$

Next, by the Îto lemma for both options, V and V_1, we have

$$\begin{aligned} dV = &\left(\frac{\partial V}{\partial t} + \tilde{L}V + \mu S\frac{\partial V}{\partial S}\right)dt + \sigma S\frac{\partial V}{\partial S}\,dX_t + b\frac{\partial V}{\partial v}\,dW_t \\ &+ \left[V(t, e^J S, v) - V(t, S, v)\right]dQ_t\,, \end{aligned} \tag{8.109}$$

where $\tilde{L}$ is a second-order linear partial differential operator defined by

$$\tilde{L} = \frac{1}{2}\sigma^2 S^2\frac{\partial^2}{\partial S^2} + \sigma S b\rho\frac{\partial^2}{\partial S\partial v} + \frac{1}{2}b^2\frac{\partial^2}{\partial v^2} + a\frac{\partial}{\partial v}\,. \tag{8.110}$$

Therefore, the instantaneous profit/loss is

$$
\begin{aligned}
dR = &\left[\frac{\partial V}{\partial t} + \tilde{L}V + \mu S\frac{\partial V}{\partial S} - \mu S\Delta - \Delta_1\left(\frac{\partial V_1}{\partial t} + \tilde{L}V_1 + \mu S\frac{\partial V_1}{\partial S}\right)\right]dt \\
&+\sigma S\left[\frac{\partial V}{\partial S} - \Delta - \Delta_1\frac{\partial V_1}{\partial S}\right]dX_t + b\left[\frac{\partial V}{\partial v} - \Delta_1\frac{\partial V_1}{\partial v}\right]dW_t \\
&+\Bigg\{\big[V(t,e^J S,v) - V(t,S,v)\big] - \Delta(e^J-1)S \\
&-\Delta_1\big[V_1(t,e^J S,v) - V_1(t,S,v)\big]\Bigg\}dQ_t\,. \qquad (8.111)
\end{aligned}
$$

To eliminate all randomness from the portfolio we need to choose the parameters Δ and Δ_1 such that the stochastic terms proportional to dX_t, dW_t and dQ_t vanish. Obviously, this is impossible since we only have two parameters. This means that *randomness cannot be fully hedged away.* One way to deal with this is to hedge the diffusion and leave the random jumps. Then we can choose, as before, Δ_1 so that

$$
\Delta_1 = \left(\frac{\partial V_1}{\partial v}\right)^{-1}\frac{\partial V}{\partial v}\,, \qquad (8.112)
$$

(which is always possible if $\frac{\partial V_1}{\partial v} \neq 0$) and then to choose Δ so that

$$
\Delta = \frac{\partial V}{\partial S} - \Delta_1\frac{\partial V_1}{\partial S}\,. \qquad (8.113)
$$

Then the change in the portfolio is

$$
\begin{aligned}
dR = &\left(\frac{\partial V}{\partial t} + \tilde{L}V\right)dt + \left[V(t,e^J S,v) - V(t,S,v) - (e^J-1)S\frac{\partial V}{\partial S}\right]dQ_t \\
&-\Delta_1\Bigg\{\left(\frac{\partial V_1}{\partial t} + \tilde{L}V_1\right)dt \\
&+\left[V_1(t,e^J S,v) - V_1(t,S,v) - (e^J-1)S\frac{\partial V_1}{\partial S}\right]dQ_t\Bigg\}\,. \qquad (8.114)
\end{aligned}
$$

Now, since there is still some randomness left in the portfolio we cannot apply the no-arbitrage principle directly. However, it can be argued [79] that it can be applied to the *expectation value of the portfolio*, that is, we require that

$$
E(dR) = r\Pi dt\,. \qquad (8.115)
$$

By using this equation we obtain

$$\left(\frac{\partial V}{\partial t}+\tilde{L}V+rS\frac{\partial V}{\partial S}-rV\right)$$
$$+\lambda E\left[V(t,e^J S,v)-V(t,S,v)-(e^J-1)S\frac{\partial V}{\partial S}\right]$$
$$=\Delta_1\left\{\left(\frac{\partial V_1}{\partial t}+\tilde{L}V_1+rS\frac{\partial V_1}{\partial S}-rV_1\right)\right.$$
$$\left.+\lambda E\left[V_1(t,e^J S,v)-V_1(t,S,v)-(e^J-1)S\frac{\partial V_1}{\partial S}\right]\right\}, \quad (8.116)$$

where the expectation value is taken over the random jump amplitude with the distribution function $\omega(J)$, that is,

$$E[f(J)]=\int_{-\infty}^{\infty} dJ\,\omega(J)f(J)\,. \quad (8.117)$$

Now, by taking into account eq. (8.112) we obtain that both options (V and V_1) must satisfy the same equation

$$\frac{\partial V}{\partial t}+\tilde{L}V+rS\frac{\partial V}{\partial S}+\gamma\frac{\partial V}{\partial v}-rV$$
$$+\lambda E\left[V(t,e^J S,v)-V(t,S,v)-(e^J-1)S\frac{\partial V}{\partial S}\right]=0\,, \quad (8.118)$$

where the function $\gamma=\gamma(S,v)$ is the *risk-neutral drift rate*; it is related to the *market price of volatility risk* $\varphi=\varphi(S,v)$ by

$$\gamma=a-b\varphi\,. \quad (8.119)$$

Thus the option price satisfies the integro-differential equation

$$\left(\frac{\partial}{\partial t}+L\right)V=0\,, \quad (8.120)$$

where L is the *integro-differential* (*pseudo-differential*) operator of the form

$$L=L_{\rm diff}+\lambda L_J\,, \quad (8.121)$$

with $L_{\rm diff}$ being the partial differential operator

$$L_{\rm diff}=\frac{1}{2}\sigma^2S^2\frac{\partial^2}{\partial S^2}+\rho b\sigma S\frac{\partial^2}{\partial S\partial v}+\frac{1}{2}b^2\frac{\partial^2}{\partial v^2}+rS\frac{\partial}{\partial S}+\gamma\frac{\partial}{\partial v}-r\,, \quad (8.122)$$

and L_J being the integral operator that acts on functions of S as follows

$$(L_J f)(S) = -mS\frac{\partial}{\partial S}f(S) - f(S) + \int_{-\infty}^{\infty} dJ\, \omega(J) f(e^J)\,, \qquad (8.123)$$

recall that $m = E(e^J - 1)$ is the average jump amplitude. The operator L_J can also be expressed in terms of the characteristic function as follows

$$L_J = -mS\frac{\partial}{\partial S} - 1 + \hat{\omega}\left(-iS\frac{\partial}{\partial S}\right)\,. \qquad (8.124)$$

8.6 Solution of Two-Dimensional Models

8.6.1 Black-Scholes Model

Let us consider a European call option of an asset with strike price K, the spot price S and the expiration time T. Let σ be the volatility of the underlying asset and r be the interest rate of the risk-free investment. Then the price of the option $C(t, S)$ satisfies the valuation equation (8.27)

$$(\partial_t - L)\, C(t, S) = 0\,, \qquad (8.125)$$

where

$$L = -\frac{\sigma^2}{2}S^2\frac{\partial^2}{\partial S^2} - rS\frac{\partial}{\partial S} + r\,, \qquad (8.126)$$

with the terminal condition

$$C(T, S) = (S - K)_+\,. \qquad (8.127)$$

Here we changed the sign of the operator L to make it positive.

