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Analytic and Geometric Methods for Heat Kernel Applications in Finance

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Chapter 1

Stochastic Models in Mathematical Finance

1.1 Preface

In present lectures we will review some of the advanced methods for solving second-order parabolic partial differential equations. Such equations arise in many applications in physics, applied and pure mathematics, engineering, and, in particular, in modeling stochastic processes, such as financial markets. I am not an expert neither in financial mathematics nor in stochastic partial differential equations. That is why the financial models that I have drawn from the literature will serve for illustration only.

Our primary concern in these lectures will be rather a systematic development of effective methods for various approximation schemes for parabolic differential equations. Since these methods make an extensive use of differential geometric and analytical concepts we will start by building up a background in differential geometry and geometric analysis that will be needed later. The heart of these lectures will be the development of a short-time asymptotic expansion for the heat kernel. We will explain it in details and give explicit examples of some advanced calculations.

A remark about the level and the style of the presentation is in order. Since most of the time we will start from scratch, the level of the presentation will be necessarily uneven. We will start from very elementary introductory concepts (that should be boring for a specialist) and will 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, we intentionally sacrifice rigor for clarity and availability for a wider audience. So, the style will be rather informal. Most of the time we will not discuss and state precise conditions (which are, of course, of primary interest for pure mathematicians) under which the statements and results are valid.

We will provide the references to the original papers I will review for those who would like to study the material even deeper. Of course, the subject is so huge that it is impossible to give a more or less comprehensive review of the literature. No such attempt will be made. These lectures are rather a tutorial for non-specialists than a review for people working in this area.

1.2 Black-Scholes Model

1.2.1 One-dimensional Model

We follow here [34]. Wiener process (or Brownian motion) is a normalized real-valued stochastic process $W(t)$ such that, in particular,

$$E(dW) = 0\,, \qquad \text{and} \qquad E[(dW)^2] = dt\,. \tag{1.1}$$

More generally, for n Wiener processes $W_i(t)$, $i = 1, 2 \ldots, n$, there holds

$$E(dW_i) = 0\,, \qquad \text{and} \qquad E[dW_i dW_j] = \rho_{ij} dt\,, \tag{1.2}$$

where ρ_{ij} is $n \times n$ correlation matrix.

Let us consider a stock whose price at time t is $S(t) \geq 0$. Let $S_0 = S(0)$ be the initial price, $\mu > 0$ be the drift and $\sigma \neq 0$ be the volatility. Suppose that $S(t)$ evolves according to the stochastic differential equation

$$dS(t) = \mu S(t) dt + \sigma S(t) dW(t)\,, \tag{1.3}$$

where $W(t)$ is a Wiener process.

Let us consider the European call option, which is the right to buy one share of the stock S at the strike price K at the strike time T. Let $V(t, S)$ be the price of the option at time t and the stock price $S(t) = S$. The range of the variables t and S is

$$0 \leq t \leq T \qquad \text{and} \qquad 0 \leq S < \infty\,. \tag{1.4}$$

Assume that for $S \geq 0$

$$V(T,S) = (S-K)_+ \,, \tag{1.5}$$

where

$$(S-K)_+ = \max(S-K,0)\,, \tag{1.6}$$

and for $0 \leq t \leq T$

$$V(t,0) = 0\,. \tag{1.7}$$

Let r be the interest rate of a risk-free investment. Then the price of the option satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) V = 0\,, \tag{1.8}$$

where L is Black-Scholes partial differential operator defined by

$$L = \frac{1}{2}\sigma^2 S^2 \frac{\partial^2}{\partial S^2} + rS\frac{\partial}{\partial S} - r\,. \tag{1.9}$$

1.2.2 Multi-dimensional Model

We follow here [31]. Let us consider n stocks whose prices at time t are $S_i(t) \geq 0$, $i = 1,2,\ldots,n$. Let $S_{i,0} = S_i(0)$ be the initial prices, $\mu_i > 0$ be the drifts and $\sigma_i \neq 0$ be the volatilities. Suppose that $S_i(t)$ evolve according to the stochastic differential equations

$$dS_i(t) = \mu_i S_i(t)dt + \sigma_i S_i(t) dW_j(t)\,, \tag{1.10}$$

where $W_i(t)$ are Wiener processes with the correlation matrix ρ_{ij}.

Let us consider an option, which is the right to buy shares of the stocks $S_1,\ldots,S_n$ at the strike time T. Let $V(t,S_1,\ldots,S_n)$ be the price of the option at time t and the stock prices $S_i(t) = S_i$. The range of the variables t and S_i is

$$0 \leq t \leq T \qquad \text{and} \qquad 0 \leq S_i < \infty\,. \tag{1.11}$$

Assume that for $S_i \geq 0$

$$V(T,S_1,\ldots,S_n) = P(S_1,\ldots,S_n)\,, \tag{1.12}$$

where $P(S_1,\ldots,S_n)$ is some given expiration condition, and for $0 \leq t \leq T$ and for each S_i the price of the option is equal to zero if any $S_i = 0$, i.e.

$$V(t,S_1,\ldots,S_n)\Big|_{S_i=0} = 0\,. \tag{1.13}$$

Let r be the interest rate of a risk-free investment and q_i be the dividend rate for stock S_i. Let C_{ij} be a matrix defined by

$$C_{ij} = \rho_{ij}\sigma_i\sigma_j\,. \tag{1.14}$$

Then the price of the option satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) V = 0\,, \tag{1.15}$$

where L is multi-dimensional Black-Scholes partial differential operator

$$L = \frac{1}{2}\sum_{i,j=1}^{n} C_{ij}S_iS_j\frac{\partial^2}{\partial S_i\partial S_j} + \sum_{i=1}^{n}(r-q_i)S_i\frac{\partial}{\partial S_i} - r\,. \tag{1.16}$$

1.3 Stochastic Volatility Models

1.3.1 Valuation Equation

We follow [36] here. Let the stock price $S(t)$ and its variance $v(t)$ satisfy the stochastic differential equations

$$\begin{aligned} dS(t) &= \mu(t)\,S(t)\,dt + \sqrt{v(t)}\,S(t)\,dW_1(t)\,, & (1.17)\\ dv(t) &= \alpha(t,S,v)\,dt + \eta\,\beta(t,S,v)\,\sqrt{v(t)}\,dW_2(t)\,, & (1.18)\end{aligned}$$

where $\mu = \mu(t)$ is the deterministic instantaneous drift, η is the volatility of volatility (which is assumed to be constant), $\alpha = \alpha(t,S,v)$ and $\beta = \beta(t,S,v)$ are some functions of S, v and t, and $dW_1(t)$ and $dW_2(t)$ are Wiener processes with correlation ρ.

Let $V(t,S,v)$ be the price of an option and r be the interest rate of a risk-free investment. Then the option price satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) V = 0\,, \tag{1.19}$$

where L is the second-order partial differential operator

$$\begin{aligned} L &= \frac{1}{2}vS^2\frac{\partial^2}{\partial S^2} + \rho\eta\beta(t,S,v)vS\frac{\partial^2}{\partial S\partial v} + \frac{1}{2}\eta^2\beta^2(t,S,v)v\frac{\partial^2}{\partial v^2}\\ &\quad + rS\frac{\partial}{\partial S} + [\alpha(t,S,v) - \varphi(t,S,v)\beta(t,S,v)]\frac{\partial}{\partial v} - r\,, \end{aligned} \tag{1.20}$$

and $\varphi = \varphi(t, S, v)$ is the market price of volatility risk. The range of the variables t, S and v is

$$0 \le t \le T\,, \qquad 0 \le S < \infty\,, \qquad 0 \le v < \infty\,. \tag{1.21}$$

Therefore, this equation should be supplemented by appropriate initial (or expiration) condition at $t = T$ as well as boundary conditions at $S = 0$ and $v = 0$.

Let $S(t)$ and $v(t)$ satisfy the following initial conditions

$$S(0) = S'\,, \qquad v(0) = v'\,. \tag{1.22}$$

Then the conditional probability $p(t, S, v|S', v')$ satisfies the same partial differential equation and the initial condition

$$p(0, S, v|S', v') = \delta(S - S')\delta(v - v')\,. \tag{1.23}$$

It enables one to compute the local volatility simply as the mean value of the stochastic volatility $\sigma_S(S, v) = \sqrt{v}S$ [42]

$$\sigma^2_{\rm loc}(S, t) = \frac{\int\limits_0^\infty dv\; p(t, S, v|S', v')\sigma^2_S(S, v)}{\int\limits_0^\infty dv\; p(t, S, v|S'v')}\,. \tag{1.24}$$

1.3.2 Dupire Model

Suppose the stock price $S(t)$ evolves according to the stochastic differential equation

$$dS(t) = \mu(t)\, S(t)\, dt + \sigma(t, S)\, S(t)\, dW(t)\,, \tag{1.25}$$

where $\mu = \mu(t)$ is the risk-neutral drift, $\sigma = \sigma(t, S)$ is the local volatility and $dW(t)$ is the Wiener process.

Let $C = C(T, S_0, K)$ be the value of the European option with strike K and expiration T and given current stock price S_0. Here $T, S_0, K > 0$. Let $r = r(T)$ be the risk-free rate and $D = D(T)$ be the dividend yield. Then the undiscounted option price C satisfies the partial differential equation [36]

$$\left(\frac{\partial}{\partial T} - L\right) C = 0\,, \tag{1.26}$$

where L is the second-order differential operator

$$L = \frac{1}{2}\sigma^2 K^2 \frac{\partial^2}{\partial K^2} - [r(T) - D(T)]K\frac{\partial}{\partial K} + r(T) - D(T)\,. \tag{1.27}$$

1.3.3 Heston Model

Heston model corresponds to choosing the functions $\alpha(t,S,v)$ and $\beta(t,S,v)$ in the general stochastic volatility model as follows [36]

$$\beta(t,S,v) = 1\,, \qquad \text{and} \qquad \alpha(t,S,v) = -\lambda(v-\bar{v})\,, \tag{1.28}$$

where the constant λ is the speed of reversion of v and $\bar{v}$ is its long term mean, and by choosing the market price of volatility by

$$\varphi(t,S,v) = \theta v \tag{1.29}$$

with some constant θ.

Then the stock price $S(t)$ and the volatility $v(t)$ evolve according to the stochastic differential equations

$$\begin{aligned} dS(t) &= \mu(t)\,S(t)\,dt + \sqrt{v(t)}\,S(t)\,dW_1(t)\,, & (1.30)\\ dv(t) &= -\lambda[v(t)-\bar{v}]\,dt + \eta\,\sqrt{v(t)}\,dW_2(t)\,. & (1.31) \end{aligned}$$

The process followed by $v(t)$ is a special case of the so-called affine jump diffusion [36].

The option price then satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) V = 0\,, \tag{1.32}$$

with the operator L defined by

$$L = \frac{1}{2}vS^2\frac{\partial^2}{\partial S^2} + \rho\eta vS\frac{\partial^2}{\partial S\partial v} + \frac{1}{2}\eta^2 v\frac{\partial^2}{\partial v^2} + rS\frac{\partial}{\partial S} - \lambda'(v-\bar{v}')\frac{\partial}{\partial v} - r\,, \tag{1.33}$$

where $\lambda' = \lambda - \theta$ and $\bar{v}' = \lambda\bar{v}/(\lambda-\theta)$. Of course, this equation has to be supplemented by the terminal condition at $t = T$ and by boundary conditions at $S = 0$ and $v = 0$.

1.3.4 SABR Model

We follow [37] here. Let us consider a European option on a forward asset expiring T years from today. The forward rate process is assumed to satisfy the stochastic differential equations

$$\begin{aligned} dF(t) &= \sigma(t)C(F)\,dW_1(t)\,, & (1.34)\\ d\sigma(t) &= v\sigma(t)\,dW_2(t)\,, & (1.35) \end{aligned}$$

where v is a constant parameter (volatility of volatility) and $W_1(t)$ and $W_2(t)$ are Wiener processes with the constant correlation ρ. The parameter v is assumed to such that v^2T is small. Here the function $C(F)$ is supposed to be positive monotone non-decreasing and smooth. It is extended to negative values of the argument by

$$C(-F) = -C(F)\,. \tag{1.36}$$

Let $G(t, f, \sigma; T, F, \Sigma)$ be the price of Arrow-Debreu securitiy whose payoff at time T is given by Dirac delta-function. For time $0 < t < T$ it satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) G = 0\,, \tag{1.37}$$

where

$$L = \frac{1}{2}\sigma^2 \left(C(f)^2 \frac{\partial^2}{\partial f^2} + 2v\rho C(f) \frac{\partial^2}{\partial f \partial \sigma} + v^2 \frac{\partial^2}{\partial \sigma^2} \right), \tag{1.38}$$

with the terminal condition

$$G(T, f, \sigma; T, F, \Sigma) = \delta(f - F)\delta(\sigma - \Sigma)\,. \tag{1.39}$$

This equation should be also supplemented by appropriate boundary conditions at zero and at infinity. In particular, it is assumed that

$$\lim_{F,\Sigma\to\infty} G(t, f, \sigma; T, F, \Sigma) = 0\,. \tag{1.40}$$

In a very special case (called the normal SABR model)

$$C(f) = 1, \qquad \rho = 0\,, \tag{1.41}$$

the operator L takes an especially simple form

$$L = \frac{1}{2}\sigma^2 \left(\frac{\partial^2}{\partial f^2} + v^2 \frac{\partial^2}{\partial \sigma^2} \right), \tag{1.42}$$

If the function $G(t, f, \sigma; T, F, \Sigma)$ is known, then the price of a European call option struck at K and expiring time T is

$$C(t, f, \sigma) = \int_{-\infty}^{\infty} dF \int_{0}^{\infty} d\Sigma\; G(t, f, \sigma; T, F, \Sigma)(F - K)_+\,. \tag{1.43}$$

1.3.5 Bourgade-Croissant Model

We follow [30] here. Let δ, λ' and μ' be constant parameters, and $W_1(t)$ and $W_2(t)$ be Wiener processes with the constant correlation ρ. We consider the following process with stochastic volatility

$$\begin{aligned} dF(t) &= \sigma^\delta(t) C(F(t))\, dW_1(t)\,, && (1.44)\\ d\sigma(t) &= \lambda'[\mu' - \sigma(t)]dt + \nu\sigma^\delta(t)\, dW_2(t)\,. && (1.45) \end{aligned}$$

This model includes the SABR model for

$$\delta = 1, \qquad C(F) = F^\beta, \qquad \text{and} \qquad \lambda' = 0\,, \tag{1.46}$$

and Heston model for

$$\delta = \frac{1}{2} \qquad \text{and} \qquad C(F) = F\,. \tag{1.47}$$

Let $G(\tau; f, \sigma, F, \Sigma)$ be the density of probability to get to the point (F, Σ) leaving from the point (f, σ) after a time τ. Then G follows the partial differential equation

$$\left(\frac{\partial}{\partial\tau} - L\right) G = 0\,, \tag{1.48}$$

where

$$L = \frac{1}{2}\sigma^{2\delta}\left(C(f)^2\frac{\partial^2}{\partial f^2} + 2\rho\nu C(f)\frac{\partial^2}{\partial f\partial\sigma} + v^2\frac{\partial^2}{\partial\sigma^2} + \lambda'(\sigma - \mu')\frac{\partial}{\partial\sigma}\right), \tag{1.49}$$

A more general model, so called bi-delta model, involves four Wiener processes W_i, $i = 1, 2, 3, 4$, with the correlation matrix ρ_{ij}. It is described by the following system of stochastic differential equations

$$\begin{aligned} dx(t) &= \alpha^\delta(t) C(x)\, dW_1(t)\,, && (1.50)\\ d\alpha(t) &= \lambda[\alpha_\infty - \alpha(t)]dt + \nu\alpha^\delta(t)\, dW_2(t)\,, && (1.51)\\ dy(t) &= \beta^\gamma(t) C(y)\, dW_3(t) && (1.52)\\ d\beta(t) &= \lambda[\beta_\infty - \beta(t)]dt + \nu\beta^\gamma(t)\, dW_4(t)\,, && (1.53) \end{aligned}$$

where $\delta, \lambda, \nu, \alpha_\infty$ and β_∞ are some constant parameters.

1.3.6 Hull-White Model

We follow here [1]. Let $S(t)$ be the price of a traded asset, such as stock, at time t, r be the interest rate of a risk-free asset, $\sigma(t) = f(Y(t))$ be volatility process, which is some function of a process $Y(t)$, and $W_1(t)$ and $W_2(t)$ be two Wiener processes with correlation ρ. Then the model evolves according to the following stochastic differential equations

$$dS(t) = \alpha S(t)\, dt + f(Y)S(t)\, dW_1(t) \tag{1.54}$$

$$dY(t) = [a + bY(t)]dt + cY(t)\, dW_2(t) \tag{1.55}$$

where α, a, b, c are some constants.

Then the price $V(t, S, Y)$ of the corresponding derivative satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) V = 0\,, \tag{1.56}$$

where L is the second-order partial differential operator

$$L = \frac{1}{2}f^2(Y)S^2\frac{\partial^2}{\partial S^2} + c\rho f(Y)S\frac{\partial^2}{\partial S \partial Y} + \frac{1}{2}c^2\frac{\partial^2}{\partial Y^2} + rS\frac{\partial}{\partial S} - k(t, S, Y)\frac{\partial}{\partial Y} - r\,, \tag{1.57}$$

with

$$k(t, S, Y) = a + bY - c\left[\rho\frac{\alpha - r}{f(Y)} + \gamma(t, S, Y)\sqrt{1 - \rho^2}\right]. \tag{1.58}$$

Here $\gamma(t, S, Y)$ is an unknown function called the market price of risk.

The Hull-White model is a special case of the above model when

$$f(Y) = \sqrt{Y}\,, \qquad a = 0\,, \qquad b < 0\,, \qquad \rho = 0\,. \tag{1.59}$$

1.3.7 Multidimensional Stochastic Volatility Models

We follow here [29]. Let $S(t)$ be the price of an underlying asset. We assume that the volatility of this asset is a function of $(n-1)$ stochastic factors $y^i(t)$, $i = 1, 2, \ldots, (n-1)$. More precisely, we consider n Wiener processes $W_0(t)$, $W_1(t)$, ..., $W_{n-1}(t)$ with the correlation matrix ρ_{ij}. Then the model is described by the following system

of stochastic differential equations

$$dS(t) = rS(t)\,dt + \sigma(S,y,t)S(t)\,dW_0(t) \tag{1.60}$$

$$dy^i(t) = \theta^i(t,y)\,dt + \sum_{j=1}^{n-1}\nu^{ij}(t,y)\,dW_j(t)\,, \qquad i=1,\dots,n-1 \tag{1.61}$$

where $\theta^i(t,y)$ are drift coefficients and $\nu^{ij}(t,y)$ is a diffusion matrix. We assume that $S>0$ and the variables y^i range either in the whole space $\mathbb{R}^{n-1}$ or in the half-space $y^i>0$.

Let $C(t,S,y,;T,K)$ the price of the option with maturity T and strike K. Let

$$A^k(y,t) = \sum_{j=1}^{n-1}\nu^{kj}(y,t)\rho_{j0}\,, \tag{1.62}$$

$$B^{kl}(y,t) = \frac{1}{2}\sum_{i,j=1}^{n-1}\nu^{ki}(y,t)\rho_{ij}\nu^{jl}(y,t) \tag{1.63}$$

Then C satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t}+L\right)C = 0\,, \tag{1.64}$$

where L is the second-order partial differential operator

$$\begin{aligned} L &= \frac{1}{2}\sigma^2(S,y,t)S^2\frac{\partial^2}{\partial S^2} + \sum_{j,k=1}^{n-1}A^k(y,t)\sigma(S,y,t)S\frac{\partial^2}{\partial S\partial y^k} \\ &\quad + \frac{1}{2}\sum_{k,l=1}^{n-1}B^{kl}(y,t)\frac{\partial^2}{\partial y^k\partial y^l} + rS\frac{\partial}{\partial S} + \sum_{i=1}^{n-1}\theta^i(t,y)\frac{\partial}{\partial y^i} - r\,, \end{aligned} \tag{1.65}$$

with the initial condition

$$C(T,S,y;K,T) = (S-K)_+\,. \tag{1.66}$$

Chapter 2

Methods for Solution of Linear Partial Differential Equations

2.1 Parabolic Partial Differential Equations

Differential Equation

As we have seen above all models of stochastic processes lead to a linear partial differential equation of the general form

$$\left(\frac{\partial}{\partial t} + L\right) V(t;x) = 0 \tag{2.1}$$

where L is a second-order partial differential operator of the form

$$L = L(t,x,\partial_x) = -\sum_{i,j=1}^{n} \alpha^{ij}(t,x)\frac{\partial^2}{\partial x^i \partial x^j} + \sum_{i=1}^{n} \beta^i(t,x)\frac{\partial}{\partial x^i} + \gamma(t,x)\,, \tag{2.2}$$

where the coefficients $\alpha^{ij}(t,x)$, $\beta^i(t,x)$ and $\gamma(t,x)$ are some real valued functions of n variables x^i, $i = 1,\ldots,n$, that we will call space variables, and, in general, time t. Henceforth, we will use the notation $x = (x^1,\ldots,x^n)$ and we will denote the partial derivatives with respect to the time and space variables simply by

$$\partial_t = \frac{\partial}{\partial t}\,, \qquad \partial_i = \frac{\partial}{\partial x^i}\,. \tag{2.3}$$

In particular, such equations arise in studying heat conduction and diffusion; therefore, we call this equation a *(generalized) heat equation*. This equation has to be supplemented with some initial (or terminal) conditions. 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, $t > 0$, and the initial condition is set at $t = 0$, i.e.

$$V(0; x) = f(x)\,, \tag{2.4}$$

where $f(x)$ is a given function of x.

Boundary Conditions

The range of space variables is a more complicated issue. It depends on their precise meaning. Some of them are typically stock prices or volatilities and they should be positive. We will simply assume that the space variables range in some open subset M of the Euclidean space $\mathbb{R}^n$ with or without boundary ∂M, which is a hypersurface in $\mathbb{R}^n$. If the boundary is present, then the above equation has 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, again on the model under consideration. We will assume that the boundary conditions have the form

$$BV(t, x)\Big|_{\partial M} = 0\,, \tag{2.5}$$

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

$$B = \sum_{i=1}^{n} v^i(t, x)\partial_i + u(t, x)\,, \tag{2.6}$$

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

$$B_D = 1\,. \tag{2.7}$$

Let N^i be the inward pointing 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

$$B_N = \frac{\partial}{\partial N} = \sum_{i=1}^{n} N^i(x)\partial_i \,. \tag{2.8}$$

Heat Kernel

The fundamental solution of the equation (2.1) is 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'. It is the solution of the differential equation

$$(\partial_t + L)U(t, x|t', x') = 0 \,, \tag{2.9}$$

with initial condition in form of Dirac delta-function

$$U(t', x|t', x') = \delta(x - x') \,, \tag{2.10}$$

and the boundary conditions

$$BU(t, x|t', x')\Big|_{x\in\partial M} = 0 \,. \tag{2.11}$$

Here $\delta(x - x')$ is the n-dimensional delta-function

$$\delta(x - x') = \delta(x^1 - x'^1)\cdots\delta(x^n - x'^n) \,. \tag{2.12}$$

In the case when the operator L does not depend on time t, the fundamental solution $U(t, x; t'x')$ depends on just one time variable, $t - t'$, that is,

$$U(t, x|t', x') = \tilde{U}(t - t'; x, x') \,, \tag{2.13}$$

where $\tilde{U}(t; x, x')$ satisfies the equation

$$(\partial_t + L)\tilde{U}(t; x, x') = 0 \,, \tag{2.14}$$

with the initial condition

$$\tilde{U}(0; x, x') = \delta(x - x') \,. \tag{2.15}$$

By slightly abusing notation we will omit tilde here and denote this function by $U(t; x, x')$. This should not cause any confusion since from the number of arguments it is always clear what function is used.

The function $U(t, x|t', x')$ is called the *heat kernel* of the operator L and is the primary object of interest of the present lectures.

Similarity Transformation

Let $\omega(x)$ be a smooth function. It should be clear that if $U(t,x|t',x')$ is the heat kernel of the operator L, that is, it satisfies the heat equation (2.9) with initial condition (2.10), then the function

$$U_\omega(t,x|t',x') = e^{-\omega(x)}U(t,x|t',x')e^{\omega(x')} \tag{2.16}$$

is the heat kernel of the operator

$$\begin{aligned} L_\omega &= L_\omega(t,x,\partial_x) = e^{-\omega(x)}L(t,x,\partial_x)e^{\omega(x)} \\ &= L(t,x,\partial_i+\omega_{,i})\,, \end{aligned} \tag{2.17}$$

where $\omega_{,i}=\partial_i\omega$, since it satisfies the equation

$$(\partial_t + L_\omega)U_\omega(t,x|t',x') = 0\,, \tag{2.18}$$

with initial condition

$$U_\omega(t',x|t',x') = \delta(x-x')\,. \tag{2.19}$$

We call the transformation $L\mapsto L_\omega = e^{-\omega}Le^{\omega}$ a *similarity transformation* and two operators related by a similarity transformation *similar operators*. Their heat kernels differ just by a trivial factor. That is why the operators L and L_ω have many common properties. In particular, the similarity transformation is *isospectral*, that is, similar operators have the same spectrum. The similarity transformation can be used to simplify the form of the operator L.

Cauchy Problem

If the fundamental solution is given then the solution of the original problem is

$$V(t,x) = \int\limits_M dx'\; U(t,x|0,x')f(x')\,, \tag{2.20}$$

where dx is the n-dimensional volume element

$$dx = dx^1\cdots dx^n\,. \tag{2.21}$$

That is why, instead of studying various problems with different initial conditions one can study one problem with delta-function initial condition. In the stochastic models described above the function

$U(t;x,x')$ is nothing but the conditional probability of reaching the point x at the time t if one starts at the point x' at the time $t=0$.

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

$$(\partial_t + L)V(t,x) = g(t,x)\,, \tag{2.22}$$

$$V(0,x) = f(x)\,, \tag{2.23}$$

is given by

$$V(t,x) = \int\limits_M dx'\; U(t,x|0,x')f(x') + \int\limits_0^t dt' \int\limits_M dx'\; U(t,x|t',x')g(t',x')\,. \tag{2.24}$$

Elliptic Operators

The question arises whether there exists a function $V(t,x)$ that satisfies the 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 heat kernel. The answer to this question depends, of course, on the type of the operator L and on the boundary conditions. Roughly speaking, this problem does indeed have a unique solution, at least for small times, if all coefficient functions are smooth and the problem is *elliptic*. This means that the operator L is elliptic and the boundary conditions are elliptic. Then the partial differential equation under study belongs to a wide class of equations called *parabolic partial differential equations*.

In most of these lectures 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 in the last lecture.

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 $\mathbb{R}^n$. The

expression

$$\sigma(x,p) = L(x,ip) = \sum_{j,k=1}^{n} \alpha^{jk}(x) p_j p_k + i \sum_{j=1}^{n} \beta^j(x) p_j + \gamma(x)\,. \qquad (2.25)$$

is called the *symbol* of the operator L and expression

$$\sigma_L(x,p) = \sum_{j,k=1}^{n} \alpha^{jk}(x) p_j p_k\,. \qquad (2.26)$$

is called the *leading symbol* (or the *principal symbol*) of the operator L.

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

$$\sigma_L(x,p) = \sum_{j,k=1}^{n} \alpha^{jk}(x) p_j p_k > 0 \qquad \text{for any} \quad x \qquad \text{and} \quad p \neq 0\,. \qquad (2.27)$$

Such operators are called *elliptic operators with positive-definite leading symbol*.

The ellipticity of general boundary conditions is a much more complicated issue. Let us just note that the classical boundary conditions (Dirichlet and Neumann) are elliptic.

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

$$\Delta = \sum_{j=1}^{n} \partial_j^2\,, \qquad (2.28)$$

which is obtained by choosing the identity matrix $\alpha^{jk} = \delta_{jk}$ and $\beta^i = \gamma = 0$. Here

$$\delta_{jk} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases} \qquad (2.29)$$

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

$$\sigma(x,p) = \sum_{j=1}^{n} (p_j)^2\,. \qquad (2.30)$$

2.2 Spectral Theory of Operators in Hilbert Spaces

2.2.1 Hilbert Spaces

Partial differential operators act on some 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. 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, g) to two vectors f and g. It is linear in the second argument and anti-linear in the first argument and satisfies the relation

$$(f, g) = \overline{(g, f)}\,, \tag{2.31}$$

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

$$||f|| = \sqrt{(f, f)}\,. \tag{2.32}$$

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 (φ_n) is said to be *orthonormal* if it consists of mutually orthogonal unit vectors. The complex numbers

$$a_n = (f, \varphi_n) \tag{2.33}$$

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

$$f = \sum_{n=1}^{\infty} a_n \varphi_n \,, \tag{2.34}$$

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

$$||f||^2 = \sum_{n=1}^{\infty} |a_n|^2 \,. \tag{2.35}$$

Functional L^2 Hilbert 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 and the L^2 norm are defined by

$$(f, g) = \int_a^b dx \; \overline{f(x)} g(x) \,, \tag{2.36}$$

$$||f||^2 = (f, f) = \int_a^b dx \; |f(x)|^2 \,. \tag{2.37}$$

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

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

$$(f, g) = \int_a^b dx \; \mu(x) \; \overline{f(x)} g(x) \,. \tag{2.38}$$

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 $\mu(x)$ be a positive function on M. Then the inner product can be defined by

$$(f, g) = \int_M dx \; \mu(x) \; \overline{f(x)} g(x) \,. \tag{2.39}$$

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*.

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

$$\varphi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}, \qquad n = 0, \pm 1, \pm 2, \ldots \tag{2.40}$$

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

$$f(x) = \sum_{n=-\infty}^{\infty} a_n \varphi_n(x), \tag{2.41}$$

where

$$a_n = \int_{-\pi}^{\pi} dt\; f(t)\varphi_n(t), \tag{2.42}$$

is nothing but the classical Fourier series. The scalars a_n are the Fourier coefficients. 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.

2.2.2 Self-Adjoint Operators on Hilbert Spaces

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

$$[A,B] = AB - BA\,. \tag{2.43}$$

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 and *non-commuting* otherwise.

Let $(\varphi_n)_{n=1}^{\infty}$ be an orthonormal basis in H. Then every operator can be represented by an infinite-dimensional matrix

$$A_{kj} = (\varphi_k, A\varphi_j)\,. \tag{2.44}$$

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

$$\mathrm{Tr}\, A = \sum_{k=1}^{n} (\varphi_k, A\varphi_k) = \sum_{k=1}^{n} A_{kk}\,. \tag{2.45}$$

Of course, the trace, when it exists, does not depend on the chosen orthonormal basis. An operator A is called *trace-class* if it has a finite trace. The trace has a nice cyclic property, that is, if the operators A, B, AB and BA are trace class, then

$$\mathrm{Tr}\, AB = \mathrm{Tr}\, BA\,, \tag{2.46}$$

in particular,

$$\mathrm{Tr}\,[A, B] = 0\,. \tag{2.47}$$

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

$$(A^* f, g) = (f, Ag)\,. \tag{2.48}$$

The matrix of the adjoint operator is Hermitian conjugate of the matrix of the original operator, that is,

$$(A^*)_{jk} = (\overline{A_{kj}})\,. \tag{2.49}$$

An operator A is called *self-adjoint* if

$$A = A^* \tag{2.50}$$

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

$$(A^*)^* = A\,, \tag{2.51}$$

$$(AB)^* = B^* A^*\,. \tag{2.52}$$

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

$$AA^{-1} = A^{-1}A = I\,, \tag{2.53}$$

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

$$\begin{aligned} (A^{-1})^{-1} &= A\,, & (2.54)\\ (AB)^{-1} &= B^{-1}A^{-1}\,, & (2.55)\\ (A^*)^{-1} &= (A^{-1})^*. & (2.56) \end{aligned}$$

An operator U is called *unitary* if

$$UU^* = U^*U = I\,, \tag{2.57}$$

or

$$U^{-1} = U^*. \tag{2.58}$$

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

$$(Uf, Ug) = (f, U^*Ug) = (f, g). \tag{2.59}$$

Every unitary operator U can be represented in the form

$$U = \exp(A)\,, \tag{2.60}$$

with some anti-self-adjoint operator A.

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

$$(f, Af) > 0\,. \tag{2.61}$$

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

$$(f, A^*Af) = (Af, Af) = ||Af||^2 \geq 0\,, \tag{2.62}$$

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

$$(f, A^{-1}f) = (Ag, g) > 0\,, \tag{2.63}$$

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

An operator P is called *idempotent* if

$$P^2 = P\,. \tag{2.64}$$

A self-adjoint idempotent operator is called a *projection*. Given a vector subspace S, the *orthogonal complement* $S^\perp$ of S is the vector subspace 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,

$$Pf = \begin{cases} f & \text{if } f \text{ is in } S\,, \\ 0 & \text{if } f \text{ is in } S^\perp\,. \end{cases} \tag{2.65}$$

It is easy to see that if P is a projection operator onto a subspace S, then the operator $(I - P)$ is a projection operator onto the orthogonal complement $S^\perp$. If the subspace S is finite-dimensional, then the projection operator P is trace-class and the dimension of the subspace S is equal to the trace of the projection

$$\dim S = \operatorname{Tr} P\,. \tag{2.66}$$

Integral Operators

Let G be an operator on the Hilbert space $L^2([a,b])$ defined by

$$(Gf)(x) = \int_a^b dx'\, G(x,x') f(x')\,, \tag{2.67}$$

where $G(x,y)$ is some function of two variables called the *integral kernel* of the operator G.

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 $G(x,x')$ be a function of two points x and x'. Then the integral

$$(Gf)(x) = \int_M dx'\, \mu(x')\, G(x,x') f(x')\,, \tag{2.68}$$

defines an integral operator G on $L^2(M,\mu)$ with the integral kernel $G(x,x')$.

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

$$G^{\mathrm{diag}}(x) = G(x,x)\,. \tag{2.69}$$

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

$$\mathrm{Tr}\; G = \int\limits_M dx\,\mu(x) G(x,x)\,. \tag{2.70}$$

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

$$(G^*)(x,x') = \overline{G(x',x)}\,. \tag{2.71}$$

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

$$G(x,x') = \overline{G(x',x)}\,. \tag{2.72}$$

Partial Differential Operators

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

First of all, we can only differentiate differentiable (or smooth functions). However, the spaces of smooth functions 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 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, for example, the trace, may diverge. So, one has to make sure at each step that everything is well-defined and converges and so on. This is one of the main differences between finite-dimensional linear algebra and functional

analysis. In these lecture we will care 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.

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

$$L = -\sum_{i,j=1}^{n} \alpha^{ij}(x)\partial_i\partial_j + \sum_{j=1}^{n} \beta^j(x)\partial_j + \gamma(x)\,. \tag{2.73}$$

with real-valued coefficients.

We study the conditions on the coefficients of this operator so that it is self-adjoint. The adjoint L^* of the operator L is defined by

$$(Lf, g) = (f, L^*g) \tag{2.74}$$

for any functions f and g satisfying the boundary conditions. Recall that we only consider either Dirichlet or Neumann boundary conditions. In more details this equation means

$$\int\limits_M dx\,\mu(x)\overline{(Lf)(x)}g(x) = \int\limits_M dx\,\mu(x)\overline{f(x)}L^*g(x)\,. \tag{2.75}$$

To find the adjoint operator L^* we need to integrate by parts twice. Of course, in doing so, we will get some boundary terms, and the purpose of boundary conditions is exactly to make these boundary term vanish. It is easy to check that for both Dirichlet and Neumann boundary conditions this indeed happens. What remains is an expression for the operator L^*

$$\begin{aligned} L^* &= -\sum_{i,j=1}^{n} \mu^{-1}(x)\partial_i\partial_j\alpha^{ij}\mu(x) - \sum_{j=1}^{n} \mu^{-1}(x)\partial_j\beta^j(x)\mu(x) + \gamma(x) \\ &= -\sum_{i,j=1}^{n} \alpha^{ij}(x)\partial_i\partial_j - \sum_{j=1}^{n} \tilde{\beta}^j(x)\partial_j + \tilde{\gamma}(x)\,, \end{aligned} \tag{2.76}$$

where

$$\tilde{\beta}^j = -\beta^j - 2\sum_{i=1}^{n} \mu^{-1}\partial_i(\mu\alpha^{ij})\,, \tag{2.77}$$

$$\tilde{\gamma} = \gamma - \sum_{i,j=1}^{n} \mu^{-1}\partial_i\partial_j(\mu\alpha^{ij}) - \sum_{i=1}^{n} \mu^{-1}\partial_i(\mu\beta^i)\,. \tag{2.78}$$

Thus, the operator L is self-adjoint, that is, $L = L^*$, if the coefficient functions β^i satisfy the following conditions

$$\beta^j = -\sum_{i=1}^{n} \mu^{-1}\partial_i(\mu\alpha^{ij})\,. \tag{2.79}$$

It is easy to see that in this case

$$\tilde{\beta}^i = \beta^i\,, \tag{2.80}$$

and

$$\tilde{\gamma} = \gamma\,. \tag{2.81}$$

Therefore, a self-adjoint operator is determined by the matrix α^{ij} and the scalar γ. It can be written in an explicitly self-adjoint form

$$L = -\sum_{i,j=1}^{n} \mu^{-1}(x)\ \partial_i\mu(x)\alpha^{ij}(x)\partial_j + \gamma(x)\,. \tag{2.82}$$

When we write a differential operator in such a form, then the order of functions and derivatives does matter. It is assumed that the operator acts on a function f in the following way

$$(Lf)(x) = -\sum_{i,j=1}^{n} \mu^{-1}(x)\ \partial_i\left[\mu(x)\alpha^{ij}(x)\partial_j f(x)\right] + \gamma(x)f(x)\,. \tag{2.83}$$

A remark has to be made here. Note that 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 $\alpha^{ij}(x)$ and $\beta^i(x)$ the question is whether it is possible to find a function $\mu(x)$ such that the equation (2.79) is satisfied.

Let us also note that the form of the operator can be simplified by a similarity transformation. Let

$$\mu = e^{-2\omega}\,. \tag{2.84}$$

Then the operator $L_\omega = e^{-\omega} L e^{\omega}$ has the form

$$L_\omega = -\sum_{i,j=1}^{n} \partial_i \alpha^{ij}(x) \partial_j + \gamma_\omega(x)\,, \tag{2.85}$$

where

$$\gamma_\omega = \gamma + \sum_{i,j=1}^{n} \left[\alpha^{ij}(\partial_i\omega)(\partial_j\omega) - \partial_i(\alpha^{ij}\partial_j\omega)\right]\,. \tag{2.86}$$

More generally, any operator of the form (2.73) can be written as follows. Suppose that the matrix α^{ij} is non-degenerate. Let us denote the entries of this matrix by

$$g^{ij} = \alpha^{ij} \tag{2.87}$$

and the entries of the inverse matrix by

$$(g_{ij}) = (\alpha^{ij})^{-1}\,. \tag{2.88}$$

Let g denote the determinant of the matrix g_{ij},

$$g = \det g_{ij} = (\det \alpha^{ij})^{-1}\,. \tag{2.89}$$

Further, let

$$\mathcal{A}_i = -\sum_{j=1}^{n} \frac{1}{2} g_{ij}\beta^j - \sum_{j,k=1}^{n} \frac{1}{2} g_{ij} g^{-1/2} \partial_k (g^{1/2} g^{jk}) \tag{2.90}$$

$$Q = \gamma + \sum_{i,j=1}^{n} \left[g^{ij}\mathcal{A}_i\mathcal{A}_j + g^{-1/2}\partial_i(g^{1/2}g^{ij}\mathcal{A}_j)\right]\,. \tag{2.91}$$

Then the operator L takes the form

$$L = -\sum_{i,j=1}^{n} g^{-1/2}(\partial_i + \mathcal{A}_i) g^{1/2} g^{ij} (\partial_j + \mathcal{A}_j) + Q\,. \tag{2.92}$$

This form of the operator enables one a nice geometric interpretation that we will discuss in the next lecture.

Note that if the vector $\mathcal{A}_i$ is non-zero, then the operator is not self-adjoint. It can still be equivalent (similar) to a self-adjoint operator. Let ω be a smooth function and let us make a similarity transformation $L \to L_\omega = e^{-\omega} L e^{\omega}$. We want to study the question

whether there exists a function ω such that the operator L_ω is self-adjoint. We have

$$L_\omega = -g^{-1/2}(\partial_i + \mathcal{A}_i + \omega_{;i})g^{1/2}g^{ij}(\partial_j + \mathcal{A}_j + \omega_{;j}) + Q\,, \tag{2.93}$$

where $\omega_{;i} = \partial_i\omega$. We want to find function ω such that

$$\partial_i\omega = -\mathcal{A}_i\,. \tag{2.94}$$

Obviously such a function exists only if the vector $\mathcal{A}_i$ is a gradient, that is, if it satisfies the equation

$$\partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i = 0\,. \tag{2.95}$$

Thus the quantity

$$\mathcal{R}_{ij} = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i = 0\,. \tag{2.96}$$

measures the extent to which the operator L is non-self-adjoint.

2.2.3 Resolvent and Spectrum

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

$$A\varphi = \lambda\varphi\,. \tag{2.97}$$

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 is 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 is also called the degree of degeneracy.

The operator

$$G(\lambda) = (A - \lambda I)^{-1}$$

is called the *resolvent* of the operator A. The complex numbers λ for which the resolvent $G(\lambda)$ is well defined (bounded) are called *regular points* of A. The set of 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 A.

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 reacher 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 axis.

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 a projection can only be either 1 or 0.

Spectral Theorem for Self-Adjoint Operators

A very important fact about self-adjoint operators in Hilbert spaces is the following. If all the eigenvalues are simple, that is all eigenspaces are one-dimensional, then the set of all normalized eigenvectors forms an orthonormal basis. When the eigenspaces are more than one-dimensional, then the eigenvectors belonging to the same eigenspace are not necessarily orthogonal, but can be always 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 A. Then the matrix of the operator A diagonalizes

$$(\varphi_k, A\varphi_j) = \lambda_k \delta_{kj}\,, \tag{2.98}$$

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

$$f = \sum_{n=1}^{\infty} a_n \varphi_n \tag{2.99}$$

we have

$$Af = \sum_{n=1}^{\infty} \lambda_n a_n \varphi_n \,. \tag{2.100}$$

This can be rephrased as follows. Let $(P_n)_{n=1}^{\infty}$ be the projection operators onto the eigenspaces Then

$$\sum_{n=1}^{\infty} P_n = I \tag{2.101}$$

and

$$A = \sum_{n=1}^{\infty} \lambda_n P_n \,. \tag{2.102}$$

Functions of Operators

This enables one to define pretty general functions of operators by

$$f(A) = \sum_{n=1}^{\infty} f(\lambda_n) P_n \,. \tag{2.103}$$

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

For example, for a self-adjoint positive operator A one can define the complex power of A

$$A^{-s} = \sum_{n=1}^{\infty} \lambda_n^{-s} P_n \,, \tag{2.104}$$

where s is a complex variable, and the exponential of A

$$U(t) = \exp(-tA) = \sum_{n=1}^{\infty} e^{-t\lambda_n} P_n \,, \tag{2.105}$$

where $t > 0$.

Spectral Theorem for Self-adjoint Partial Differential Operators on Compact Manifolds

We list here without proof some properties of elliptic partial differential operators on compact manifolds. We will describe the manifold theory in more details in the next lectures. 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 (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 L is real.

2. The spectrum of L is bounded from below.

3. 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.

4. The eigenvalues have finite multiplicities, $(d_k)_{k=1}^{\infty}$, and, therefore, the eigenspaces are finite-dimensional.

5. The projections $(P_k)_{k=1}^{\infty}$ to the eigenspaces are trace-class operators and their traces are equal to the multiplicities of the eigenvalues
$$\operatorname{Tr} P_k = d_k \,. \tag{2.106}$$

6. The eigenvalues form an increasing sequence $(\lambda_k)_{k=1}^{\infty}$, that is,
$$\lambda_1 < \lambda_2 < \cdots < \lambda_k < \lambda_{k+1} < \cdots \,. \tag{2.107}$$
To simplify notation in subsequent formulas we relabel the eigenvalues in such a way that each eigenvalue is repeated according to its multiplicity. Then the projections P_k are one-dimensional and the eigenvalues form a monotone non-decreasing sequence
$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \leq \lambda_{k+1} \leq \cdots \,. \tag{2.108}$$

7. The operator L is either positive or has only finitely many non-positive eigenvalues.

8. As $k \to \infty$ the eigenvalues grow to infinity as k^2, more precisely, they have the following asymptotics

$$\lambda_k = ck^2 + O(k)\,, \tag{2.109}$$

where c is some positive constant.

9. The eigenfunctions $(\varphi_k(x))_{k=1}^{\infty}$ are smooth functions that form a basis in $L^2(M,\mu)$, which can be made orthonormal.

10. The resolvent and the heat kernel of the operator L are given by

$$G(\lambda; x, x') = \sum_{k=1}^{\infty} \frac{1}{\lambda_k - \lambda} \varphi_k(x)\overline{\varphi_k(x')}\,, \tag{2.110}$$

$$U(t; x, x') = \sum_{k=1}^{\infty} e^{-t\lambda_k} \varphi_k(x)\overline{\varphi_k(x')}\,. \tag{2.111}$$

2.2.4 Spectral Functions

The traces of various functions of an operator A

$$\operatorname{Tr} f(A) = \sum_{k=1}^{\infty} d_k f(\lambda_k) \tag{2.112}$$

define so-called spectral functions. They can be used to study the spectrum of the operator A.

Of particular importance in the study of partial differential operators are the *zeta-function* and the *heat trace*. Let L be an elliptic operator with a positive leading symbol and with a purely point spectrum $(\lambda_k)_{k=1}^{\infty}$. 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

$$\zeta(s) = \operatorname{Tr} L^{-s} = \sum_{k=1}^{\infty} d_k \lambda_k^{-s}\,. \tag{2.113}$$

The *heat trace* is defined as the trace of the heat semi-group of the operator L for $t > 0$

$$\operatorname{Tr} \exp(-tL) = \sum_{k=1}^{\infty} d_k e^{-t\lambda_k}\,. \tag{2.114}$$

Since the differential operators are unbounded, the sequence of eigenvalues λ_k grows without bound as $k \to \infty$. This ensures the convergence of the spectral sum for the heat trace 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 $\operatorname{Re} s$. Then the zeta-function is defined by analytical continuation to the whole complex plane.

The zeta function can be used to define another very important spectral function, namely, the functional determinant. It is easy to check that for a positive symmetric finite-dimensional matrix A the determinants can be written in the form

$$\det A = \exp\left(-\frac{d}{ds}\operatorname{tr} A^{-s}\right)\Bigg|_{s=0}. \tag{2.115}$$

One can show that for differential operators the zeta-function $\zeta(s)$ is analytic at $s = 0$. Therefore, the above formula can be used to *define* the *functional determinant* $\operatorname{Det} L$ of a differential operator L,

$$\operatorname{Det} L = \exp\left[-\zeta'(0)\right]. \tag{2.116}$$

2.3 Operators with Constant Coefficients

2.3.1 Fourier Transform

First, let us recall the definition of Fourier transform. Let f be a function of a real variable $x \in \mathbb{R}$. Then Fourier transform of f is a function $\hat{f}(p) = (\mathcal{F}f)(p)$ of a real variable $p \in \mathbb{R}$ defined by

$$\hat{f}(p) = (\mathcal{F}f)(p) = \int_{-\infty}^{\infty} dx\; e^{-ipx} f(x)\,, \tag{2.117}$$

so that

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx} \hat{f}(p)\,. \tag{2.118}$$

Properties of Fourier Transform

Fourier transform of the derivatives is particularly simple. We have

$$(\mathcal{F}[\partial_x f(x)])(p) = ip\hat{f}(p)\,. \tag{2.119}$$

and

$$(\mathcal{F}[\partial_x^2 f(x)])(p) = -p^2 \hat{f}(p)\,. \tag{2.120}$$

More generally, we have

$$(\mathcal{F}[xf(x)])(p) = i\partial_p \hat{f}(p)\,, \tag{2.121}$$

$$(\mathcal{F}[x\partial_x f(x)])(p) = -\partial_p[p\hat{f}(p)] = -(p\partial_p + 1)\hat{f}(p)\,, \tag{2.122}$$

and

$$(\mathcal{F}[x\partial_x^2 f(x)])(p) = -i\partial_p[p^2\hat{f}(p)] = -i(p^2\partial_p + 2p)\hat{f}(p)\,. \tag{2.123}$$

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

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{for } x < 0 \end{cases} \tag{2.124}$$

can be obtained this way

$$\theta(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi i} e^{ipx} \frac{1}{p - i\varepsilon}\,, \tag{2.125}$$

where $\varepsilon > 0$ is an infinitesimal positive parameter. Indeed, for $x > 0$ the contour is closed in the upper half plane and there is a simple pole there at $p = i\varepsilon$ with residue 1. For $x < 0$ the contour is 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.

The formula for inverse Fourier transform can be interpreted as Fourier transform of a constant. It gives then

$$\delta(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx}\,. \tag{2.126}$$

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

$$\partial_x \theta(x) = \delta(x)\,. \tag{2.127}$$

Multi-dimensional Fourier Transform

Fourier transform can be obviously generalized to n dimensions. Let f be a function of n real variables x^j. 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 Fourier transform of f is a function $\hat{f}(p) = (\mathcal{F}f)(p)$ of real variables ω^j defined by

$$\hat{f}(p) = (\mathcal{F}f)(p) = \int\limits_{\mathbb{R}^n} dx\; e^{-i\langle p,x\rangle} f(x)\,, \tag{2.128}$$

where $dx = dx^1 \ldots dx^n$, and

$$\langle p, x\rangle = \sum_{j=1}^{n} p_j x^j\,. \tag{2.129}$$

The inverse Fourier transform is then defined by

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,x\rangle}\, \hat{f}(p)\,, \tag{2.130}$$

where $dp = dp_1 \ldots dp_n$.

The n-dimensional delta-function

$$\delta(x) = \delta(x^1) \cdots \delta(x^n)\,, \tag{2.131}$$

can be represented as the Fourier integral

$$\delta(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,x\rangle}\,. \tag{2.132}$$

2.3.2 Green Functions of Elliptic Operators

Solving Differential Equations by Fourier Transform

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 differential differential operator

$$L = -\alpha\partial_x^2 + \beta\partial_x + \gamma\,, \tag{2.133}$$

with real coefficients α, β and γ. We will assume that $\alpha > 0$. The symbol of this operator is

$$\sigma(p) = \alpha p^2 + i\beta p + \gamma\,. \tag{2.134}$$

The operator L is self-adjoint if $\beta = 0$.

Let λ be a complex number, $g(x)$ be a known function of x and $f(x)$ be an unknown function satisfying the differential equation

$$(L - \lambda)f = g\,, \tag{2.135}$$

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

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

$$[\sigma(p) - \lambda]\hat{f}(p) = \hat{g}(p)\,, \tag{2.136}$$

which we immediately solve

$$\hat{f}(p) = \frac{\hat{g}(p)}{\sigma(p) - \lambda}\,. \tag{2.137}$$

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

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx} \frac{\hat{g}(p)}{\sigma(p) - \lambda}\,. \tag{2.138}$$

Resolvent

We can now rewrite this solution in the form

$$f(x) = \int_{-\infty}^{\infty} dx'\; G(\lambda; x, x')g(x')\,, \tag{2.139}$$

where

$$G(\lambda; x, x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')} \frac{1}{\sigma(p) - \lambda}\,. \tag{2.140}$$

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

$$(L - \lambda)G(x, x') = \delta(x - x')\,, \tag{2.141}$$

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

$$\sigma(p) - \lambda = 0\,. \tag{2.142}$$

Obviously, the solutions are

$$p_{1,2}(\lambda) = i[\nu \pm \Delta(\lambda)]\,, \tag{2.143}$$

where

$$\nu = -\frac{\beta}{2\alpha} \tag{2.144}$$

and

$$\Delta(\lambda) = \frac{1}{2\alpha}\sqrt{\beta^2 + 4\alpha(\gamma - \lambda)}\,. \tag{2.145}$$

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 $\operatorname{Im}\Delta(\lambda) > 0$.

For the purpose of the calculation of the integral we will assume that λ has a sufficiently large negative real part, more precisely,

$$\operatorname{Re}\lambda < \gamma\,, \tag{2.146}$$

so that the roots $p_{1,2}(\lambda)$ are distinct and

$$\nu - \operatorname{Re}\Delta(\lambda) < 0 < \nu + \operatorname{Re}\Delta(\lambda)\,, \tag{2.147}$$

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:

$$G(\lambda; x, x') = \begin{cases} \dfrac{1}{2\alpha\Delta(\lambda)} \exp\left\{-[\nu + \Delta(\lambda)](x - x')\right\} & \text{for } x > x' \\ \dfrac{1}{2\alpha\Delta(\lambda)} \exp\left\{-[\nu - \Delta(\lambda)](x - x')\right\} & \text{for } x < x' \end{cases}. \tag{2.148}$$

This can also be written in the form

$$G(\lambda; x, x') \;=\; \frac{1}{2\alpha\Delta(\lambda)} \exp\left\{-\nu(x - x') - \Delta(\lambda)|x - x'|\right\}\,. \tag{2.149}$$

Notice that if λ satisfies the condition (2.146) 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 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 parabolic curve in the complex plane of $\lambda(p)$ described by the equation

$$\lambda(p) = (\alpha p^2 + \gamma) + i\beta p\,, \tag{2.150}$$

where p is a real parameter. Let

$$\lambda = u + iv\,. \tag{2.151}$$

If $\beta \neq 0$, then the spectral curve is described explicitly by

$$u = \frac{\alpha}{\beta^2} v^2 + \gamma\,. \tag{2.152}$$

Note that the resolvent cannot be analytically continued through this curve to large real positive values of λ. In the case when $\beta = 0$ 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.

Green Functions in Higher Dimension

Similarly to the one-dimensional case, 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 matrix, β^j be a real constant vector and γ be a real constant. Let L be an elliptic linear second-order partial differential differential operator with constant coefficients of the form

$$L = -\sum_{j,k=1}^{n} \alpha^{jk} \partial_j \partial_k + \sum_{j=1}^{n} \beta^j \partial_j + \gamma\,, \tag{2.153}$$

The symbol and the leading symbol of the operator L are given by

$$\sigma(p) = \sum_{j,k=1}^{n} \alpha^{jk} p_j p_k + i \sum_{j=1}^{n} \beta^j p_j + \gamma\,, \tag{2.154}$$

$$\sigma_L(p) = \sum_{j,k=1}^{n} \alpha^{jk} p_j p_k \,. \tag{2.155}$$

Since the operator L is elliptic the leading symbol $\sigma_L(p)$ is positive definite for any real $p \neq 0$, that is,

$$\sigma_L(p) = \sum_{j,k=1}^{n} \alpha^{jk} p_j p_k > 0 \qquad \text{for any real} \qquad p \neq 0 \,. \tag{2.156}$$

The operator L is self-adjoint if $\beta^i = 0$.

Let λ be a complex number, $g(x)$ be a known function of x and $f(x)$ be an unknown function satisfying the differential equation

$$(L - \lambda) f = g \,, \tag{2.157}$$

and the boundary condition that f goes to zero at $x \to \pm\infty$. Let $\hat{g}(p)$ be Fourier transform of the function g. Then by applying Fourier transform to this equation we obtain the solution

$$f(x) = (\mathcal{F}^{-1}\hat{f})(x) = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,x\rangle} \frac{\hat{g}(p)}{\sigma(p) - \lambda} \,. \tag{2.158}$$

This can be now written in the form

$$f(x) = \int\limits_{\mathbb{R}^n} dx'\, G(\lambda; x, x') g(x') \,, \tag{2.159}$$

where

$$G(\lambda; x, x') = \int\limits_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} e^{i\langle p,(x-x')\rangle} \frac{1}{\sigma(p) - \lambda} \,, \tag{2.160}$$

is the resolvent of the operator L satisfying the equation

$$(L - \lambda) G(x, x') = \delta(x - x') \,. \tag{2.161}$$

2.3.3 Heat Kernel

This integral can be computed as follows. Let us assume that λ has a sufficiently large negative real part so that

$$\sigma(p) - \operatorname{Re}\lambda > 0 \qquad \text{for any real} \qquad p \,. \tag{2.162}$$

Then we have

$$\frac{1}{\sigma(p)-\lambda} = \int_0^\infty dt\; e^{-t[\sigma(p)-\lambda]} \tag{2.163}$$

Now, let A be a symmetric non-degenerate positive definite $n \times n$ matrix and x be a n-vector, We recall the *Gaussian integrals* in n dimensions

$$\begin{aligned}\int_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} \exp\left\{-t\left\langle p, Ap\right\rangle + i\left\langle x, p\right\rangle\right\} \\ = (4\pi t)^{-n/2}(\det A)^{-1/2} \exp\left\{-\frac{1}{4t}\left\langle x, A^{-1}x\right\rangle\right\}.\end{aligned} \tag{2.164}$$

By using this formula we obtain an integral representation of the resolvent

$$G(\lambda; x, x') = \int_0^\infty dt\; e^{t\lambda} U(t; x, x') \tag{2.165}$$

where

$$\begin{aligned} U(t;x,x') &= \int_{\mathbb{R}^n} \frac{dp}{(2\pi)^n} \exp\left\{-t\sigma(p) + i\left\langle p, (x-x')\right\rangle\right\} \\ &= (4\pi t)^{-n/2}[\det A]^{-1/2} \exp\left\{\frac{1}{2}\left\langle (x-x'), A^{-1}\beta\right\rangle\right\} \\ &\quad \times \exp\left\{-t\left[\gamma + \frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle\right]\right\} \\ &\quad \times \exp\left\{-\frac{1}{4t}\left\langle (x-x'), A^{-1}(x-x')\right\rangle\right\}, \end{aligned} \tag{2.166}$$

and A is the positive definite matrix $A = (\alpha^{ij})$.

By using Fourier integral representation it is easy to see that the function $U(t; x, x')$ satisfies the differential equation

$$(\partial_t + L)U(t; x, x') = 0\,. \tag{2.167}$$

Also, by using Fourier integral representation of the delta-function we see that

$$\lim_{t\to 0^+} (4\pi t)^{-n/2}[\det A]^{-1/2} \exp\left\{-\frac{1}{4t}\left\langle x, A^{-1}x\right\rangle\right\} = \delta(x)\,, \tag{2.168}$$

and, hence, we obtain the initial condition

$$U(0;x,x') = \delta(x-x')\,. \tag{2.169}$$

This equation is called the heat equation (or diffusion equation). The function $U(t;x,x')$ is so-called fundamental solution of the heat equation called the *heat kernel*.

The integral over t can be computed by using the formula

$$\int_0^\infty dt\; t^{-p} \exp\left(-at - \frac{b}{4t}\right) = 2^p \left(\frac{a}{b}\right)^{(p-1)/2} K_{p-1}(\sqrt{ab})\,, \tag{2.170}$$

where $a,b>0$ $K_\alpha(x)$ is the modified Bessel function of an imaginary argument called the Macdonald function. We obtain then for the resolvent

$$\begin{aligned} G(\lambda;x,x') &= (4\pi)^{-n/2}[\det A]^{-1/2} \exp\left\{\frac{1}{2}\left\langle (x-x'), A^{-1}\beta\right\rangle\right\} \\ &\quad \times 2^{n/2}\left(\frac{a}{b}\right)^{(n-2)/2} K_{(n-2)/2}(\sqrt{ab})\,, \end{aligned} \tag{2.171}$$

where

$$b = \left\langle (x-x'), A^{-1}(x-x')\right\rangle\,, \tag{2.172}$$

$$a = \frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle + \gamma - \lambda\,. \tag{2.173}$$

This, of course, is only true for λ with sufficiently large negative real part so that

$$\mathrm{Re}\,\lambda < \gamma\,. \tag{2.174}$$

The study of the spectrum of non-self-adjoint operators is, in general, a much more complicated problem. What we know for sure is that the spectrum is located in the half-plane

$$\mathrm{Re}\,\lambda < \gamma\,. \tag{2.175}$$

Since the operator L acts on a non-compact space we can also say that 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.

2.3.4 Indegro-Differential Equations

Fourier transform can also be applied to integro-differential equations with convolution kernel. Such equations appear, in particular, in modeling of so-called jump-diffusion processes. To be specific let L be a differential operator of the form

$$L = -\alpha\partial_x^2 + \beta\partial_x + \gamma \tag{2.176}$$

acting on functions on the real line. The symbol of this operator is, of course,

$$\sigma(p) = \alpha p^2 + i\beta p + \gamma\,. \tag{2.177}$$

Let K be an integral operator defined by

$$(Kf)(x) = \int_{-\infty}^{\infty} dx'\; K(x-x')f(x')\,. \tag{2.178}$$

Let $g(x)$ be a given function, λ be a complex number and $f(x)$ be an unknown function satisfying the integro-differential equation

$$(L + K - \lambda)f = g\,. \tag{2.179}$$

Let $\hat{f}(p)$ and $\hat{g}(p)$ be Fourier transforms of the functions f and g. Let $\hat{K}(p)$ be Fourier transform of the kernel $K(x)$, that is,

$$\hat{K}(p) = \int_{-\infty}^{\infty} dx\; e^{-ipx}K(x)\,, \tag{2.180}$$

so that the kernel is

$$K(x-x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x-x')}\hat{K}(p)\,. \tag{2.181}$$

Then Fourier transform $\widehat{(Kf)}(p)$ of the function $(Kf)(x)$ is

$$\widehat{(Kf)}(p) = \hat{K}(p)\hat{f}(p)\,. \tag{2.182}$$

By applying Fourier transform to this equation we obtain a linear algebraic equation

$$[\sigma(p) + \hat{K}(p) - \lambda]\hat{f}(p) = \hat{g}(p)\,, \tag{2.183}$$

the solution of which is, of course,

$$\hat{f}(p) = \frac{\hat{g}(p)}{\sigma(p) + \hat{K}(p) - \lambda} \,. \tag{2.184}$$

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

$$f(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi}\, e^{ipx} \frac{\hat{g}(p)}{\sigma(p) + \hat{K}(p) - \lambda} \,. \tag{2.185}$$

Of course, this can be written in the form

$$f(x) = \int\limits_{-\infty}^{\infty} dx'\, G(\lambda; x, x') g(x') \,, \tag{2.186}$$

where

$$G(\lambda; x, x') = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi}\, e^{ip(x-x')} \frac{1}{\sigma(p) + \hat{K}(p) - \lambda} \tag{2.187}$$

is the resolvent of the integro-differential operator $L + K$.

Let us consider an integral operator T defined by

$$(Tf)(x) = \int\limits_{-\infty}^{\infty} dx'\, \omega(x') \left[f(x + x') - f(x) \right] \,, \tag{2.188}$$

where $\omega(x)$ is some probability distribution, in particular, $\omega(x)$ is non-negative and

$$\int\limits_{-\infty}^{\infty} dx\, \omega(x) = 1 \,. \tag{2.189}$$

Such an operator can be called a *jump operator*. Fourier transform of the probability distribution $\omega(x)$,

$$\hat{\omega}(p) = \int\limits_{-\infty}^{\infty} dx\, e^{-ipx} \omega(x) \tag{2.190}$$

is called the *characteristic function*.

Since the action of the operator T can be written as

$$(Tf)(x) = \int_{-\infty}^{\infty} dx' \, \omega(x' - x) f(x') - f(x) \,, \tag{2.191}$$

the jump operator has the form

$$T = K - I \,, \tag{2.192}$$

where I is the identity operator and K is a convolution operator with the kernel

$$K(x) = \omega(-x) \,. \tag{2.193}$$

Let us consider an integro-differential equation

$$(L + \mu T - \lambda) f = g \,, \tag{2.194}$$

where μ is a constant. Then by using the solution to the convolution integro-differential equation above we obtain

$$f(x) = \int_{-\infty}^{\infty} dx' \, G(\lambda; x, x') g(x') \,, \tag{2.195}$$

where the resolvent is now

$$G(\lambda; x, x') = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \, e^{ip(x-x')} \frac{1}{\sigma(p) + \mu\hat{\omega}(-p) - \mu - \lambda} \,. \tag{2.196}$$

2.3.5 Laplace Transform

We will also use 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 $F(s) = (\mathcal{L}f)(s)$ of a complex variable $s \in \mathbb{C}$ defined by

$$F(s) = (\mathcal{L}f)(s) = \int_{0}^{\infty} dt \, e^{-st} f(t) \,. \tag{2.197}$$

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 constant γ such that Laplace transform $F(s)$ converges in

the half-plane $\mathrm{Re}\, s > \gamma$. Then inverse Laplace transform is defined by

$$f(t) = (\mathcal{L}^{-1}F)(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} F(s)\,. \tag{2.198}$$

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

Properties of Laplace Transform

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

$$(\mathcal{L}[\partial_t f(t)])(s) = sF(s) - f(0)\,, \tag{2.199}$$

$$(\mathcal{L}[\partial_t^2 f(t)])(s) = s^2F(s) - sf(0) - f'(0)\,. \tag{2.200}$$

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

$$(\mathcal{L}[tf(t)])(s) = -\partial_s F(s)\,. \tag{2.201}$$

More generally, one can get

$$(\mathcal{L}[t\partial_t f(t)])(s) = -\partial_s[sF(s)] = -(s\partial_s + 1)F(s)\,, \tag{2.202}$$

and

$$(\mathcal{L}[t\partial_t^2 f(t)])(s) = -\partial_s[s^2F(s) - sf(0)] = -(s^2\partial_s + 2s)F(s) + f(0)\,. \tag{2.203}$$

Parabolic Partial Differential Equations

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 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

$$L = -\sum_{j,k=1}^{n} \alpha^{jk}(x)\partial_j\partial_k + \sum_{j=1}^{n} \beta^j(x)\partial_j + \gamma(x)\,. \tag{2.204}$$

Let $g(x)$ be a function of $x \in \mathbb{R}^n$ that goes to zero at infinity. We consider parabolic partial differential equation of the form

$$(\partial_t + L)f(t,x) = 0 \tag{2.205}$$

with initial condition

$$f(0,x) = g(x) \tag{2.206}$$

and the boundary conditions at infinity

$$\lim_{x\to\pm\infty} f(t,x) = 0\,. \tag{2.207}$$

Let $F(s;x)$ be Laplace transform of the function $f(t,x)$ with respect to the time variable. By applying Laplace transform to this equation we obtain an elliptic equation

$$(L+s)F(s;x) = g(x) \tag{2.208}$$

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,

$$(L+s)G(-s;x,x') = \delta(x-x')\,. \tag{2.209}$$

Then the solution of the elliptic equation can be written in the form

$$F(s;x) = \int\limits_{\mathbb{R}^n} dx'\; G(-s;x,x')g(x')\,, \tag{2.210}$$

and the solution of the original problem is obtained by inverse Laplace transform

$$f(t,x) = \int\limits_{\mathbb{R}^n} dx' U(t;x,x')g(x')\,, \tag{2.211}$$

where

$$U(t;x,x') = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} G(-s;x,x')\,, \tag{2.212}$$

and c is a sufficiently large real constant. This is nothing but the heat kernel; it satisfies the heat equation

$$(\partial_t + L)U(t;x,x') = 0 \tag{2.213}$$

and the initial condition

$$U(0; x, x') = \delta(x - x')\,. \tag{2.214}$$

Both the resolvent $G(-s; x, x')$ of the operator L, and the heat kernel $U(t; x, x')$ satisfy the boundary condition at infinity. Obviously, the resolvent $G(-s; x, x')$ is nothing but Laplace transform of the heat kernel

$$G(-s; x, x') = \int_0^\infty dt\; e^{-st} U(t; x, x')\,. \tag{2.215}$$

Second-order Equations

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

$$L = \alpha\partial_t^2 + \beta\partial_t + \gamma\,, \tag{2.216}$$

with real coefficients α, β and γ. We will assume that $\alpha \neq 0$, say $\alpha > 0$.

Let $g(t)$ be a known function of t and $f(t)$ be an unknown function satisfying the differential equation

$$Lf = g\,, \tag{2.217}$$

with some initial conditions

$$f(0) = a\,, \qquad f'(0) = b\,. \tag{2.218}$$

Let $F(s)$ and $G(s)$ be Laplace transforms of the functions f and g. Applying Laplace transform to this equation we get an algebraic equation

$$\sigma(s)F(s) = G(s) + \alpha(as + b) + a\beta\,, \tag{2.219}$$

where

$$\sigma(s) = \alpha s^2 + \beta s + \gamma\,. \tag{2.220}$$

Then we immediately obtain

$$F(s) = \frac{G(s) + \alpha(as + b) + a\beta}{\sigma(s)}\,, \tag{2.221}$$

and, therefore, the solution of the original differential equation is obtained by inverse Laplace transform

$$f(t) = (\mathcal{L}^{-1}F)(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} \frac{G(s) + \alpha(as+b) + a\beta}{\sigma(s)}\,, \tag{2.222}$$

where c is a sufficiently large positive real constant.

We can now rewrite this solution in the form

$$f(t) = \int\limits_0^\infty dt'\; G(t,t')g(t') + h(t)\,, \tag{2.223}$$

where

$$G(t,t') = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s(t-t')} \frac{1}{\sigma(s)}\,, \tag{2.224}$$

and

$$h(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{st} \frac{\alpha(as+b) + a\beta}{\sigma(s)}\,. \tag{2.225}$$

Of course, $G(t,t')$ is a Green function of the operator L satisfying the equation

$$LG(t,t') = \delta(t-t') \tag{2.226}$$

and $h(t)$ is nothing but the solution of the homogeneous equation

$$Lf = 0 \tag{2.227}$$

with the initial conditions (2.218).

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

$$\sigma(s) = 0\,. \tag{2.228}$$

They are given by

$$s_{1,2} = \nu \pm \Delta\,, \tag{2.229}$$

where

$$\nu = -\frac{\beta}{2\alpha} \tag{2.230}$$

and

$$\Delta = \frac{1}{2\alpha}\sqrt{\beta^2 - 4\alpha\gamma}\,. \tag{2.231}$$

Let us assume for simplicity that $\Delta \neq 0$ 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:

$$G(t,t') = \begin{cases} \dfrac{1}{2\alpha\Delta}\left\{\exp[(\nu+\Delta)(t-t') - \exp[(\nu-\Delta)(t-t')]\right\} & \text{for } t > t' \\ 0 & \text{for } t < t' \end{cases}, \tag{2.232}$$

which can also be written in the form

$$G(t,t') = \theta(t-t')\frac{1}{2\alpha\Delta}\left\{\exp[(\nu+\Delta)(t-t') - \exp[(\nu-\Delta)(t-t')]\right\}\,. \tag{2.233}$$

Similarly, we compute the function $h(t)$,

$$h(t) = c_1 e^{(\nu+\Delta)t} + c_2 e^{(\nu-\Delta)t}\,, \tag{2.234}$$

where

$$c_1 = \frac{\alpha(\nu+\Delta)a + \alpha b + \beta a}{2\alpha\Delta}\,, \tag{2.235}$$

$$c_2 = -\frac{\alpha(\nu-\Delta)a + \alpha b + \beta a}{2\alpha\Delta}\,. \tag{2.236}$$

Equations with Linear Coefficients

Laplace transform can be also applied for solving equation with non-constant coefficients. Let L be a second-order differential operator with of the form

$$L = -(\alpha_0 + \alpha_1 x)\partial_x^2 + (\beta_0 + \beta_1 x)\partial_x + \gamma_0 + \gamma_1 x \tag{2.237}$$

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

$$\sigma_L(x,\omega) = (\alpha_0 + \alpha_1 x)\omega^2 \tag{2.238}$$

is positive definite.

Then the equation

$$Lf = g \tag{2.239}$$

is a second-order differential equation with non-constant coefficients. Now, let us apply 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

$$[p(s)\partial_s + q(s)]\, F(s) = \tilde{G}(s)\,, \tag{2.240}$$

where $p(s)$ and $q(s)$ are quadratic polynomials defined by

$$p(s) = \alpha_1 s^2 - \beta_1 s - \gamma_1\,, \tag{2.241}$$

$$q(s) = -\alpha_0 s^2 + (\beta_0 + 2\alpha_1)s + \gamma_0 - \beta_1\,. \tag{2.242}$$

and

$$\tilde{G}(s) = G(s) - \alpha_0 as - \alpha_0 b + \alpha_1 a + \beta_0 a \tag{2.243}$$

where $a = f(0)$ and $b = f'(0)$.

This equation can be easily solved. First we define

$$\mu(s) = \exp\left(\int ds\, \frac{q(s)}{p(s)}\right)\,. \tag{2.244}$$

Then the solution is

$$F(s) = \frac{1}{\mu(s)}\left\{\int ds\; \mu(s)\frac{\tilde{G}(s)}{p(s)} + C\right\}\,, \tag{2.245}$$

where C is an arbitrary constant that should be determined from the boundary condition

$$\lim_{\mathrm{Im}\, s\to\pm\infty} F(s) = 0\,. \tag{2.246}$$

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

There is an elegant variation of the method of Laplace transform for such differential equations. We describe it on the example of the linear homogeneous second-order differential equation with linear coefficients

$$Lf = 0\,, \tag{2.247}$$

where L is a second-order differential operator with of the form

$$L = (\alpha_0 + \alpha_1 t)\partial_t^2 + (\beta_0 + \beta_1 t)\partial_t + \gamma_0 + \gamma_1 t \tag{2.248}$$

with coefficients that are linear functions. Let us represent the solution in the form

$$f(t) = \int\limits_C \frac{ds}{2\pi i}\, e^{st} F(s)\,, \tag{2.249}$$

where C is a contour of integration in the complex plane that will be specified later. Then

$$\partial_t f(t) = \int\limits_C \frac{ds}{2\pi i}\, e^{st} sF(s)\,, \tag{2.250}$$

$$\partial_t^2 f(t) = \int\limits_C \frac{ds}{2\pi i}\, e^{st} s^2 F(s)\,, \tag{2.251}$$

$$tf(t) = -\int\limits_C \frac{ds}{2\pi i}\, e^{st}\partial_s F(s) + \frac{1}{2\pi i}\, e^{st} F(s)\Big|_{\partial C}\,, \tag{2.252}$$

$$t\partial_t f(t) = -\int\limits_C \frac{ds}{2\pi i}\, e^{st}\partial_s [sF(s)] + \frac{1}{2\pi i}\, e^{st} sF(s)\Big|_{\partial C}\,, \tag{2.253}$$

$$t\partial_t^2 f(t) = -\int\limits_C \frac{ds}{2\pi i}\, e^{st}\partial_s [s^2 F(s)] + \frac{1}{2\pi i}\, e^{st} s^2 F(s)\Big|_{\partial C}\,, \tag{2.254}$$

where ∂C is the boundary of the contour C. Substituting these equations into the original equation we obtain

$$\int\limits_C \frac{ds}{2\pi i}\, e^{st} \left\{p(s)\partial_s + q(s)\right\} F(s) + \frac{1}{2\pi i}\, e^{st} \left(\alpha_1 s^2 + \beta_1 s + \gamma_1\right) F(s)\Big|_{\partial C} = 0\,, \tag{2.255}$$

where $p(s)$ and $q(s)$ are defined above, This equation will be satisfied if both parts are equal to zero. Thus, we obtain a differential equation

$$\left\{p(s)\partial_s + q(s)\right\} F(s) = 0 \tag{2.256}$$

and a boundary condition

$$\left(\alpha_1 s^2 + \beta_1 s + \gamma_1\right) F(s)\Big|_{\partial C} = 0\,. \tag{2.257}$$

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

$$h(s)\Big|_{\partial C} = h(s_1) - h(s_0)\,. \tag{2.258}$$

This means that we could choose a contour whose endpoints are either the roots of the equation

$$\alpha_1 s^2 + \beta_1 s + \gamma_1 = 0 \tag{2.259}$$

or the zeros of the function $F(s)$. Different contours of integration and different arbitrary constants 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.