Recall that for dividend stocks with a dividend d the valuation operator has the form

$$L = -\frac{\sigma^2}{2}S^2\frac{\partial^2}{\partial S^2} + (d - r)S\frac{\partial}{\partial S} + r\,. \qquad (8.128)$$

Also, for currency options with the foreign rate of interest r_f and for commodity options with the cost of carry q the valuation operator has the same form with $d = r_f$ and $d = -q$. Finally, the valuation operator for the options on futures for a non-dividend stock also has the same form (8.128) with $d = r$.

First of all, we introduce new variables

$$\tau = T - t\,, \qquad (8.129)$$

$$x = \log S\,. \qquad (8.130)$$

Also, we introduce parameters

$$\alpha = \frac{\sigma^2}{2}\,, \tag{8.131}$$

$$\beta = \frac{\sigma^2}{2} + d - r\,. \tag{8.132}$$

Then the option satisfies the equation

$$(\partial_\tau + L)\, C(\tau, x) = 0\,, \tag{8.133}$$

where

$$L = -\alpha\partial_x^2 + \beta\partial_x + r\,, \tag{8.134}$$

with the initial condition

$$C(0, x) = (e^x - e^{x_0})_+\,, \tag{8.135}$$

where $x_0 = \log K$.

This equation has constant coefficients. Therefore, its heat kernel is easily calculated by using Fourier transform and the Gaussian integral (1.18)

$$\begin{aligned} U_{BS}(\tau; x, x') &= \exp(-\tau L)\delta(x - x') \\ &= \int_{-\infty}^{\infty} \frac{dp}{2\pi} \exp\left\{ip(x - x') - \tau\left[\alpha p^2 + i\beta p + r\right]\right\} \\ &= (4\pi\alpha\tau)^{-1/2} e^{-r\tau} \exp\left\{-\frac{(x - x' - \beta\tau)^2}{4\alpha\tau}\right\} \\ &= (4\pi\alpha\tau)^{-1/2} \exp\left\{-\tau\left(r + \frac{\beta^2}{4\alpha}\right)\right\} \exp\left\{\frac{\beta}{2\alpha}(x - x')\right\} \\ &\quad \times \exp\left\{-\frac{(x - x')^2}{4\alpha\tau}\right\}\,. \end{aligned} \tag{8.136}$$

This is the Black-Scholes heat kernel.

Now the price of the Black-Scholes call option is calculated by computing the integral

$$C_{BS}(\tau, x) = \int_{x_0}^{\infty} dx'\, U_{BS}(\tau; x, x')(e^{x'} - e^{x_0})\,. \tag{8.137}$$

This integral can be expressed in terms of the standard cumulative normal distribution

$$N(x) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{x} dt \, \exp\left(-\frac{t^2}{2}\right) = \frac{1}{2}\left[1 + \text{ erf } \left(\frac{x}{\sqrt{2}}\right)\right], \tag{8.138}$$

where erf (x) is the error function. Indeed, by using the integral

$$\int\limits_{0}^{\infty} dx \, e^{-px^2+qx} = \sqrt{\pi}\, p^{-1/2} \exp\left(\frac{q^2}{4p}\right) N\left(\frac{q}{\sqrt{2p}}\right), \tag{8.139}$$

we obtain

$$C_{BS}(\tau, x) = e^{-r\tau}\left\{ e^{x+(\alpha-\beta)\tau} N\left(\frac{x - x_0}{\sqrt{2\alpha\tau}} + \frac{2\alpha - \beta}{\sqrt{2\alpha}}\sqrt{\tau}\right) \right.$$
$$\left. - e^{x_0} N\left(\frac{x - x_0}{\sqrt{2\alpha\tau}} - \frac{\beta}{\sqrt{2\alpha}}\sqrt{\tau}\right)\right\}. \tag{8.140}$$

8.6.2 Higher Dimensional Black-Scholes Model

Let us consider n assets whose prices at time t are S^i, $i = 1, 2, \ldots, n$. Let $V(t, S) = V(t, S^1, \ldots, S^n)$ be the price of an option at time t with the expiration time T. Let r be the interest rate of a risk-free investment and d_i be the dividend rates for underlying assets S_i. Let σ_i be the volatility of the stock S_i and ρ^{ij} be the correlation matrix of the corresponding Wiener processes. Then the valuation equation for the option is

$$(\partial_t - L)\, V(t, S) = 0\,, \tag{8.141}$$

where the valuation operator is (8.41)

$$L = -\frac{1}{2}\sum_{i,j=1}^{n} C_{ij} S^i S^j \frac{\partial^2}{\partial S^i \partial S^j} - \sum_{i=1}^{n} (r - d_i) S^i \frac{\partial}{\partial S^i} + r\,, \tag{8.142}$$

and the matrix C_{ij} is defined by (no summation over the repeated indices i, j here)

$$C_{ij} = \rho^{ij} \sigma_i \sigma_j\,. \tag{8.143}$$

The type of the option is specified by the payoff function $P(S)$ in the terminal condition

$$V(T, S) = P(S)\,. \tag{8.144}$$

We introduce new variables

$$\tau = T - t\,, \tag{8.145}$$

$$x^i = \log S^i\,. \tag{8.146}$$

Also, we introduce the matrix

$$\alpha^{ij} = \frac{1}{2} C_{ij} = \frac{1}{2}\rho^{ij}\sigma_i\sigma_j\,, \tag{8.147}$$

and the vector

$$\beta^i = \frac{1}{2} C_{ii} + d_i - r = \frac{1}{2}(\sigma_i)^2 + d_i - r\,, \tag{8.148}$$

where we used the fact that the diagonal entries of the correlation matrix are equal to 1, $\rho^{ii} = 1$. Then the valuation equation becomes

$$(\partial_\tau + L)\, V = 0\,, \tag{8.149}$$

where the valuation operator is

$$L = -\alpha^{ij}\partial_i\partial_j + \beta^i\partial_i + r\,, \tag{8.150}$$

with $\partial_i = \frac{\partial}{\partial x^i}$. This equation has constant coefficients. Therefore, the corresponding heat kernel can be easily obtained by Fourier transform. In fact, we have already computed this heat kernel many times in the book; it has the form (see, for example, eq. (2.196))

$$\begin{aligned} U_{BS}(\tau; x, x') = (4\pi\tau)^{-n/2} (\det A)^{-1/2} \exp\left\{-\tau\left[r + \frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle\right]\right\} \\ \times \exp\left\{\frac{1}{2}\left\langle (x - x'), A^{-1}\beta\right\rangle\right\} \\ \times \exp\left\{-\frac{1}{4\tau}\left\langle (x - x'), A^{-1}(x - x')\right\rangle\right\}\,, \end{aligned} \tag{8.151}$$

where $A = (\alpha^{ij})$ and $A^{-1} = (\alpha_{ij})$ is the inverse matrix. The price of the option can now be computed by

$$V(\tau, S) = \int\limits_{\mathbb{R}^n} dx'\; U_{BS}(\tau; x, x') P(x')\,. \tag{8.152}$$