2.4 Homogeneous Differential Operators

2.4.1 Mellin Transform

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

$$F(s) = (\mathcal{M}f)(s) = \int_0^\infty dt\; t^{s-1} f(t)\,. \tag{2.260}$$

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 $\lim_{|\mathrm{Im} s| \to \infty} F(s) = 0$. Then inverse Mellin transform is defined by

$$f(t) = (\mathcal{M}^{-1}F)(t) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} t^{-s} F(s)\,, \tag{2.261}$$

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 Mellin transform, are determined by the rate at which the function f decreases or increases at 0 and ∞.

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

$$\begin{aligned}(\mathcal{M}f(t))(s) &= \int_{-\infty}^{\infty} dx\; e^{sx} f(e^x) \\ &= (\mathcal{F}f(e^x))(is)\,, \end{aligned} \tag{2.262}$$

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

$$\begin{aligned}(\mathcal{F}f(x))(p) &= \int_{0}^{\infty} dt\; t^{-ip-1} f(\log t) \\ &= (\mathcal{M}f(\log t))(-ip)\,, \end{aligned} \tag{2.263}$$

which is Mellin transform of the function $f(\log t)$ evaluated at $s = -ip$. This means, in particular, that Fourier transform of the function $f(x)$ is well defined if the imaginary axis is in the strip of analyticity of Mellin transform of the function $f(\log t)$.

Properties of Mellin Transform

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

$$[\mathcal{M}(tf(t))](s) = (\mathcal{M}f)(s+1)\,. \tag{2.264}$$

Further, by integration by parts we obtain

$$[\mathcal{M}(\partial_t f(t))](s) = -(s-1)(\mathcal{M}f)(s-1)\,. \tag{2.265}$$

Therefore,

$$[\mathcal{M}(t\partial_t f(t))](s) = -s(\mathcal{M}f)(s)\,, \tag{2.266}$$

and

$$[\mathcal{M}(t^2\partial_t^2 f(t))](s) = s(s+1)(\mathcal{M}f)(s)\,. \tag{2.267}$$

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

$$\Gamma(s) = \int_0^\infty dt\; t^{s-1} e^{-t}\,. \tag{2.268}$$

It satisfies the functional equation

$$s\Gamma(s) = \Gamma(s+1)\,, \tag{2.269}$$

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

$$\operatorname{Res}\Gamma(s)\Big|_{s=-k} = \frac{(-1)^k}{k!}\,. \tag{2.270}$$

Let $\Omega(t)$ be a function of t such that for any $\alpha > 0$ and any $N \geq 0$

$$\lim_{t\to 0,\infty} t^\alpha \partial_t^N \Omega(t) = 0\,. \tag{2.271}$$

Let $b(s)$ be a function defined by

$$b(s) = \frac{1}{\Gamma(-s)}(\mathcal{M}\Omega)(-s) = \frac{1}{\Gamma(-s)}\int_0^\infty dt\; t^{-s-1}\Omega(t)\,. \tag{2.272}$$

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

$$b(s) = \frac{1}{\Gamma(-s+N)}\int_0^\infty dt\; t^{-s-1+N}(-\partial_t)^N\Omega(t)\,, \tag{2.273}$$

where N is a positive integer. Moreover, by using the analytical properties of the gamma function we can also obtain the values of the function $b(s)$ at the non-negative integer points

$$b(k) = (-1)^k \partial_t^k \Omega(t)\Big|_{t=0}\,, \qquad k = 0, 1, 2, \dots\,, \tag{2.274}$$

which are nothing but the Taylor coefficients of the function $\Omega(t)$ at $t = 0$.

Now we can invert the Mellin transformation to get

$$\Omega(t) = \frac{1}{2\pi i} \int\limits_{c-i\infty}^{c+i\infty} ds\; t^s \Gamma(-s) b(s) \tag{2.275}$$

where c is a negative constant. Deforming the contour of integration here we obtain then

$$\Omega(t) = \sum_{k=0}^{N-1} \frac{(-t)^k}{k!} b(k) + R_N(t) \tag{2.276}$$

where

$$R_N(t) = \frac{1}{2\pi i} \int\limits_{c_N-i\infty}^{c_N+i\infty} ds\; t^s \Gamma(-s) b(s) \tag{2.277}$$

where $N - 1 < c_N < N$. 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 $\Omega(t)$ at $t \to 0$

$$\Omega(t) \sim \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} b(k) \tag{2.278}$$

Note that this series is convergent only in case when the rest term $R_N(t)$ vanishes at $N \to \infty$ 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 rest term $R_N(t)$ does not vanish at $N \to \infty$ 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.

Homogeneous Differential Equations

Let L be a linear second-order differential homogeneous differential operator

$$L = -\alpha x^2 \partial_x^2 + \beta x \partial_x + \gamma\,, \tag{2.279}$$

with real coefficients α, β and γ, acting on functions of x with $x > 0$. We will assume that $\alpha > 0$.

The leading symbol of the operator L,

$$\sigma(x,p) = \alpha x^2 p^2 \,, \tag{2.280}$$

is positive but fails to be elliptic at $x = 0$. The function

$$\sigma^{\mathcal{M}}(s) = -\alpha s^2 - (\alpha+\beta)s + \gamma \,. \tag{2.281}$$

can be called *Mellin symbol* of the operator L.

Let λ be a complex number, $g(x)$ be a known function of x and $f(x)$ be an unknown function satisfying the differential equation

$$(L-\lambda)f = g \,, \tag{2.282}$$

and the boundary condition

$$\lim_{x\to 0} f(x) = \lim_{x\to\infty} f(x) = 0 \,. \tag{2.283}$$

This equation can be easily solved by using Mellin transform. Let $F(s)$ and $G(s)$ be Mellin transforms of the functions f and g. Then by applying Mellin transform to this equation we obtain an algebraic equation

$$[\sigma^{\mathcal{M}}(s) - \lambda]F(s) = G(s) \,. \tag{2.284}$$

Then we immediately obtain

$$F(s) = \frac{G(s)}{\sigma^{\mathcal{M}}(s) - \lambda} \,, \tag{2.285}$$

and, therefore, the solution of the original differential equation is obtained by inverse Mellin transform

$$f(t) = (\mathcal{M}^{-1}F)(t) = \int\limits_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} t^{-s} \frac{G(s)}{\sigma^{\mathcal{M}}(s) - \lambda} \,, \tag{2.286}$$

where c is a constant that will be specified below.

Resolvent

We can now rewrite this solution in the form

$$f(x) = \int\limits_0^\infty \frac{dx'}{x'}\, G(\lambda; x, x') g(x') \,, \tag{2.287}$$

where

$$G(\lambda; x, x') = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \left(\frac{x}{x'}\right)^{-s} \frac{1}{\sigma^{\mathcal{M}}(s) - \lambda}\,, \tag{2.288}$$

is the resolvent of the operator L satisfying the equation

$$(L - \lambda)G(\lambda; x, x') = x'\delta(x - x')\,, \tag{2.289}$$

where $\delta(x - x')$ is the Dirac delta-function.

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

$$\sigma^{\mathcal{M}}(s) = 0\,, \tag{2.290}$$

given by

$$s_{1,2} = \nu \pm \Delta(\lambda)\,, \tag{2.291}$$

where

$$\nu = -\frac{\beta + \alpha}{2\alpha} \tag{2.292}$$

and

$$\Delta(\lambda) = \frac{1}{2\alpha}\sqrt{(\alpha + \beta)^2 + 4\alpha(\gamma - \lambda)}\,. \tag{2.293}$$

We will assume that λ has a sufficiently large negative real part, that is,

$$\operatorname{Re}\lambda < \gamma\,, \tag{2.294}$$

so that the roots are distinct and

$$\operatorname{Re} s_2 < 0 < \operatorname{Re} s_1\,. \tag{2.295}$$

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:

$$G(\lambda; x, x') = \begin{cases} \dfrac{1}{2\alpha\Delta(\lambda)} \left(\dfrac{x}{x'}\right)^{-\nu-\Delta} & \text{for } x > x' \\ \dfrac{1}{2\alpha\Delta(\lambda)} \left(\dfrac{x}{x'}\right)^{-\nu+\Delta} & \text{for } x < x' \end{cases}\,. \tag{2.296}$$

This can also be written in the form

$$G(\lambda; x, x') = \frac{1}{2\alpha\Delta(\lambda)} \left\{ \theta(x - x') \left(\frac{x}{x'}\right)^{-\nu-\Delta} + \theta(x' - x) \left(\frac{x}{x'}\right)^{-\nu+\Delta} \right\}. \tag{2.297}$$

Notice that the resolvent goes to zero as $x \to 0$ and $x \to \infty$.

2.5 Asymptotic Expansion of Integrals

2.5.1 Asymptotic Expansions

First of all, we remind some definitions of asymptotic analysis. Let us consider two functions f and g of real variable x. We consider limits 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

$$f(x) = o(g(x)) \tag{2.298}$$

if

$$\lim_{x\to a} \frac{f(x)}{g(x)} = 0\,. \tag{2.299}$$

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

$$f(x) = O(g(x)) \tag{2.300}$$

if

$$\lim_{x\to a} \frac{f(x)}{g(x)} = C\,, \tag{2.301}$$

with some constant C. In particular, $f(x) = o(1)$ means that $f(x)$ is *infinitesimal* as $x \to a$ and $f(x) = O(1)$ means that $f(x)$ is *bounded* as $x \to a$. Finally, we write

$$f(x) \sim g(x) \tag{2.302}$$

if

$$\lim_{x\to a} \frac{f(x)}{g(x)} = 1\,, \tag{2.303}$$

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

$$\varphi_{n+1}(x) = o(\varphi_n(x))\,. \tag{2.304}$$

Such a sequence is called an *asymptotic sequence* at $x \to a$. For example, a 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 a function f is *expanded in an asymptotic series* and write

$$f(x) \sim \sum_{n=1}^{\infty} a_n \varphi_n(x), \tag{2.305}$$

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

$$f(x) - \sum_{n=1}^{N} a_n \varphi_n(x) = o(\varphi_N(x)) \,. \tag{2.306}$$

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

$$R_N(x) = f(x) - \sum_{n=1}^{N} a_n \varphi_n(x) \tag{2.307}$$

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

$$\lim_{x \to a} R_N(x) = 0 \,. \tag{2.308}$$

However, if for some fixed x

$$\lim_{N \to \infty} R_N(x) \neq 0 \tag{2.309}$$

then the asymptotic series diverges. In general, there are three possibilities: a) asymptotic series converges to the original function; b) asymptotic series converges to a different function; c) 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.

2.5.2 Gaussian Integrals

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

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \, e^{-x^2} = 1 \,. \tag{2.310}$$

By scaling the variable $x \to \alpha x$ with a positive constant $\alpha > 0$ we also get

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}} \, e^{-\alpha x^2} = \alpha^{-1/2} \,, \tag{2.311}$$

and now by shifting the variable $x \to x - i\beta/(2\alpha)$ we get

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}}\, e^{-\alpha x^2 + i\beta x} = \alpha^{-1/2} \exp\left(-\frac{\beta^2}{4\alpha}\right) . \tag{2.312}$$

By expanding both sides of this equation in a power series in β we finally obtain the following Gaussian integrals

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}}\, e^{-\alpha x^2} x^{2k+1} = 0 \tag{2.313}$$

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}}\, e^{-\alpha x^2} x^{2k} = \frac{(2k)!}{2^{2k} k!} \alpha^{-k-1/2} . \tag{2.314}$$

Multidimensional Gaussian integrals are computed similarly. Let $A = (a_{ij})$ be an $n \times n$ 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 p there holds

$$\int_{\mathbb{R}^n} \frac{dx}{\pi^{n/2}} \exp\left(-\langle x, Ax \rangle + i \langle p, x \rangle\right) = (\det A)^{-1/2} \exp\left(-\frac{1}{4} \langle p, A^{-1} p \rangle\right) . \tag{2.315}$$

This formula can be proved by diagonalizing the matrix A and using the one-dimensional Gaussian integrals.

By expanding both sides of this equation in Taylor series in p we also obtain

$$\int_{\mathbb{R}^n} \frac{dx}{\pi^{n/2}} \exp\left(-\langle x, Ax \rangle\right) x^{i_1} \cdots x^{i_{2k+1}} = 0 \tag{2.316}$$

$$\int_{\mathbb{R}^n} \frac{dx}{\pi^{n/2}} \exp\left(-\langle x, Ax \rangle\right) x^{i_1} \cdots x^{i_{2k}} = (\det A)^{-1/2} \frac{(2k)!}{2^{2k} k!} G^{(i_1 i_2} \cdots G^{i_{2k-1} i_{2k})} . \tag{2.317}$$

Here $G = A^{-1}$ is the inverse matrix and and the parenthesis denote complete symmetrization over all indices included. A very important

property of Gaussian integrals is that the right-hand side 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 in the last lecture.

2.5.3 Laplace Integrals in One Dimension

Let S and φ be real-valued smooth functions on an interval $[a, b]$ and λ be a large positive parameter. Consider the integrals of the form

$$F(\lambda) = \int_a^b dx\ \varphi(x) e^{-\lambda S(x)}\,. \tag{2.318}$$

Such integrals are called *Laplace integrals*. We will study the asymptotics of Laplace integrals as $\lambda \to \infty$.

Suppose that the function S has a minimum at an interior point x_0 of the interval $[a, b]$, i.e. $a < x_0 < b$. Then $S'(x_0) = 0$. 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

$$S(x) = S(x_0) + S''(x_0)\frac{(x - x_0)^2}{2} + O((x - x_0)^3)\,. \tag{2.319}$$

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 and becomes a standard Gaussian integral. Thus, we obtain the main term of the asymptotics as $\lambda \to \infty$

$$F(t) \sim \left(\frac{2\pi}{\lambda}\right)^{1/2} \left[S''(x_0)\right]^{-1/2}\ e^{-\lambda S(x_0)} \varphi(x_0)\,. \tag{2.320}$$

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

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{1/2} \left[S''(x_0)\right]^{-1/2}\ e^{-\lambda S(x_0)} \sum_{k=0}^{\infty} a_k \lambda^{-k}\,, \tag{2.321}$$

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 $S^{(k)}(x_0)$, $k \geq 3$, and derivatives $\varphi^{(l)}(x_0)$, $l \geq 0$, and involve inverse powers of $S''(x_0)$.

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

$$x = x_0 + \lambda^{-1/2} y \,. \tag{2.322}$$

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 getting

$$S(x_0 + \lambda^{-1/2} y) = S(x_0) + \frac{1}{2}\lambda^{-1} S''(x_0) y^2 + \sum_{n=3}^{\infty} \frac{S^{(n)}(x_0)}{n!} y^n \lambda^{-n/2} \,, \tag{2.323}$$

$$\varphi(x_0 + \lambda^{-1/2} y) = \sum_{n=0}^{\infty} \frac{\varphi^{(n)}(x_0)}{n!} y^n \lambda^{-n/2} \,. \tag{2.324}$$

Then the quadratic term in the exponent is of order $O(1)$. So we leave it in the exponent and expand the exponent of the rest in a power series. Then the integrand becomes

$$\lambda^{-1/2} \exp\left\{ -\lambda S(x_0) - \frac{1}{2} S''(x_0) y^2 \right\} V(x_0, y, \lambda) \,, \tag{2.325}$$

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

$$V(x_0, y, \lambda) = \sum_{k=0}^{\infty} b_k(x_0, y) \lambda^{-k/2} \,. \tag{2.326}$$

The coefficients $b_k(x_0, y)$ are polynomials in y with coefficients that are polynomial in the derivatives of the function S of order greater or equal than three and all derivatives of the function φ evaluated at x_0.

Next, 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 a power series in inverse powers of λ.

2.5.4 Laplace Integral in Multiple Dimensions

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

$$F(\lambda) = \int\limits_M dx\ \varphi(x) \exp[-\lambda S(x)]\,. \tag{2.327}$$

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

$$\partial_i S(x_0) = 0\,. \tag{2.328}$$

The $n \times n$ real symmetric matrix,

$$H = (\partial_i \partial_j S(x_0))\,, \tag{2.329}$$

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,

$$\det H \neq 0\,. \tag{2.330}$$

By standard analytic arguments one can show that non-degenerate critical points are isolated.

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

$$S(x) = S(x_0) + \frac{1}{2}\,\langle (x - x_0), H(x - x_0)\rangle + O((x - x_0)^3)\,. \tag{2.331}$$

Then as $\lambda \to \infty$ the main contribution to the integral comes from a small neghborhood of 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 we get the leading asymptotics of the integral $F(\lambda)$ as $\lambda \to \infty$

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{n/2} [\det H]^{-1/2} \exp[-\lambda S(x_0)] \varphi(x_0)\,. \tag{2.332}$$

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

$$F(\lambda) \sim \left(\frac{2\pi}{\lambda}\right)^{n/2} [\det H]^{-1/2} \exp[-\lambda S(x_0)] \sum_{k=0}^{\infty} a_k \lambda^{-k} . \tag{2.333}$$

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 derivatives $[\partial_{i_1} \cdots \partial_{i_m} \varphi(x_0)]$, $m \geq 0$, of the function φ evaluated at the point x_0 and the inverse Hessian matrix H^{-1}.

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

$$x^i = x_0^i + \lambda^{-1/2} y^i . \tag{2.334}$$

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 getting

$$\begin{aligned} S(x_0 + \lambda^{-1/2} y) &= S(x_0) + \frac{1}{2} \lambda^{-1} \langle y, Hy \rangle \\ &\quad + \sum_{m=3}^{\infty} \sum_{i_1,\ldots,i_m=1}^{n} \frac{\lambda^{-m/2}}{i_1! \cdots i_m!} [\partial_{i_1} \cdots \partial_{i_m} S(x_0)] \, y^{i_1} \cdots y^{i_m} , \end{aligned} \tag{2.335}$$

$$\varphi(x_0 + \lambda^{-1/2} y) = \sum_{m=0}^{\infty} \sum_{i_1,\ldots,i_m=1}^{n} \frac{\lambda^{-m/2}}{i_1! \cdots i_m!} [\partial_{i_1} \cdots \partial_{i_m} \varphi(x_0)] \, y^{i_1} \cdots y^{i_m} . \tag{2.336}$$

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 a power series in inverse powers of λ.

Each term in the asymptotic expansion can be represented by a graph, known as a *Feynmann diagram*, as follows. Let us represent the derivatives $[\partial_{i_1} \cdots \partial_{i_m} S(x_0)]$, $m \geq 3$, by *vertices* with m lines attached to it and the derivatives $[\partial_{i_1} \cdots \partial_{i_m} \varphi(x_0)]$, $m \geq 0$, by another type of vertices with m lines attached to them. Let us represent the

inverse Hessian 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.

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

Chapter 3

Introduction to Differential Geometry

In this lecture we give a very 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.

3.1 Differentiable Manifolds

A manifold is a general space that looks locally like a Euclidean space of the same dimension. This allows 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 in 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 continuously deformed everywhere to $\mathbb{R}^n$. 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*

$$x'^i = f^i(x)\,, \qquad i = 1, \dots, n\,. \tag{3.1}$$

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*.

Example. The n-sphere S^n of radius r can be realized as a hypersurface in $\mathbb{R}^{n+1}$ described by

$$(x^1)^2 + \cdots + (x^{n+1})^2 = r^2 \,. \tag{3.2}$$

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*.

Vector Fields

Let us consider a curve in M described in some local coordinates by

$$x^i = x^i(t) \,. \tag{3.3}$$

The *velocity vector* is described in these coordinates by

$$(\dot{x}^i) = \left(\dot{x}^1, \ldots, \dot{x}^n\right) \,, \tag{3.4}$$

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

$$\dot{x}'^i = \sum_{j=1}^{n} \frac{\partial x'^i}{\partial x^j} \dot{x}^j \,. \tag{3.5}$$

This motivates the following definition. A *tangent vector* at a point $p_0 \in M$ 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

$$v'^i = \sum_{j=1}^{n} \left(\frac{\partial x'^i}{\partial x^j} \right) (p_0) v^j \,. \tag{3.6}$$

The *tangent space* T_pM to M at p is the real vector space of all tangent vectors 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 $x \mapsto x(t)$, called a *flow*, as the solution of the system of ordinary first-order differential equations

$$\frac{dx^j}{dt} = v^j(x(t))\,, \qquad j = 1, \ldots, n, \tag{3.7}$$

with the initial conditions

$$x^j(0) = x^j\,. \tag{3.8}$$

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

$$\partial'_j f = \sum_{i=1}^{n} \frac{\partial x^i}{\partial x'^j} \partial_i f\,. \tag{3.9}$$

This motivates the following definition. A *covector* at a point $p_0 \in M$ 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

$$\alpha'_j = \sum_{j=1}^{n} \left(\frac{\partial x^i}{\partial x'^j} \right) (p_0) \alpha_i\,. \tag{3.10}$$

The *cotangent space* T^*_pM to M at p is the real vector space of all covectors on 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 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

$$\langle \alpha, v \rangle = \sum_{i=1}^{n} \alpha_i v^i\,. \tag{3.11}$$

Notation. In differential geometry upper and lower indices play different roles: upper indices are used to denote components of vectors (or contravariant vectors) and lower indices are used to denote components of covectors (or covariant vectors).

Riemannian Metric

A positive definite inner product in the tangent and cotangent spaces is defined with the help of a *metric* g_{ij}, which is a symmetric positive definite matrix, and its inverse, $g^{ij} = (g_{ij})^{-1}$. The inner product of two vectors is given then by

$$(v, w) = \sum_{i,j=1}^{n} g_{ij} v^i w^j \,, \tag{3.12}$$

and the inner product of two covectors is

$$(\alpha, \beta) = \sum_{i,j=1}^{n} g^{ij} \alpha_i \beta_j \,. \tag{3.13}$$

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

$$v_i = \sum_{j=1}^{n} g_{ij} v^j \,. \tag{3.14}$$

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 such that

$$\alpha^i = \sum_{j=1}^{n} g^{ij} \alpha_j \,. \tag{3.15}$$

This operation is called *raising the index of a covector*.

Let M be a manifold. A *Riemannian metric* on M is a differentiable assignment of a positive definite inner product in each tangent space T_pM to the manifold at each point $p \in M$. A *Riemannian*

manifold is a manifold with a Riemannian metric on it. The components of the metric tensor transform under the local diffeomorphisms as follows

$$g'_{ij}(x') = \sum_{k,l=1}^{n} \frac{\partial x^k}{\partial x'^i} \frac{\partial x^l}{\partial x'^j} g_{kl}(x)\,. \tag{3.16}$$

The Riemannian metric $g_{ij}(x)$ determines the *interval* (or *distance*), ds, between infinitesimmaly close points x and $x + dx$ by

$$ds^2 = \sum_{i,j=1}^{n} g_{ij}(x)\, dx^i\, dx^j\,. \tag{3.17}$$

Riemannian Volume Element

We introduce the notation for the determinant of the metric

$$g = \det g_{ij}\,. \tag{3.18}$$

Although this function does not have any indices it is not a scalar! Indeed, by taking the determinant of the eq. (3.16) we obtain

$$\sqrt{g'(x')} = \det\left(\frac{\partial x^k}{\partial x'^i}\right) \sqrt{g(x)}\,. \tag{3.19}$$

A scalar function f does not change under the change of coordinates

$$f'(x') = f(x)\,. \tag{3.20}$$

Therefore, the determinant of the metric is not a scalar. A function that transforms like this is called a *scalar density* of weight 1. Recall that the integration volume element transforms under the local diffeomorphisms as

$$dx' = \det\left(\frac{\partial x'^k}{\partial x^i}\right) dx\,. \tag{3.21}$$

This means that the quantity

$$\sqrt{g(x)}\, dx \tag{3.22}$$

remains invariant under the change of coordinates. This quantity is called *Riemannian volume element*.

Tensor Fields

A *tensor* of type (p, q) at a point $p_0 \in M$ of a manifold M is a map that assigns to each local coordinate system an 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

$$T'^{i_1 \dots i_p}_{j_1 \dots j_q} = \sum_{k_1,\dots,k_p=1}^{n} \sum_{l_1,\dots,l_q=1}^{n} \frac{\partial x'^{i_1}}{\partial x^{k_1}} \cdots \frac{\partial x'^{i_p}}{\partial x^{k_p}} \frac{\partial x^{l_1}}{\partial x'^{l_q}} \cdots \frac{\partial x^{j_1}}{\partial x'^{j_q}} T^{k_1 \dots k_p}_{l_1 \dots l_q} \tag{3.23}$$

A *tensor field* on a manifold M is a smooth assignment of a tensor to each point p in M. In local coordinates a tensor field of type (p, q) is described by a collection of smooth functions $T^{k_1 \dots k_p}_{l_1 \dots l_q}(x)$.

Einstein Summation Convention

As you have seen there is a huge amount of 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. In any expression there are two types of indices: *free indices* and *repeated indices*. Free indices appear only once in an expression; they are assumed to take all possible values from 1 to n. The position of all free indices in all terms in an equation must be the same. Repeated indices appear 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 a *contraction* of indices. 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. 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. There cannot be indices occuring three or more times in any expression.

3.1.1 Lie Derivative

Lie Derivative of a Vector Field

Let v be a vector field on a manifold M. Let $\varphi_t : M \to M$ be the flow generated by v. Let $x \in M$. Then $\varphi_t(x)$ is the point on the integral

curve of the vector field v going through x and such that

$$\varphi_0(x) = x \tag{3.24}$$

and

$$\frac{d\varphi_t(x)}{dt} = v(\varphi_t(x))\,. \tag{3.25}$$

In local coordinates for small t we have

$$\varphi_t^i(x) = x^i + tv^i(x) + O(t^2)\,, \tag{3.26}$$

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,

$$L_v f = v^i \partial_i f\,. \tag{3.27}$$

Lie derivative of a vector field w with respect to the vector field v is the vector field $L_v w$ defined by

$$(L_v w)^i = v^j \partial_j w^i - w^j \partial_j v^i\,. \tag{3.28}$$

The expression

$$[v, w]^i = v^j \partial_j w^i - w^j \partial_j v^i \tag{3.29}$$

is called *Lie bracket* of the vector fields v and w.

Lie Derivative of Tensors

Lie derivative of a 1-form α with respect to the vector field v is a 1-form $L_v\alpha$ defined by

$$(L_v\alpha)_i = v^j \partial_j \alpha_i + \alpha_j \partial_i v^j\,. \tag{3.30}$$

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

$$\begin{aligned}(L_v T)^{k_1\ldots k_p}_{i_1\ldots i_q} \;=\;& v^j \partial_j T^{k_1\ldots k_p}_{i_1\ldots i_q} + T^{k_1\ldots k_p}_{j i_2\ldots i_q}\partial_{i_1} v^j + \cdots + T^{k_1\ldots k_p}_{i_1\ldots i_{q-1} j}\partial_{i_q} v^j \\ & - T^{j k_2\ldots k_p}_{i_1 i_2\ldots i_q}\partial_j v^{k_1} - \cdots - T^{k_1\ldots k_{p-1} j}_{i_1\ldots i_q}\partial_j v^{k_p}\end{aligned}$$

In particular, Lie derivative of the metric tensor g_{ij} is

$$(L_v g)_{ij} = v^k \partial_k g_{ij} + g_{ik}\partial_j v^k + g_{kj}\partial_i v^k\,. \tag{3.31}$$

If the metric remains invariant under the flow generated by the vector field v, then the vector field v is called a *Killing vector field* and its flow is called an *isometry*. In other words, Killing vector fields are solutions of the differential equations

$$L_v g = 0\,. \tag{3.32}$$

3.2 Connection and Curvature

3.2.1 Covariant Derivative

Let M be a Riemannian manifold with the metric g_{ij}. Then Christoffel symbols are defined by

$$\Gamma^i{}_{jk} = \frac{1}{2} g^{im} \left(\partial_j g_{mk} + \partial_k g_{jm} - \partial_m g_{jk} \right) . \tag{3.33}$$

The covariant derivative of vectors v^i and covectors α_i is defined by

$$\nabla_j v^i = \partial_j v^i + \Gamma^i{}_{kj} v^k\,. \tag{3.34}$$

$$\nabla_j \alpha_i = \partial_j \alpha_i - \Gamma^k{}_{ij} \alpha_k\,. \tag{3.35}$$

More generally, the covariant derivative of a tensor T of type (p, q) is a tensor of type $(p, q+1)$ defined by

$$\begin{aligned} \nabla_j T^{i_1 \ldots i_p}_{k_1 \ldots k_q} &= \partial_j T^{i_1 \ldots i_p}_{k_1 \ldots k_q} + \Gamma^{i_1}{}_{mj} T^{m i_1 \ldots i_p}_{k_1 \ldots k_q} + \cdots + \Gamma^{i_p}{}_{mj} T^{i_1 \ldots i_{p-1} m}_{k_1 \ldots k_q} \\ &\quad - \Gamma^m{}_{i_1 j} T^{i_1 \ldots i_p}_{m k_2 \ldots k_q} - \cdots - \Gamma^m{}_{i_q j} T^{i_1 \ldots i_p}_{k_1 \ldots k_{q-1} m}\,. \end{aligned} \tag{3.36}$$

Christoffel symbols are not components of a $(1, 2)$ tensor! They do not transform as a tensor under diffeomorphisms. They are rather the coefficients of so-called *affine connection*. The connection is called *compatible with the metric* if

$$\nabla_j g_{ik} = 0\,, \tag{3.37}$$

and *torsion-free* (or symmetric) if the torsion is equal to zero, that is,

$$\Gamma^i{}_{jk} - \Gamma^i{}_{kj} = 0\,. \tag{3.38}$$

An affine connection that is torsion-free and compatible with the metric is called *Levi-Civita connection*. Each Riemannian manifold

has a unique Levi-Civita connection. By using the definition of Christoffel symbols it is not difficult to see that both these conditions are satisfied. Thus, Christoffel symbols are exactly the coefficients of Levi-Civita connection.

The covariant derivative is also denoted by a semi-colon, that is,

$$\nabla_i v^j = v^j{}_{;i} \tag{3.39}$$

and so on.

3.2.2 Riemann Tensor and Ricci Identities

Now let us define the quantities

$$R^i{}_{jkl} = \partial_k \Gamma^i{}_{jl} - \partial_l \Gamma^i{}_{jk} + \Gamma^i{}_{mk}\Gamma^m{}_{jl} - \Gamma^i{}_{ml}\Gamma^m{}_{jk}\,. \tag{3.40}$$

Then one can show that these coefficients form a tensor called *Riemann curvature tensor*.

The commutators of covariant derivatives of tensors are expressed in terms of the curvature. We have the following identities (called the *Ricci identities*):

$$[\nabla_i, \nabla_j] v^k = R^k{}_{lij} v^l \tag{3.41}$$

$$[\nabla_i, \nabla_j] \alpha_k = -R^l{}_{kij} \alpha_l \tag{3.42}$$

$$[\nabla_i, \nabla_j] T^{j_1 \ldots j_p}_{k_1 \ldots k_q} = \sum_{m=1}^{p} R^{j_m}{}_{lij} T^{j_1 \ldots j_{m-1} l j_{m+1} \ldots j_p}_{k_1 \ldots k_q} - \sum_{n=1}^{q} R^l{}_{k_n ij} T^{j_1 \ldots j_p}_{k_1 \ldots k_{n-1} l k_n k_q}\,. \tag{3.43}$$

Properties of the Curvature Tensor

By using Riemann tensor one can define new tensors, *Ricci tensor*

$$R_{ij} = R^k{}_{ikj}\,, \tag{3.44}$$

scalar curvature

$$R = g^{ij} R_{ij} = g^{ij} R^k{}_{ikj}\,, \tag{3.45}$$

and finally *Weyl tensor* (for $n > 2$)

$$C^{ij}{}_{kl} \;=\; R^{ij}{}_{kl} - \frac{4}{n-2} R^{[i}{}_{[k} \delta^{j]}{}_{l]} + \frac{2}{(n-1)(n-2)} R \delta^{[i}{}_{[k} \delta^{j]}{}_{l]}\,. \tag{3.46}$$

Here the square brackets mean anti-symmetrization over the indices included.

The Riemann tensor has the following symmetry properties

$$R_{ijkl} = -R_{ijlk} \tag{3.47}$$

$$R_{ijkl} = -R_{jikl} \tag{3.48}$$

$$R_{ijkl} = R_{klij} \tag{3.49}$$

$$R^{i}{}_{[jkl]} = R^{i}{}_{jkl} + R^{i}{}_{klj} + R^{i}{}_{ljk} = 0 \tag{3.50}$$

$$R_{ij} = R_{ji} \tag{3.51}$$

The Weyl tensor has the same symmetry properties as the Riemann tensor and all its contractions vanish, that is,

$$C^{i}{}_{jik} = 0\,. \tag{3.52}$$

By using these symmetry properties one can show that the number of algebraically independent components of Riemann tensor is

$$\frac{n^2(n^2-1)}{12}\,. \tag{3.53}$$

In dimension $n = 2$ Riemann tensor has only one independent component determined by the scalar curvature called *Gauss curvature*

$$R^{12}{}_{12} = \frac{1}{2}R\,. \tag{3.54}$$

Therefore

$$R^{ij}{}_{kl} = R\delta^{[i}{}_{[k}\delta^{j]}{}_{l]}\,, \tag{3.55}$$

$$R_{ij} = \frac{1}{2}Rg_{ij}\,. \tag{3.56}$$

In dimension $n = 3$ Riemann tensor has six independent components determined by the Ricci tensor R_{ij}. The Weyl tensor C_{ijkl} vanishes, that is,

$$R^{ij}{}_{kl} = 4R^{[i}{}_{[k}\delta^{j]}{}_{l]} + R\delta^{[i}{}_{[k}\delta^{j]}{}_{l]}\,. \tag{3.57}$$

Weyl tensor measures anisotropy of the metric in the following sense. If Weyl tensor is equal to zero, then there exist a scalar function $\omega(x)$ such that the metric has the form

$$g_{ij}(x) = e^{\omega(x)}\delta_{ij}\,. \tag{3.58}$$

Such metrics are called *conformally flat*.

Riemann tensor satisfies the following identities

$$\nabla_{[m} R^{ij}{}_{kl]} = \nabla_m R^{ij}{}_{kl} + \nabla_k R^{ij}{}_{lm} + \nabla_l R^{ij}{}_{mk} = 0\,, \tag{3.59}$$

called *Bianci identities*. By contraction one gets from here

$$\nabla_i R^{ij}{}_{kl} = \nabla_k R^j_l - \nabla_l R^j_k\,, \tag{3.60}$$

$$\nabla_i R^i_j = \frac{1}{2}\nabla_j R\,. \tag{3.61}$$

Symmetric Spaces

A Riemannian manifold M is called a *locally symmetric space* if the curvature is covariantly constant, that is,

$$\nabla_j R^i{}_{klm} = 0\,. \tag{3.62}$$

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 lecture.

3.2.3 Geometry of Two-dimensional Manifolds

Let us specify the above machinery for two-dimensional manifolds, $n = \dim M = 2$. In this case our tensor indices will run over $1, 2$. In this case the curvature tensor has just one independent component, K, called *Gauss curvature*. More precisely, it is defined as follows. Because of the symmetries of the curvature tensor it can only have the form

$$R^i{}_j{}^k{}_l = K\left(\delta^i{}_k\delta^j{}_l - \delta^i{}_l\delta^j{}_k\right)\,, \tag{3.63}$$

where K is a scalar function. The Ricci tensor and the scalar curvature are then

$$R^i{}_j = K\delta^i{}_j\,, \tag{3.64}$$

$$R = 2K\,. \tag{3.65}$$

That is, Gauss curvature is just one half of the scalar curvature, and the only non-zero components of the curvature tensor and the Ricci tensor are

$$R^1{}_2{}^1{}_2 = R^2{}_1{}^2{}_1 = R^1{}_1 = R^2{}_2 = K\,. \tag{3.66}$$

In particular, this means that every two-dimensional manifold is conformally flat.

A very important class of manifolds consists of manifolds with constant curvature. In dimension two there are just two types of such manifolds, the sphere, S^2, with positive constant curvature, and the hyperbolic plane, H^2, with negative constant curvature.