Notice that we used the heat kernel in the density form; that is why it contains the factor $(\det A)^{-1/2}$.

8.6.3 Two-dimensional Stochastic Volatility Models

Let S be the price of the underlying asset. We assume that the volatility $\sigma(S, v)$ of this asset is stochastic and depends on just one stochastic factor v with volatility $b(v)$ that does not depend on S and drift $a(S, v)$. All models discussed in Chap. 1 are of this type. Let r be the interest rate of a risk-free investment and ρ be the correlation of the corresponding Wiener processes. Let $\gamma = \gamma(S, v)$ be the risk-neutral drift defined by

$$\gamma(S, v) = a(S, v) - b(v)\varphi(S, v), \tag{8.153}$$

where $\varphi(S, v)$ is the market price of the volatility risk (see Sec. 8.4 for details). Recall also that the correlation ρ is varied between -1 and 1, that is,

$$-1 < \rho < 1\,. \tag{8.154}$$

Then the valuation equation for a European call option $C(t, S, v)$ with strike K and the expiration time T satisfies the usual equation

$$(\partial_t - L)C(t, S, v) = 0\,, \tag{8.155}$$

where the valuation operator L has the form (8.73)

$$\begin{aligned} L = &-\frac{1}{2}\sigma^2(S, v)S^2\frac{\partial^2}{\partial S^2} - \rho b(v)\sigma(S, v)S\frac{\partial^2}{\partial S \partial v} - \frac{1}{2}b^2(v)\frac{\partial^2}{\partial v^2} \\ &-rS\frac{\partial}{\partial S} - \gamma(S, v)\frac{\partial}{\partial v} + r\,, \end{aligned} \tag{8.156}$$

Here we changed the sign of the valuation operator to make it positive.

First of all, we need to specify the range of variables. Obviously,

$$0 \le t \le T, \qquad 0 < S < \infty\,. \tag{8.157}$$

As to the range of the variable v it could be different in different models. In any case it should vary in such a range that both functions $\sigma(S, v)$ and $b(v)$ are non-negative

$$\sigma(S, v) > 0, \qquad b(v) > 0\,. \tag{8.158}$$

To be specific we assume that

$$v_1 < v < v_2\,. \tag{8.159}$$

Next, we need to impose a terminal condition

$$C(T, S, v) = (S - K)_+\,, \tag{8.160}$$

and, in general, some boundary conditions.

It is worth stressing that in the limiting case when the volatility σ is constant and

$$b = \gamma = 0 \tag{8.161}$$

this model degenerates to the standard Black-Scholes model. The Black-Scholes model serves as a canonical model; all other models are compared to it. In particular, one defines so called *implied volatility* as an implicit function $\sigma_{BS}(t, S, v)$ such that if one replaces the constant volatility σ in the standard Black-Scholes formula (8.140) for the call option $C_{BS}(t, S)$ by $\sigma_{BS}(t, S, v)$ then one gets precisely the price of the option in a more general model, that is,

$$C(t, S, v) = C_{BS}(t, S)\Big|_{\sigma=\sigma_{BS}(t,S,v)} . \tag{8.162}$$

In fact, all models are discussed and compared not in terms of the option price $C(t, S, v)$ but in terms of the implied volatility.

We introduce new coordinates by

$$\tau = T - t\,, \tag{8.163}$$

$$x = \log S\,; \tag{8.164}$$

obviously,

$$0 \le \tau \le T, \qquad -\infty < x < \infty\,. \tag{8.165}$$

We denote $x^1 = x$ and $x^2 = v$. Then the valuation equation becomes

$$(\partial_\tau + L)C(\tau, x) = 0\,, \tag{8.166}$$

where the valuation operator is

$$\begin{aligned} L = &-\frac{1}{2}\sigma^2\partial_1^2 - \rho b\sigma\partial_1\partial_2 - \frac{1}{2}b^2\partial_2^2 \\ &+\frac{1}{2}\left(\sigma^2 - 2r\right)\partial_1 - \gamma\partial_2 + r\,; \end{aligned} \tag{8.167}$$

here, as usual, $\partial_i = \frac{\partial}{\partial x^i}$.

The operator (8.167) defines a two-dimensional Riemannian metric g^{ij} with contravariant components

$$g^{11} = \frac{1}{2}\sigma^2\,, \tag{8.168}$$

$$g^{12} = \frac{1}{2}\rho b\sigma\,, \tag{8.169}$$

$$g^{22} = \frac{1}{2}b^2\,. \tag{8.170}$$

The matrix (g^{ij}) is invertible and positive definite. The determinant of this matrix determines the inverse of the determinant of the metric g_{ij},

$$g = (\det g^{ij})^{-1} = \frac{4}{(1-\rho^2)\sigma^2 b^2}\,. \tag{8.171}$$

This means, in particular, that for $\rho = \pm 1$ the metric is not invertible, which means, in turn, that the operator L is not elliptic. Also, the metric becomes singular at the points where $\sigma(S,v) = 0$ or $b(v) = 0$. That is why we need to require the positivity of the functions $\sigma(S,v)$ and $b(v)$.