We give below explicit formulas for Gauss curvature in various coordinate systems. Let us consider first an orthogonal coordinate system such that the metric is given by

$$ds^2 = g_{11}(dx^1)^2 + g_{22}(dx^2)^2\,, \tag{3.67}$$

that is, the non-diagonal components, g_{12}, of the metric vanish. Then a straightforward calculation gives

$$K = -\frac{1}{2}(g_{11}g_{22})^{-1/2}\left\{\partial_1\left[(g_{11}g_{22})^{-1/2}\partial_1 g_{22}\right] + \partial_2\left[(g_{11}g_{22})^{-1/2}\partial_2 g_{11}\right]\right\}. \tag{3.68}$$

Since every two-dimensional manifold is conformally flat, this means that there always exists so called *conformal coordinates*, in which the metric has the form

$$ds^2 = e^{2\omega}\left[(dx^1)^2 + (dx^2)^2\right]\,, \tag{3.69}$$

that is, the non-vanishing components of the metric are given by

$$g_{11} = g_{22} = e^{2\omega}\,. \tag{3.70}$$

In this case the above formula gives

$$K = -e^{-2\omega}\left(\partial_1^2 + \partial_2^2\right)\omega\,. \tag{3.71}$$

A particular case of this metric is

$$ds^2 = \frac{4}{(1+\kappa\rho^2)^2}\left[(dx^1)^2 + (dx^2)^2\right]\,, \tag{3.72}$$

where $\varkappa$ is a constant and

$$\rho = \sqrt{(x^1)^2 + (x^2)^2}\,. \tag{3.73}$$

with Gauss curvature

$$K = \varkappa\,. \tag{3.74}$$

In so-called *geodesic polar coordinates* the metric has the form

$$ds^2 = dr^2 + a^2(r,\theta)d\theta^2\,, \tag{3.75}$$

where $a(r,\theta)$ is some function. Therefore, Gauss curvature can be written as

$$K = -\frac{1}{a}\partial_r^2 a\,. \tag{3.76}$$

Notice the following important particular cases

$$K = 1 \qquad \text{for } a = \sin r\,, \tag{3.77}$$

and

$$K = -1 \qquad \text{for } a = \sinh r\,. \tag{3.78}$$

3.2.4 Parallel Transport and Geodesic Distance

Let T be a tensor field and v be a vector field on a manifold M. Then the *directional derivative along the vector field* v is defined by

$$\nabla_v T = v^i \nabla_i T\,. \tag{3.79}$$

Let x and x' be two points on a manifold M and C be a smooth curve connecting these points described locally by $x^i(\tau)$, where $\tau \in [0,t]$, so that $x(0) = x'$ and $x(t) = x$. In the following we denote indices at 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. 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 tangent vector to C is defined by

$$v^i = \dot{x}^i(\tau), \tag{3.80}$$

where the dot denotes the derivative with respect to τ. The *length of the curve* C (or the distance between the points x' and x along the curve C) is defined as

$$d_C(x,x') = \int_0^t d\tau\, \sqrt{g_{ij}(x(\tau))\dot{x}^i\dot{x}^j}\,. \tag{3.81}$$

We say that a tensor T is *parallel transported along* C if

$$v^i \nabla_i T = 0\,. \tag{3.82}$$

A curve C such that the tangent vector $\dot{x}$ to C (in some parametrization) is transported parallel along C, that is,

$$\dot{x}^j \nabla_j \dot{x}^i = 0, \tag{3.83}$$

is called a *geodesics*. Then such parameter τ is called an *affine parameter*. The coordinates of the geodesics $x = x(\tau)$ satisfy the non-linear second-order ordinary differential equation

$$\ddot{x}^i + \Gamma^i{}_{jk}(x(\tau))\dot{x}^k \dot{x}^j = 0\,. \tag{3.84}$$

A very important fact about the geodesics is that any two sufficiently close points, x and x', can be connected by a single geodesics. Another fact that is often used as a definition of the geodesics is that the geodesics 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 $d(x, x')$.

The parallel transport of vector field along a geodesic connecting the points x and x' from the point x' to the point x is described by the *parallel transport operator*, $g^i{}_{j'}(x, x')$. It is a *bi-vector*, which means that it is a vector at the point x and a covector at the point x'. It is defined by the linear first order differential equation

$$\dot{x}^k \nabla_k g^i{}_{j'} = 0\,, \tag{3.85}$$

or, in components,

$$\frac{d}{d\tau} g^i{}_{j'}(x(\tau), x') + \Gamma^i{}_{kl}(x(\tau))\dot{x}^k g^l{}_{j'}(x(\tau), x') = 0\,, \tag{3.86}$$

with the initial condition

$$g^i{}_{j'}(x(\tau), x')\Big|_{x=x'} = g^i{}_{j'}(x(\tau), x')\Big|_{\tau=0} = \delta^i{}_j\,. \tag{3.87}$$

The parallel transport of any tensor can be easily expressed in terms of the operator of parallel transport. Let $\mathcal{G}T(x, x')$ denote the result of the parallel transport of a tensor T from the point x' to the point x. Then we have, for example,

$$(\mathcal{G}v)^i(x, x') = g^i{}_{j'}(x, x')v^{j'}(x')\,, \tag{3.88}$$

$$(\mathcal{G}T)^{i}{}_{k}(x,x') = g_{k}{}^{m'}(x,x')g^{i}{}_{j'}(x,x')T^{j'}{}_{m'}(x') \tag{3.89}$$

and so on.

Note that, in general, if the tensor field T is not parallel, then the value $T(x)$ of the tensor field T at the point x is different from the value $(\mathcal{G}T)(x,x')$ obtained by the parallel transport along the geodesic from the point x' .

3.2.5 World Function and Van Vleck Determinant

Let x' be a fixed point in a manifold M. Let us consider a sufficiently small neighborhood of this point and connect every other point x in this region with the point x' by a geodesic $x = x(\tau)$, with an affine parameter τ so that $x(0) = x'$ and $x(t) = x$. The Synge *world function* is defined then just as half of the square of the geodesic distance

$$\sigma(x,x') = \frac{1}{2}d^2(x,x')\,. \tag{3.90}$$

It can also be written in the form

$$\sigma(x,x') = \frac{1}{2}t^2 g_{ij}(x(t))\dot{x}^i(t)\dot{x}^j(t), \tag{3.91}$$

where $\dot{x}(\tau)$ is the tangent vector to the geodesic connecting the points x' and x. This is a *bi-scalar* function that determines the local geometry of the manifold. The derivatives of this function

$$\sigma_i = \nabla_i\sigma = \partial_i\sigma\,, \qquad \sigma_{i'} = \nabla_{i'}\sigma = \partial_{i'}\sigma\,, \tag{3.92}$$

are exactly the tangent vectors to the geodesic at the points x and x' respectively pointing in opposite directions, that is,

$$\sigma^i = t\dot{x}^\mu(t)\,, \qquad \sigma^{i'} = -t\dot{x}^{i'}(0)\,. \tag{3.93}$$

The two-point quantity $\sigma_i(x,x')$ is a scalar at the point x' and a covector at the point x, and the two-point quantity $\sigma_{i'}(x,x')$ is a scalar at the point x and a covector at the point x'. That is, the vector σ^i is obtained from the vector $\sigma^{i'}$ by parallel transport along the geodesic from the point x' and reversing its direction

$$\sigma^i = -g^i{}_{j'}\sigma^{j'}\,. \tag{3.94}$$

The norm of these tangent vectors is the same and is equal to length of the geodesic (that is, the geodesic distance). In other

words, the world function satisfies the first-order differential equations

$$\sigma(x,x') = \frac{1}{2} g^{ij}(x)\sigma_i(x,x')\sigma_j(x,x') = \frac{1}{2} g^{i'j'}(x')\sigma_{i'}(x,x')\sigma_{j'}(x,x') \,. \quad (3.95)$$

and the initial conditions

$$\sigma\Big|_{x=x'} = \sigma_i\Big|_{x=x'} = \sigma_{i'}\Big|_{x=x'} = 0 \,. \quad (3.96)$$

We define the second derivatives of the world function

$$\sigma_{ij} = \nabla_i \nabla_j \sigma \,, \qquad \sigma_{ij'} = \nabla_i \nabla_{j'} \sigma = \partial_i \partial_{j'} \sigma \,. \quad (3.97)$$

Then, by analyzing the behavior of the world function at $x \to x'$ one can show that the second derivatives satisfy the following initial conditions

$$\sigma_{ij}\Big|_{x=x'} = g_{ij} \,, \qquad \sigma_{ij'}\Big|_{x=x'} = -g_{ij} \,. \quad (3.98)$$

Finally, we define a two-point scalar $\Delta(x,x')$ called Van Vleck-Morette determinant

$$\Delta(x,x') = g^{-1/2}(x) \det\left[-\sigma_{ij'}(x,x')\right] g^{-1/2}(x') \,. \quad (3.99)$$

Then by using the above equations one can show that $\Delta(x,x')$ satisfies the following differential equation

$$\sigma^i \nabla_i \Delta^{1/2} = \frac{1}{2}(n - \sigma^i{}_i)\Delta^{1/2} \quad (3.100)$$

with the initial condition

$$\Delta\Big|_{x=x'} = 1 \,. \quad (3.101)$$

We will need this equation to study the heat kernel on Riemannian manifolds.

3.3 Covariant Expansions on Riemannian Manifolds

3.3.1 Equations for Derivatives of World Function and Operator of Parallel Transport

We follow here our papers [3, 6, 17]. 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 geodesics. Then all two-points functions defined above are 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,

$$[f(x,x')] = \lim_{x \to x'} f(x,x')\,. \tag{3.102}$$

First of all, we show that the coincidence limits of higher order symmetrized derivatives ($n \geq 2$) of the tangent vectors to the geodesics vanish,

$$[\nabla_{(i_1} \cdots \nabla_{i_n)} \sigma^j] = [\nabla_{(i_1} \cdots \nabla_{i_n)} \sigma^{j'}] = 0\,, \tag{3.103}$$

Similarly, we get for the higher symmetrized derivatives ($n \geq 1$) of the operator of parallel transport

$$[\nabla_{(i_1} \cdots \nabla_{i_n)} g^j{}_{k'}] = 0\,. \tag{3.104}$$

Now, let us define the operator of differentiation along the geodesics

$$D = \sigma^i \nabla_i\,. \tag{3.105}$$

Then the defining equation for the world function can be rewritten in the form

$$D\sigma^i = \sigma^i\,, \qquad D\sigma^{j'} = \sigma^{j'}\,. \tag{3.106}$$

Let us define the matrices $\xi = (\xi^i{}_j(x,x'))$ and $\eta = (\eta^{i'}{}_j(x,x'))$ by

$$\xi^i{}_j = \nabla_j \sigma^i = \nabla_j \nabla^i \sigma\,, \tag{3.107}$$

$$\eta^{i'}{}_j = \nabla_j \sigma^{i'} = \nabla_j \nabla^{i'} \sigma\,, \tag{3.108}$$

Then, the above equations can be rewritten in the form

$$\xi^i{}_j \sigma^j = \sigma^i\,, \tag{3.109}$$

$$\eta^{i'}{}_j \sigma^j = \sigma^{i'}\,, \qquad \eta^{i'}{}_j \sigma_{i'} = \sigma_j \tag{3.110}$$

Now, let us define another matrix $K = (K^i{}_j(x,x'))$ by

$$K^i{}_j = R^i{}_{kjl} \sigma^k \sigma^l\,. \tag{3.111}$$

Then by differentiating these equations and commuting the derivatives we get the following equations for the matrices ξ and η

$$D\xi + \xi(\xi - 1) + K = 0\,, \tag{3.112}$$
$$D\eta + \eta(\xi - 1) = 0\,. \tag{3.113}$$

One can easily show that the coincidence limits of third derivatives of the world function vanish, that is,

$$[\sigma_{;ijk}] = [\sigma_{;ijk'}] = 0\,. \tag{3.114}$$

Therefore, the initial conditions for the matrices ξ and η are

$$[\xi] = I\,, \qquad [\nabla_i \xi] = 0\,, \tag{3.115}$$

$$[\eta] = -I\,, \qquad [\nabla_i \eta] = 0\,, \tag{3.116}$$

where I is the unit matrix.

Let $\gamma = \eta^{-1}$ be the inverse of the matrix η. Then it obviously satisfies the equations

$$\gamma^i{}_{j'}\eta^{j'}{}_k = \delta^i{}_k\,, \qquad \eta^{j'}{}_i\gamma^i{}_{k'} = \delta^{j'}{}_{k'}\,, \tag{3.117}$$

and

$$\gamma^i{}_{j'}\sigma^{j'} = \sigma^i\,, \qquad \gamma^i{}_{j'}\sigma_i = \sigma_{j'}\,. \tag{3.118}$$

We can express the matrix ξ in terms of the matrix η (or γ) from eq. (3.113)

$$\xi = 1 + (D\gamma)\gamma^{-1}\,. \tag{3.119}$$

Finally, by substituting this equation into eq (3.112) we obtain the following equation for the matrix γ

$$\left(D^2 + D + K\right)\gamma = 0 \tag{3.120}$$

with the initial conditions

$$[\gamma] = -1\,, \qquad [\nabla_i \gamma] = 0\,. \tag{3.121}$$

It is this equation that is the most important ingredient in our approach. First of all, it is a linear second-order differential equation. Therefore, it has a unique solution satisfying the initial conditions (3.121).

We will solve this equation in form of a covariant Taylor series (see below). Moreover, this equation can be solved exactly in symmetric spaces when the curvature tensor is covariantly constant. This equation is the most convenient basis to find all of two-point quantities since all those quantities are expressible in terms of γ. For example, by noticing first that the determinant of the parallel transport operator is

$$\det\left[g^{i}{}_{j'}(x,x')\right] = g^{-1/2}(x)g^{1/2}(x'), \tag{3.122}$$

it is easy to see that Van Vleck-Morette determinant is equal to

$$\Delta = \det\left(-g_{i}{}^{k'}\gamma^{i}{}_{j'}\right)^{-1}. \tag{3.123}$$

We derive some new equations for the matrices η and γ. By using the above equations we obtain

$$\nabla_{[l}\eta^{i'}{}_{j]} = 0\,, \qquad \gamma^{k}{}_{[l'}\nabla_{|k|}\gamma^{i}{}_{j']} = 0\,. \tag{3.124}$$

$$\gamma^{k}{}_{i'}\nabla_{k}\left(\Delta^{-1}\eta^{i'}{}_{j}\right) = 0\,. \tag{3.125}$$

Here, as usual, the square brackets mean the anti-symmetrization over all indices included; the vertical lines denote the indices excluded from the anti-symmetrization. We will use these equations for computation of heat kernel asymptotics in the next sections.

Now, we derive an equation for the parallel transport operator. Let us introduce the following notation for the first derivative of the operator of parallel transport

$$\mathcal{G}^{k'}{}_{j'i'} = \gamma^{m}{}_{i'}g_{l}{}^{k'}\nabla_{m}g^{l}{}_{j'}\,, \tag{3.126}$$

and also the following notation for the curvature tensor parallel transported to the point x

$$\mathcal{B}^{i'}{}_{k'j} = g_{n}{}^{i'}g^{l}{}_{k'}R^{n}{}_{ljm}\sigma^{m}\,. \tag{3.127}$$

Then by differentiating the equation of parallel transport,

$$Dg^{i}{}_{j'} = 0\,, \tag{3.128}$$

commuting the derivatives and using eq. (3.119) we obtain a first-order differential equation

$$(D+1)\mathcal{G}^{k'}{}_{m'i'} = -\gamma^{j}{}_{i'}\mathcal{B}^{k'}{}_{m'j} \tag{3.129}$$

with the initial condition

$$[\mathcal{G}^{j'}{}_{k'i'}] = 0\,. \tag{3.130}$$

This equation can be written in the following simple matrix form.

Let us introduce the following matrices

$$\mathcal{G}_{i'} = \left(\mathcal{G}^{j'}{}_{k'i'}\right) \tag{3.131}$$

and

$$\mathcal{B}_i = \left(\mathcal{B}^{j'}{}_{k'i}\right)\,. \tag{3.132}$$

Then we have the equation

$$(D+1)\mathcal{G}_{i'} = -\gamma^{j}{}_{i'}\mathcal{B}_j \tag{3.133}$$

with the initial condition

$$[\mathcal{G}_{i'}] = 0\,. \tag{3.134}$$

Now, let us consider a vector field $\mathcal{A}_i$. We define a two-point function $\mathcal{P}(x,x')$ by

$$\mathcal{P}(x,x') = \exp\left(-\int_0^t d\tau\ \dot{x}^i(\tau)\mathcal{A}_i(x(\tau))\right)\,, \tag{3.135}$$

where $\dot{x}^i = \frac{dx^i}{d\tau}$ and the integral is taken along the geodesic $x(\tau)$ connecting the points x' and x so that $x(0) = x'$ and $x(t) = x$. This function satisfies the equation

$$D^{\mathcal{A}}\mathcal{P} = 0\,, \tag{3.136}$$

where

$$D^{\mathcal{A}} = \sigma^i\nabla_i^{\mathcal{A}}\,, \tag{3.137}$$

$$\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i\,, \tag{3.138}$$

and the initial condition

$$[\mathcal{P}] = 1\,. \tag{3.139}$$

Note that here $\nabla_i = \partial_i$.

Next, let

$$\hat{\mathcal{A}}_{i'} = \gamma^m{}_{i'}\mathcal{P}^{-1}\nabla_m^{\mathcal{A}}\mathcal{P}\,, \tag{3.140}$$

and

$$\mathcal{L}_j = \mathcal{R}_{jm}\sigma^m\,, \tag{3.141}$$

where

$$\mathcal{R}_{ij} = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i\,. \tag{3.142}$$

Then by differentiating the equation (3.136) we obtain a first-order differential equation

$$(D+1)\hat{\mathcal{A}}_{i'} = -\gamma^j{}_{i'}\mathcal{L}_j \tag{3.143}$$

with the initial condition

$$[\hat{\mathcal{A}}_{i'}] = 0\,. \tag{3.144}$$

It is not difficult to see also that the function $\mathcal{P}$ has the following coincidence limits

$$[\nabla^{\mathcal{A}}_{(i_1}\cdots\nabla^{\mathcal{A}}_{i_n)}\mathcal{P}] = 0\,. \tag{3.145}$$

3.3.2 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 $f(x)$ as a function of the affine parameter t, that is, $f(x(t))$. Then we can expand it in Taylor series in t at $t=0$

$$f(x(t)) = \sum_{n=0}^{\infty}\frac{1}{n!}t^n\left[\frac{d^n}{d\tau^n}f(x(\tau))\right]_{\tau=0}\,. \tag{3.146}$$

Now, we recall that

$$\frac{d}{d\tau} = \dot{x}^i(\tau)\nabla_i\,, \tag{3.147}$$

and use the equation of geodesic, $\dot{x}^i\nabla_i\dot{x}^j = 0$ to obtain

$$f(x) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_k)}f\right](x')\,. \tag{3.148}$$

This is 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

$$D\sigma^{i'} = \sigma^{i'} \tag{3.149}$$

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'). Similarly, the equation for the operator of parallel transport

$$Dg^{i}{}_{j'} = 0 \tag{3.150}$$

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.

First, we define the scalar eigenfunctions $|n\rangle$, $(n = 0, 1, 2, \dots)$, by

$$|0\rangle = 1 \tag{3.151}$$

$$|n\rangle = |i'_1 \cdots i'_n\rangle = \frac{(-1)^n}{n!}\sigma^{i'_1} \cdots \sigma^{i'_n}\,. \tag{3.152}$$

Then, obviously,

$$D|n\rangle = n|n\rangle\,. \tag{3.153}$$

Then 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

$$\frac{(-1)^n}{n!}g^{k}{}_{l'}\sigma^{i'_1} \cdots \sigma^{i'_n}\,. \tag{3.154}$$

Note also that by adding the factor $\mathcal{P}$ we get the eigenfunctions of the operator $D^{\mathcal{A}}$,

$$D^{\mathcal{A}}\mathcal{P}|n\rangle = n\mathcal{P}|n\rangle\,. \tag{3.155}$$

Let us define also the dual functions $\langle m|$ as operators acting on functions as

$$\langle m|f\rangle = \langle i_1 \cdots i_m|f\rangle = \left[\nabla_{(i_1} \cdots \nabla_{i_m)}f\right]\,, \tag{3.156}$$

in other words, the operator $\langle m|$ maps a function to its symmetrized covariant derivative evaluated at the point $x = x'$.

Now, it is not difficult to see that these operators satisfy the following duality property

$$\langle m|n\rangle = \delta_{mn}\delta^{i_1\cdots i_n}_{j_1\cdots j_n}\,, \tag{3.157}$$

where

$$\delta^{i_1\cdots i_n}_{j_1\cdots j_n} = \delta^{i_1}_{(j_1}\cdots\delta^{i_n}_{j_n)}\,. \tag{3.158}$$

Now it is almost obvious that our set of eigenfunctions is complete due to the fact that there is no 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 0. Of course, we restrict ourselves here to functions which are analytic in the neighborhood of the point x'.

Then we have the following completeness relation

$$\sum_{n=0}^{\infty}|n\rangle\langle n| = \mathrm{Id}\,, \tag{3.159}$$

where Id is the identity operator. Finally, by using this relation we obtain covariant Taylor series for any scalar field f

$$f = \sum_{n=0}^{\infty}|n\rangle\langle n|f\rangle \tag{3.160}$$

$$= \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}f\right](x')\,. \tag{3.161}$$

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

$$v^j = g^j{}_{k'}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}v^k\right](x')\,. \tag{3.162}$$

We also mention a more general expansion

$$f = \mathcal{P}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}\mathcal{P}^{-1}f\right](x')\,. \tag{3.163}$$

3.3.3 Covariant Fourier Transform

In order to study non-localities 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 define covariant Fourier transform of a scalar function f as follows

$$\hat{f}(k;x') = \int\limits_M dx\; g^{1/2}(x)\Delta(x,x')\exp\left[ik_{j'}\sigma^{j'}(x,x')\right] f(x)\,, \tag{3.164}$$

where $k_{j'}$ is a covector in the cotangent space at the point x'.

Remark. We should make a remark here. First, we defined all two-point functions in a sufficiently small neighborhood of the 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 on geodesic with the point x'. At such points Van Vleck 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* of 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 in the integral above over a sufficiently small geodesic ball of 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 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.

By using the equations for the functions $\Delta(x,x')$ and $\sigma^{i'}(x,x')$ one can show then that inverse Fourier transform is given by

$$f(x) = \int\limits_{\mathbb{R}^n} \frac{dk}{(2\pi)^n} g^{-1/2}(x') \exp\left[-ik_{j'}\sigma^{j'}(x,x')\right] \hat{f}(k;x')\,, \tag{3.165}$$

where $dk = dk_{1'}\dots dk_{n'}$, and the integration goes over the whole cotangent space at x'. In particular, covariant Fourier integral representation of the scalar delta-function has the form

$$\begin{aligned}\delta(x,y) &= \Delta^{1/2}(x,x')\Delta^{1/2}(y,x') \\ &\times \int\limits_{\mathbb{R}^n} \frac{dk}{(2\pi)^n} g^{-1/2}(x') \exp\left\{ik_{j'}\left[\sigma^{j'}(y,x') - \sigma^{j'}(x,x')\right]\right\}.\end{aligned} \tag{3.166}$$

The derivatives of Fourier transform are easy to compute since

$$\nabla_l f(x) = -i\,\eta^{m'}{}_l(x,x') \int\limits_{\mathbb{R}^n} \frac{dk}{(2\pi)^n} g^{-1/2}(x') \exp\left[-ik_{j'}\sigma^{j'}(x,x')\right] k_{m'}\hat{f}(k;x')\,. \tag{3.167}$$

Covariant Fourier transform of tensors is defined similarly. First, we parallel transform the 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

$$\hat{v}^{l'}(k;x') = \int\limits_M dx\; g^{1/2}(x)\Delta(x,x') \exp\left[ik_{j'}\sigma^{j'}(x,x')\right] g_m{}^{l'}(x,x')v^m(x)\,, \tag{3.168}$$

$$v^m(x) = g^m{}_{l'}(x,x') \int\limits_{\mathbb{R}^n} \frac{dk}{(2\pi)^n} g^{-1/2}(x') \exp\left[-ik_{j'}\sigma^{j'}(x,x')\right] \hat{v}^{l'}(k;x')\,. \tag{3.169}$$

3.3.4 Covariant Taylor Series of Two-Point Functions

We will need covariant Taylor series of the two-point functions introduced above. Let us calculate the two-point functions in form of covariant Taylor series.

First of all let us find the solution of the basic equation for the matrix γ. Let $V = (g^{i}{}_{j'})$ be the matrix of the operator of parallel transport. Then by taking into consideration the initial condition for the matrix γ we obtain the formal operator solution

$$\begin{aligned} \gamma &= -V\left\{1 + (D^2 + D)^{-1}\bar{K}\right\}^{-1} \\ &= V\sum_{n=0}^{\infty}(-1)^{n+1}\left\{(D^2 + D)^{-1}\bar{K}\right\}^{n}, \end{aligned} \tag{3.170}$$

where

$$\bar{K} = V^{-1}KV \tag{3.171}$$

is the matrix K parallel transported to the point x'. Now we expand the matrix K defined by (3.111) in covariant Taylor series

$$K = V\sum_{n=2}^{\infty}\frac{(-1)^n}{(n-2)!}K_{(n)}V^{-1} \tag{3.172}$$

where

$$K_{(n)} = \left(K_{(n)}{}^{i'}{}_{j'}\right) \tag{3.173}$$

are matrices defined by

$$K_{(n)}{}^{i'}{}_{j'} = K^{i'}{}_{j'l'_1\cdots l'_n}\sigma^{l'_1}\cdots\sigma^{l'_n}, \tag{3.174}$$

with tensor coefficients given by

$$K^{i}{}_{jl_1\cdots l_n} = \nabla_{(l_1}\cdots\nabla_{l_{n-2}}R^{i}{}_{l_{n-1}|j|l_n)}. \tag{3.175}$$

Here, as usual, the parenthesis denote complete symmetrization over all indices included except those separated by the vertical lines.

Next, let f be a function with zero coincidence limit $[f] = \langle 0|f\rangle = 0$. Then the action of the inverse operator $(D^2+D)^{-1}$ on the function f is well defined and can be represented by the spectral sum

$$(D^2 + D)^{-1}f = \sum_{n=1}^{\infty}\frac{1}{n(n+1)}|n\rangle\langle n|f\rangle. \tag{3.176}$$

Now by noticing that the matrix K has zero coincidence limit, i.e. $\langle 0|K\rangle = 0$, we obtain

$$\gamma = V\left(-1 + \sum_{n=2}^{\infty} \frac{(-1)^n}{n!}\gamma_{(n)}\right). \tag{3.177}$$

The matrix coefficients $\gamma_{(n)}$ are given by

$$\gamma_{(n)} = \sum_{k=1}^{[\frac{n}{2}]}(-1)^{k+1} \sum_{\substack{n_1,\cdots,n_k\geq 2 \\ n_1+\cdots+n_k=n}} N^{-1}(n_1,\cdots,n_k)K_{(n_k)}K_{(n_{k-1})}\cdots K_{(n_2)}K_{(n_1)}\,, \tag{3.178}$$

where $[x]$ denotes the integer part of the real number x, and $N(n_1,\ldots,n_k)$ is a combinatorial coefficient defined by

$$\begin{aligned} N(n_1,\cdots,n_k) &= \frac{(n+1)}{(n-1)!}(n_1-2)!\cdots(n_k-2)! \\ &\quad \times n_1(n_1+1)(n_1+n_2)(n_1+n_2+1)\cdots \\ &\quad \times(n_1+\cdots+n_{k-1})(n_1+\cdots+n_{k-1}+1)\,. \end{aligned} \tag{3.179}$$

We see that the matrices

$$\gamma_{(n)} = \left({\gamma_{(n)}}^{i'}{}_{j'}\right) \tag{3.180}$$

have the form

$${\gamma_{(n)}}^{i'}{}_{j'} = {\gamma^{i'}}_{j'l'_1\cdots l'_n}\sigma^{l'_1}\cdots\sigma^{l'_n}\,. \tag{3.181}$$

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

$${\gamma^i}_{jk_1k_2} = \frac{1}{3}R^i{}_{(k_1|j|k_2)}\,, \tag{3.182}$$

$${\gamma^i}_{jk_1k_2k_3} = \frac{1}{2}\nabla_{(k_1}R^i{}_{k_2|j|k_3)}\,, \tag{3.183}$$

$${\gamma^i}_{jk_1k_2k_3k_4} = \frac{3}{5}\nabla_{(k_1k_2}R^i{}_{k_3|j|k_4)} - \frac{1}{5}R^i{}_{(k_1|m|k_2}R^m{}_{k_3|j|k_4)}\,. \tag{3.184}$$

Using this solution for the matrix γ one can easily calculate all other two-point functions. For example, for the matrix η we obtain

$$\eta = \left(-1 + \sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\eta_{(n)}\right)V^{-1} \tag{3.185}$$

where

$$\eta_{(n)} = -\sum_{k=1}^{[\frac{n}{2}]} \sum_{\substack{n_1,\cdots,n_k\geq 2 \\ n_1+\cdots+n_k=n}} \frac{n!}{n_1!\cdots n_k!}\gamma_{n_k}\cdots\gamma_{n_1}\,. \tag{3.186}$$

Thus the matrices

$$\eta_{(n)} = \left(\eta_{(n)}{}^{i'}{}_{j'}\right)\,, \tag{3.187}$$

have the form

$$\eta_{(n)}{}^{i'}{}_{j'} = \eta^{i'}{}_{j'k'_1\cdots k'_n}\sigma^{k'_1}\cdots\sigma^{k'_n}\,, \tag{3.188}$$

with tensor coefficients determined by the above formula. A couple of first coefficients are given by Some first coefficients (2.73) equal

$$\eta^{i}{}_{jk_1k_2} = -\frac{1}{3}R^{i}{}_{(k_1|j|k_2)}\,, \tag{3.189}$$

$$\eta^{i}{}_{jk_1k_2k_3} = -\frac{1}{2}\nabla_{(k_1}R^{i}{}_{k_2|j|k_3)}\,, \tag{3.190}$$

$$\eta^{i}{}_{jk_1k_2k_3k_4} = -\frac{3}{5}\nabla_{(k_1}\nabla_{k_2}R^{i}{}_{k_3|j|k_4)} - \frac{7}{15}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|j|k_4)}\,. \tag{3.191}$$

Similarly, we represent Van Vleck-Morette determinant in the form

$$\Delta = \exp(2\zeta)\,, \tag{3.192}$$

where ζ is given by the series

$$\zeta = \sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\zeta_{(n)} \tag{3.193}$$

with the coefficients

$$\zeta_{(n)} = \sum_{k=1}^{[\frac{n}{2}]}\frac{1}{2k}\sum_{\substack{n_1,\cdots,n_k\geq 2 \\ n_1+\cdots+n_k=n}}\frac{n!}{n_1!\cdots n_k!}\,\mathrm{tr}\,\left(\gamma_{(n_1)}\cdots\gamma_{(n_k)}\right)\,. \tag{3.194}$$

These coefficients have the form

$$\zeta_{(n)} = \zeta_{i'_1\cdots i'_n}\sigma^{i'_1}\cdots\sigma^{i'_n} \tag{3.195}$$

with the tensor coefficients determined by the above equation. In particular, a couple of first coefficients are

$$\zeta_{k_1k_2} = \frac{1}{6}R_{k_1k_2}, \tag{3.196}$$

$$\zeta_{k_1k_2k_3} = \frac{1}{4}\nabla_{(k_1}R_{k_2k_3)}, \tag{3.197}$$

$$\zeta_{k_1k_2k_3k_4} = \frac{3}{10}\nabla_{(k_1}\nabla_{k_2}R_{k_3k_4)} + \frac{1}{15}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|i|k_4)}\,. \tag{3.198}$$

Therefore, Taylor expansion of Van Vleck determinant is given by

$$\Delta^{1/2} = \sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\Delta^{1/2}_{(n)} \tag{3.199}$$

with the coefficients

$$\Delta^{1/2}_{(n)} = \Delta^{1/2}_{i'_1\cdots i'_n}\sigma^{i'_1}\cdots\sigma^{i'_n}\,. \tag{3.200}$$

In particular, a couple of first coefficients are

$$\Delta^{1/2}_{k_1k_2} = \frac{1}{6}R_{k_1k_2}, \tag{3.201}$$

$$\Delta^{1/2}_{k_1k_2k_3} = \frac{1}{4}\nabla_{(k_1}R_{k_2k_3)}, \tag{3.202}$$

$$\Delta^{1/2}_{k_1k_2k_3k_4} = \frac{3}{10}\nabla_{(k_1}\nabla_{k_2}R_{k_3k_4)} + \frac{1}{15}R^{i}{}_{(k_1|m|k_2}R^{m}{}_{k_3|i|k_4)} + \frac{1}{12}R_{(k_1k_2}R_{k_3k_4)}\,. \tag{3.203}$$

Finally, we compute Taylor series for the derivative of the operator of parallel transport in form of the matrix $\mathcal{A}_{i'}$ defined by eqs. (3.131) and (3.140). In order to do this let us expand the matrix $\mathcal{L}_m$ in covariant Taylor series

$$\mathcal{B}_m = g_m{}^{l'}\sum_{n=1}^{\infty}\frac{(-1)^n}{(n-1)!}\mathcal{B}_{(n)\,l'}\,, \tag{3.204}$$

where

$$\mathcal{B}_{(n)\,l'} = \left(\mathcal{B}_{(n)}{}^{i'}{}_{j'l'}\right) \tag{3.205}$$

are matrices defined by

$$\mathcal{B}_{(n)}{}^{i'}{}_{j'l'} = \mathcal{B}^{i'}{}_{j'l'k'_1\cdots k'_n}\sigma^{k'_1}\cdots\sigma^{k'_n}\,, \tag{3.206}$$

with tensor coefficients given by

$$\mathcal{B}^{i}{}_{jmk_1\cdots k_n} = \nabla_{(k_1}\cdots\nabla_{k_{n-1}}R^{i}{}_{|jm|k_n)}\,. \tag{3.207}$$

Now, the formal operator solution of the eq.(3.133) is

$$\mathcal{G}_{i'} = -(D+1)^{-1}\mathcal{B}_m\gamma^m{}_{i'}\,. \tag{3.208}$$

Next, by defining the inverse operator in form of the spectral sum

$$(D+1)^{-1} = \sum_{n=0}^{\infty}\frac{1}{n+1}|n\rangle\langle n| \tag{3.209}$$

we obtain

$$\mathcal{G}^{i'}{}_{j'm'} = \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\mathcal{G}^{i'}{}_{j'm'k'_1\cdots k'_n}\sigma^{k'_1}\cdots\sigma^{k'_n}\,, \tag{3.210}$$

where the tensor coefficients are given by

$$\mathcal{G}^{i}{}_{jmk_1\cdots k_n} = \frac{n}{n+1}\left\{\mathcal{B}^{i}{}_{jmk_1\cdots k_n} - \sum_{p=1}^{n-2}\binom{n-1}{p-1}\mathcal{B}^{i}{}_{jl(k_1\cdots k_p}\gamma^{l}{}_{|m|k_{p+1}\cdots k_n)}\right\}. \tag{3.211}$$

We list here the first three coefficients

$$\mathcal{G}^{i}{}_{jmk_1} = \frac{1}{2}R^{i}{}_{jmk_1}\,, \tag{3.212}$$

$$\mathcal{G}^{i}{}_{jmk_1k_2} = \frac{2}{3}\nabla_{(k_1}R^{i}{}_{j|m|k_2)}\,, \tag{3.213}$$

$$\mathcal{G}^{i}{}_{jmk_1k_2k_3} = \frac{3}{4}\nabla_{(k_1}\nabla_{k_2}R^{i}{}_{j|m|k_3)} - \frac{1}{4}R^{i}{}_{jl(k_1}R^{l}{}_{k_2|m|k_3)}\,. \tag{3.214}$$

Next, we find the formal operator solution of the eq.(3.143)

$$\hat{\mathcal{A}}_{i'} = -\left(D^{\mathcal{A}}+1\right)^{-1}\mathcal{L}_j\gamma^j{}_{i'} \tag{3.215}$$

Defining the inverse operator as

$$\left(D^{\mathcal{A}}+1\right)^{-1} = \sum_{n=}^{\infty}\frac{1}{n+1}\mathcal{P}|n\rangle\langle n|\mathcal{P}^{-1}\,, \tag{3.216}$$

and expanding the vector $\mathcal{L}_j$

$$\mathcal{L}_j = \sum_{n=1}^{\infty}\frac{(-1)^n}{(n-1)!}g_j{}^{k'}\mathcal{R}_{k'i'_1\cdots i'_n}\sigma^{i'_1}\cdots\sigma^{i'_n}\,, \tag{3.217}$$

where

$$\mathcal{R}^{k}{}_{i_1\cdots i_n} = \nabla_{(i_1}\cdots\nabla_{i_{n-1}}\mathcal{R}^{k}{}_{i_n)}\,, \tag{3.218}$$

we obtain

$$\hat{\mathcal{A}}_{j'} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \mathcal{A}_{j'i'_1\cdots i'_n} \sigma^{i'_1} \cdots \sigma^{i'_n} , \tag{3.219}$$

where

$$\mathcal{A}_{ji_1\cdots i_n} = \frac{n}{n+1} \left\{ \mathcal{R}_{ji_1\cdots i_n} - \sum_{k=1}^{n-2} \binom{n-1}{k-1} \mathcal{R}_{l(i_1\cdots i_k} \gamma^l{}_{|j|i_{k+1}\cdots i_n)} \right\} . \tag{3.220}$$

We list below some low-order coefficients

$$\mathcal{A}_{mk_1} = \frac{1}{2} \mathcal{R}^i{}_{mk_1} , \tag{3.221}$$

$$\mathcal{A}_{mk_1k_2} = \frac{2}{3} \nabla_{(k_1} \mathcal{R}_{|m|k_2)} , \tag{3.222}$$

$$\mathcal{A}_{mk_1k_2k_3} = \frac{3}{4} \nabla_{(k_1} \nabla_{k_2} \mathcal{R}_{|m|k_3)} - \frac{1}{4} \mathcal{R}_{l(k_1} R^l{}_{k_2|m|k_3)} . \tag{3.223}$$

3.3.5 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 of symmetric spaces when

$$\nabla_m R^i{}_{jkl} = 0 . \tag{3.224}$$

Neglecting all terms with derivatives of curvatures we find from Taylor series for the matrix γ that all odd order coeficients vanish,

$$\gamma_{(2m+1)} = 0 , \tag{3.225}$$

and the even order coefficients are

$$\gamma_{(2m)} = \frac{(-1)^{m+1}}{2m+1} \bar{K}^m , \tag{3.226}$$

where $\bar{K} = (\bar{K}^{i'}{}_{j'})$ is a matrix defined by

$$\bar{K}^{i'}{}_{j'} = R^{i'}{}_{k'j'l'} \sigma^{k'} \sigma^{l'} . \tag{3.227}$$

Now, Taylor series can be summed up giving a closed formula for the matrix γ

$$\gamma = -V \frac{\sin \sqrt{\bar{K}}}{\sqrt{\bar{K}}} . \tag{3.228}$$

The other functions are simply computed from this result and we obtain

$$\eta = -\frac{\sqrt{\bar{K}}}{\sin\sqrt{\bar{K}}} V^{-1}\,, \tag{3.229}$$

and

$$\Delta = \det \frac{\sqrt{\bar{K}}}{\sin\sqrt{\bar{K}}}\,. \tag{3.230}$$

Similarly, we can also sum up Taylor series for the matrix $\mathcal{G}_{m'}$ to obtain a closed formula

$$\mathcal{G}^{i'}{}_{j'm'} = -R^{i'}{}_{j'l'p'}\sigma^{p'} \left(\frac{1-\cos\sqrt{\bar{K}}}{\bar{K}}\right)^{l'}{}_{m'}\,. \tag{3.231}$$

Finally, the vector $\hat{\mathcal{A}}_{i'}$ has the form

$$\hat{\mathcal{A}}_{m'} = -\mathcal{R}_{l'p'}\sigma^{p'} \left(\frac{1-\cos\sqrt{\bar{K}}}{\bar{K}}\right)^{l'}{}_{m'}\,. \tag{3.232}$$

These formulas may be useful in 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

$$R^{i}{}_{jkl} = \Lambda(\delta^i_k g_{jl} - \delta^i_l g_{jk})\,, \tag{3.233}$$

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 matrix $\bar{K}$ in this case has the form

$$\bar{K}^{i'}{}_{j'} = 2\Lambda\sigma\Pi_\perp{}^{i'}{}_{j'}\,, \tag{3.234}$$

where $\Pi_\perp$ is an orthogonal projection to the plane orthogonal to the vector $\sigma^{i'}$ defined by

$$\Pi_\perp{}^{i'}{}_{j'} = \delta^{i'}_{j'} - \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}\,. \tag{3.235}$$

Indeed, it is not difficult to check that

$$\Pi_\perp{}^2 = \Pi_\perp, \tag{3.236}$$

and

$$\Pi_{\perp}{}^{j'}{}_{i'}\sigma^{i'} = \sigma_{j'}\Pi_{\perp}{}^{j'}{}_{i'} = 0\,. \tag{3.237}$$

Using this projection we can easily compute any function of the matrix $\bar{K}$

$$f(\bar{K}) = f(0)(I - \Pi_{\perp}) + f(2\Lambda\sigma)\Pi_{\perp}\,. \tag{3.238}$$

Thus the formal expressions obtained above for arbitrary symmetric spaces take the concrete form

$$\gamma^{l}{}_{j'} = g^{l}{}_{i'}\left\{-\delta^{i'}{}_{j'}\Phi + \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}(\Phi - 1)\right\}\,, \tag{3.239}$$

$$\eta^{i'}{}_{l} = g_{l}{}^{j'}\left\{-\delta^{i'}{}_{j'}\Phi^{-1} + \frac{\sigma^{i'}\sigma_{j'}}{2\sigma}(\Phi^{-1} - 1)\right\}\,, \tag{3.240}$$

where

$$\Phi = \frac{\sinh\sqrt{-2\Lambda\sigma}}{\sqrt{-2\Lambda\sigma}}\,, \tag{3.241}$$

and

$$\mathcal{G}^{i'}{}_{j'm'} = -\Psi R^{i'}{}_{j'm'k'}\sigma^{k'}\,, \tag{3.242}$$

$$\hat{\mathcal{A}}_{m'} = -\Psi\mathcal{R}_{m'k'}\sigma^{k'}\,, \tag{3.243}$$

where

$$\Psi = \frac{1 - \cosh\sqrt{-2\Lambda\sigma}}{2\Lambda\sigma}\,. \tag{3.244}$$

We will also need the matrix $\xi^{i}{}_{k} = \nabla_{k}\sigma^{i}$. We know that

$$\xi = 1 + (D\gamma)\eta\,. \tag{3.245}$$

By using the above formulas for the matrices γ and η we immediately obtain

$$\xi^{i}{}_{k} = \delta^{i}{}_{j}(1 + F) - \frac{\sigma^{i}\sigma_{k}}{2\sigma}F\,, \tag{3.246}$$

where

$$F = \Phi^{-1}D\Phi\,. \tag{3.247}$$

Now, we notice that when acting on functions that depend only on σ the operator D takes the form

$$Df(\sigma) = 2\sigma\frac{\partial}{\partial\sigma}f(\sigma)\,. \tag{3.248}$$

Therefore, we obtain

$$F = \sqrt{-2\Lambda\sigma}\coth\left(\sqrt{-2\Lambda\sigma}\right) - 1\,. \tag{3.249}$$

In particular, the trace of the matrix ξ determines the Laplacian of the function σ

$$\sigma^{;i}_{;i} = n + (n-1)F\,. \tag{3.250}$$

Using these formulas Van Vleck determinant can be easily computed as well

$$\Delta = \Phi^{-n+1}\,. \tag{3.251}$$

Notice that for hyperbolic space, when $\Lambda < 0$, Van Vleck determinant does not become neither zero nor infinity.

We will need the Laplacian of the square root of Van Vleck determinant. First of all, when Laplacian acts of a scalar function that depends only on σ it takes a very simple form

$$\nabla^i\nabla_i f(\sigma) = \left[2\sigma\frac{\partial^2}{\partial\sigma^2} + \sigma^{;i}_{;i}\frac{\partial}{\partial\sigma}\right] f(\sigma)\,. \tag{3.252}$$

Omitting intermediate calculations we quote the result

$$\Delta^{-1/2}\nabla^i\nabla_i\Delta^{1/2} = \frac{(n-1)}{2}\Lambda\left[\frac{(n-3)}{2}\left(\coth^2\left(\sqrt{-2\Lambda\sigma}\right) + \frac{1}{2\Lambda\sigma}\right) + 1\right]. \tag{3.253}$$

3.4 Geometric Interpretation of Partial Differential Operators

3.4.1 Laplacian

The *Laplacian* Δ is an invariant second-order partial differential operator acting on tensor fields defined by

$$\Delta = g^{ij}\nabla_i\nabla_j\,. \tag{3.254}$$

By using explicit formulas for Christoffel symbols one can obtain for scalar Laplacian acting on functions the following expression in local coordinates

$$\Delta f = g^{-1/2}\partial_i(g^{1/2}g^{ij}\partial_j f)\,. \tag{3.255}$$

3.4.2 Laplace Type Partial Differential Operators

Let M be a manifold and μ be a weight function on M. Let us consider an elliptic second-order partial differential operator L acting in $L^2(M,\mu)$ of the form

$$L = -\alpha^{ij}(x)\partial_i\partial_j + \beta^j(x)\partial_j + \gamma(x)\,. \tag{3.256}$$

Recall that we do not write sums anymore. If we want the operator to be self-adjoint then the operator becomes

$$L = -\mu^{-1}(x)\partial_i\mu(x)\alpha^{ij}(x)\partial_j + \gamma(x)\,, \tag{3.257}$$

with some weight function $\mu(x)$. Since the operator is elliptic, the matrix α^{ij} is positive. Therefore, it can be identified with some Riemannian metric g^{ij}

$$\alpha^{ij} = g^{ij}\,. \tag{3.258}$$

The measure, in general, remains arbitrary. It can be parametrized by

$$\mu = g^{1/2}e^{-2\omega}\,, \tag{3.259}$$

where ω is some scalar function. Then the operator L takes the form

$$L = -e^{2\omega}g^{ij}\nabla_i e^{-2\omega}\nabla_j + \gamma\,, \tag{3.260}$$

which can also be written in a similar form

$$L = e^{\omega}\left(-\Delta + Q\right)e^{-\omega}\,, \tag{3.261}$$

where

$$Q = \gamma + g^{ij}\omega_{;i}\omega_{;j} - (\Delta\omega)\,. \tag{3.262}$$

Thus, every second-order self-adjoint operator is equivalent (similar) to an operator of the form

$$L = -\Delta + Q \tag{3.263}$$

with some function Q. Such operators are called *Laplace type operators*.

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, change of local coordinates. Now one can apply the whole machinery of differential geometry, which makes the study of partial differential operators much more efficient.

Matrix Valued Operators and Connections

Let us consider more general operators acting on sections of vector bundles over manifolds. For simplicity, one can think of those as simply matrix-valued operators acting on vector-valued functions. Such vector-valued functions can be described as a column N-vector of functions $\varphi = (\varphi^A)$, $A = 1, \dots, N$. Let us consider operators of the form

$$L = -I\alpha^{ij}(x)\partial_i\partial_j + \beta^j(x)\partial_j + \gamma(x)\,, \tag{3.264}$$

where I is the identity $N \times N$ matrix and β^j and γ are some $N \times N$ matrices. That is, we assume that the leading symbol

$$\sigma(x,p) = \alpha^{ij}(x)p_ip_j \tag{3.265}$$

is a *positive scalar*. Such operators are also called Laplace type operators with *positive definite scalar leading symbol*.

Let us assume also that the operator L is self-adjoint. Then there exists a metric g_{ij}, a matrix-valued covector $\mathcal{A}_i$ (called the *connection* on the vector bundle), and a matrix-valued function Q such that the operator can be written in form of a Laplace type operator

$$\begin{aligned} L &= -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q \\ &= -g^{ij}(\nabla_i + \mathcal{A}_i)(\nabla_j + \mathcal{A}_j) + Q \\ &= -g^{-1/2}(\partial_i + \mathcal{A}_i)g^{1/2}g^{ij}(\partial_j + \mathcal{A}_j) + Q\,. \end{aligned} \tag{3.266}$$

Here

$$\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i \tag{3.267}$$

is the *(generalized) covariant derivative* on the vector bundle. The new ingredients are defined by

$$g^{ij} = \alpha^{ij} \tag{3.268}$$

$$\mathcal{A}_i = -\frac{1}{2}g_{ij}\beta^j - \frac{1}{2}g_{ij}g^{-1/2}\partial_k(g^{1/2}g^{jk}) \tag{3.269}$$

$$Q = \gamma + g^{ij}\mathcal{A}_i\mathcal{A}_j + g^{-1/2}\partial_i(g^{1/2}g^{ij}\mathcal{A}_j)\,. \tag{3.270}$$

It is important to realize the following. Although it is always possible to rewrite any second-order operator in such form, it is *not always self-adjoint*. To get a self-adjoint operator, the matrix-valued vector $\mathcal{A}_i$ should be a true connection, which means that it should be an anti-Hermitian matrix, that is,

$$\mathcal{A}_i^* = -\mathcal{A}_i\,. \tag{3.271}$$

Then the matrix-valued tensor

$$\mathcal{R}_{ij} = \partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i + [\mathcal{A}_i, \mathcal{A}_j] \tag{3.272}$$

determines the *curvature* of the connection $\mathcal{A}_i$ on the vector bundle.

In particular, this means that for scalar functions this is only possible if the connection is *purely imaginary*, which means that the class of functions under study must be complex. In other words, there is no one-dimensional real valued vector bundle with real-valued connection.

In these lectures we restrict ourselves to second-order elliptic scalar operators with real coefficients. Every such operator can be written in the Laplace type form (3.266). However, if the vector $\mathcal{A}_i$ is non-zero, then the operator is not self-adjoint. It is equivalent (similar) to a self-adjoint operator if the tensor $\mathcal{R}_{ij}$ is equal to zero. Thus this tensor measures the extent to which the operator L is non-self-adjoint.

Chapter 4

Asymptotics of Singularly Perturbed Partial Differential Equations

4.1 Physical 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*.

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.

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.

We will explain in this lecture how this method can be applied

to obtain approximate asymptotic solutions of the heat equation, which is of our primary interest.

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.

4.1.1 Examples

Schrödinger Equation

Let us consider an n-dimensional Euclidean space $\mathbb{R}^n$ with Cartesian coordinates $x = (x_1, \dots, x_n)$. Let Δ be the scalar Laplacian defined by

$$\Delta = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2} \tag{4.1}$$

Let us consider a quantum particle of mass m moving in a potential $V(x)$. Then the *Hamiltonian* H is a differential operator defined by

$$H = -\frac{\hbar^2}{2m}\Delta + V(x)\,, \tag{4.2}$$

where $\hbar$ is Planck constant, and the quantum dynamics of the particle is described by the wave function $\psi(x)$ that satisfies the *Schrödinger Equation*

$$\left[i\hbar\frac{\partial}{\partial t} - H\right]\psi = 0\,. \tag{4.3}$$

This is a singularly perturbed partial differential equation since the Planck constant $\hbar$ is considered a small parameter. The approximate solution of this equation as $\hbar \to 0$ are called the *semi-classical asymptotics*.

Helmholtz Equation

Let us consider now a problem in wave optics and wave acoustics. Let $n(x)$ be the refraction coefficient and k be the wave number. The main equation of the wave optics if *Helmhotz Equation*

$$\left[\Delta + k^2 n^2(x)\right] u(x) = 0\,. \tag{4.4}$$

Then the approximate solutions of this equation as $k \to \infty$ are called the *short-wave* (or *high-frequency*) *asymptotics*.

Many other equations of mathematical physics have similar form, in particular, Maxwell equations, Dirac equation, equations of elasticity theory, etc.

4.2 Semi-classical Ansatz

Let $x = (x^i)$ be a point in $\mathbb{R}^n_x$. Let us consider a linear second-order partial differential operator acting on functions on $\mathbb{R}^n$ of the form

$$L(x, \partial) = -\alpha^{jk}(x)\partial_j\partial_k + \beta^j(x)\partial_j + \gamma(x)\,, \tag{4.5}$$

with some non-constant coefficients. Remember that a summation is always understood over repeated indices. We will assume that all coefficient functions are smooth and go to some constant values at infinity.

Let $p = (p_i)$ be the dual coordinates that take values in $\mathbb{R}^n_p$. We will call the variables p *momenta* and the space $\mathbb{R}^{2n}_{x,p} = \mathbb{R}^n_x \times \mathbb{R}^n_p$ of the points (x, p) the *phase space*. We will denote the natural pairing (scalar product) between momenta p and coordinates x by

$$\langle p, x\rangle = p_i x^i\,. \tag{4.6}$$

The symbol of the operator L is

$$\sigma(x, p) = \alpha^{jk}(x)p_j p_k + i\beta^j(x)p_j + \gamma(x)\,, \tag{4.7}$$

and the principal symbol reads

$$\sigma_P(x, p) = \alpha^{ij}(x)p_i p_j\,. \tag{4.8}$$

Let $\varepsilon > 0$ be a small positive parameter. Let us rescale all derivatives by the small parameter ε, that is, we replace

$$\partial_i \mapsto \varepsilon\partial_i\,. \tag{4.9}$$

Then

$$L(x, \varepsilon\partial) = -\varepsilon^2\alpha^{jk}(x)\partial_j\partial_k + \varepsilon b^j(x)\partial_j + \gamma(x)\,, \tag{4.10}$$

is a singularly perturbed 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 values at $\varepsilon = 0$.

Let us consider the equation

$$L(x, \varepsilon\partial)\varphi = 0\,. \tag{4.11}$$

For constant coefficients this equation has the following plane wave solution

$$\varphi(x) = \exp\left(\frac{i}{\varepsilon}\,\langle p, x\rangle\right)\,, \tag{4.12}$$

with some constant momentum p. The main idea of the semi-classical approximation for non-constant coefficients is to replace this plane wave in the limit $\varepsilon \to 0$ by a *distorted plane wave*

$$\exp\left[\frac{i}{\varepsilon}S(x)\right]\,. \tag{4.13}$$

where $S(x)$ is some function called the *action*. More precisely, one looks for the solution of this equation as $\varepsilon \to 0$ in form of the following asymptotic ansatz

$$\varphi(x) \sim \exp\left[\frac{i}{\varepsilon}S(x)\right]\sum_{k=0}^{\infty}\varepsilon^k a_k(x)\,, \tag{4.14}$$

with some coefficients a_k.

Then the algorithm for determining the function S and the coefficients a_k is rather simple. One just substitutes the ansatz in the differential equation and equate 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 *Hamiltonian System*. Then one solves the Hamiltonian system (in principle) and finds the action $S(x)$. Second, for $k \geq 1$ one gets a system of differential recursion relations for $a_k(x)$, called the *transport equations*, and finds as many coefficients $a_k(x)$ as needed.

4.3 Hamilton-Jacobi Equation

We assume that the coefficients of the operator L do not depend on ε. Then we have the following *commutation formula*

$$\exp\left(-\frac{i}{\varepsilon}S\right) L(x,\varepsilon\partial) \exp\left(\frac{i}{\varepsilon}S\right) = \sigma\left(x, \frac{\partial S}{\partial x}\right) - i\varepsilon\left\{\left[2\alpha^{jk}(\partial_j S) + i\beta^k\right]\partial_k + \alpha^{jk}(\partial_k\partial_j S)\right\} - \varepsilon^2\alpha^{kj}\partial_k\partial_j\,. \tag{4.15}$$

Therefore, in the leading order in the parameter ε we see that the action S has to satisfy the Hamilton-Jacobi equation (or the *characteristic equation*)

$$\sigma\left(x, \frac{\partial S}{\partial x}\right) = 0\,, \tag{4.16}$$

or, in more detail,

$$\alpha^{jk}(x)(\partial_j S)(\partial_k S) + i\beta^j(x)\partial_j S + \gamma(x) = 0\,, \tag{4.17}$$

which is a first-order partial differential equation. 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. Alternatively, we could assume that $\beta^j(x,\varepsilon)$ depends on ε in such a way that $\beta^j(x,0) = 0$. Then the action has to satisfy the equation

$$\alpha^{jk}(x)(\partial_j S)(\partial_k S) + \gamma(x) = 0\,. \tag{4.18}$$

If the matrix α^{ij} is supposed to be positive, then this equation will have a non-trivial solution only if $\gamma \geq 0$. One can go even further and assume that the function $\gamma(x,\varepsilon)$ also depends on ε is such a way that $\gamma(x,0) = 0$. The the Hamilton-Jacobi equation has the form

$$\alpha^{jk}(x)(\partial_j S)(\partial_k S) = 0\,. \tag{4.19}$$

Of course, this equation can have a real solution only if the matrix α^{ij} is not definite.

In particular, Hamilton-Jacobi equation for the Schrödinger Equation in quantum mechanics is

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\delta^{ij}(\partial_i S)(\partial_j S) + V(x) = 0\,, \tag{4.20}$$

which is an equation of classical mechanics for a particle of mass m moving in the potential $V(x)$. Similarly Hamilton-Jacobi equation for Helmholtz Equation of wave optics is the *eikonal equation*

$$\delta^{ij}(\partial_i S)(\partial_j S) = n^2(x) \tag{4.21}$$

of geometrical optics for a light ray propagating in a medium with the refraction coefficient $n(x)$.

To specify a unique solution of the Hamilton-Jacobi equations one has to impose some initial conditions (Cauchy problem) on a *Cauchy hypersurface* (an $(n-1)$-dimensional submanifold of $\mathbb{R}^n$) Σ in $\mathbb{R}^n_x$. Let $\hat{x} = (\hat{x}^\mu)$, $\mu = 1, \ldots, (n-1)$ be the parameters taking values in some domain in $\mathbb{R}^{n-1}$, so that the hypersurface Σ is described by

$$x^i = f^i(\hat{x})\,. \tag{4.22}$$

Then the initial conditions are

$$S(x)\Big|_\Sigma = S_0(\hat{x})\,, \tag{4.23}$$

where $S_0(\hat{x})$ is a given function of the parameters $\hat{x}$.

4.4 Hamiltonian System

A fundamental result of analysis of partial differential equations is that the integration of a first-order nonlinear partial differential equation can be reduced to the integration of a system of ordinary differential equations.

$$\frac{dx^k}{dt} = \frac{\partial\sigma(x,p)}{\partial p_k} = 2\alpha^{jk}p_j + i\beta^k, \tag{4.24}$$

$$\frac{dp^j}{dt} = -\frac{\partial\sigma(x,p)}{\partial x^j}\,, \tag{4.25}$$

with the initial conditions

$$x^i\Big|_{t=0} = f^i(\hat{x})\,, \tag{4.26}$$

$$p_i\Big|_{t=0} = p_i^{(0)}(\hat{x})\,, \tag{4.27}$$

where $f^i(\hat{x})$ are the functions that describes the hypersurface Σ and the functions $p_i^{(0)}(\hat{x})$ are such that

$$p_i^{(0)}(\hat{x})\frac{\partial f^i(\hat{x})}{\partial \hat{x}^\mu} = \frac{\partial S_0(\hat{x})}{\partial \hat{x}^\mu}\,. \tag{4.28}$$

Then the symbol $\sigma(x,p)$ is called a Hamiltonian and this system is called a *Hamiltonian system*.

For example, for the stationary Schrödinger Operator (no time derivative) for a quantum particle of mass m in a potential $V(x)$ the symbol (Hamiltonian) has the form

$$\sigma(x,p) = \frac{\delta^{ij} p_i p_j}{2m} + V(x)\,, \tag{4.29}$$

and the Hamiltonian system

$$\frac{dx^i}{dt} = \frac{p^i}{m}, \tag{4.30}$$

$$\frac{dp^i}{dt} = -\frac{\partial V(x)}{\partial x^i} \tag{4.31}$$

describes a classical particle of mass m in a potential $V(x)$.

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

$$x = x(t,\hat{x}), \qquad p = p(t,\hat{x})\,. \tag{4.32}$$

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

An important remark is due here. Contrary to the phase trajectories that are smooth curves in the phase space (that do not intersect), the classical trajectories in the coordinate space do intersect, touch, collect at a single point etc., forming so called *focal points* or *caustics*.

The solution of the Hamiltonian system defines a local diffeomorphism $x^i = x^i(t,\hat{x})$ with the Jacobian

$$J(t,\hat{x}) = \det \frac{\partial x(t,\hat{x})}{\partial(t,\hat{x})}\,. \tag{4.33}$$

The *focal points* are the points along the trajectory $x = x(t,\hat{x})$ such that the Jacobian vanishes

$$J(t,\hat{x}) = \det \frac{\partial x(t,\hat{x})}{\partial(t,\hat{x})} = 0\,. \tag{4.34}$$

The *caustics* are sets of focal points. As a consequence the semiclassical approximation breaks down at caustics.

Along the phase trajectories the action varies according to the equation

$$dS = \langle p, dx \rangle \ . \tag{4.35}$$

Therefore, the solution of Hamilton-Jacobi equation is

$$S(x(t,\hat{x})) = S_0(\hat{x}) + \int\limits_0^t \left\langle p(\tau,\hat{x}), \frac{dx(\tau,\hat{x})}{d\tau} \right\rangle d\tau \,, \tag{4.36}$$

where the integral is taken along the phase trajectory with corresponding initial conditions.

4.5 Transport Equations

To compute the coefficients a_k of the asymptotic expansion one needs to find the corresponding differential equations. By using the commutation formula (4.15) we obtain the equation for the leading order coefficient a_0

$$\left\{ \left[2\alpha^{jk}(\partial_j S) + i\beta^k \right] \partial_k + \alpha^{jk}(\partial_k \partial_j S) \right\} a_0 = 0 \,. \tag{4.37}$$

Note that along the phase trajectory $x = x(t,\hat{x})$ we have

$$\frac{d}{dt} = \frac{dx^k}{dt}\partial_k = \left[2\alpha^{jk}(\partial_j S) + i\beta^k \right] \partial_k \,. \tag{4.38}$$

Therefore, the above equation takes the form

$$\left\{ \frac{d}{dt} + \alpha^{jk}(\partial_k \partial_j S) \right\} a_0 = 0 \,. \tag{4.39}$$

This is a first-order ordinary differential equation along the phase trajectory; that is why is is called a *transport equation*.

To solve this equation we recall the Lioville formula. Let us consider an autonomous system of ordinary differential equations

$$\frac{dx^i}{dt} = F^i(x) \,. \tag{4.40}$$

Let $x^i(t,x_0)$ be the solution of this system with the initial conditions

$$x(0,x_0) = x_0 \,. \tag{4.41}$$

Let $J = J(t, x_0)$ be the Jacobian

$$J(t, x_0) = \det \left(\frac{\partial x^i(t, x_0)}{\partial x_0^j} \right) . \tag{4.42}$$

Then it satisfies the differential equation

$$\frac{d}{dt} J(t, x_0) = \frac{\partial F^i(x(t, x_0))}{\partial x^i} J(t, x_0) . \tag{4.43}$$

Applied to our Hamiltonian system it just says that the Jacobian $J = J(t, \hat{x})$ satisfies the transport equation

$$\left\{ \frac{d}{dt} - \alpha^{ij}(\partial_i \partial_j S) - M \right\} J^{1/2} = 0 , \tag{4.44}$$

where

$$M = (\partial_k S)(\partial_j \alpha^{jk}) + i \frac{1}{2} \partial_j \beta^j . \tag{4.45}$$

Recall that the derivative of the action is given by the solution of the Hamiltonian system, i.e. $\partial_i S = p_i(t, \hat{x})$. By using this equation the transport equation for a_0 can be written now in the form

$$\left[\frac{1}{\sqrt{J}} \frac{d}{dt} \sqrt{J} - M \right] a_0 = 0 . \tag{4.46}$$

This equation can be now integrated along the trajectories

$$a_0(x) = f_0(\hat{x}) \left(\frac{J(0, \hat{x})}{J(t, \hat{x})} \right)^{1/2} \exp \left\{ \int_0^t d\tau \; M(x(\tau, \hat{x})) \right\} , \tag{4.47}$$

where $f_0(\hat{x})$ is an arbitrary function that should be determined from some initial or boundary conditions. Thus, finally, we obtain the leading asymptotics

$$\varphi = f_0(\hat{x}) \left(\frac{J(0, \hat{x})}{J(t, \hat{x})} \right)^{1/2} \exp \left\{ \frac{i}{\varepsilon} S_0(\hat{x}) + \int_0^t d\tau \; \left[\frac{i}{\varepsilon} p_j(\tau, \hat{x}) \frac{dx^j}{d\tau} + M(x(\tau, \hat{x})) \right] \right\} . \tag{4.48}$$

The next coefficients can be computed similarly by solving the transport equations.

4.6 Asymptotics of Singularly Perturbed Evolution Equation

Now let us consider a more interesting question of finding approximate solutions of singularly perturbed evolution equation. Let $L(x, \partial)$ be a second-order partial differential operator with the symbol $\sigma(x, p)$ of the type considered above acting on functions in $\mathbb{R}^n$. Let us assume now that it is *elliptic*, that is the matrix $\alpha^{ij}(x)$ is positive definite for any x.

Let $\varepsilon > 0$ be a small parameter and let us consider the following singularly perturbed evolution equation

$$[-i\varepsilon\partial_t + L(x, \varepsilon\partial_x)]\,\varphi = 0\,, \tag{4.49}$$

with some fast oscillating initial conditions

$$\varphi(t, x)\Big|_{t=0} = \varphi_0(x) \exp\left[\frac{i}{\varepsilon} S_0(x)\right]\,, \tag{4.50}$$

describing a localized wave packet.

Then applying the general method described above we look for a solution in the form of an asymptotic series

$$\varphi(t, x) \sim \exp\left[\frac{i}{\varepsilon} S(t, x)\right] \sum_{k=0}^{\infty} \varepsilon^k a_k(t, x)\,. \tag{4.51}$$

By substituting this ansatz into the equation and expanding in powers of ε we obtain Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \sigma\left(x, \frac{\partial S}{\partial x}\right) = 0\,. \tag{4.52}$$

with initial conditions

$$S(t, x)\Big|_{t=0} = S_0(x)\,. \tag{4.53}$$

Further, to this problem we associate the corresponding Hamiltonian system

$$\frac{dx^j}{dt} = \frac{\partial\sigma(x, p)}{\partial p_j}\,, \tag{4.54}$$

$$\frac{dp_k}{dt} = -\frac{\partial\sigma(x, p)}{\partial x^k} \tag{4.55}$$

with initial conditions

$$x^i\Big|_{t=0} = x_0, \qquad p_i\Big|_{t=0} = \frac{\partial S_0(x)}{\partial x^i}\Big|_{x=x_0} \tag{4.56}$$

Let $x = x(t, x_0)$ and $p = p(t, x_0)$ be the solution of the Hamiltonian system. Then the solution of Hamilton-Jacobi equation is expressed in terms of the Hamiltonian system as

$$S(t,x) = S_0(x_0) + \int_0^t d\tau \left[\left\langle p(\tau, x_0), \frac{dx(\tau, x_0)}{d\tau} \right\rangle - \sigma(x(\tau, x_0), p(\tau, x_0)) \right], \tag{4.57}$$

where the integral is taken along the trajectories of the Hamiltonian system. Of course, here x_0 should be expressed as a function of x and t.

Next, for the function a_0 we obtain a transport equation

$$\left[\frac{1}{\sqrt{J}} \frac{d}{dt} \sqrt{J} - M \right] a_0 = 0\,, \tag{4.58}$$

where M is given by the same formula (4.45) as before. Here $J = J(t,x)$ is the Jacobian

$$J(t,x) = \det \left(\frac{\partial x^i(t, x_0)}{\partial x_0^j} \right). \tag{4.59}$$

We impose the following initial conditions for the function a_0

$$a_0\Big|_{t=0} = \varphi_0(x)\,. \tag{4.60}$$

Then the solution of the transport equation is

$$a_0(t,x) = \varphi_0(x) \left(\frac{J(0,x_0)}{J(t,x_0)} \right)^{1/2} \exp\left\{ \int_0^t d\tau\ M(x(t,x_0)) \right\} \tag{4.61}$$

and the leading asymptotics of the solution of the Cauchy problem is

$$\begin{aligned} \varphi(t,x) \quad &= \quad \varphi_0(x) \left(\frac{J(0,x_0)}{J(t,x_0)} \right)^{1/2} \\ &\times \exp\left\{ \frac{i}{\varepsilon} S_0(x_0) + \int_0^t d\tau\ \left[\frac{i}{\varepsilon} p_j(\tau, x_0) \frac{dx^j}{d\tau} + M(x(\tau, x_0)) \right] \right\}. \end{aligned} \tag{4.62}$$

4.7 Asymptotics of Singularly Perturbed Heat Equation

The method of semi-classical approximation was developed initially 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 a second-order partial differential operator with the symbol $\sigma(x,p)$ of the type considered above,

$$L = -\alpha^{ij}(x)\partial_i\partial_j + \beta^i(x)\partial_i + \gamma(x)\,, \tag{4.63}$$

acting on functions in $\mathbb{R}^n$. Let us assume now that it is *elliptic*, that is the matrix $\alpha^{ij}(x)$ is positive definite for any x.

Let $\varepsilon > 0$ be a small parameter and let us consider the following singularly perturbed heat equation

$$[\varepsilon\partial_t + L(x,\varepsilon\partial_x)]\,U(t;x,x') = 0\,, \tag{4.64}$$

with the initial conditions

$$U(0;x,x') = \delta(x-x')\,. \tag{4.65}$$

Then applying the general method described above we look for a solution in the form of an asymptotic series

$$U(t;x,x') \sim \exp\left[-\frac{1}{\varepsilon}S(t;x,x')\right]\sum_{k=0}^{\infty}\varepsilon^k b_k(t;x,x')\,. \tag{4.66}$$

The leading asymptotics of the heat kernel is

$$U(t;x,x') \sim \exp\left[-\frac{1}{\varepsilon}S(t;x,x')\right] b_0(t;x,x')\,. \tag{4.67}$$

Thus the initial condition for the function S should be such that as $t\to 0$

$$\lim_{t\to 0}\exp\left[-\frac{1}{\varepsilon}S(t;x,x')\right] b_0(t;x,x') = \delta(x-x')\,. \tag{4.68}$$

This means that we can normalize the functions S and b_0 as $t \to 0$ as follows. We require that there must exist well-defined limits

$$\Phi(x,x') = \lim_{t\to 0} 4tS(t;x,x')\,, \tag{4.69}$$

$$\psi(x,x') = \lim_{t\to 0}(4\pi t)^{n/2} b_0(t;x,x')\,, \tag{4.70}$$

and that the function $\Phi(x,x')$ has non-degenerate Hessian, that is, the matrix of mixed derivatives,

$$\det\left[\partial_i\partial_{j'}\Phi(x,x')\right] \neq 0\,, \tag{4.71}$$

at least for x close to x'. Then

$$\psi(x,x') = \left(\det\left[\partial_i\partial_{j'}\Phi(x,x')\right]\right)^{1/2}\,. \tag{4.72}$$

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'.

We will need the commutation formula

$$\exp\left(\frac{1}{\varepsilon}S\right)\left[\varepsilon\partial_t + L(x,\varepsilon\partial_x)\right]\exp\left(-\frac{1}{\varepsilon}S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 T_2\,, \tag{4.73}$$

where T_0 is a function,

$$T_0 = -\partial_t S - \alpha^{ij}(\partial_i S)(\partial_j S) - \beta^j\partial_j S + \gamma\,, \tag{4.74}$$

T_1 is a first order partial differential operator

$$T_1 = \partial_t + [\beta^j + 2\alpha^{ij}(\partial_j S)]\partial_i + \alpha^{ij}(\partial_i\partial_j S)\,, \tag{4.75}$$

and T_2 is a second-order differential operator

$$T_2 = -\alpha^{ij}\partial_i\partial_j\,. \tag{4.76}$$

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)

$$\partial_t S + H(x,\partial_x S) = 0\,, \tag{4.77}$$

where

$$H(x,p) = \alpha^{ij}(x)p_i p_j + \beta^j(x)p_j - \gamma(x)\,, \tag{4.78}$$

and the recurrence relations (transport equations) for the coefficients b_k for $k = 0, 1, \ldots,$

$$T_1 b_0 = 0 \tag{4.79}$$
$$T_1 b_{k+1} = -T_2 b_k \,. \tag{4.80}$$

The solution of Hamilton-Jacobi equation can be obtained as follows. Let us introduce the corresponding Hamiltonian system

$$\frac{dx^i}{d\tau} = \frac{\partial H(x,p)}{\partial p^i} = 2\alpha^{ij}(x)p_j + \beta^i(x)\,, \tag{4.81}$$
$$\frac{dp_k}{d\tau} = -\frac{\partial H(x,p)}{\partial x^k} = -\partial_k \alpha^{ij}(x)p_i p_j - \partial_k \beta^j(x)p_j + \partial_k \gamma(x)\,. \tag{4.82}$$

Let $[x(\tau), p(\tau)]$ be the solution of this system with the following boundary conditions

$$x(0) = x'\,, \qquad x(t) = x\,. \tag{4.83}$$

Of course, $x(\tau)$ and $p(\tau)$ depend on 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

$$\begin{aligned} S(t,x,x') &= \int_0^t d\tau \, \left[p_i(\tau)\frac{dx^i(\tau)}{d\tau} - H(x(\tau),p(\tau)) \right] \\ &= \int_0^t d\tau \, \left[\frac{1}{4}\alpha_{ij}(x(\tau))\frac{dx^i(\tau)}{d\tau}\frac{dx^j(\tau)}{d\tau} - \frac{1}{2}\alpha_{ij}(x(\tau))\beta^j(x(\tau))\frac{dx^i(\tau)}{d\tau} \right. \\ &\left. + \frac{1}{4}\alpha_{ij}(x(\tau))\beta^i(x(\tau))\beta^j(x(\tau)) + \gamma(x(\tau)) \right], \end{aligned} \tag{4.84}$$

where α_{ij} is the matrix inverse to α^{ij} and the integral is taken along the phase trajectory.

Then one can show that

$$\frac{\partial S(t,x,x')}{\partial x^i} = p_i(t)\,, \tag{4.85}$$
$$\frac{\partial S(t,x,x')}{\partial x'^i} = -p_i(0)\,, \tag{4.86}$$

and that $S(t,x,x')$ satisfies Hamilton-Jacobi equation. It also satisfies Hamilton-Jacobi equation with respect to the coordinates x', that is,

$$-\partial_t S + H(x', \partial_{x'} S) = 0\,. \tag{4.87}$$

Now, it should be clear that the differential operator T_1 has the form

$$T_1 = \frac{d}{dt} + \alpha^{ij}(\partial_i \partial_j S)\,, \tag{4.88}$$

where d/dt is the total derivative (along the trajectories of the Hamiltonian system) of a function that depends on t and x, that is,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{dx^i}{dt}\frac{\partial}{\partial x^i}\,. \tag{4.89}$$

Another important property of the function S consists in the following. Let us define the determinant

$$Z(t;x,x') = \det\left[-\partial_i \partial_{j'} S(t;x,x')\right]. \tag{4.90}$$

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,

$$S_i = \partial_i S\,, \qquad S_{ij} = \partial_i \partial_j S\,, \qquad S_{ij'} = \partial_i \partial_{j'} S\,, \qquad S_{ijk'} = \partial_i \partial_j \partial_{k'} S\,. \tag{4.91}$$

Then by differentiating Hamilton-Jacobi equation with respect to x and x' we obtain

$$\partial_t S_{k'm} + 2(\partial_m \alpha^{ij}) S_i S_{jk'} + 2\alpha^{ij}(S_i S_{k'jm} + S_{k'j} S_{im}) + (\partial_m \beta^i) S_{k'i} + \beta^i S_{k'im} = 0\,. \tag{4.92}$$

Let $B^{k'm}$ be the inverse of the matrix $S_{k'm}$. We notice that

$$\partial_t Z = B^{k'm}(\partial_t S_{k'm}) Z \tag{4.93}$$

and

$$\partial_i Z = B^{k'm} S_{k'mi} Z\,. \tag{4.94}$$

Now, by multiplying this equation by $B^{k'm}$ and contracting the indices k' and m we obtain the *continuity equation* for the determinant Z

$$\left\{\partial_t + (2\alpha^{ij} S_j + \beta^j)\partial_i + 2\alpha^{ij} S_{ij} + 2(\partial_i \alpha^{ij}) S_j + (\partial_i \beta^i)\right\} Z = 0\,. \tag{4.95}$$

or, in a more compact form

$$\left[\partial_t + \partial_i(2\alpha^{ij}S_j + \beta^j)\right] Z = 0\,. \tag{4.96}$$

We will need the equation for the square root $Z^{1/2}$

$$\left\{\partial_t + (2\alpha^{ij}S_j + \beta^j)\partial_i + \alpha^{ij}S_{ij} + (\partial_i\alpha^{ij})S_j + \frac{1}{2}(\partial_i\beta^i)\right\} Z^{1/2} = 0\,. \tag{4.97}$$

By using the transport operator T_1 this equation can be written as

$$(T_1 + M)Z^{1/2} = 0 \tag{4.98}$$

where

$$M = (\partial_i\alpha^{ij})S_j + \frac{1}{2}(\partial_i\beta^i)\,. \tag{4.99}$$

Therefore, the operator T_1 can be written as

$$T_1 = Z^{1/2}\left(\frac{d}{dt} - M\right) Z^{-1/2}\,. \tag{4.100}$$

Thus, by integrating the transport equation we get the coefficient b_0

$$b_0(t,x,x') = (2\pi)^{-n/2} Z^{1/2}(t,x,x') \exp\left\{\int_0^t d\tau M(\tau,t,x,x')\right\}\,. \tag{4.101}$$

The normalization factor is chosen here in such a way to satisfy the initial condition.