By inverting this matrix we obtain the covariant components

$$g_{11} = \frac{2}{(1-\rho^2)\sigma^2}\,, \tag{8.172}$$

$$g_{12} = -\frac{2\rho}{(1-\rho^2)\sigma b}\,, \tag{8.173}$$

$$g_{22} = \frac{2}{(1-\rho^2)b^2}\,. \tag{8.174}$$

This defines the interval

$$\begin{aligned} ds^2 &= \frac{2}{1-\rho^2}\left(\frac{dx^2}{\sigma^2(x,v)} - 2\rho\frac{dx\,dv}{\sigma(x,v)b(v)} + \frac{dv^2}{b^2(v)}\right) \\ &= \frac{2}{1-\rho^2}\left(\frac{dx}{\sigma(x,v)} - \rho\frac{dv}{b(v)}\right)^2 + 2\frac{dv^2}{b^2(v)}\,. \end{aligned} \tag{8.175}$$

Next, we compute the quantities

$$g^{1/2}g^{11} = \frac{1}{\sqrt{1-\rho^2}}\frac{\sigma}{b}\,, \tag{8.176}$$

$$g^{1/2}g^{12} = \frac{\rho}{\sqrt{1-\rho^2}}\,, \tag{8.177}$$

$$g^{1/2}g^{22} = \frac{1}{\sqrt{1-\rho^2}}\frac{b}{\sigma}\,. \tag{8.178}$$

This allows us to compute the quantity $\Gamma^i = g^{-1/2}\partial_j(g^{1/2}g^{ij})$ (3.610),

$$\Gamma^1 = \frac{1}{2}\sigma\partial_1\sigma\,, \tag{8.179}$$

$$\Gamma^2 = -\frac{b^2}{2}\frac{\partial_2\sigma}{\sigma}\,. \tag{8.180}$$

Therefore, the Laplacian of this metric has the form

$$\begin{aligned}\Delta &= g^{-1/2}\partial_i g^{1/2} g^{ij}\partial_j \\ &= \frac{1}{2}\sigma^2\partial_1^2 + \rho b\sigma\partial_1\partial_2 + \frac{1}{2}b^2\partial_2^2 + \frac{1}{2}\sigma\sigma_1\partial_1 - \frac{b^2}{2}\frac{\sigma_2}{\sigma}\partial_2\,, \end{aligned} \tag{8.181}$$

where $\sigma_i = \partial_i\sigma$. Now, we can decompose the operator L accordingly, (3.617), (3.622),

$$L = -\Delta + L_1 + r\,, \tag{8.182}$$

where L_1 is the first-order differential operator

$$L_1 = A\partial_1 + B\partial_2\,, \tag{8.183}$$

with

$$A = \frac{\sigma^2}{2} + \frac{1}{2}\sigma\sigma_1 - r\,, \tag{8.184}$$

$$B = -\gamma - \frac{b^2}{2}\frac{\sigma_2}{\sigma}\,. \tag{8.185}$$

Omitting lengthy but straightforward calculations we also obtain the scalar curvature of the above metric

$$\begin{aligned} R &= \sigma b\partial_2\left(b\frac{\partial_2\sigma}{\sigma^2}\right) + \rho\sigma b\partial_2\left(\frac{\partial_1\sigma}{\sigma}\right) \\ &= \sigma b\partial_2\left(\rho\partial_1\log\sigma - b\partial_2\frac{1}{\sigma}\right)\,. \end{aligned} \tag{8.186}$$

Let us consider a class of models in which the volatility factorizes

$$\sigma(x,v) = f(x)h(v)\,, \tag{8.187}$$

where f and h are some positive functions. Then the metric is defined by

$$ds^2 = \frac{2}{h^2(v)}\left[\frac{1}{(1-\rho^2)}\left(\frac{dx}{f(x)} - \rho\frac{h(v)}{b(v)}dv\right)^2 + \frac{h^2(v)}{b^2(v)}dv^2\right]\,. \tag{8.188}$$

This dictates the introduction of natural local coordinates $(y^1, y^2) = (y, u)$ by

$$y = \frac{1}{\sqrt{1-\rho^2}}\left[\int_{x_0}^{x}\frac{dx'}{f(x')} - \rho\int_{v_0}^{v}\frac{h(v')}{b(v')}dv'\right]\,, \tag{8.189}$$

$$u = \int_{v_0}^{v}\frac{h(v')}{b(v')}dv'\,, \tag{8.190}$$

where x_0 and v_0 are some constants. Then the derivatives are related by

$$\partial_1 = \partial_x = \frac{1}{\sqrt{1-\rho^2}} \frac{1}{f} \partial_y \tag{8.191}$$

$$\partial_2 = \partial_v = -\frac{\rho}{\sqrt{1-\rho^2}} \frac{h}{b} \partial_y - \frac{h}{b} \partial_u \,. \tag{8.192}$$

In these coordinates the metric takes a very simple conformal form

$$ds^2 = \frac{2}{h^2} \left(dy^2 + du^2 \right) \,. \tag{8.193}$$

Therefore, the curvature in these coordinates is

$$R = -hb\partial_v \left(b\partial_v \frac{1}{h} \right) = h^2 \partial_u^2 \log h \,. \tag{8.194}$$

Note that the curvature does not depend on the function f at all. This means that the arbitrariness of this function just reflects the possibility to make an arbitrary change of coordinates; it does not change the geometry.

A wide class of models is covered by the following functions

$$f(x) = 1, \tag{8.195}$$

$$h(v) = \xi v^\alpha, \tag{8.196}$$

$$b(v) = \eta v^\beta \,, \tag{8.197}$$

where $\alpha > 0$ and $\beta > 0$. Then the curvature is

$$R = -\eta^2 \alpha(\alpha + 1 - \beta) \frac{1}{v^{2-2\beta}} \,. \tag{8.198}$$

Notice that for $\beta < 1 + \alpha$ the curvature is negative, $R < 0$ and for $\beta = 1$ it is constant, $R = -\eta^2\alpha^2$. Also, for $\beta < 1$ the curvature is singular at $v = 0$.

This equation means that $R > 0$ if the function $\log h$ is a convex function of u and $R < 0$ if the function $\log h$ is concave; in all models considered in Chap. 1 the function $\log h$ is indeed a concave function of u so that $R < 0$. Notice that there is a big difference between manifolds with positive and negative curvatures, in particular, in terms of the geodesic flow. The fact that the curvature is negative already tells us something about the properties of the heat kernel.