Finally, the leading asymptotics of the singularly perturbed heat kernel as $\varepsilon \to 0$ has the form

$$U(t;x,x') \sim (2\pi)^{-n/2} Z^{1/2}(t,x,x') \exp\left\{-\frac{1}{\varepsilon}S(t,x,x') + \int_0^t d\tau M(\tau,t,x,x')\right\}\,. \tag{4.102}$$

In the next lecture 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.

Chapter 5

Asymptotic Expansion of the Heat Kernel

5.1 Asymptotic Ansatz

We follow here [3, 6, 17]. As we have seen above every elliptic second-order partial differential operator can be put 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 Riemannian manifold without boundary with a Riemannian metric g_{ij}. Let L be an elliptic second-order partial differential operator of Laplace type (not necessarily self-adjoint). Then it must have the form

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q\,, \tag{5.1}$$

where $\nabla_i^{\mathcal{A}} = \nabla_i + \mathcal{A}_i$, $\mathcal{A}_i$ is some real vector field and $Q = Q(x)$ is some smooth real function on M. In local coordinates this operator takes the form

$$L = -g^{-1/2}(\partial_i + \mathcal{A}_i)g^{1/2}g^{ij}(\partial_j + \mathcal{A}_j) + Q\,. \tag{5.2}$$

The adjoint of this operator is

$$\begin{aligned} L^* &= -g^{ij}(\nabla_i - \mathcal{A}_i)(\nabla_j - \mathcal{A}_j) + Q \\ &= -g^{-1/2}(\partial_i - \mathcal{A}_i)g^{1/2}g^{ij}(\partial_j - \mathcal{A}_j) + Q\,. \end{aligned} \tag{5.3}$$

The heat kernel $U(t; x, x')$ is the fundamental solution of the heat equation, that is, it is required to satisfy the equation

$$(\partial_t + L_x)U(t; x, x') = 0\,, \tag{5.4}$$

and the initial condition

$$U(0;x,x') = \delta(x,x')\,. \tag{5.5}$$

It also satisfies the adjoint equation with respect to the coordinates of the point x'

$$(\partial_t + L^*_{x'})U(t;x,x') = 0\,. \tag{5.6}$$

Here $\delta(x,x')$ is the covariant delta-function defined by

$$\delta(x,x') = g^{-1/4}(x)\delta(x-x')g^{-1/4}(x')\,. \tag{5.7}$$

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

$$\int\limits_M dx\; g^{1/2}(x)\delta(x,x')f(x) = f(x')\,. \tag{5.8}$$

In such 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.

Then one can show that for $t > 0$ the heat kernel is a smooth function of the coordinates of both points x and x'. Recall the form of the heat kernel in flat Euclidean space $\mathbb{R}^n$,

$$U(t;x,x') = (4\pi t)^{-n/2}\exp\left(-\frac{|x-x'|^2}{4t}\right)\,. \tag{5.9}$$

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. We define

$$U(t;x,x') = (4\pi t)^{-n/2}\mathcal{P}(x,x')\Delta^{1/2}(x,x')\exp\left(-\frac{\sigma(x,x')}{2t}\right)\Omega(t;x,x')\,, \tag{5.10}$$

where $\sigma(x,x')$ is the world function and $\Delta(x,x')$ is the corresponding Van Vleck-Morette determinant and $\mathcal{P}(x,x')$ is a two-point function defined in the previous section. 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.

By using the equations for the functions σ, Δ and $\mathcal{P}$ we find that the function $\Omega(t;x,x')$ satisfies the equation

$$\left(\frac{\partial}{\partial t}+\frac{1}{t}D+\hat{L}\right)\Omega(t;x,x')=0\,, \tag{5.11}$$

where

$$\begin{aligned} D &= \sigma^i\nabla_i\,, && (5.12)\\ \sigma_i &= \nabla_i\sigma\,, && (5.13)\\ \hat{L} &= \mathcal{P}^{-1}\Delta^{-1/2}L\Delta^{1/2}\mathcal{P}\,, && (5.14) \end{aligned}$$

and the initial conditions

$$\Omega(0;x,x')=1\,. \tag{5.15}$$

We will assume the function $Q(x)$ to be bounded below by a sufficiently large positive parameter m^2, tht is, for any x

$$Q(x)\geq m^2\,. \tag{5.16}$$

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 $N\geq 0$

$$\lim_{t\to\infty,0}\ t^\alpha\left(\frac{\partial}{\partial t}\right)^N\Omega(t;x,x')=0\,. \tag{5.17}$$

5.2 Mellin Transform of the Heat Kernel

Now let us consider the Mellin transformation of $\Omega(t)$

$$b_q(x,x')=\frac{1}{\Gamma(-q)}\int\limits_0^\infty dt\ t^{-q-1}\Omega(t;x,x')\,, \tag{5.18}$$

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

$$b_q(x,x') = \frac{1}{\Gamma(-q+N)} \int_0^\infty dt\; t^{-q-1+N} \left(-\frac{\partial}{\partial t}\right)^N \Omega(t;x,x')\,, \tag{5.19}$$

where N is an arbitrary positive integer.

Moreover, by making use of the asymptotic properties 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 $q=k$, $(k=0,1,2,...)$,

$$b_k(x,x') = \left(-\frac{\partial}{\partial t}\right)^k \Omega(t;x,x')\Big|_{t=0}\,. \tag{5.20}$$

It is also not difficult to establish the crucial asymptotic property of b_q, namely, for any $N>0$

$$\lim_{|q|\to\infty\,,\mathrm{Re}\, q<N} \Gamma(-q+N) b_q(x,x') = 0\,. \tag{5.21}$$

Now we can invert the Mellin transform and write down

$$\Omega(t;x,x') = \int_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i}\; t^q \Gamma(-q) b_q(x,x')\,, \tag{5.22}$$

where c is a negative constant.

5.2.1 Minackshisundaram-Pleijel Expansion

Deforming the contour of integration in (5.22) and taking into account the properties (5.20) and (5.21) we obtain

$$\Omega(t;x,x') = \sum_{k=0}^{N-1} \frac{(-t)^k}{k!} b_k(x,x') + R_N(t;x,x')\,, \tag{5.23}$$

where

$$R_N(t;x,x') = \int_{c_N-i\infty}^{c_N+i\infty} \frac{dq}{2\pi i}\; t^q \Gamma(-q) b_q(x,x')\,, \tag{5.24}$$

where $N-1 < c_N < N$.

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. (5.23) gives the asymptotic expansion of $\Omega(t;x,x')$ as $t \to 0$

$$\Omega(t;x,x') \sim \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} b_k(x,x') \,. \tag{5.25}$$

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). 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 (5.25) is convergent only in the case when the remainder term $R_N(t;x,x')$ (5.24) 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 (5.25) diverges for any finite $t > 0$. Thus the asymptotic ansatz (5.25) is useful 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 (5.22).

5.3 Recurrence Relations for Heat Kernel Coefficients

By substituting the ansatz (5.22) into the equation (5.11) we obtain a functional equation for the function $b_q(x,x')$

$$\left(1 + \frac{1}{q} D\right) b_q(x,x') = \hat{L} b_{q-1}(x,x') \,. \tag{5.26}$$

For positive integer $q = 1, 2, \ldots$ this equation gives a differential recursive system for the heat kernel coefficients b_k. For $q = 0$ it gives

$$D b_0 = 0 \,. \tag{5.27}$$

From the initial condition (5.15) by taking into account eq. (5.20) we get the initial condition of the recursion

$$b_0(x,x') = 1 \,. \tag{5.28}$$

Thus instead of the differential equation (5.11) for the function $\Omega(t;x,x')$ with the initial condition (5.15) we obtained the functional equation (5.26) for the function $b_q(x,x')$ with the initial condition (5.28). One also has the asymptotic property (5.21) of the function $b_q(x,x')$ which reflects the property (5.19) for the function $\Omega(t;x,x')$.

5.4 Green Function of Laplace Type Operator

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

$$G^p(x,x') = \frac{1}{\Gamma(p)} \int\limits_0^\infty dt\; t^{p-1} U(t;x,x') \tag{5.29}$$

Then by using our ansatz (5.10) for the heat kernel and integrating over t we obtain

$$\begin{aligned} G^p(x,x') &= (4\pi)^{-n/2} \Delta^{1/2}(x,x') \\ &\times \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i} \frac{\Gamma(-q)\Gamma\left(-p+\frac{n}{2}-q\right)}{\Gamma(p)} \left(\frac{\sigma(x,x')}{2}\right)^{p-\frac{n}{2}+q} b_q(x,x')\,, \end{aligned} \tag{5.30}$$

where c is a sufficiently large negative constant satisfying the condition $c < \frac{n}{2} - \mathrm{Re}\, p$.

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

$$G^p(x,x) = (4\pi)^{-n/2} \frac{\Gamma\left(p-\frac{n}{2}\right)}{\Gamma(p)} b_{\frac{n}{2}-p}(x,x)\,. \tag{5.31}$$

Further, by setting $p = 1$ we obtain the Green function of the operator L,

$$\begin{aligned} G(x,x') &= (4\pi)^{-n/2} \Delta^{1/2}(x,x') \\ &\times \int\limits_{c-i\infty}^{c+i\infty} \frac{dq}{2\pi i} \Gamma(-q)\Gamma\left(\frac{n}{2}-q-1\right) \left(\frac{\sigma(x,x')}{2}\right)^{1-\frac{n}{2}+q} b_q(x,x')\,, \end{aligned} \tag{5.32}$$

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 (5.32) 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 (5.32) to the right to the infinity one can obtain an expansion of the Green function in powers of σ (*Hadamard series*). We obtain

$$G = G^{\text{sing}} + G^{\text{non-anal}} + G^{\text{reg}}. \tag{5.33}$$

Here G^{sing} is the *singular part* which is polynomial in the inverse powers of $\sqrt{\sigma}$

$$G^{\text{sing}} = (4\pi)^{-n/2}\Delta^{1/2} \sum_{k=0}^{\left[\frac{(n+1)}{2}\right]-2} \frac{(-1)^k}{k!}\Gamma\left(\frac{n}{2} - k - 1\right)\left(\frac{2}{\sigma}\right)^{\frac{n}{2}-k-1} b_k\,. \tag{5.34}$$

Further, in odd dimension $n = 1, 3, \dots$ we have

$$G^{\text{non-anal}} \sim (-1)^{\frac{n-1}{2}}(4\pi)^{-\frac{n}{2}}\Delta^{\frac{1}{2}} \sum_{k=0}^{\infty} \frac{\pi}{\Gamma\left(k + \frac{n+1}{2}\right)\Gamma\left(k + \frac{3}{2}\right)}\left(\frac{\sigma}{2}\right)^{k+\frac{1}{2}} b_{k+\frac{n-1}{2}} \tag{5.35}$$

$$G^{\text{reg}} \sim (-1)^{\frac{(n+1)}{2}}(4\pi)^{-\frac{n}{2}}\Delta^{\frac{1}{2}} \sum_{k=0}^{\infty} \frac{\pi}{k!\Gamma\left(k + \frac{n}{2}\right)}\left(\frac{\sigma}{2}\right)^{k} b_{k-1+\frac{n}{2}}\,. \tag{5.36}$$

And in even dimension $n = 2, 4, \dots$ we have

$$\begin{aligned} G^{\text{non-anal}} \quad \sim \quad & (-1)^{\frac{n}{2}-1}(4\pi)^{-\frac{n}{2}}\Delta^{\frac{1}{2}} \log\left(\frac{\sigma}{2}\right) \\ & \times \sum_{k=0}^{\infty} \frac{1}{k!\Gamma\left(k + \frac{n}{2}\right)}\left(\frac{\sigma}{2}\right)^{k} b_{k-1+\frac{n}{2}} \end{aligned} \tag{5.37}$$

$$G^{\rm reg} \sim (-1)^{\frac{n}{2}-1}(4\pi)^{-\frac{n}{2}}\Delta^{\frac{1}{2}}\sum_{k=0}^{\infty}\frac{1}{k!\Gamma\left(k+\frac{n}{2}\right)}\left(\frac{\sigma}{2}\right)^k \times\left\{b'_{k-1+\frac{n}{2}}-\left[\Psi(k+1)+\Psi\left(k+\frac{n}{2}\right)\right]b_{k-1+\frac{n}{2}}\right\}, \tag{5.38}$$

where $\Psi(z)=(d/dz)\log\Gamma(z)$ is the logarithmic derivative of the gamma-function and

$$b'_q=\frac{\partial b_q}{\partial q}\,. \tag{5.39}$$

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 $b_{k+\frac{1}{2}}$ 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 $(n=1,3,\dots)$:

$$G^{\rm reg}(x,x) = (-1)^{\frac{(n+1)}{2}}(4\pi)^{-\frac{n}{2}}\frac{\pi}{\Gamma\left(\frac{n}{2}\right)}b_{\frac{n}{2}-1}(x,x)\,, \tag{5.40}$$

and in even dimensions $(n=2,4,\dots)$

$$G^{\rm reg}(x,x)=(-1)^{\frac{n}{2}-1}\frac{(4\pi)^{-n/2}}{\Gamma\left(\frac{n}{2}\right)}\left\{b'_{\frac{n}{2}-1}(x,x)-\left[\Psi\left(\frac{n}{2}\right)-\mathbb{C}\right]b_{\frac{n}{2}-1}(x,x)\right\}, \tag{5.41}$$

where $\mathbb{C}=-\Psi(1)=0.577\dots$ is the Euler's constant.

5.5 Non-recursive Solution of Recurrence Relations

Let us apply expounded method of covariant expansions 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

$$b_k = \left(1+\frac{1}{k}D\right)^{-1}\hat{L}\left(1+\frac{1}{k-1}D\right)^{-1}\hat{L}\cdots(1+D)^{-1}\hat{L}\cdot 1\,. \qquad (5.42)$$

Now, by expanding the coefficients b_k in covariant Taylor series

$$\begin{aligned} b_k &= \sum_{n=0}^{\infty}|n\rangle\langle n|b_k\rangle \\ &= \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sigma^{i'_1}\cdots\sigma^{i'_n}\left[\nabla_{(i_1}\cdots\nabla_{i_n)}b_k\right](x') \end{aligned} \qquad (5.43)$$

(recall that square brackets mean the coincidence limit of a two-point function $[f(x,x')]=f(x,x)$) and defining the inverse operator $\left(1+\frac{1}{k}D\right)^{-1}$ by

$$\left(1+\frac{1}{k}D\right)^{-1} = \sum_{n=0}^{\infty}\left(1+\frac{n}{k}\right)^{-1}|n\rangle\langle n| \qquad (5.44)$$

we obtain from (5.42)

$$\begin{aligned} \langle n|b_k\rangle &= \sum_{n_1,\cdots,n_{k-1}\geq 0} N(n,k;n_1,\ldots,n_k) \\ &\quad\times\langle n|\hat{L}|n_{k-1}\rangle\langle n_{k-1}|\hat{L}|n_{k-2}\rangle\cdots\langle n_1|\hat{L}|0\rangle\,, \end{aligned} \qquad (5.45)$$

where

$$N(n,k;n_1,\ldots,n_k) = \frac{k}{(k+n)}\cdot\frac{(k-1)}{(k-1+n_{k-1})}\cdots\frac{2}{(2+n_2)}\cdot\frac{1}{(1+n_1)}\,, \qquad (5.46)$$

and $\langle m|\hat{L}|n\rangle$ are the *matrix elements* of the operator $\hat{L}$ defined by

$$\begin{aligned} \langle m|\hat{L}|n\rangle &= \langle i_1\cdots i_m|\hat{L}|j_1\cdots j_n\rangle \\ &= \left[\nabla_{(i_1}\cdots\nabla_{i_m)}\hat{L}\frac{(-1)^n}{n!}\sigma^{j'_1}\cdots\sigma^{j'_n}\right]_{x=x'}\,. \end{aligned} \qquad (5.47)$$

Note that $\langle n|b_k\rangle$ is a symmetric tensor of type $(0,n)$

$$\langle n|b_k\rangle = b_{(k)i_1\ldots i_n}\,, \qquad (5.48)$$

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

$$\langle m|\hat{L}|n\rangle = L^{j_1\dots j_n}_{i_1\dots i_m}\,. \tag{5.49}$$

Of course, the matrix element $\langle m|\hat{L}|0\rangle$ is just a symmetric tensor of type $(0,m)$

$$\langle m|\hat{L}|0\rangle = L_{i_1\dots i_m} \tag{5.50}$$

The product of matrix elements is defined then as an inner product in the space of symmetric tensors, that is,

$$\langle m|\hat{L}|n\rangle\langle n|\hat{L}|p\rangle = L^{j_1\dots j_n}_{i_1\dots i_m} L^{l_1\dots l_p}_{j_1\dots j_n}\,, \tag{5.51}$$

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

$$\begin{aligned} b_{(k)i_1\dots i_n} \;=\; & \sum_{n_1,\cdots,n_{k-1}\geq 0} N(n,k;n_1,\dots,n_k) \\ & \times L^{j_1\dots j_{n_{k-1}}}_{i_1\dots i_n} L^{l_1\dots l_{n_{k-2}}}_{j_1\dots j_{n_{k-1}}} \cdots L^{p_1\dots p_{n_1}}_{m_1\dots m_{n_2}} L_{p_1\dots p_{n_1}}\,. \end{aligned} \tag{5.52}$$

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 world function σ. 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. (5.45) is limited from above, that is, $n_1\geq 0$ and

$$n_i \leq n_{i+1}+2\,, \qquad i=1,2,\dots,k-1\,, \tag{5.53}$$

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 (5.47) 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

$$\mathcal{D}_{i'} = \gamma^{j}{}_{i'} \nabla_j \,. \tag{5.54}$$

These operators have a nice property that

$$\mathcal{D}_{i'} \sigma^{j'} = \delta^{j'}{}_{i'} \,. \tag{5.55}$$

That is why, it is convenient to express the operator $\hat{L}$ in terms of this operator. By using the equations (3.124) and (3.125) we obtain

$$\hat{L} = -(\mathcal{D}_{i'} - \zeta_{i'} + \hat{\mathcal{A}}_{i'}) X^{i'j'} (\mathcal{D}_{j'} + \zeta_{j'} + \hat{\mathcal{A}}_{j'}) + Q \,, \tag{5.56}$$

where

$$X^{i'j'} = \eta^{i'}{}_{k} \eta^{j'k} \,. \tag{5.57}$$

Recall also that

$$\begin{aligned} \zeta_{i'} &= \mathcal{D}_{i'} \zeta \,, & (5.58)\\ \zeta &= \log \Delta^{1/2} \,, & (5.59)\\ \hat{\mathcal{A}}_{i'} &= \gamma^{j}{}_{i'} \mathcal{P}^{-1} \nabla^{\mathcal{A}}_{j} \mathcal{P} \,. & (5.60) \end{aligned}$$

This can be further written in the form

$$\hat{L} = -X^{i'j'} \mathcal{D}_{i'} \mathcal{D}_{j'} - Y^{i'} \mathcal{D}_{i'} + Z \tag{5.61}$$

where

$$\begin{aligned} Y^{i'} &= \mathcal{D}_{j'} X^{i'j'} + 2 X^{i'j'} \hat{\mathcal{A}}_{j'} & (5.62)\\ Z &= X^{i'j'} (\zeta_{i'} \zeta_{j'} - \hat{\mathcal{A}}_{i'} \hat{\mathcal{A}}_{j'}) - \mathcal{D}_{j'} \left[X^{i'j'} \left(\zeta_{i'} + \hat{\mathcal{A}}_{i'} \right) \right] + Q \,. & (5.63) \end{aligned}$$

Inserting the operator $\hat{L}$ in the form (5.61) into the definition of the matrix elements (5.47) we obtain

$$\begin{aligned} \langle i_1 \cdots i_m | \hat{L} | j_1 \cdots j_n \rangle &= \frac{(-1)^n}{n!} & (5.64)\\ &\times \left[\nabla_{(i_1} \cdots \nabla_{i_m)} \left(-X^{i'j'} \mathcal{D}_{i'} \mathcal{D}_{j'} - Y^{i'} \mathcal{D}_{i'} + Z \right) \sigma^{j'_1} \cdots \sigma^{j'_n} \right]_{x=x'} \,. \end{aligned}$$

Now by using the coincidence limits (5.74) and eqs. (5.55), (3.157) we obtain the matrix elements

$$\langle m|\hat{L}|n\rangle = 0 \tag{5.65}$$

for $n > m+2$ and $n = m+1$,

$$\langle i_1 \cdots i_m|\hat{L}|j_1 \cdots j_{m+2}\rangle = -\delta^{(j_1 \cdots j_m}_{i_1 \cdots i_m} g^{j_{m+1} j_{m+2})}\,, \tag{5.66}$$

and

$$\langle i_1 \cdots i_m|\hat{L}|j_1 \cdots j_n\rangle = \binom{m}{n}\delta^{j_1 \cdots j_n}_{(i_1 \cdots i_n} Z_{i_{n+1} \cdots i_m)} \tag{5.67}$$

$$+\binom{m}{n-1}\delta^{(j_1 \cdots j_{n-1}}_{(i_1 \cdots i_{n-1}} Y^{j_n)}{}_{i_n \cdots i_m)} - \binom{m}{n-2}\delta^{(j_1 \cdots j_{n-2}}_{(i_1 \cdots i_{n-2}} X^{j_{n-1} j_n)}{}_{i_{n-1} \cdots i_m)}\,,$$

for $n \leq m$, where

$$X^{ij}{}_{l_1 \cdots l_n} = \left[\nabla_{(l_1} \cdots \nabla_{l_n)} X^{i'j'}\right]\,, \tag{5.68}$$

$$Y^{j}{}_{l_1 \cdots l_n} = \left[\nabla_{(l_1} \cdots \nabla_{l_n)} Y^{j'}\right] \tag{5.69}$$

$$Z_{l_1 \cdots l_n} = \left[\nabla_{(l_1} \cdots \nabla_{l_n)} Z\right] \tag{5.70}$$

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 (5.45) is limited from above

$$0 \leq n_1 \leq n_2 + 2 \leq \cdots \leq n_{k-1} + 2(k-2) \leq n + 2(k-1)\,, \tag{5.71}$$

and, therefore,this sum contains a finite number of terms.

Finally, by using the explicit expressions (5.57)–(5.63) we obtain

from (5.68)–(5.70)

$$X^{ij}{}_{l_1\cdots l_n} = \sum_{k=0}^{n} \binom{n}{k} \eta^{(i}{}_{m(l_1\cdots l_k} \eta^{j)m}{}_{l_{k+1}\cdots l_n)} \,, \tag{5.72}$$

$$Y^{j}{}_{l_1\cdots l_n} = -X^{ji}{}_{il_1\cdots l_n} + 2\sum_{k=0}^{n} \binom{n}{k} X^{j}{}_{m(l_1\cdots l_k} \mathcal{A}^{m}{}_{l_{k+1}\cdots l_n)} \,, \tag{5.73}$$

$$\begin{aligned} Z_{l_1\cdots l_n} &= Q_{l_1\cdots l_n} + \sum_{k=0}^{n} \binom{n}{k} \Big\{ X_{ij(l_1\cdots l_k} \left[\zeta^{ij}{}_{l_{k+1}\cdots l_n)} - \mathcal{A}^{ij}{}_{l_{k+1}\cdots l_n)}\right] \\ &\quad + X^{i}{}_{ji(l_1\cdots l_k} \left[\zeta^{j}{}_{l_{k+1}\cdots l_n)} - \mathcal{A}^{j}{}_{l_{k+1}\cdots l_n)}\right] \Big\} \\ &\quad + \sum_{k=0}^{n}\sum_{m=0}^{n-k} \frac{n!}{k!m!(n-k-m)!} X_{ij(l_1\cdots l_k} \Big[\mathcal{A}^{i}{}_{l_{k+1}\cdots l_{k+m}} \mathcal{A}^{j}{}_{l_{k+m+1}\cdots l_n)} \\ &\quad - \zeta^{i}{}_{l_{k+1}\cdots l_{k+m}} \zeta^{j}{}_{l_{k+m+1}\cdots l_n)} \Big] \,, \end{aligned} \tag{5.74}$$

where

$$Q_{l_1\cdots l_n} = \nabla_{(l_1} \cdots \nabla_{l_n)} Q \tag{5.75}$$

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 (3.187), (3.194) and (3.220).

So, by using the coincidence limits of symmetrized derivatives of two-point quantities from previous lectures one can calculate the matrix elements (5.47) of the operator $\hat{L}$ and, therefore, Taylor coefficients of the heat kernel coefficients b_k (5.45).

From the dimensional arguments it is obvious that for $m = n$ the matrix elements $\langle m|\hat{L}|n\rangle$ given by eq. (5.67) 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 (5.45), turns out to be very convenient.

The matrix elements $\langle m|L|n\rangle$ are presented by some blocks with m lines coming in from the left and n lines going out to the right (Fig. 1),

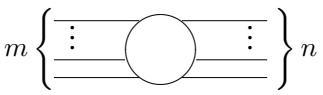


Fig. 1

and the product of the matrix elements $\langle m|L|k\rangle\langle k|L|n\rangle$ — by two blocks connected by k intermediate lines (Fig. 2),

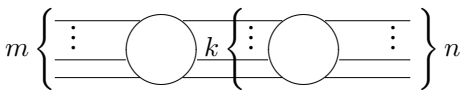


Fig. 2

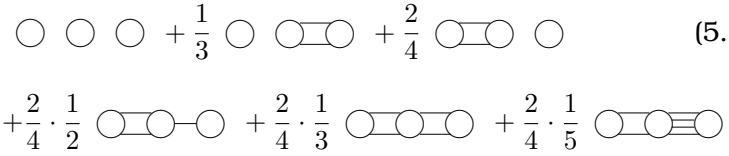
that represents the contractions of the corresponding tensor indices (the inner product).

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. (5.46). 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.

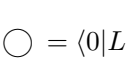
For example, the diagrams for the diagonal values of the heat kernel coefficients $[b_k] = \langle 0|b_k\rangle$ for $k = 1, 2, 3$ have the form,

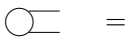
$$[b_1] = \quad \bigcirc \tag{5.76}$$

$$[b_2] = \quad \bigcirc \quad \bigcirc \quad + \frac{1}{3} \quad \bigcirc\!\!-\!\!\bigcirc \tag{5.77}$$

$[b_3]$ =  (5.78)

As an illustration let us compute the coefficients $[b_1]$ and $[b_2]$. We have

 $= \langle 0|L|0\rangle = Z_{(0)} = Q - \frac{1}{6}R\,,$ (5.79)

 $= \langle 0|L|j_1 j_2\rangle = -g^{j_1 j_2}$ (5.80)

 $= \langle i_1 i_2|L|0\rangle = Z_{(2)i_1 i_2}$ (5.81)

 $= \langle 0|L|2\rangle\langle 2|L|0\rangle = -g^{ij} Z_{(2)ij}\,,$ (5.82)

where

$$Z_{(2)ij} = \nabla_{(i}\nabla_{j)}Q - \frac{1}{2}\mathcal{R}_{k(i}\mathcal{R}^{k}{}_{j)} + \frac{1}{2}\nabla_{(i}\nabla_{|k|}\mathcal{R}^{k}{}_{j)} - \frac{3}{20}\nabla_i\nabla_j R \quad (5.83)$$
$$-\frac{1}{20}\Delta R_{ij} + \frac{1}{15}R_{il}R^{l}{}_{j} - \frac{1}{30}R_{iklm}R_{j}{}^{klm} - \frac{1}{30}R_{kl}R^{k}{}_{i}{}^{l}{}_{j}\,.$$

Here the symbol Δ denotes the Laplacian $\Delta = g^{ij}\nabla_i\nabla_j$ and not the Van Vleck determinant.

This immediately gives

$$[b_1] = Q - \frac{1}{6}R\,, \quad (5.84)$$

and, by taking the trace of $Z_{(2)ij}$ we obtain the well known result

$$[b_2] = \left(Q - \frac{1}{6}R\right)^2 - \frac{1}{3}\Delta Q + \frac{1}{6}\mathcal{R}_{ij}\mathcal{R}^{ij} + \frac{1}{15}\Delta R - \frac{1}{90}R_{ij}R^{ij} + \frac{1}{90}R_{ijkl}R^{ijkl}\,. \quad (5.85)$$

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 resricted 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

$$R^i{}_{jkl} = \Lambda(\delta^i{}_k g_{jl} - \delta^i{}_l g_{jk}) \,, \tag{5.86}$$

enables one to compute the heat kernel coefficients in closed form simply by integrating the recursion relation along geodesics. Let us restrict ourselves for simplicity to pure Laplacian

$$L = -g^{ij}\nabla_i \nabla_j \,. \tag{5.87}$$

Van Vleck determinant as well as all other two-point functions are known explicitly as functions of σ and the Laplacian becomes a second-order ordinary differential operator. 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

$$\sigma = \frac{1}{2} r^2 \,. \tag{5.88}$$

Let also

$$\Lambda = -\rho^2 \,. \tag{5.89}$$

Then by using the equations of a previous lecture one can show that the operator D and the Laplacian when applied to radial functions are

$$Df(r) = r\partial_r f(r) \tag{5.90}$$

$$Lf(r) = -\left[\partial_r^2 + (n-1)\rho \coth(\rho r)\partial_r\right] f(r) \,. \tag{5.91}$$

We recall that

$$\Delta^{1/2} = \left(\frac{\sinh(\rho r)}{\rho r}\right)^{-(n-1)/2} \,. \tag{5.92}$$

Therefore the recursion relations can be written now as

$$\left(1 + \frac{1}{k} r\partial_r\right) b_k = \hat{L} b_{k-1} \,, \tag{5.93}$$

where

$$\hat{L} = \Delta^{-1/2} L \Delta^{1/2} \,. \tag{5.94}$$

with the initial condition $b_0 = 1$. These relations can be easily integrated to get

$$b_k(r) = k \frac{1}{r^k} \int_0^r dr' \; r'^{k-1} \hat{L}_{r'} b_{k-1}(r') \,, \tag{5.95}$$

where the operator $\hat{L}_{r'}$, of course, acts on the variable r'.

Since the first coefficient is known exactly, $b_0 = 1$, we can compute the coefficient b_1 simply by integrating the derivative of the van Vleck determinant

$$b_1(r) = \frac{1}{r} \int_0^r dr' \; \Delta^{-1/2}(r') L_{r'} \Delta^{1/2}(r') \cdot 1 \,. \tag{5.96}$$

We remind that

$$\Delta^{-1/2} L \Delta^{1/2} = \frac{(n-1)}{4} \rho^2 \left\{ (n-3) \left[\coth^2(\rho r) - \frac{1}{\rho^2 r^2} \right] + 2 \right\} . \tag{5.97}$$

This integral can be computed exactly; we obtain

$$b_1 = \frac{(n-1)}{4} \rho^2 \left\{ n - 1 - \frac{(n-3)}{\rho^2 r^2} \left[\rho r \coth(\rho r) - 1 \right] \right\} . \tag{5.98}$$

Notice that when $r = 0$ this gives the coincidence limit

$$[b_1] = \frac{n(n-1)}{6} \rho^2 \,. \tag{5.99}$$

Since the scalar curvature is now

$$R = n(n-1)\Lambda = -n(n-1)\rho^2, \tag{5.100}$$

this coincides with the coincidence limit obtained above for a general case

$$b_1 = -\frac{1}{6} R \,. \tag{5.101}$$

Thus the heat kernel on spaces of constant negative curvature, that is, hyperbolic spaces is approximated by

$$\begin{aligned} U(t;x,x') &= (4\pi t)^{-n/2}\left(\frac{\sinh(\rho r)}{\rho r}\right)^{-(n-1)/2}\exp\left(-\frac{r^2}{4t}\right) \\ &\quad\times\left\{1-\frac{(n-1)}{4}\rho^2\left[n-1-\frac{(n-3)}{\rho^2 r^2}\left[\rho r\coth(\rho r)-1\right]\right]t\right. \\ &\quad\left.+O(t^2)\right\}. \end{aligned} \tag{5.102}$$

Finally, we evaluate this result for $n=2$,

$$\begin{aligned} U(t;x,x') &= \frac{1}{4\pi t}\sqrt{\frac{\rho r}{\sinh(\rho r)}}\exp\left(-\frac{r^2}{4t}\right) \\ &\quad\times\left\{1-\frac{t}{4r^2}\left[\rho^2 r^2+\rho r\coth(\rho r)-1\right]+O(t^2)\right\}. \end{aligned} \tag{5.103}$$

This is precisely the formula used in [37] in the derivation of Hagan formula for SABR model. We should warn that reader that there is a notational difference with that paper. The authors of that paper used the heat kernel in the density form, whereas we used the heat kernel in an invariant scalar form. they are related by the square root of the determinant of the metric tensor.

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

$$L=-\partial_x^2+Q\,, \tag{5.104}$$

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 $t\to 0$

$$\begin{aligned} U(t;x,x') &\sim (4\pi t)^{-1/2}\exp\left[-\frac{1}{4t}(x-x')^2\right] \\ &\quad\times\sum_{k=0}^{\infty}\frac{(-t)^k}{k!}b_k(x,x'). \end{aligned} \tag{5.105}$$

By substituting this into the heat equation we get the recursion system

$$b_0(x,x') = 1 \tag{5.106}$$

$$\left[1 + \frac{1}{k}(x-x')\frac{\partial}{\partial x}\right] b_k = La_{k-1}\,. \tag{5.107}$$

We look for solution of this recursion system in form of a Taylor series

$$b_k(x,x') = \sum_{n=0}^{\infty} \frac{1}{n!}(x-x')^n b_k^{(n)}(x')\,. \tag{5.108}$$

Then the solution is

$$\begin{aligned} b_k^{(n)} &= \sum_{n_1,\cdots,n_{k-1}\geq 0} \frac{k}{k+n}\cdot\frac{k-1}{k-1+n_{k-1}}\cdots\frac{1}{1+n_1} \\ &\quad \times L_{nn_{k-1}}L_{n_{k-1}n_{k-2}}\cdots L_{n_1 0}\,. \end{aligned} \tag{5.109}$$

Here L_{mn} are the matrix elements of the operator L ($m,n\geq 0$)

$$L_{mn} = -\delta_{n,(m+2)} + \binom{m}{n} Q^{(m-n)}\,, \tag{5.110}$$

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

$$0 \leq n_1 \leq n_2 + 2 \leq \cdots \leq n_{k-1} + 2(k-1) \leq n + 2(k-1)\,. \tag{5.111}$$

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* [27]. It has the form

$$b_k^{(n)} = \sum_{d=1}^{k} \sum_{|\mathbf{m}|=n+2k-2d} c(\mathbf{m}) Q^{(m_d)}\cdots Q^{(m_2)}Q^{(m_1)}\,, \tag{5.112}$$

where the second sum goes over multi-indices $\mathbf{m} = (m_1, m_2, \ldots, m_d)$ with non-negative integer components such that

$$|\mathbf{m}| = m_1 + m_2 + \cdots + m_d = n + 2k - 2d\,, \tag{5.113}$$

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,

$$|\mathbf{m}|_p = m_1 + m_2 + \cdots + m_p\,. \tag{5.114}$$

Then, after some combinatorial gymnastics, one can obtain

$$c(\mathbf{m}) = \sum_{i_1,\cdots,i_{d-1}} \prod_{p=1}^{d} \binom{i_p}{i_{p-1}} \frac{\binom{|\mathbf{m}|_p - 2i_{p-1}+2p}{m_p}}{\binom{|\mathbf{m}|_p - i_{p-1}+2p+1}{i_p - i_{p-1}}}\,, \tag{5.115}$$

where the summation goes now over all non-negative $i_1, \ldots, i_{d-1}$ such that

$$0 \equiv i_0 < i_1 < i_2 < \cdots < i_{d-1} < i_d \equiv k, \tag{5.116}$$

and

$$2i_p \leq |\mathbf{m}|_{p+1} + 2p\,. \tag{5.117}$$

Let us also list some low-order coefficients

$$[b_1] = Q\,, \tag{5.118}$$

$$[b_2] = Q^2 - \frac{1}{3}Q''\,, \tag{5.119}$$

$$[b_3] = Q^3 - \frac{1}{2}\left(QQ'' + Q''Q + Q'Q'\right) + \frac{1}{10}Q^{(4)}\,. \tag{5.120}$$

Chapter 6

Non-Perturbative Methods for Calculation of the Heat Kernel

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 on 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 lecture 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.

6.1 Some Approaches for Calculating Heat Kernel

6.1.1 Operator Method

This is a rather formal approach pioneered by Schwinger and generalized to curved manifolds by De Witt. We define operators $\hat{x}^i$, $i = 1, 2 \ldots, n$, called *coordinate operators*, acting on some abstract Hilbert space. Suppose that the operators $\hat{x}^i$ are self-adjoint and commute with each other

$$[\hat{x}^i, \hat{x}^j] = 0\,. \tag{6.1}$$

Let $|x'\rangle$ be the eigenvectors of these operators with the eigenvalues x', that is,

$$\hat{x}^i|x'\rangle = x'^i|x'\rangle\,, \tag{6.2}$$

normalized by

$$\langle x''|x'\rangle = \delta(x'' - x')\,. \tag{6.3}$$

The vectors $|x'\rangle$ transform as scalar densities of weight $1/2$ under diffeomorphisms. We assume that they form a basis in the Hilbert space.

Next, let $\hat{p}_i$ be a set of self-adjoint operators, called *momentum operators*, such that

$$[\hat{p}_i, \hat{p}_j] = 0\,, \tag{6.4}$$

$$[\hat{x}^k, \hat{p}_j] = i\delta^k_j\,. \tag{6.5}$$

and the matrix elements of the momentum operators are

$$\langle x''|\hat{p}_j|x'\rangle = -i\partial_{j'}\delta(x'' - x')\,. \tag{6.6}$$

Let us consider the differential operator

$$L(x, \partial) = -g^{-1/2}(x)(\partial_i + \mathcal{A}_i)g^{1/2}(x)g^{ij}(x)(\partial_j + \mathcal{A}_j) + Q(x)\,, \tag{6.7}$$

where g_{ij} is a Riemannian metric, $\mathcal{A}_i$ is a covertor field and Q is a smooth function. Then we define the operator

$$\begin{aligned} H(\hat{x}, \hat{p}) &= g^{1/4}(\hat{x})L(\hat{x}, i\hat{p})g^{-1/4}(\hat{x}) \\ &= g^{-1/4}(\hat{x})\Pi_i g^{1/2}(\hat{x})g^{ij}(\hat{x})\Pi_j g^{-1/4}(\hat{x}) + Q(\hat{x})\,, \end{aligned} \tag{6.8}$$

where

$$\Pi_k = \hat{p}_k - i\mathcal{A}_k(\hat{x})\,. \tag{6.9}$$

Here we just replaced the coordinates x and momenta by the operators

$$x^i \mapsto \hat{x}^i\,, \qquad \partial_j \mapsto i\hat{p}_j\,. \tag{6.10}$$

The operator H is treated naturally as the Hamiltonian of an abstract dynamical system. Notice that the Hamiltonian $H(\hat{x},\hat{p})$ is essentially the symbol $\sigma(x,p)$ of the operator $L(x,\partial)$, where we have replaced the momenta p by the operators $\hat{p}$.

The operators $\hat{x}^i$ and Π_j satisfy the commutation relations

$$[\hat{x}^j,\Pi_k] = i\delta^j{}_k\,, \tag{6.11}$$

and

$$[\Pi_i,\Pi_j] = -\mathcal{R}_{ij}\,, \tag{6.12}$$

where

$$\mathcal{R}_{ij} = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i\,. \tag{6.13}$$

Now, let us define time-dependent operators

$$\hat{x}^i(t) = \exp(tH)\hat{x}^i\exp(-tH) \tag{6.14}$$

and

$$\hat{\Pi}_j(t) = \exp(tH)\hat{\Pi}_j\exp(-tH)\,. \tag{6.15}$$

These operators satisfy the operator differential equations (Heisenberg equations)

$$\frac{dx^i(t)}{dt} = [H,x^i(t)] \tag{6.16}$$

$$\frac{d\Pi_j(t)}{dt} = [H,\Pi_j(t)] \tag{6.17}$$

and the initial conditions

$$\hat{x}^i(0) = \hat{x}^i\,, \qquad \hat{\Pi}_j(0) = \hat{\Pi}_j\,. \tag{6.18}$$

It is clear that the Hamiltonian is conserved under this (quantum) dynamics,

$$H(\hat{x}(t),\Pi(t)) = H(\hat{x},\Pi)\,. \tag{6.19}$$

Also, let us introduce the time dependent vectors

$$|x'(t)\rangle = \exp(tH)|x'\rangle\,, \tag{6.20}$$

and their adjoints

$$\langle x'(t)| = \langle x''|\exp(-tH)\,. \tag{6.21}$$

Then it is obvious that these vectors are the eigenvectors of the time-dependent coordinate operators $x(t)$, that is,

$$\hat{x}(t)|x'(t)\rangle = x'|x'(t)\rangle\,, \tag{6.22}$$

and

$$\langle x''(t)|\hat{x}(t) = x''\langle x''(t)|\,. \tag{6.23}$$

Finally, let us introduce the matrix element

$$\begin{aligned} U(t;x'',x') &= g^{-1/4}(x'')g^{-1/4}(x')\langle x''(t)|x'\rangle \\ &= g^{-1/4}(x'')g^{-1/4}(x')\langle x''|x'(t)\rangle \\ &= g^{-1/4}(x'')g^{-1/4}(x')\langle x''|\exp[-tH]|x'\rangle\,. \end{aligned} \tag{6.24}$$

Formally, this means that

$$U(t;x'',x') = \exp[-tL(x'',\partial_{x''})]\delta(x'',x')\,, \tag{6.25}$$

where $\delta(x'',x')$ is the covariant delta-function defined by

$$\delta(x'',x') = g^{-1/4}(x'')\delta(x'-x')g^{-1/4}(x')\,. \tag{6.26}$$

Therefore, the matrix element $U(t;x'',x')$ is nothing but the heat kernel. It satisfies the equation

$$[\partial_t + L(x'',\partial_{x''})]U(t;x'',x') = 0 \tag{6.27}$$

and the initial condition

$$U(0;x'',x') = \delta(x'',x')\,. \tag{6.28}$$

The main idea of this approach is to solve the operator equations (6.16), (6.17) and use the commutation relations to compute the heat kernel. By using the definition of the time-dependent operators and the formula for commutators we can rewrite them in the form

$$\hat{x}^i(t) = \exp(tAd_H)\hat{x} = \sum_{k=0}^{\infty}\frac{t^k}{k!}\underbrace{[H,[H,\cdots,[H,\hat{x}^i]\cdots]]}_{k}\,., \tag{6.29}$$

$$\Pi_j(t) = \exp(tAd_H)\Pi = \sum_{k=0}^{\infty}\frac{t^k}{k!}\underbrace{[H,[H,\cdots,[H,\Pi_j]\cdots]]}_{k}\,, \tag{6.30}$$

where, as usual, Ad_H is the operator defined by

$$Ad_H B = [H, B] \,. \tag{6.31}$$

Now, suppose that we could integrate the operator equations (or sum the above series) in the form

$$\hat{x}(t) = f_1(t; \hat{x}, \Pi) \,. \tag{6.32}$$

$$\Pi(t) = f_2(t; \hat{x}, \Pi) \,, \tag{6.33}$$

where f_1 and f_2 are some functions. Then, one can express the initial momentums in terms of coordinate operators

$$\Pi = f_3(t; \hat{x}(t), \hat{x}) \,, \tag{6.34}$$

where f_3 is some other function. Next, one could substitute them into the expression for the Hamiltonian and order them using the commutation relations so that all $\hat{x}(t)$ would be placed to the left and all $\hat{x}$ to the right. Then, as a result the Hamiltonian takes the form

$$H(\hat{x}, \Pi) = \mathrm{T}\, h(t; \hat{x}(t), \hat{x}) \,, \tag{6.35}$$

where h is some function and the symbol T means the time ordering from the right to the left with respect to time t.

Further, we have

$$\partial_t U(t; x'', x') = -\langle x''(t) | H(\hat{x}, \Pi) | x' \rangle \,. \tag{6.36}$$

Finally, by substituting the representation (6.35) of the Hamiltonian into this equation we obtain

$$\partial_t U(t; x'', x') = -h(t; x'', x') U(t; x'', x') \,. \tag{6.37}$$

This equation can be easily integrated to give

$$U(t; x'', x') = C(x'', x') \exp\left(- \int dt\, h(t; x'', x') \right) \,, \tag{6.38}$$

where $C(x'', x')$ is an arbitrary function that should be determined from the initial condition

$$U(0; x'', x') = \delta(x'' - x') \,. \tag{6.39}$$

Linear Connection

We illustrate this method on a simple example. Let us consider the operator L

$$L = -\delta^{jk} \left(\partial_j + \mathcal{A}_j\right) \left(\partial_k + \mathcal{A}_k\right) , \tag{6.40}$$

where the vector $\mathcal{A}_i$ is linear function,

$$\mathcal{A}_i = -\frac{1}{2}\mathcal{R}_{ij} x^j , \tag{6.41}$$

and $\mathcal{R}_{jk}$ is an anti-symmetric constant 2-tensor. Since the metric is Euclidean $g_{ij} = \delta_{ij}$ there is no difference between upper and lower indices.

Since the Hamiltonian of this model is simply

$$H = \hat{\Pi}_j \hat{\Pi}^j , \tag{6.42}$$

the operator equations take the form

$$\frac{d\hat{x}^j}{dt} = -2i\hat{\Pi}^j , \tag{6.43}$$

$$\frac{d\hat{\Pi}_j}{dt} = 2\mathcal{R}_{jk}\hat{\Pi}^k . \tag{6.44}$$

These equations are linear and can be easily solved. We obtain

$$\hat{\Pi}^j(t) = \left[\exp(2t\mathcal{R})\right]^j{}_k \hat{\Pi}^k , \tag{6.45}$$

$$\hat{x}^j(t) = \hat{x}^j - i\left[\frac{\exp(2t\mathcal{R}) - 1}{\mathcal{R}}\right]^j{}_k \hat{\Pi}^k , \tag{6.46}$$

where $\mathcal{R} = (\mathcal{R}_{ij})$ is the anti-symmetric matrix of the tensor $\mathcal{R}_{ij}$. Thus, we can express the initial momenta operators in term of the coordinate operators,

$$\hat{\Pi}^j = i\left[\frac{\mathcal{R}}{\exp(2t\mathcal{R}) - 1}\right]^j{}_k [\hat{x}(t) - \hat{x}]^k . \tag{6.47}$$

Now, by using the anti-symmetry of the matrix $\mathcal{R}$ we can rewrite the Hamiltonian in the form

$$H = -\frac{1}{4}[\hat{x}(t) - \hat{x}]^j \left(\frac{\mathcal{R}^2}{\sinh^2(t\mathcal{R})}\right)_{jk} [\hat{x}(t) - \hat{x}]^k . \tag{6.48}$$

Finally, we compute the commutator

$$[\hat{x}^j(t), \hat{x}^k] = -\left[\frac{\exp(2t\mathcal{R}) - 1}{\mathcal{R}}\right]^{jk} . \tag{6.49}$$

By using this commutator we can reorder the operators $\hat{x}(t)$ and $\hat{x}$ to obtain

$$\begin{aligned} h(t; x'', x') &= \langle x''(t)|H|x'\rangle \\ &= -\frac{1}{4}(x'' - x')^j \left(\frac{\mathcal{R}^2}{\sinh^2(t\mathcal{R})}\right)_{jk} (x'' - x')^k + \frac{1}{2}\mathrm{tr}\left[\mathcal{R}\coth(t\mathcal{R})\right] , \end{aligned} \tag{6.50}$$

where tr is the matrix trace.

The solution of the heat equation with initial condition takes now the form

$$\begin{aligned} U(t|x'', x') &= (4\pi t)^{-n/2}\mathcal{P}(x'', x')\det\left(\frac{t\mathcal{R}}{\sinh(t\mathcal{R})}\right)^{1/2} \\ &\quad \times \exp\left(-\frac{1}{4}(x'' - x')^i \left[\mathcal{R}\coth(t\mathcal{R})\right]_{ij} (x'' - x')^j\right) \end{aligned} \tag{6.51}$$

where $\det$ means the matrix determinant 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

$$(x - x')^j \partial_j \mathcal{P}(x, x') = \frac{1}{2}\mathcal{R}_{jm} x^m \mathcal{P}(x, x') \tag{6.52}$$

and the initial condition

$$\mathcal{P}(x, x) = 1 . \tag{6.53}$$

Therefore,

$$\mathcal{P}(x'', x') = \exp\left(\frac{1}{2}\mathcal{R}_{jk} x''^j x'^k\right) . \tag{6.54}$$

The case of a harmonic oscillator

$$L = -\partial_i \partial^i + \frac{1}{2}P_{ij} x^i x^j , \tag{6.55}$$

where P_{ij} is a constant symmetric tensor, can be treated similarly. Both these cases are solvable because the operator equations are linear.

6.1.2 Covariant Fourier Transform Method

In this section we use extensively the machinery developed in a previous lecture about the covariant asymptotic expansion of the heat kernel. We refer to that section for notation and definition of various differential-geometric objects.

Let L be a Laplace type differential operator acting on scalar functions on a Riemannian manifold of the form

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_i^{\mathcal{A}} + Q\,, \tag{6.56}$$

where Q is some function. This method is based on the formal representation of the heat kernel in the form

$$U(t;x,x') = \exp(-tL)\delta(x,x') \tag{6.57}$$

Using the representation of the δ-function in form of a covariant Fourier integral

$$\delta(x,x') = \Delta^{1/2}(x,x')\int\limits_{\mathbb{R}^n}\frac{dk}{(2\pi)^n}g^{-1/2}(x')\exp\left[ik_{j'}\sigma^{j'}(x,x')\right] \tag{6.58}$$

we get

$$\begin{aligned} U(t;x,x') &= \Delta^{1/2}(x,x')\int\limits_{\mathbb{R}^n}\frac{dk}{(2\pi)^n}g^{-1/2}(x')\exp\left[ik_{j'}\sigma^{j'}(x,x')\right] \\ &\quad\times\exp(-tA)\cdot 1\,, \end{aligned} \tag{6.59}$$

where A is an operator defined by

$$A = \exp\left(-ik_{j'}\sigma^{j'}\right)\hat{L}\exp\left(ik_{l'}\sigma^{l'}\right)\,, \tag{6.60}$$

and the operator $\hat{L}$ is defined by

$$\hat{L} = \mathcal{P}^{-1}\Delta^{-1/2}L\Delta^{1/2}\mathcal{P}\,. \tag{6.61}$$

We remind the definition of some objects that we will need. For more details see the lecture on differential geometry. We will use the operators $\mathcal{D}_{i'}$

$$\mathcal{D}_{i'} = \gamma^{j}{}_{i'}\nabla_j\,,\,, \tag{6.62}$$

where $\gamma^{i}{}_{j'}$ is the inverse of the matrix $\eta^{i'}{}_{j} = \nabla_j \sigma^{i'}$. These operators are very convenient in curved space since they satisfy the following commutation relations

$$[\mathcal{D}_{i'}, \mathcal{D}_{j'}] = 0\,, \qquad \left[\mathcal{D}_{i'}, \sigma^{j'}\right] = \delta^{j'}{}_{i'}\,. \tag{6.63}$$

Thus, the operators $\mathcal{D}_{i'}$ and the vectors $\sigma^{j'}$ play the role of usual derivatives and coordinates in flat space.

We can express the operator $\hat{L}$ in terms of the operators $\mathcal{D}_{i'}$, (5.61)

$$\hat{L} = -X^{i'j'}\mathcal{D}_{i'}\mathcal{D}_{j'} - Y^{i'}\mathcal{D}_{i'} + Z\,, \tag{6.64}$$

where the functions $X^{i'j'}$, $Y^{i'}$ and Z are defined by

$$X^{i'j'} = \eta^{i'}{}_{k}\eta^{j'k} \tag{6.65}$$

$$Y^{i'} = \mathcal{D}_{j'}X^{i'j'} + 2X^{i'j'}\hat{\mathcal{A}}_{j'} \tag{6.66}$$

$$Z = X^{i'j'}(\zeta_{i'}\zeta_{j'} - \hat{\mathcal{A}}_{i'}\hat{\mathcal{A}}_{j'}) - \mathcal{D}_{j'}\left[X^{i'j'}\left(\zeta_{i'} + \hat{\mathcal{A}}_{i'}\right)\right] + Q\,, \tag{6.67}$$

and

$$\hat{\mathcal{A}}_{i'} = \mathcal{P}^{-1}\mathcal{D}^{\mathcal{A}}_{i'}\mathcal{P}\,, \qquad \zeta_{i'} = \mathcal{D}_{i'}\zeta\,. \tag{6.68}$$

Recall also that $\eta^{i'}{}_{j} = \nabla_j \sigma^{i'}$ and $\zeta = \log \Delta^{1/2}$.

Therefore, the operator A can be written in the form

$$A = \hat{L} - ik_{i'}T^{i'} + k_{j'}k_{l'}X^{j'l'}\,, \tag{6.69}$$

where $T^{i'}$ is a first-order differential operator defined by

$$T^{i'} = 2X^{i'j'}\mathcal{D}_{j'} + Y^{i'}\,. \tag{6.70}$$

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 asymptotic expansion as $t \to 0$ and $x \to x'$

$$\begin{aligned} U(t;x,x') &= (4\pi t)^{-n/2}\Delta^{1/2}(x,x')\int\limits_{\mathbb{R}^n}\frac{dk}{\pi^{n/2}}g^{-1/2}(x')\exp\left[it^{-1/2}k_{j'}\sigma^{j'}\right] \\ &\quad \times \exp\left\{-k_{i'}k_{j'}X^{i'j'} + ik_{j'}\sqrt{t}\,T^{j'} - t\hat{L}\right\}\cdot 1\,. \end{aligned} \tag{6.71}$$

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 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.

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

$$U(t;x,x) = (4\pi t)^{-n/2} \tag{6.72}$$
$$\times \lim_{x\to x'} \int\limits_{\mathbb{R}^n} \frac{dk}{\pi^{n/2}} g^{-1/2}(x') \exp\left\{-k_{i'}k_{j'}X^{i'j'} + ik_{j'}\sqrt{t}T^{j'} - t\hat{L}\right\}\cdot 1\,.$$

Let us separate the value of the function $X^{i'j'}$ at x', that is,

$$X^{i'j'} = g^{i'j'}(x') + \tilde{X}^{i'j'}\,. \tag{6.73}$$

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

$$\langle f(k)\rangle = \lim_{x\to x'} \int \frac{dk}{\pi^{n/2}} g^{-1/2} \exp\left[-g^{i'j'}(x')k_{i'}k_j\right] f(k)\,, \tag{6.74}$$

so that

$$\langle k_{i_1}\cdots k_{i_{2n+1}}\rangle = 0 \tag{6.75}$$
$$\langle k_{i_1}\cdots k_{i_{2n}}\rangle = \frac{(2n)!}{2^{2n}n!} g_{(i_1i_2}\cdots g_{i_{2n-1}i_{2n})}\,. \tag{6.76}$$

Further, let

$$A_0 = \hat{L}\,, \tag{6.77}$$
$$A_1 = -ik_{j'}\,T^{j'}\,, \tag{6.78}$$
$$A_2 = k_{i'}k_{j'}\tilde{X}^{i'j'}\,. \tag{6.79}$$

Then the heat kernel diagonal takes the form

$$U(t;x,x) = (4\pi t)^{-n/2}\Omega(t;x,x)\,, \tag{6.80}$$

where

$$\Omega(t;x,x) = \left\langle \exp\left(-A_2 - \sqrt{t}A_1 - tA_0\right)\cdot 1\right\rangle . \tag{6.81}$$

By expanding it in the asymptotic series as $t \to 0$

$$\Omega(t;x,x) \sim \sum_{k=0}^{\infty} \frac{(-t)^k}{k!}[b_k] , \tag{6.82}$$

we obtain the heat kernel coefficients in the form

$$[b_k] \;=\; \sum_{N=0}^{\infty} \frac{k!}{N!} \sum_{\substack{0\le k_1,\ldots,k_N\le 2\\ k_1+\cdots+k_N=k}} \langle A_{k_1}\cdots A_{k_N}\cdot 1\rangle , \tag{6.83}$$

where 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.

6.2 Approximation Schemes for Calculation of the Heat Kernel

6.2.1 Asymptotic Expansions

We consider the scalar Laplace type operator

$$L = -g^{ij}\nabla_j^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q . \tag{6.84}$$

In this lecture we are going to investigate the general structure of the heat kernel coefficients b_k. 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, i.e. the covariant derivatives of the curvature. Let us call the Riemann curvature tensor R_{ijkl} and the potential Q the *background fields* and denote them by $\Re = \{R_{ijkl}, \mathcal{R}_{ij}, Q\}$. Let us introduce, in addition, the infinite set of all covariant derivatives of the curvatures, so-called *covariant jets*,

$$\Re_{(i)} = \nabla_{(j_1}\cdots\nabla_{j_i)}\Re . \tag{6.85}$$

i will be called the order of a jet $\Re_{(i)}$. It is worth noting that the jets are defined by symmetrized covariant derivatives. This makes them well defined as ordering 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

$$g_{ij} \mapsto g_{ij}(\alpha,\varepsilon), \tag{6.86}$$
$$\mathcal{A}_i \mapsto \mathcal{A}_i(\alpha,\varepsilon)\,, \tag{6.87}$$
$$Q \mapsto Q(\alpha,\varepsilon)\,, \tag{6.88}$$

in such a way that the jets transform uniformly

$$\mathfrak{R}_{(i)} \mapsto \alpha\varepsilon^i\mathfrak{R}_{(i)}. \tag{6.89}$$

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

$$L \mapsto L(\alpha,\varepsilon) \tag{6.90}$$

and the heat kernel

$$U(t) \mapsto U(t;\alpha,\varepsilon). \tag{6.91}$$

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, $\nabla_i\mathfrak{R} \to 0$.

More precisely, we recognize two cases: i) the short-wave approximation,

$$\nabla\nabla\mathfrak{R} \gg \mathfrak{R}\mathfrak{R} \qquad \text{or} \qquad \varepsilon^2 \gg \alpha, \tag{6.92}$$

which correspond to the situation when the curvatures are small but rapidly varying, and ii) the long-wave approximation,

$$\nabla\nabla\mathfrak{R} \ll \mathfrak{R}\mathfrak{R} \qquad \text{or} \qquad \varepsilon^2 \ll \alpha\,, \tag{6.93}$$

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.)

Short-time Approximation

As we have seen in the previous lectures there is an asymptotic expansion of the heat kernel as $t \to 0$

$$[U(t;\alpha,\varepsilon)] \sim (4\pi t)^{-n/2} \sum_{k\geq 0} \frac{(-t)^k}{k!} b_k(\alpha,\varepsilon). \tag{6.94}$$

The coefficients b_k are polynomial in the jets. The first two coefficients have the well known form

$$b_0 = 1\,, \qquad b_1 = Q - \frac{1}{6}R\,.$$

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

$$b_k(\alpha,\varepsilon) = \sum_{n=0}^{k} \alpha^n \varepsilon^{2k-2n} b_{k,n}. \tag{6.95}$$

Here $b_{k,n}$ are the homogeneous parts of a_k of order n in the curvatures that can be symbolically written in the form

$$b_{k,n} = \sum_{\substack{i_1,\ldots,i_n\geq 0 \\ i_1+\cdots+i_n=k-2n}} \sum \Re_{(i_1)} \cdots \Re_{(i_n)}, \tag{6.96}$$

where the second summation is over different invariant structures. The first coefficient reads simply

$$b_0 = 1,. \tag{6.97}$$

The higher order coefficients $[b_k]$, $(k \geq 2)$ have the following homogeneous parts [5,6]

$$
\begin{aligned}
b_{k,0} &= 0, && (6.98)\\
b_{k,1} &= \alpha_k^{(1)}\Delta^{k-1}Q + \alpha_k^{(2)}\Delta^{k-1}R, && (6.99)\\
b_{k,2} &= \beta_k^{(1)}Q\Delta^{k-2}Q + 2\beta_k^{(2)}\mathcal{R}^i{}_j\nabla_i\Delta^{k-3}\nabla_m\mathcal{R}^{mj} - 2\beta_k^{(3)}Q\Delta^{k-2}R \\
&\quad +\beta_k^{(4)}R_{ij}\Delta^{k-2}R^{ij} + \beta_k^{(5)}R\Delta^{k-2}R \\
&\quad +\nabla\left(\sum_{i=0}^{2k-3}\sum\nabla^i\Re\nabla^{2k-3-i}\Re\right), && (6.100)\\
&\cdots && (6.101)\\
b_{k,k} &= \sum\Re^k, && (6.102)
\end{aligned}
$$

where $\alpha_k^{(i)}$ and $\beta_k^{(i)}$ are some universal numerical constants. Note that $\Delta = \nabla^i\nabla_i$ is the Laplacian and not 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 $\Re^k$.

Short-wave Approximation

Let us consider now the asymptotic expansion in the limit $\alpha \to 0$ of the perturbation theory. One can show that it has the form

$$[U(t;\alpha,\varepsilon)] \sim (4\pi t)^{-n/2}\sum_{n=0}^{\infty}(\alpha t)^n h_n(t;\varepsilon), \qquad (6.103)$$

where $h_n(t,\varepsilon)$ are some *nonlocal* functionals that have the following asymptotic expansion as $t \to 0$

$$h_n(t;\varepsilon) \sim \sum_{l=0}^{\infty}\frac{(-1)^{n+l}}{(n+l)!}(\varepsilon^2 t)^l b_{n+l,n}. \qquad (6.104)$$

The first functionals h_n are

$$\begin{aligned} h_0(t;\varepsilon) &= 1, && (6.105)\\ h_1(t;\varepsilon) &= t\left\{F_{(1)}(\varepsilon^2 t\Delta)Q - F_{(2)}(\varepsilon^2 t\Delta)R\right\}, && (6.106)\\ h_2(t;\varepsilon) &= \frac{t^2}{2}\Big\{QF_{(1)}(\varepsilon^2 t\Delta)Q + 2\mathcal{R}^i{}_j\nabla_i\Delta^{-1}F_{(3)}(\varepsilon^2 t\Delta)\nabla_m\mathcal{R}^{mj} \\ &\quad -2QF_{(2)}(\varepsilon^2 t\Delta)R + R_{ij}F_{(4)}(\varepsilon^2 t\Delta)R^{ij} + RF_{(5)}(\varepsilon^2 t\Delta)R\Big\} \\ &\quad +\text{total derivative}, && (6.107) \end{aligned}$$

where $F_{(i)}(z)$ are some analytic functions.

Long-wave Approximation

The long-wave approximation corresponds to the asymptotic expansion of the deformed heat kernel as $\varepsilon \to 0$

$$[U(t;\alpha,\varepsilon)] \sim (4\pi t)^{-n/2}\sum_{l=0}^{\infty}(\varepsilon^2 t)^l u_l(t;\alpha). \qquad (6.108)$$

The coefficients u_l are essentially *non-perturbative* functionals that have the following perturbative asymptotic expansion as $t \to 0$

$$u_l(t;\alpha) \sim \sum_{n=0}^{\infty}\frac{(-1)^{n+l}}{(n+l)!}(\alpha t)^n a_{l+n,n}. \qquad (6.109)$$

The zeroth order of this approximation,

$$[U(t;\alpha,\varepsilon)]\Big|_{\varepsilon=0} \sim (4\pi t)^{-n/2}u_0(t;\alpha), \qquad (6.110)$$

corresponds to covariantly constant background

$$\Re_{(i)} = 0 \qquad \text{for } i \geq 1, \qquad (6.111)$$

or, more explicitly,

$$\nabla_m R_{ijkl} = 0, \qquad \nabla_m\mathcal{R}_{ij} = 0\,, \qquad \nabla_m Q = 0. \qquad (6.112)$$

The zeroth order functional $u_0(t;\alpha)$ has the following perturbative asymptotic expansion

$$u_0(t;\alpha) \sim \sum_{n\geq 0}\frac{(-1)^n}{n!}(\alpha t)^n b_{n,n}, \qquad (6.113)$$

or, symbolically,

$$u_0(t;\alpha) \sim \sum_{n=0}^{\infty} \sum (\alpha t \Re)^n, \tag{6.114}$$

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.

6.3 Leading Derivatives and Nonlocality

In this section we show how the leading derivatives in the heat kernel coefficients can be computed by the technique developed in the previous lecture. 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 calculational 'diagrammatic' technique developed in the previous lecture. 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

$$\langle m|\hat{L}|m+2\rangle = -\delta^{(i_1\cdots i_m}_{j_1\cdots j_m} g^{i_{m+1}i_{m+2})}\,. \tag{6.115}$$

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 (5.45) (and some heavy com-

binatorics) one obtains

$$\begin{aligned}\langle n|b_k\rangle &= \sum_{N=1}^{k}(-1)^{N-k}\sum_{1\le i_1<i_2<\cdots<i_{N-1}\le k-1}\ \sum_{n_1,\cdots,n_{N-1}\ge 0}\\ &\times N(i_1,n_1,\cdots i_{N-1},n_{N-1},k,n)\\ &\times\langle n;k-i_{N-1}-1|\hat{L}|n_{N-1}\rangle\langle n_{N-1};i_{N-1}-i_{N-2}-1|\hat{L}|n_{N-2}\rangle\cdots\\ &\times\langle n_2;i_2-i_1-1|\hat{L}|n_1\rangle\langle n_1;i_1-1|\hat{L}|0\rangle\,, \end{aligned}\tag{6.116}$$

where

$$\langle n;k|\hat{L}|m\rangle = g^{i_1i_2}\cdots g^{i_{2k-1}i_{2k}}\langle i_1\cdots i_{2k}i_{2k+1}\cdots i_{n+2k}|\hat{L}|j_1\cdots j_m\rangle\,,\tag{6.117}$$

$$\begin{aligned}&N(i_1,n_1\cdots i_{N-1},n_{N-1},k,n) =\\ &\frac{1}{\binom{2k+n-1}{k}}\frac{\binom{2i_2+n_2-1}{i_1}}{\binom{2i_1+n_1-1}{i_1}}\cdots\frac{\binom{2i_{N-1}+n_{N-1}-1}{i_{N-2}}}{\binom{2i_{N-2}+n_{N-2}-1}{i_{N-2}}}\frac{\binom{2k+n-1}{i_{N-1}}}{\binom{2i_{N-1}+n_{N-1}-1}{i_{N-1}}}\end{aligned}\tag{6.118}$$

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,

$$\begin{aligned}&n_1+2(i_1-1)\ge 0,\quad n_2+2(i_2-i_1-1)\ge n_1,\qquad\cdots\qquad,\\ &n+2(k-i_{N-1}-1)\ge n_{N-1}\,.\end{aligned}\tag{6.119}$$

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 (6.116) for the coincidence limit of heat kernel coefficients

$$\begin{aligned}[b_k] &= \frac{(-1)^{k-1}}{\binom{2k-1}{k}}\langle 0;k-1|\hat{L}|0\rangle\\ &+(-1)^k\sum_{i=1}^{k-1}\sum_{n_i=0}^{2(k-i-1)}\frac{\binom{2k-1}{i}}{\binom{2k-1}{k}\binom{2i+n_i-1}{i}}\langle 0;k-i-1|\hat{L}|n_i\rangle\langle n_i;i-1|\hat{L}|0\rangle\\ &+O(\Re^3)\,.\end{aligned}\tag{6.120}$$

Here we have taken into account in (6.116) the first diagram $(N = 1)$ and the second class of diagrams $(N = 2)$.

Now we should make use of the formulas of the previous lectures to calculate the matrix elements $\langle n; k|\hat{L}|m\rangle$ within the same accuracy $O(\Re^3)$, substitute them in eq. (6.120) and carry out the summation.

Omitting these very cumbersome calculations we write down the result (for $k \geq 2$)

$$\begin{aligned}[b_k] &= \frac{2}{k+1}\left(F^{(1)}_{k+1}(\Delta)Q - F^{(3)}_{k+1}(\Delta)R\right) \qquad (6.121)\\ &+QF^{(1)}_k(\Delta)Q + 2\mathcal{R}^i{}_j\nabla_i\Delta^{-1}F^{(2)}_k(\Delta)\nabla_m\mathcal{R}^{mj} - 2QF^{(3)}_k(\Delta)R\\ &+R_{ij}F^{(4)}_k(\Delta)R^{ij} + RF^{(5)}_k(\Delta)R + O(\nabla(\Re^2)) + O(\Re^3)\,,\end{aligned}$$

where the total derivatives and terms of order higher than two are omitted. Here Δ is the Laplacian and $F^{(i)}_k(\Delta)$ are differential operators of order $(2k-4)$

$$F^{(i)}_k(\Delta) = \frac{1}{2}\frac{k!(k-2)!}{(2k-3)!}f^{(i)}_k(-\Delta)^{k-2}\,, \qquad (6.122)$$

where $f^{(i)}_k$ are numerical coefficients defined by

$$f^{(1)}_k = 1\,, \qquad (6.123)$$

$$f^{(2)}_k = \frac{1}{2(2k-1)}\,, \qquad (6.124)$$

$$f^{(3)}_k = \frac{k-1}{2(2k-1)}\,, \qquad (6.125)$$

$$f^{(4)}_k = \frac{1}{2(4k^2-1)}\,, \qquad (6.126)$$

$$f^{(5)}_k = \frac{k^2-k-1}{4(4k^2-1)}\,. \qquad (6.127)$$

It is not difficult to show that $F^{(i)}_k(\Delta)$ (6.122) can be represented in an integral form which will be very useful for further consideration

$$F^{(i)}_k(\Delta) = \frac{1}{2}k(k-1)\int\limits_0^1 d\xi\, f^{(i)}(\xi)(1-\xi^2)^{k-2}\left(-\frac{\Delta}{4}\right)^{k-2}\,, \qquad (6.128)$$

where

$$f^{(1)}(\xi) = 1\,, \tag{6.129}$$

$$f^{(2)}(\xi) = \frac{1}{2}\xi^2\,, \tag{6.130}$$

$$f^{(3)}(\xi) = \frac{1}{4}(1-\xi^2)\,, \tag{6.131}$$

$$f^{(4)}(\xi) = \frac{1}{6}\xi^4\,, \tag{6.132}$$

$$f^{(5)}(\xi) = \frac{1}{48}(3-6\xi^2-\xi^4)\,. \tag{6.133}$$

Now we can make an 'analytical continuation' of the heat kernel coefficients (6.121) to the whole complex plane of their order (keeping in mind all the reservations made in the previous lecture) and obtain the function b_q (5.19). The result of such an analytical continuation has the form (6.121) 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 (6.128), with k being replaced by q. This can also be written by using the gamma-function

$$F_q^{(i)}(\Delta) = \frac{1}{2}\frac{\Gamma(q+1)\Gamma(q-1)}{\Gamma(2q-2)} f_q^{(i)}(-\Delta)^{q-2}\,. \tag{6.134}$$

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 or from the general formula (2.15)

$$\begin{aligned}[U(t)] &= (4\pi t)^{-n/2}\Big\{1 - t\left[\gamma^{(1)}(t\Delta)Q - \gamma^{(3)}(t\Delta)R\right] \\ &\quad + \frac{t^2}{2}\Big[Q\gamma^{(1)}(t\Delta)Q + 2\mathcal{R}^i{}_j\nabla_i\Delta^{-1}\gamma^{(2)}(t\Delta)\nabla_m\mathcal{R}^{mj} \\ &\quad -2Q\gamma^{(3)}(t\Delta)R + R_{ij}\gamma^{(4)}(t\Delta)R^{ij} + R\gamma^{(5)}(t\Delta)R\Big] \\ &\quad + O(\nabla(RR)) + O(R^3)\Big\}\,,\end{aligned} \tag{6.135}$$

where $\gamma^{(i)}(t\Delta)$ are some non-local (pseudo-differential) operators de-

fined by

$$\gamma^{(i)}(t\Delta) = \int_0^1 d\xi\, f^{(i)}(\xi) \exp\left(\frac{1-\xi^2}{4} t\Delta\right) \tag{6.136}$$

with $f^{(i)}(\xi)$ given by (6.133).

This formulas are 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.

6.4 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 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 the operator

$$L = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q\,, \tag{6.137}$$

where $\nabla_i^{\mathcal{A}}$ are some first-order differential operators (covariant derivatives) and Q is a function.