The Laplacian takes especially simple form

$$\Delta = \frac{1}{2} h^2 \left(\partial_y^2 + \partial_u^2 \right) \,. \tag{8.199}$$

In the new coordinates the operator L_1 becomes

$$L_1 = C\partial_y + D\partial_u \,, \tag{8.200}$$

where

$$C = \frac{1}{\sqrt{1-\rho^2}} \left\{ \frac{1}{2} h^2 \left(f_x + f \right) - \frac{r}{f} + \rho\gamma \frac{h}{b} + \frac{\rho}{2} bhv \right\} ,$$

$$D = h \left(\frac{\gamma}{b} + \frac{v}{2} b \right) , \tag{8.201}$$

where $f_x = \partial_x f$. In many models the function f is constant, say $f(x) = 1$. Then the coefficients of this operator take the form

$$C = \frac{1}{\sqrt{1-\rho^2}} \left\{ \frac{1}{2} h^2 - r + \rho\gamma \frac{h}{b} + \frac{\rho}{2} bhv \right\} ,$$

$$D = h \left(\frac{\gamma}{b} + \frac{v}{2} b \right) . \tag{8.202}$$

Thus the operator L reads

$$L = -\frac{1}{2} h^2 \left(\partial_y^2 + \partial_u^2 \right) + C\partial_y + D\partial_u \,. \tag{8.203}$$

The heat kernel of the operator L is now defined by

$$(\partial_\tau + L) U(\tau; x, v, x', v') = 0 \,, \tag{8.204}$$

with the initial condition

$$U(0; x, v, x', v') = \frac{1}{2} \sqrt{1-\rho^2} f(x) h(v) b(v) \delta(x - x') \delta(v - v') \,. \tag{8.205}$$

Then the option price is given in terms of the heat kernel by

$$C(\tau, x, v) = \frac{2}{\sqrt{1-\rho^2}} \int_{x_0}^{\infty} dx' \int_{v_1}^{v_2} dv' \frac{1}{f(x') h(v') b(v')} U(\tau; x, v, x', v') (e^{x'} - e^{x_0}) \,, \tag{8.206}$$

where $x_0 = \log K$ and v_1 and v_2 are the constants determining the range of the variable v in (8.159).

8.6.4 Models on Hyperbolic Plane

Let us compute the curvature, the Laplacian and the operator L_1 for various models described in Sec. 8.4. In all these models η is a constant parameter. In all the following models the hyperbolic coordinates (y, u) range over the

whole upper half-plane

$$-\infty < y < \infty, \qquad u > 0\,. \tag{8.207}$$

The function $h(v)$ has the form in new coordinates

$$h(v) = \eta u\,, \tag{8.208}$$

and, therefore, the metric reads

$$ds^2 = \frac{2}{\eta^2 u^2}\left(dy^2 + du^2\right) \tag{8.209}$$

Therefore, the curvature is constant and negative

$$R = -\eta^2\,, \tag{8.210}$$

and the Laplacian has the form

$$\Delta = \frac{\eta^2}{2} u^2 \left(\partial_y^2 + \partial_u\right)^2\,. \tag{8.211}$$

Thus, we see that in all these models the curvature is constant and negative which means that the corresponding manifold has locally the geometry of the hyperbolic plane H^2. Moreover, since the coordinates (y, u) range over the upper half-plane they cover the whole hyperbolic plane. Therefore, we could use here powerful geometric methods (in addition to the perturbation theory) to compute the heat kernel of these models.

We have already found the heat kernel of Laplacian in the hyperbolic plane H^2 in the previous chapter, at least in the limit $\tau \to 0$. Let r be the geodesic distance between (y, u) and (y', u'); it is given by (3.197)

$$r = \frac{1}{\varkappa} \cosh^{-1}\varphi\,, \tag{8.212}$$

where

$$\varkappa = \frac{\eta}{\sqrt{2}} \tag{8.213}$$

and

$$\varphi = 1 + \frac{(y - y')^2 + (u - u')^2}{2uu'}\,. \tag{8.214}$$

Then the heat kernel of the Laplacian reads

$$U_0(\tau; x, v, x', v') = \frac{1}{4\pi\tau}\sqrt{\frac{\varkappa r}{\sinh(\varkappa r)}}\exp\left(-\frac{r^2}{4\tau}\right) \times\left\{1 - \tau b_1(r) + \frac{\tau^2}{2} b_2(r) + O(\tau^3)\right\}, \tag{8.215}$$

where the functions $b_1(r)$ and $b_2(r)$ are given by (5.156) and (5.157).

By treating the operator L_1 as a perturbation and using the eq. (1.215), we get the heat kernel of the operator L

$$U(\tau; x, v, x', v') \tag{8.216}$$
$$= e^{-r\tau}\left\{1 - \tau L_1 + \frac{\tau^2}{2}\left(L_1^2 + [L_1, \Delta]\right) + O(\tau^3)\right\} U_0(\tau; x, v, x', v')\,.$$

This is a generalization of the formula used in [48, 49] in the derivation of the so-called *Hagan formula* for the SABR model. If we restrict ourselves to the linear order in L_1 and substitute here an expression for the geodesic distance as a function of coordinates, then this equation reduces to the Hagan formula. Of course, the operator L_1 has different forms in these models.

Below we specify the formula (8.206) for different models. In all these cases $U(t; x, v, x', v')$ is the heat kernel given by eq. (8.216).

8.6.4.1 GARCH Model and Hull-White Model

For the GARCH model and the Hull-White model the functions $\sigma(S, v)$ and $b(v)$ have the same form (8.83), (8.84), and (8.85), (8.86),

$$\sigma(S, v) = h(v) = v^\alpha\,, \tag{8.217}$$

$$b(v) = \frac{\eta}{\alpha} v\,. \tag{8.218}$$

Here the variable v ranges over the real half-axis

$$0 < v < \infty, \tag{8.219}$$

and α is a non-negative parameter,

$$0 < \alpha \leq 1\,. \tag{8.220}$$

The hyperbolic coordinates can be easily computed

$$y = \frac{1}{\sqrt{1-\rho^2}}\left(x - \frac{\rho}{\eta} v^\alpha\right), \tag{8.221}$$

$$u = \frac{1}{\eta} v^\alpha\,. \tag{8.222}$$

The option price is given by (8.206)

$$C(\tau,x,v)=\frac{2\alpha}{\eta\sqrt{1-\rho^2}}\int\limits_{x_0}^{\infty}dx'\int\limits_{0}^{\infty}dv'v'^{-1-\alpha}U(t;x,v,x',v')(e^{x'}-e^{x_0})\,. \quad (8.223)$$

8.6.4.2 Ornstein-Uhlenbeck Model

For the Ornstein-Uhlenbeck model the functions $\sigma(S,v)$ and $b(v)$ have the form (8.85), (8.86)

$$\sigma(S,v)=h(v)=e^v\,, \quad (8.224)$$

$$b(v)=\eta\,. \quad (8.225)$$

The variable v ranges now over the whole real axis

$$-\infty<v<\infty\,. \quad (8.226)$$

The hyperbolic coordinates are now

$$y=\frac{1}{\sqrt{1-\rho^2}}\left(x-\frac{\rho}{\eta}e^v\right)\,, \quad (8.227)$$

$$u=\frac{1}{\eta}e^v\,. \quad (8.228)$$

The option price is given now by (8.206)

$$C(\tau,x,v)=\frac{2}{\eta\sqrt{1-\rho^2}}\int\limits_{x_0}^{\infty}dx'\int\limits_{-\infty}^{\infty}dv'e^{-v'}U(\tau;x,v,x',v')(e^{x'}-e^{x_0})\,. \quad (8.229)$$

8.6.4.3 SABR Model

For the SABR model the functions $\sigma(S,v)$ and $b(v)$ have the form (8.87), (8.88)

$$\sigma(S,v)=vf(x)\,, \quad (8.230)$$

$$b(v)=\eta v\,, \quad (8.231)$$

where f is a positive monotone function so that

$$h(v)=v\,. \quad (8.232)$$

and the variable v ranges over the real half-axis

$$0 < v < \infty\,. \tag{8.233}$$

The hyperbolic coordinates are now

$$y = \frac{1}{\sqrt{1-\rho^2}}\left(\int_0^x \frac{dx'}{f(x')} - \frac{\rho}{\eta}v\right)\,, \tag{8.234}$$

$$u = \frac{1}{\eta}v\,. \tag{8.235}$$

A popular choice of the function f is

$$f(x) = e^{-\alpha x} \tag{8.236}$$

with $0 \le \alpha \le 1$. Then

$$y = \frac{1}{\sqrt{1-\rho^2}}\left(\frac{e^{\alpha x}}{\alpha} - \frac{\rho}{\eta}v\right)\,. \tag{8.237}$$

Note that these coordinates do not cover the whole hyperbolic plane. The coordinates y and u are restricted by

$$\sqrt{1-\rho^2}\,y + \rho u \ge 0\,. \tag{8.238}$$

Therefore, they only cover a portion of the upper half plane

$$u > 0, \qquad u > -\frac{\sqrt{1-\rho^2}}{\rho}y, \qquad -\infty < y < \infty. \tag{8.239}$$

Nevertheless, the heat kernel on the hyperbolic plane gives the heat kernel of the SABR model in the first approximation as $\tau \to 0$. Thus, the full heat kernel can be still computed by (8.216).

The option price is given by now by (8.206)

$$C(\tau,x,v) = \frac{2}{\eta\sqrt{1-\rho^2}}\int_{x_0}^{\infty} dx' \int_0^{\infty} dv' \frac{1}{f(x')v'^2}U(\tau;x,v,x',v')(e^{x'} - e^{x_0})\,. \tag{8.240}$$

8.6.5 Heston Model

For the Heston model the functions $\sigma(S,v)$ and $b(v)$ have the form (8.75), (8.76)

$$\sigma(S,v) = h(v) = \sqrt{v}\,, \tag{8.241}$$

$$b(v) = \eta\sqrt{v}\,. \tag{8.242}$$

Therefore, by using the eq. (8.186) (or (8.194), 8.198) we obtain the curvature of the corresponding metric

$$R = -\frac{\eta^2}{2v}\,. \tag{8.243}$$

In the Heston model the curvature has a singularity at the boundary $v = 0$. This poses serious problems in dealing with this equation. The whole geometric approach breaks down at the singularity and one needs some other methods to explore the region close to the boundary.

Therefore, we will not use the geometric approach in this section but will instead work directly with the valuation operator. To be specific we assume that the following form of the risk-neutral drift

$$\gamma = -\lambda(v - \bar{v})\,, \tag{8.244}$$

where λ and $\bar{v}$ are constant parameters. Then the valuation operator has the form

$$L = -\frac{1}{2}v\left[\partial_x^2 + 2\rho\eta\partial_x\partial_v + \eta^2\partial_v^2\right] + \frac{1}{2}(v - 2r)\,\partial_x + \lambda(v - \bar{v})\partial_v + r\,. \tag{8.245}$$

The heat kernel $U(\tau; x, v, x', v')$ of the operator L is now defined by the equation

$$(\partial_\tau + L)\,U(\tau; x, v, x', v') = 0\,, \tag{8.246}$$

with the initial condition

$$U(0; x, u, x', u') = \delta(x - x')\delta(v - v')\,, \tag{8.247}$$

and the appropriate boundary conditions at the singularity.

Now, since the coefficients of the operator do not depend on x we can apply a generalized Fourier transform in x. Thus we represent the heat kernel in the form

$$U(\tau; x, v, x', v') = \int\limits_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} e^{ip(x-x')}\hat{U}(\tau; p, v, v')\,. \tag{8.248}$$

Here a is a real constant that must be chosen in such a way that the integral converges. Note that we shifted the integration contour from the real axis for the convergence of Fourier integral. This is equivalent to a Mellin transform in the variable S with a contour of integration in the strip of analyticity. That is why Fourier integral in the variable x also have a strip of analyticity. So, the constant a is the imaginary part of the momentum p chosen in the strip of analyticity.

Thus, we obtain the equation for $\hat{U}$

$$\left(\partial_\tau + \hat{L}\right) \hat{U}(\tau; p, v, v') = 0\,, \tag{8.249}$$

where

$$\hat{L} = -\frac{\eta^2}{2} v \partial_v^2 + \left[(\lambda - \eta\rho ip)v - \lambda\bar{v}\right] \partial_v + \frac{1}{2}\left(p^2 + ip\right) v + r(1 - ip)\,, \tag{8.250}$$

with the initial condition

$$\hat{U}(0; p, v, v') = \delta(v - v')\,. \tag{8.251}$$

Further, since the coefficients of the operator $\hat{L}$ are linear in v we can apply Laplace transform in the variable v (see Sec. 2.6). Thus we represent the heat kernel in the form

$$U(\tau; x, v, x', v') = \int\limits_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i} \exp\left[ip(x - x') + qv\right] F(\tau; p, q, v')\,, \tag{8.252}$$

where c is a sufficiently large positive constant. Substituting this form of the heat kernel into the equation (8.246) we obtain a *first-order* partial differential equation

$$\left[\partial_\tau + f(q)\partial_q + \varphi(q)\right] F(\tau; p, q, v') = 0\,, \tag{8.253}$$

where

$$f(q) = \frac{\eta^2}{2} q^2 - (\lambda - \eta\rho ip)q - \frac{1}{2}\left(p^2 + ip\right), \tag{8.254}$$

$$\varphi(q) = (\eta^2 - \lambda\bar{v})q + (\eta\rho - r)ip + r - \lambda\,. \tag{8.255}$$

The initial condition for the function F has the form

$$F(0; p, q, v') = e^{-qv'}\,. \tag{8.256}$$

This equation is of the Hamilton-Jacobi type; it can be solved by the method described in Chap. 4 (see also Sec. 2.1). We write

$$F = e^{\Psi}\,. \tag{8.257}$$

Then the above equation takes the form

$$\left[\partial_\tau + f(q)\partial_q\right] \Psi(\tau; p, q, v') = -\varphi(q)\,, \tag{8.258}$$

with the initial condition

$$\Psi(0; p, q, v') = -qv'\,. \tag{8.259}$$

The corresponding characteristic Hamiltonian system is

$$\frac{d\hat{q}}{d\tau} = f(\hat{q})\,, \tag{8.260}$$

$$\frac{d\hat{\Psi}}{d\tau} = -\varphi(\hat{q})\,. \tag{8.261}$$

These equations are separable and can be easily integrated. First, we obtain

$$\tau = \int_{q_0}^{q} \frac{d\hat{q}}{f(\hat{q})}, \tag{8.262}$$

and then

$$\Psi(\tau; p, q, v') = -q_0 v' - \int_{q_0}^{q} d\hat{q}\ \frac{\varphi(\hat{q})}{f(\hat{q})}\,. \tag{8.263}$$

Here $q_0 = q_0(\tau, q)$ is a function of τ and q that is implicitly defined by the first equation, that is, $\tau(q_0) = 0$.

Now, we compute these integrals. Let q_1 and q_2 be the roots of the function $f(q)$, that is, the solutions of the equation

$$\eta^2 q^2 - 2(\lambda - \eta\rho i p)q - p^2 - ip = 0\,. \tag{8.264}$$

Then

$$q_{1,2} = q_{1,2}(p) = \frac{1}{\eta^2}\left(\lambda - \eta\rho i p \pm \delta\right)\,, \tag{8.265}$$

where

$$\delta = \delta(p) = \sqrt{\eta^2(1-\rho^2)p^2 + (\eta^2 - 2\eta\rho\lambda)ip + \lambda^2}\,. \tag{8.266}$$

Then by using the integral

$$\int \frac{dq}{f(q)} = \frac{1}{\delta}\left[\log(q - q_1) - \log(q - q_2)\right] \tag{8.267}$$

we obtain

$$\tau = \frac{1}{\delta}\log\left[\frac{(q-q_1)(q_0-q_2)}{(q_0-q_1)(q-q_2)}\right]\,. \tag{8.268}$$

Therefore, by solving this equation for q_0 we get

$$q_0 = q_0(\tau; p, q) = \frac{1}{\eta^2}\left(\lambda - \eta\rho i p\right) + \frac{\delta}{\eta^2}\frac{1+R}{1-R}\,, \tag{8.269}$$

where

$$R = R(\tau; p, q) = \frac{q - q_1}{q - q_2}e^{-\delta\tau}\,. \tag{8.270}$$

Further, by using the integral

$$\int dq \frac{q}{f(q)} = \frac{1}{\delta} \left[q_1 \log (q - q_1) - q_2 \log (q - q_2) \right] , \tag{8.271}$$

we obtain

$$\Psi = -q_0 v' - a_1 \log \frac{q - q_1}{q_0 - q_1} - a_2 \log \frac{q - q_2}{q_0 - q_2} , \tag{8.272}$$

where

$$a_1 = a_1(p) = 1 - \frac{\lambda \bar{v}}{\eta^2} + (\lambda \bar{v} \rho - r\eta) \frac{ip}{\eta \delta} + \left(r\eta^2 - \lambda^2 \bar{v} \right) \frac{1}{\eta^2 \delta} , \tag{8.273}$$

$$a_2 = a_2(p) = 1 - \frac{\lambda \bar{v}}{\eta^2} - (\lambda \bar{v} \rho - r\eta) \frac{ip}{\eta \delta} - \left(r\eta^2 - \lambda^2 \bar{v} \right) \frac{1}{\eta^2 \delta} . \tag{8.274}$$

Then the heat kernel takes the form

$$U(\tau; x, v, x', v') = \int\limits_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i} \exp \left[ip(x - x') + qv - q_0 v' \right] \times \left(\frac{q_0 - q_1}{q - q_1} \right)^{a_1} \left(\frac{q_0 - q_2}{q - q_2} \right)^{a_2} . \tag{8.275}$$

Now, by substituting this heat kernel into the eq. (8.206) we can obtain the price of the call option with the initial condition

$$C(0; x, v) = \left(e^x - e^{x_0} \right)_+ . \tag{8.276}$$

It is given in terms of the functions

$$P_n(\tau; x, v) = \int\limits_0^\infty dx' \int\limits_0^\infty dv' \, U(\tau; x, v, x', v') e^{nx'} . \tag{8.277}$$

satisfying the heat equation (8.246) with the initial condition

$$P_n(0; x, v) = e^{nx} \theta(x) = \begin{cases} e^{nx} & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases} , \tag{8.278}$$

where $n \geq 0$ and $\theta(x)$ is the step-function. By using these functions the option price can be written in the form

$$C(\tau; x, v) = P_1(\tau; x, v) - e^{x_0} P_0(\tau; x, v) . \tag{8.279}$$

Now, by using the above heat kernel and computing the integrals over x' and v' we obtain

$$P_n(\tau;x,v)=\int\limits_{ia-\infty}^{ia+\infty}\frac{dp}{2\pi}\int\limits_{c-i\infty}^{c+i\infty}\frac{dq}{2\pi i}e^{ipx+qv}\frac{1}{(ip-n)q_0}\left(\frac{q_0-q_1}{q-q_1}\right)^{a_1}\left(\frac{q_0-q_2}{q-q_2}\right)^{a_2}. \tag{8.280}$$

This formula gives a complete solution for the heat kernel. However, it is pretty complicated since it involves two complex integrals. Recall that all parameters here depend on p as well. This integral can be computed by residue theory. However, it is much easier to solve the heat equation (8.246) directly without Laplace transform. We use the Fourier transform in x only

$$P_n(\tau;x,v)=\int\limits_{ia-\infty}^{ia+\infty}\frac{dp}{2\pi}e^{ipx}\hat{P}_n(\tau;p,v)\,, \tag{8.281}$$

where a is a sufficiently large negative real constant, so that $a<-n$. The Fourier transformed function $\hat{P}_n(\tau;p,v)$ satisfies the heat equation (8.249) with the initial condition

$$\hat{P}_n(0;p,v)=\frac{1}{ip-n}\,. \tag{8.282}$$

Now, we use the singular perturbation technique (see Chap. 4). We rescale all derivatives

$$\left\{\varepsilon\partial_\tau-\varepsilon^2\frac{\eta^2}{2}v\partial_v^2+\varepsilon\left[(\lambda-\eta\rho ip)v-\lambda\bar{v}\right]\partial_v\right.$$
$$\left.+\frac{1}{2}\left(p^2+ip\right)v+r(1-ip)\right\}\hat{P}_n(\tau;p,v)=0\,, \tag{8.283}$$

and look for a solution in the form

$$\hat{P}_n(\tau;p,v)=\exp\left[\frac{1}{\varepsilon}\Phi(\tau;p,v)\right]\Omega(\tau;p,v)\,, \tag{8.284}$$

where

$$\Omega(\tau;p,v)=\sum_{k=0}^{\infty}\varepsilon^k\Omega_k(\tau;p,v)\,. \tag{8.285}$$

These functions satisfy the initial conditions

$$\Phi(0;p,v)=0\,, \tag{8.286}$$

$$\Omega(0;p,v)=\frac{1}{ip-n}\,. \tag{8.287}$$

Substituting this ansatz into the equation we obtain the Hamilton-Jacobi equation for the function Φ, the action,

$$\partial_\tau \Phi - \frac{\eta^2}{2} v (\partial_v \Phi)^2 + \left[(\lambda - \eta\rho i p) v - \lambda \bar{v} \right] \partial_v \Phi + \frac{1}{2} \left(p^2 + ip \right) v + r(1 - ip) = 0 \,, \tag{8.288}$$

and a recursive system for the coefficients Ω_k

$$\left\{ \partial_\tau + \left[(\lambda - \eta\rho i p - \eta^2 (\partial_v \Phi)) v - \lambda \bar{v} \right] \partial_v - \frac{\eta^2}{2} v (\partial_v^2 \Phi) \right\} \Omega_k = \frac{\eta^2}{2} v \partial_v^2 \Omega_{k-1} \,. \tag{8.289}$$

The first equation (8.288) is solved by the linear ansatz

$$\Phi(\tau; p, v) = v A(\tau; p) + B(\tau; p) \,, \tag{8.290}$$

with initial conditions

$$A(0; p) = B(0; p) = 0 \,. \tag{8.291}$$

Substituting this into the Hamilton-Jacobi equation (8.288) we obtain the following equations for the functions A and B

$$\partial_\tau A = \frac{\eta^2}{2} A^2 - (\lambda - \eta\rho i p) A - \frac{1}{2} (p^2 + ip) \,, \tag{8.292}$$

$$\partial_\tau B = \lambda \bar{v} A - r(1 - ip) \,. \tag{8.293}$$

The eq. (8.292) is identical to eq. (8.260); the right-hand side is nothing but the function $f(A)$ defined by (8.254). The solution of this equations is obtained as follows; first, we obtain

$$\tau = \frac{1}{\delta} \log \left[\frac{(A - q_1) q_2}{q_1 (A - q_2)} \right] \,, \tag{8.294}$$

where $q_{1,2}$ are defined by (8.265). Then

$$\begin{aligned} A &= \frac{q_1 q_2 \left[\exp(\delta\tau) - 1 \right]}{q_1 \exp(\delta\tau) - q_2} \\ &= -\frac{p^2 + ip}{\lambda - \eta\rho i p + \delta \coth\left(\delta\tau / 2 \right)} \,. \end{aligned} \tag{8.295}$$

This allows one to find

$$\begin{aligned} B = {} & \frac{1}{\eta^2} \left[\lambda^2 \bar{v} - \eta^2 r + \eta \left(\eta r - \lambda\rho\bar{v} \right) ip \right] \tau \\ & - 2 \frac{\lambda \bar{v}}{\eta^2} \log \left[\cosh\left(\delta\tau / 2 \right) + \frac{1}{\delta} (\lambda - \eta\rho i p) \sinh\left(\delta\tau / 2 \right) \right] \,. \end{aligned} \tag{8.296}$$

Next, the equation for Ω_0 is

$$\left\{\partial_\tau + \left[(\lambda - \eta\rho ip - \eta^2 A)v - \lambda\bar{v}\right]\partial_v\right\}\Omega_0 = 0\,. \tag{8.297}$$

Since the initial value is constant the solution of this equation is constant

$$\Omega_0 = \frac{1}{ip - n}\,. \tag{8.298}$$

Once this is established then from the recursion system it follows that all higher-order coefficients are zero,

$$\Omega_k = 0, \tag{8.299}$$

and, therefore,

$$\hat{P}_n(\tau; p) = \frac{1}{ip - n}\exp\left[vA(\tau; p) + B(\tau; p)\right]\,. \tag{8.300}$$

Thus the solution of the initial value problem is

$$\begin{aligned} P_n(\tau; x, v) = {} & \exp\left\{\left(\frac{\lambda^2\bar{v}}{\eta^2} - r\right)\tau\right\} \\ & \times \int_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi}\frac{1}{(ip - n)}\exp\left\{\left[x + \frac{1}{\eta}\left(\eta r - \lambda\rho\bar{v}\right)\tau\right] ip\right\} \\ & \times \exp\left[-\frac{p^2 + ip}{\lambda - \eta\rho ip + \delta\coth\left(\delta\tau/2\right)}\,v\right] \\ & \times \left[\cosh\left(\delta\tau/2\right) + \frac{1}{\delta}(\lambda - \eta\rho ip)\sinh\left(\delta\tau/2\right)\right]^{-2\lambda\bar{v}/\eta^2}\,. \end{aligned} \tag{8.301}$$

This is the basis of the well-known *Heston formula*. For a more practical treatment of the Heston model we refer to an excellent book [69].

8.7 Notes

This chapter is devoted to the application of the methods developed in the previous chapters to stochastic volatility models of the mathematical finance. The general theory of financial derivatives is described in [53, 56, 62]. A very good introduction to mathematical finance can be found in the books [17, 52, 77, 78, 79, 41, 55]. The Heston model was studied in [69] and the SABR model was studied in [49, 48].

Summary

We have covered a wide range of topics in this book. The main goal of the book is the development of the machinery for the asymptotic expansion of the heat kernel and its application in some specific models in mathematical finance. We tried to make the book as complete as possible. That is why, we included some background chapters on analysis, partial differential equations and geometry.

The really interesting material was described in Part III devoted to the application of the theory of singular perturbations to the heat equation. We described in detail the semiclassical approximation of quantum mechanics and its relation to the Hamiltonian systems and considered some exactly solvable examples like systems with quadratic Hamiltonians. The chapter on the asymptotic expansion of the heat kernel is the main chapter of the book. Here we developed a very powerful technique for the calculation of the coefficients of the heat kernel asymptotic expansion and applied it to some particular cases.

We also presented some more advanced material dealing mostly with some algebraic methods that are exploiting the symmetries of the model to compute the heat kernel. This allows one to compute the heat kernel for operators with quadratic potential as well as on Lie groups and symmetric spaces. We also introduced and discussed path integrals.

The Part IV of the book is devoted to the application of the methods developed in the previous chapters to some models of mathematical finance. First, we introduced the basic concepts of finance such as options and derivatives and then presented some models focusing primarily on the stochastic volatility models. We showed that most of these models lead to a parabolic partial differential equation, a generalized heat (or diffusion) equation. The only exception are the jump-diffusion models that lead to a integro-differential equation. Finally, we showed how some of these models can be solved by employing the methods developed in this book.

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DOI 10.1007/978-3-319-26266-6

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DOI 10.1007/978-3-319-26266-6