Let us consider for a moment a trivial case of vanishing curvature, $R^i{}_{jkl} = \mathcal{R}_{ij} = 0$, and constant potential term. In this case

the operators of covariant derivatives obviously commute and form together with the potential term and the metric an Abelian algebra

$$[\nabla_i, \nabla_j] = 0, \qquad [\nabla_i, Q] = 0\,, \qquad [\nabla_i, g_{jk}] = 0\,. \tag{6.138}$$

As a result, it is easy to show that the heat-semigroup of the operator L can be presented in form of a Gaussian integral

$$\exp(-tL) = (4\pi t)^{-n/2} \exp(-tQ) \int\limits_{\mathbb{R}^n} dk g^{1/2} \exp\left(-\frac{1}{4t} k^i g_{ij} k^j\right) \exp\left(k^j \nabla_j\right), \tag{6.139}$$

Acting with this operator on the delta-function $\delta(x, x')$ and using the obvious relation

$$\exp(k^j \nabla_j)\delta(x, x') = \delta(x - x' + k) \tag{6.140}$$

one can simply integrate over k to obtain the heat kernel in coordinate representation

$$U(t; x, x') = (4\pi t)^{-n/2} \exp\left[-\frac{1}{4t}(x - x')^i g_{ij} (x - x')^j - tQ\right]. \tag{6.141}$$

The heat kernel diagonal is obtained by taking the coincidence limit $x \to x'$

$$[U(t)] = (4\pi t)^{-n/2} \exp\left(-tQ\right). \tag{6.142}$$

Of course, for non-zero curvature the covariant differential operators ∇_i^A do not commute and the commutators of them are proportional to the curvatures $\Re$. The commutators of covariant derivatives with the curvatures give the first derivatives of the curvatures, i.e. the jets $\Re_{(1)}$, the commutators of covariant derivatives with $\Re_{(1)}$ give the second jets $\Re_{(2)}$ etc.

$$\begin{aligned} [\nabla, \nabla] &= \Re, \\ [\nabla, \Re] &= \Re_{(1)}, \\ &\cdots \\ [\nabla, \Re_{(i)}] &= \Re_{(i+1)}, \\ &\cdots \end{aligned} \tag{6.143}$$

For scalar operators the commutators of jets with themselves vanish

$$[\Re_{(i)}, \Re_{(k)}] = 0\,. \tag{6.144}$$

Thus the operators of covariant differentiation ∇ together with the whole set of all jets form an *infinite* dimensional Lie algebra $\{\nabla, \Re_{(i)}\}$. 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 (6.139) would be the zeroth order approximation in the commutators of the covariant derivatives, i.e. in the curvatures. Roughly speaking, we are going to find a representation of the heat semigroup in the form

$$\exp(-tL) = \int dk\ \Psi(t,k) \exp\left\{-\frac{1}{4t} k^A \Phi_{AB}(t) k^B\right\} \exp(k^A \xi_A), \qquad (6.145)$$

where $\xi_A = \{X_a, Y_i\}$, $X_a = X_a^\mu \nabla_\mu$ are some first order differential operators and Y_i are some functions. 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, this algebra closes and becomes finite dimensional.

Using this representation one could, as above, act with $\exp(k_A \xi^A)$ 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 $k^A \xi_A$ on the delta-function than that of the exponential of the second order operator L.

6.4.1 Linear Connection in Flat Space

In this section we consider a slightly more complicated case when the metric g_{ij} is still flat, that is, $R^i{}_{jkl} = 0$, but the covariant deriva-

tives $\nabla_j^{\mathcal{A}}$ have a linear connection $\mathcal{A}_j$, which simply means that

$$\nabla_j^{\mathcal{A}} = \partial_j - \frac{1}{2}\mathcal{R}_{jk}x^k\,, \tag{6.146}$$

where $\mathcal{R}_{jk}$ is a *constant* tensor. That is, we consider an operator L that acts on scalar functions in $\mathbb{R}^n$ of the form

$$L = -\delta^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q\,, \tag{6.147}$$

with the Euclidean metric and the covariant derivatives defined above.

First we consider the case of *constant potential term*. In this case the covariant derivatives form a *nilpotent* Lie algebra

$$[\nabla_j^{\mathcal{A}}, \nabla_k^{\mathcal{A}}] = \mathcal{R}_{jk}, \tag{6.148}$$

$$[\nabla_j^{\mathcal{A}}, \mathcal{R}_{kl}] = [\nabla_j^{\mathcal{A}}, Q] = 0. \tag{6.149}$$

For this algebra one can prove a theorem expressing the heat semi-group in terms of an average over some Lie group [8]

$$\begin{aligned}\exp(-tL) &= (4\pi t)^{-n/2}\det\left(\frac{t\mathcal{R}}{\sinh(t\mathcal{R})}\right)^{1/2}\exp(-tQ) \\ &\int\limits_{\mathbb{R}^n} dk \exp\left\{-\frac{1}{4t}k^j\left[t\mathcal{R}\coth(t\mathcal{R})\right]_{lm}k^m\right\}\exp\left(k^j\nabla_j^{\mathcal{A}}\right),\end{aligned} \tag{6.150}$$

where $\mathcal{R}$ denotes the matrix $\mathcal{R} = (\mathcal{R}_{ij})$.

Further, one can show that

$$\exp(k^j\nabla_j^{\mathcal{A}})\delta(x,x') = \mathcal{P}(x,x')\delta(x-x'+k)\,, \tag{6.151}$$

where the function $\mathcal{P}(x,x')$ is defined by (6.54). Subsequently, the integral over k^j becomes trivial and we immediately obtain the heat kernel

$$\begin{aligned}U(t;x,x') &= (4\pi t)^{-n/2}\det\left(\frac{t\mathcal{R}}{\sinh(t\mathcal{R})}\right)^{1/2}\exp(-tQ) \\ &\times\mathcal{P}(x,x')\exp\left\{-\frac{1}{4t}(x-x')^j\left[t\mathcal{R}\coth(t\mathcal{R})\right]_{lm}(x-x')^m\right\}.\end{aligned} \tag{6.152}$$

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.

Quadratic Potential Term

Now we consider the case when the first and the second derivatives of the potential term do not vanish but all the higher derivatives do, that is, the potential Q is now assumed to be a quadratic function (harmonic oscillator). Thus we have a nilpotent Lie algebra $\{\nabla_j^{\mathcal{A}}, \mathcal{R}_{jk}, Q, Q_{;j}, Q_{;jk}\}$ whose non-zero commutators are

$$[\nabla_j^{\mathcal{A}}, \nabla_k^{\mathcal{A}}] = iF_{jk}, \tag{6.153}$$

$$[\nabla_i^{\mathcal{A}}, Q] = Q_{;i} \tag{6.154}$$

$$[\nabla_j^{\mathcal{A}}, Q_{;i}] = 2P_{ij} \tag{6.155}$$

where $Q_{;i} = \nabla_i Q$ and

$$P_{ij} = \frac{1}{2}\nabla_i \nabla_j Q\,. \tag{6.156}$$

For our purposes, it will be helpful to introduce the following parametrization of the potential term

$$Q = M - \beta^{\mu\nu} L_\mu L_\nu, \tag{6.157}$$

where Greek indices range over $(\mu = 1, \ldots, p)$, with some $p \leq n$, and $\beta^{\mu\nu}$ is some constant symmetric nondegenerate $p \times p$ matrix, M is a constant and L_μ are some linear functions, that is, the double commutators with the derivatives vanish,

$$[\nabla_i^{\mathcal{A}}, [\nabla_j^{\mathcal{A}}, L_\mu]] = 0\,. \tag{6.158}$$

Then

$$P_{ij} = -\beta^{\mu\nu} L_{\mu;i} L_{\nu;j}\,. \tag{6.159}$$

This gives us another nilpotent Lie algebra, $\{\nabla_i^{\mathcal{A}},\ \mathcal{R}_{ij},\ M,\ L_\mu,\ L_{\mu;j}\}$, with the following nontrivial commutators

$$[\nabla_i^{\mathcal{A}}, \nabla_j^{\mathcal{A}}] = \mathcal{R}_{ij}, \tag{6.160}$$

$$[\nabla_i^{\mathcal{A}}, L_\mu] = L_{\mu;i}\,. \tag{6.161}$$

Now, let us introduce the generators $\xi_A = (\nabla_i^{\mathcal{A}}, L_\mu)$, where the capital Latin indices range over $(A = 1, \ldots, D)$, with $D = d + p$. Then we can rewrite the commutation relations in a more compact form

$$[\xi_A, \xi_B] = \mathcal{F}_{AB}, \tag{6.162}$$

$$[\xi_A, \mathcal{F}_{CD}] = [\mathcal{F}_{AB}, \mathcal{F}_{CD}] = 0, \tag{6.163}$$

where $\mathcal{F}_{AB}$ is a $D \times D$ matrix defined by

$$(\mathcal{F}_{AB}) = \begin{pmatrix} \mathcal{R}_{kj} & L_{\mu;k} \\ -L_{\mu;j} & 0 \end{pmatrix}. \tag{6.164}$$

The operator L can now be written in the form

$$L = -\gamma^{AB}\xi_A\xi_B + M, \tag{6.165}$$

where

$$(\gamma^{AB}) = \begin{pmatrix} \delta^{jk} & 0 \\ 0 & \beta^{\mu\nu} \end{pmatrix}. \tag{6.166}$$

The matrices $\beta^{\mu\nu}$ 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.

Note that the Lie algebra (6.162) is essentially of the same type as (6.148). For algebras of this kind the heat semi-group is given by the integral over the corresponding Lie group [8]

$$\begin{aligned} \exp(-tL) \;&=\; (4\pi t)^{-D/2} \det\left(\frac{\sinh(t\mathcal{F})}{t\mathcal{F}}\right)^{-1/2} \exp(-tM) \\ &\quad \times \int\limits_{\mathbb{R}^D} dk\, \gamma^{1/2} \exp\left\{-\frac{1}{4t} k^A \left[t\mathcal{F}\coth(t\mathcal{F})\right]_{AB} k^B\right\} \exp(k^C\xi_C)\,, \end{aligned} \tag{6.167}$$

where $\gamma = \det\gamma_{AB} = \det\beta_{\mu\nu}$ and γ_{AB} is the inverse of the matrix γ^{AB} and $\beta_{\mu\nu}$ is the inverse of the matrix $\beta^{\mu\nu}$.

Thus we have expressed the heat semi-group in terms of the operator $\exp(k^A\xi_A)$. Next, we split the integration variables $(k^A) = (q^i, \omega^\mu)$, use the Campbell-Hausdorff formula to single out the non-commutative part, and integrate over ω^μ.

To describe the result let us define the matrix

$$G(z) = [1 - z\mathcal{R} - z^2 P]^{-1}\,, \tag{6.168}$$

where P is the matrix (P_{ij}) and the set of matrices

$$B(t) = \oint_C \frac{dz}{2\pi i}\frac{t}{z^2}\coth(tz^{-1})G(z), \tag{6.169}$$

$$A(t) = \oint_C \frac{dz}{2\pi i}\frac{t}{z}\coth(tz^{-1})G(z), \tag{6.170}$$

$$C(t) = \oint_C \frac{dz}{2\pi i}t\coth(tz^{-1})G(z), \tag{6.171}$$

$$K(t) = \oint_C \frac{dz}{2\pi i}\frac{t}{z^2}\sinh(tz^{-1})G(z), \tag{6.172}$$

$$S(t) = \oint_C \frac{dz}{2\pi i}\frac{t}{z}\sinh(tz^{-1})G(z), \tag{6.173}$$

$$N(t) = \oint_C \frac{dz}{2\pi i}t\sinh(tz^{-1})G(z), \tag{6.174}$$

where the integral is taken over a sufficiently small counterclockwise oriented circle C around the origin.

After some long but straightforward calculation we obtain the heat semi-group

$$\exp(-tL) = (4\pi t)^{-n/2}\exp\left\{-tQ + \Phi(t) + \frac{1}{4}t^3 Q_{;i}\Psi^{ij}(t)Q_{;j}\right\} \tag{6.175}$$
$$\times \int_{\mathbb{R}^n} dq\,\exp\left\{-\frac{1}{4t}q^i D_{ij}(t)q^j - \frac{t}{2}Q_{;i}\left[\delta^i{}_j + A^i{}_j(t)\right]q^j\right\}\exp(q^k\nabla_k^A),$$

where

$$D(t) = B(t) + t^2[1 - A(t)]P[1 + t^2C(t)P]^{-1}[1 + A(t)], \tag{6.176}$$

$$\begin{aligned}\Phi(t) &= -\frac{1}{2}\log\det\left[1 + t^2N(t)P\right] \\ &\quad -\frac{1}{2}\log\det\left\{K(t) - t^2S(t)P[1 + t^2N(t)P]^{-1}S(t)\right\} \\ &\quad -\frac{1}{2}\log\det\left[1 + t^2C(t)P\right],\end{aligned} \tag{6.177}$$

$$\Psi(t) = [1 + t^2C(t)P]^{-1}C(t)\,. \tag{6.178}$$

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. (6.151) the integration over q in (6.175) becomes trivial and we obtain the heat kernel

$$\begin{aligned} U(t;x,x') &= (4\pi t)^{-n/2}\mathcal{P}(x,x')\exp\left\{-tQ(x)+\Phi(t)\right\} \\ &\times\exp\left\{\frac{1}{4}t^3 Q_{;i}(x)\Psi^{ij}(t)Q_{;j}(x)\right\} \\ &\times\exp\left\{-\frac{1}{4t}(x-x')^i D_{ij}(t)(x-x')^j\right\} \\ &\times\exp\left\{\frac{t}{2}Q_{;i}(x)[\delta^i{}_j+A^i{}_j(t)](x-x')^j\right\}. \end{aligned} \tag{6.179}$$

Expanding this expression in a power series in $(x-x')$ one can easily get *all* coincidence limits of covariant derivatives of the heat kernel. In particular, the heat kernel diagonal has a very simple form

$$U(t;x,x)=(4\pi t)^{-n/2}\exp\left\{-tQ+\Phi(t)+\frac{1}{4}t^3 Q_{;i}\Psi^{ij}(t)Q_{;j}\right\}. \tag{6.180}$$

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 tensor $\mathcal{R}_{ij}$ and the second derivatives of the potential term, $P_{ij}=\frac{1}{2}\nabla_i\nabla_j Q$.

Let us consider the particular case of (6.179) when the matrices $\mathcal{R}$ and P commute, i.e.

$$\mathcal{R}^i{}_j P^j{}_k = P^i{}_j \mathcal{R}^j{}_k\,. \tag{6.181}$$

One can show that in this special case the heat kernel diagonal reads

$$\begin{aligned} [U(t)] &= (4\pi t)^{-n/2}\det\left(\frac{\sinh(t\Delta)}{t\Delta}\right)^{-1/2}\exp(-tQ) \\ &\times\exp\left\{\frac{1}{4}tQ_{;i}\left[\frac{1}{P}\left(\frac{\Delta}{2tP}\frac{\cosh(t\mathcal{R})-\cosh(t\Delta)}{\sinh(t\Delta)}+1\right)\right]^i{}_j Q^{;j}\right\}, \end{aligned} \tag{6.182}$$

where

$$\Delta = (4P + \mathcal{R}^2)^{1/2} \,. \tag{6.183}$$

If the second derivatives of the potential vanish, $P_{ij} = \frac{1}{2}\nabla_i \nabla_j Q = 0$, then the heat kernel diagonal simplifies even further

$$\begin{aligned} [U(t)] &= (4\pi t)^{-n/2} \det \left(\frac{\sinh(t\mathcal{R})}{t\mathcal{R}} \right)^{-1/2} \exp(-tQ) \\ &\quad \times \exp\left\{ \frac{1}{4} t Q_{;i} \left(\frac{t\mathcal{R}\coth(t\mathcal{R}) - 1}{\mathcal{R}^2} \right)^i{}_j Q^{;j} \right\} . \end{aligned} \tag{6.184}$$

In the case when $\mathcal{R}_{ij} = 0$, the heat kernel diagonal has the form

$$\begin{aligned} [U(t)] &= (4\pi t)^{-n/2} \det \left(\frac{\sinh(2t\sqrt{P})}{2t\sqrt{P}} \right)^{-1/2} \exp(-tQ) \\ &\quad \times \exp\left\{ -\frac{1}{4} Q_{;i} \left(\frac{\tanh(t\sqrt{P}) - t\sqrt{P}}{P^{3/2}} \right)^i{}_j Q^{;j} \right\} . \end{aligned} \tag{6.185}$$

This is the case of a harmonic oscillator (with a quadratic potential).

6.5 Heat Kernel on Symmetric Spaces

6.5.1 Geometric Background

Algebraic Constraints

Let us consider the operator

$$L = -g^{ij} \nabla^{\mathcal{A}} \nabla^{\mathcal{A}} + Q \,, \tag{6.186}$$

where g_{ij} is a metric, $\mathcal{A}_i$ is a vector 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 the background fields vary slowly. This does not means 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,

$$\nabla_i R^j{}_{klm} = \nabla_i \mathcal{R}_{jk} = \nabla_i Q = 0\,. \tag{6.187}$$

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 puts a rather strict constraints on the possible algebraic structure of these tensors. By taking the commutator of second covariant derivatives of these tensors we get

$$R^{ij}{}_{km}R^k{}_{nlp} - R^{ij}{}_{kn}R^k{}_{mlp} + R^{ij}{}_{kl}R^k{}_{pmn} - R^{ij}{}_{kp}R^k{}_{lmn} = 0\,, \tag{6.188}$$

and

$$\mathcal{R}_{km}R^k{}_{lij} - \mathcal{R}_{kl}R^k{}_{mij} = 0\,. \tag{6.189}$$

The condition on the Riemann curvature tensor $R^i{}_{jkl}$ determines the geometry of so-called *locally symmetric spaces*. The condition of the tensor $\mathcal{R}_{ij}$ significantly restricts possible symmetric spaces with allow the existence of covariantly constant anti-symmetric 2-tensors. For example, the n-sphere, S^n is a symmetric space with the curvature tensor given by

$$R^i{}_{jkl} = \Lambda(\delta^i{}_k g_{jl} - \delta^i{}_l g_{jk})\,, \tag{6.190}$$

with some constant Λ. Substituting this curvature tensor in eq. (6.189) and contracting the indices l and i we obtain

$$(n-2)\mathcal{R}_{jm} = 0\,. \tag{6.191}$$

This means that such covariantly constant tensor can exists only on two-dimensional sphere, S^2. In higher dimensions these constraints can be satisfied only if $\mathcal{R}_{ij} = 0$.

That is why we will restrict below to a particular case of scalar Laplacian

$$L = -\Delta\,. \tag{6.192}$$

The general case is studied in [22]. The two-dimensional case is rather special and we will discuss it separately.

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 these lectures. So, our exposition will be necessarily sketchy, in particular, we omit most of the proofs and just try to describe the general ideas and the results.

Parallel Orthonormal Frame

Let x' be a fixed point in M and 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 ${e_a}^{i'}$, $a = 1, \dots, n$, be an orthonormal basis of vectors in the tangent space at the point x', that is,

$$g_{i'j'} {e_a}^{i'} {e_b}^{j'} = \delta_{ab} \,. \tag{6.193}$$

Such basis is called an *orthonormal frame*. We will use small Latin letters from the beginning of the alphabet, $a, b, c, \dots$, to denote frame indices. Of course, they range over $1, \dots, n$. Let ${e^a}_{i'}$ the *dual orthonormal frame* of covectors in the cotangent space at the point x', which means that

$${e^b}_{i'} {e_a}^{i'} = {\delta^b}_a \,. \tag{6.194}$$

We extend the local orthonormal frame at the fixed point x' to a local orthonormal frame at the point x by parallel transport

$$\begin{aligned} {e_a}^i &= {g^i}_{j'} {e_a}^{j'} \,, & (6.195) \\ {e^a}_i &= {g_i}^{j'} {e^a}_{j'} \,, & (6.196) \end{aligned}$$

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 world function defined in the lecture on differential geometry. It is equal to one-half the square of the geodesic distance between the points x and x'. As we have seen in that lecture 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,

$$R^a{}_{bcd} = R^i{}_{jkl} e^a{}_i e_b{}^j e_c{}^k e_d{}^l \,. \tag{6.197}$$

Since our frame is parallel along geodesics it should be clear that the frame components of a covariantly constant tensor are simply constant.

Normal Coordinates

Now, let us define the quantities

$$y^a = e^a{}_i \sigma^i = -e^a{}_{j'} \sigma^{j'} \,, \tag{6.198}$$

so that

$$\sigma^i = e_a{}^i y^a \qquad \text{and} \qquad \sigma^{i'} = -e_a{}^{i'} y^a \,. \tag{6.199}$$

Notice that $y^a = 0$ at $x = x'$. Further, we have the Jacobian matrix of the change of variables $x \mapsto y$,

$$\frac{\partial y^a}{\partial x^j} = -e^a{}_{i'} \eta^{i'}{}_j \,, \tag{6.200}$$

where $\eta^{i'}{}_j = \nabla_j \sigma^{i'}$. Therefore, the Jacobian is proportional to the Van Vleck determinant and is non-degenerate. Thus, the geometric parameters y^a provide a local coordinate system, which is called the *normal coordinates*.

Two remarks are in order here. First, strictly speaking, normal coordinates can be only defined locally, in geodesic balls of radius less than the injectivity radius of the manifold. However, for symmetric spaces normal coordinates cover the whole manifold except for a set of measure zero where they become singular. This set is precisely the set of points conjugate to the fixed point x' (where $\Delta^{-1}(x,x') = 0$) and of points that can be connected to the point x' by multiple geodesics. Thus normal coordinates on symmetric spaces

are non-singular almost everywhere. Thus, we will use the normal coordinates for the whole manifold. Second, for compact manifolds (or for manifolds with compact submanifolds) the range of some normal coordinates is also compact, so that if one allows them to range over the whole real line $\mathbb{R}$, then the corresponding compact submanifolds will be covered infinitely many times.

6.5.2 Curvature Tensor and Holonomy Algebra

We assumed that the manifold M is locally symmetric. We will also assume that it 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). Let R_{ijkl} be the curvature tensor of the manifold M. Let u^i and v^j be some vectors fields on M. The *sectional curvature* $K(u,v)$ in the plane spanned by the vectors u and v is defined by

$$K(u,v) = R_{ijkl}u^i u^k v^j v^l \,. \tag{6.201}$$

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-sompact symmetric space is called a *semi-simple* symmetric space. A generic symmetric space has the structure

$$M = M_0 \times M_s \,, \tag{6.202}$$

where $M_0 = \mathbb{R}^{n_0}$ and M_s is a semi-simple symmetric space,

$$M_s = M_+ \times M_- \,, \tag{6.203}$$

with M_+ a compact symmetric space and M_- a non-compact symmetric space. We will restrict ourselves below, for simplicity, to a semi-simple symmetric space which does not have a Euclidean factor. The Euclidean part adds just a trivial factor to the heat kernel. So, without loss of generality we assume that M is semi-simple.

Then one can show that the components of the curvature tensor can be presented in the form [13]

$$R_{abcd} = \beta_{\mu\nu} E^\mu{}_{ab} E^\mu{}_{cd} \,, \tag{6.204}$$

where $\beta_{\mu\nu}$, $\mu,\nu = 1,2,\dots,p$, is a symmetric nondegenerate $p \times p$ matrix, and $E^\mu{}_{ab}$ be 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 positive definite for compact symmetric spaces and negative definite for non-compact symmetric spaces. For a general space it is indefinite.

Next, we define the traceless $n \times n$ matrices $D_\mu = (D^a{}_{\mu b})$, where

$$D^a{}_{\mu b} = -\beta_{\mu\nu} E^\nu{}_{cb} \delta^{ca} \,. \tag{6.205}$$

Then the curvature tensor can be written as

$$R^a{}_{bcd} = -D^a{}_{\mu b} E^\mu{}_{cd} \,, \tag{6.206}$$

$$R^a{}_b{}^c{}_d = \beta^{\mu\nu} D^a{}_{\mu b} D^c{}_{\nu d} \,, \tag{6.207}$$

and the Ricci tensor and the scalar curvature are

$$R^a{}_b = -\beta^{\mu\nu} D^a{}_{\mu c} D^c{}_{\nu b}, \tag{6.208}$$

$$R = -\beta^{\mu\nu} D^a{}_{\mu c} D^c{}_{\nu a} \,. \tag{6.209}$$

Also, we have identically,

$$D^a{}_{\mu[b} E^\mu{}_{cd]} = 0 \,. \tag{6.210}$$

The matrices D_μ are known to be the generators of the *holonomy algebra*, $\mathcal{H}$, i.e. the Lie algebra of the restricted *holonomy group*, H. They satisfy the commutation relations

$$[D_\mu, D_\nu] = F^\alpha{}_{\mu\nu} D_\alpha \,, \tag{6.211}$$

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, that is, they satisfy the same commutation relations,

$$[F_\mu, F_\nu] = F^\alpha{}_{\mu\nu} F_\alpha \,. \tag{6.212}$$

These commutation relations follow directly from the *Jacobi identities*

$$F^\alpha{}_{\mu[\nu} F^\mu{}_{\lambda\gamma]} = 0 \,. \tag{6.213}$$

For symmetric spaces the introduced quantities satisfy additional algebraic constraints. The most important consequence of the eq. (6.188) is the equation [13]

$$E^{\mu}{}_{ac}D^{c}{}_{\alpha b} - E^{\mu}{}_{bc}D^{c}{}_{\alpha a} = F^{\mu}{}_{\alpha\beta}E^{\beta}{}_{ab}\,. \tag{6.214}$$

Next, by using the eqs. (6.211) and (6.214) one can prove that the matrix $\beta = (\beta_{\mu\nu})$ and the matrices F_α satisfy the equation

$$(F_\alpha)^T = -\beta F_\alpha \beta^{-1}\,, \tag{6.215}$$

which means, in particular, that the matrices F_α are traceless.

Another consequence of the eq. (6.214) are the identities

$$D^{a}{}_{\mu[b}R_{c]ade} + D^{a}{}_{\mu[d}R_{e]abc} = 0, \tag{6.216}$$

$$R^{a}{}_{c}D^{c}{}_{\mu b} = D^{a}{}_{\mu c}R^{c}{}_{b}\,. \tag{6.217}$$

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

$$C^{\mu}{}_{ab} = E^{\mu}{}_{ab}, \tag{6.218}$$

$$C^{a}{}_{\mu b} = -C^{a}{}_{b\mu} = D^{a}{}_{\mu b}, \tag{6.219}$$

$$C^{\mu}{}_{\alpha\beta} = F^{\mu}{}_{\alpha\beta}\,, \tag{6.220}$$

all other components being zero. Then we define $N \times N$ matrices C_A so that $(C_A)^{B}{}_{C} = C^{B}{}_{AC}$.

Then by using the eqs. (6.210), (6.211), (6.213) and (6.214) one can show that the quantities $C^{A}{}_{BC}$ satisfy the Jacobi identities

$$C^{A}{}_{B[C}C^{C}{}_{DE]} = 0\,. \tag{6.221}$$

This means that the matrices C_A satisfy the commutation relations

$$[C_A, C_B] = C^{C}{}_{AB}C_C\,, \tag{6.222}$$

and generate the adjoint representation of some Lie algebra $\mathcal{G}$ with the structure constants $C^{A}{}_{BC}$. Note that the holonomy algebra $\mathcal{H}$ is a subalgebra of the algebra $\mathcal{G}$.

Next, we define a symmetric nondegenerate $N \times N$ matrix $\gamma = (\gamma_{AB})$

$$\gamma = (\gamma_{AB}) = \begin{pmatrix} \delta_{ab} & 0 \\ 0 & \beta_{ik} \end{pmatrix}. \tag{6.223}$$

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. (6.214) one can show that the matrix γ and the matrices C_A satisfy the equation

$$(C_A)^T = -\gamma C_A \gamma^{-1} \,. \tag{6.224}$$

which means that the adjoint and the coadjoint representations of the algebra $\mathcal{G}$ are equivalent. In particular, the matrices C_A are traceless. Thus the algebra $\mathcal{G}$ is compact.

6.5.3 Killing Vectors Fields and Lie Derivatives

The Killing vector fields ξ_i are defined by the equation

$$\nabla_a \xi_b + \nabla_b \xi_a = 0 \,. \tag{6.225}$$

By differentiating this equation, commuting derivatives and using curvature identities we obtain

$$\nabla_a \nabla_b \xi^c = -R^c{}_{bda} \xi^d \,. \tag{6.226}$$

By induction we obtain

$$\nabla_{a_{2k}} \cdots \nabla_{a_1} \xi^b = (-1)^k R^b{}_{a_1 c_1 a_2} R^{c_1}{}_{a_3 c_2 a_4} \cdots R^{c_{k-1}}{}_{a_{2k-1} c_k a_{2k}} \xi^{c_k} \,, \tag{6.227}$$

$$\nabla_{a_{2k+1}} \cdots \nabla_{a_1} \xi^b = (-1)^k R^b{}_{a_1 c_1 a_2} R^{c_1}{}_{a_3 c_2 a_4} \cdots R^{c_{k-1}}{}_{a_{2k-1} c_k a_{2k}} c_{a_{2k+1}} \xi^{c_k} \,. \tag{6.228}$$

These derivatives determine all coefficients of the covariant Taylor series for the Killing vectors, and therefore, every Killing vector in a symmetric space has the form

$$\xi^a(x) = \left(\cos\sqrt{K}\right)^a{}_b \xi^b(x') + \left(\frac{\sin\sqrt{K}}{\sqrt{K}}\right)^a{}_b y^c \xi^b{}_{;c}(x') \,, \tag{6.229}$$

where $K = (K^a{}_b)$ is the matrix defined by

$$K^a{}_b = R^a{}_{cbd} y^c y^d \,. \tag{6.230}$$

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

$$P_a{}^i = e_b{}^i \left(\cos\sqrt{K}\right)^b{}_a , \tag{6.231}$$

$$L_\mu{}^i = -e_b{}^i \left(\frac{\sin\sqrt{K}}{\sqrt{K}}\right)^b{}_a y^c D^a{}_{\mu c} . \tag{6.232}$$

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

$$\mathcal{L}_A = \xi_A{}^i \partial_i . \tag{6.233}$$

These operators take particularly simple form in normal coordinates

$$\mathcal{L}_a = \left(\sqrt{K}\cot\sqrt{K}\right)^b{}_a \frac{\partial}{\partial y^b} , \tag{6.234}$$

$$\mathcal{L}_\mu = -D^b{}_{\mu a} y^a \frac{\partial}{\partial y^b} . \tag{6.235}$$

Then one can show that the differential operators $\mathcal{L}_A$ satisfy the commutation relations

$$[\mathcal{L}_A, \mathcal{L}_B] = C^C{}_{AB} \mathcal{L}_C , \tag{6.236}$$

and generate the *isometry algebra* of the symmetric space M. For semi-simple symmetric spaces the isometry algebra is isomorphic to the Lie algebra $\mathcal{G}$ defined above. Furthermore, the operators $\mathcal{L}_\mu$ form a Lie algebra

$$[\mathcal{L}_\mu, \mathcal{L}_\nu] = F^\alpha{}_{\mu\nu} \mathcal{L}_\alpha , \tag{6.237}$$

called the *isotropy subalgebra*; for semi-simple symmetric spaces the isotropy subalgebra is isomorphic to the holonomy algebra $\mathcal{H}$ defined above.

Killing vector fields satisfy many important identities. By using one of them,

$$\gamma^{AB} \xi_A{}^i \xi_B{}^j = g^{ij} . \tag{6.238}$$

we see that the scalar Laplacian Δ can be expressed in terms of Lie derivatives by

$$\Delta = \gamma^{AB}\mathcal{L}_A\mathcal{L}_B\,. \tag{6.239}$$

Then one can easily show that Laplacian commutes with Lie derivatives

$$[\mathcal{L}_A, \Delta] = 0\,. \tag{6.240}$$

6.5.4 Geometry of the Isometry Group

Let G be the isometry group and H be its holonomy subgroup. Both these groups have compact algebras. The holonomy group is always compact and the isometry group of a semi-simple symmetric space is semi-simple, which is a product $G = G_+ \times G_-$ of a compact G_+ and a non-compact G_- subgroups.

Let C_A be generators of the isometry algebra in adjoint representation defined above. Then every element of the isometry group can be represented in the form $\exp[C(k)]$, where

$$C(k) = k^A C_A\,, \tag{6.241}$$

and k^A are some real variables called the *canonical coordinates*. In the following ∂_M means the partial derivative

$$\partial_M = \frac{\partial}{\partial k^M} \tag{6.242}$$

with respect to the canonical coordinates.

We define the matrix $X = (X_A{}^M)$ (called the *right-invariant vector fields*) by

$$X = \frac{C(k)}{1 - \exp[-C(k)]}\,, \tag{6.243}$$

and the corresponding differential operators X_A on the isometry group by

$$X_A = X_A{}^M \partial_M\,. \tag{6.244}$$

Then the operators X_A satisfy the commutation relations

$$[X_A, X_B] = C^C{}_{AB} X_C\,, \tag{6.245}$$

and form a representation of the isometry algebra.

Further, there holds the following fundamental identity

$$(\det X)^{-1/2}\gamma^{AB}X_A{}^M\partial_M X_B{}^N\partial_N(\det X)^{1/2} = \frac{1}{6}R_G\,. \tag{6.246}$$

where

$$R_G = -\frac{1}{4}\gamma^{AB}C^C{}_{AD}C^D{}_{BC},\,. \tag{6.247}$$

Now, by using the right-invariant vector fields we define the metric on the isometry group G

$$G^{MN} = \gamma^{AB}X_A{}^M X_B{}^N\,. \tag{6.248}$$

Then the right-invariant vector fields are the Killing vector fields of the metric G_{MN}, the scalar curvature of this metric is precisely the quantity R_G defined above and the Riemannian volume element on the group is

$$|G|^{1/2} = (\det G_{MN})^{1/2} = |\gamma|^{1/2}\det\left(\frac{\sinh\left[C(k)/2\right]}{C(k)/2}\right)\,, \tag{6.249}$$

where $|\gamma| = \det\gamma_{AB}$.

Next, we define the operator

$$X^2 = \gamma^{AB}X_AX_B\,. \tag{6.250}$$

One can show that X^2 is nothing but the scalar Laplacian on the group

$$X^2 = |G|^{-1/2}\partial_M|G|^{1/2}G^{MN}\partial_N\,. \tag{6.251}$$

Then, by using the commutation relations eq. (6.245) one can show that the operator X^2 commutes with the operators X_A,

$$[X_A, X^2] = 0\,. \tag{6.252}$$

Heat Kernel on the Isometry Group

Let $\Phi(t;k)$ be a function on the group G defined by

$$\begin{aligned}\Phi(t;k) &= (4\pi t)^{-N/2}\det\left(\frac{\sinh\,\left[C(k)/2\right]}{C(k)/2}\right)^{-1/2} \\ &\quad\times\exp\left(-\frac{\langle k,\gamma k\rangle}{4t}+\frac{1}{6}R_G t\right)\,,\end{aligned} \tag{6.253}$$

where $\langle k, \gamma k\rangle = \gamma_{AB} k^A k^B$.

Then one can show that $\Phi(t;k)$ satisfies the heat equation

$$\partial_t \Phi = X^2 \Phi \,, \tag{6.254}$$

with the initial condition

$$\Phi(0;k) = |\gamma|^{-1/2} \delta(k) \,. \tag{6.255}$$

6.5.5 Heat Semigroup and Heat Kernel

Heat Semi-group

Let $\mathcal{L}_A$ be the Lie derivatives and $\mathcal{L}(k)$ be a differential operator defined by

$$\mathcal{L}(k) = k^A \mathcal{L}_A \,. \tag{6.256}$$

Then by using the properties of the operators X_A, in particular,

$$X_A \exp[\mathcal{L}(k)] = \exp[\mathcal{L}(k)] \mathcal{L}_A \,, \tag{6.257}$$

$$X^2 \exp[\mathcal{L}(k)] = \exp[\mathcal{L}(k)] \Delta \,, \tag{6.258}$$

and 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

$$\exp(t\Delta) = (4\pi t)^{-N/2} \exp\left(\frac{1}{6} R_G t\right) \tag{6.259}$$
$$\times \int\limits_{\mathbb{R}^N_{\rm reg}} dk \, |\gamma|^{1/2} \det\left(\frac{\sinh\left[C(k)/2\right]}{C(k)/2}\right)^{1/2} \exp\left\{-\frac{1}{4t} \langle k, \gamma k\rangle\right\} \exp[\mathcal{L}(k)] \,.$$

Here the notation $\mathbb{R}^N_{\rm reg}$ means that the integral over the canonical variables k^A needs to be regularized. We will discuss this issue later.

Heat Kernel

The heat kernel can be obtained now by acting by the heat semigroup $\exp(t\Delta)$ on the delta-function,

$$\begin{aligned} U(t;x,x') &= \exp(t\Delta)\delta(x,x') \\ &= \int\limits_{\mathbb{R}^N_{\rm reg}} dk \, |G|^{1/2} \Phi(t;k) \exp[\mathcal{L}(k)] \delta(x,x') \,. \end{aligned} \tag{6.260}$$

In particular, the heat kernel diagonal $U(t;x,x)$ is given by

$$U(t;x,x) \;=\; \int\limits_{\mathbb{R}^N_{\rm reg}} dk\;|G|^{1/2}\Phi(t;k)\exp[\mathcal{L}(k)]\delta(x,x')\Big|_{x=x'}\,. \quad (6.261)$$

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.

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 (6.234)-(6.235) and compute the heat kernel diagonal at the point x'.

Calculation of Isometries

Let $f(x)$ 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

$$\varphi(\tau,p,\omega;x,x') = \exp[\tau\mathcal{L}(k)]f(x)\,, \quad (6.262)$$

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

$$\partial_\tau\varphi = \mathcal{L}(k)f \quad (6.263)$$

with the initial condition

$$\varphi\Big|_{\tau=0} = f\,. \quad (6.264)$$

The operator $\mathcal{L}(k)$ generates a *flow* $\psi_\tau : M \to M$ so that the curve $\hat{x}(\tau) = \psi_\tau(x)$ satisfies the equation

$$\frac{d\hat{x}^i}{d\tau} = k^A\xi_A{}^i(\hat{x}) \quad (6.265)$$

with the initial condition

$$\hat{x}^i\big|_{\tau=0} = x^i\,. \quad (6.266)$$

The solution of this equation depends on the parameters τ,p,ω,x and x', that is,

$$\hat{x} = \hat{x}(\tau,p,\omega,x,x')\,. \quad (6.267)$$

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

$$\det\left(\frac{\partial \hat{x}^\mu}{\partial p^a}\right) \neq 0 \tag{6.268}$$

is not equal to zero, and, therefore, the coordinates p can be used to parametrize the point $\hat{x}$, that is, the eq. (6.267) defines the function

$$p = p(\tau, \omega, \hat{x}, x, x')\,. \tag{6.269}$$

It is not difficult to prove that

$$\varphi(\tau, p, \omega, x, x') = f(\hat{x}(\tau, p, \omega, x, x'))\,. \tag{6.270}$$

Therefore,

$$\exp[\mathcal{L}(k)]f(x) = f(\hat{x}(1, p, \omega, x, x'))\,, \tag{6.271}$$

in particular,

$$\exp[\mathcal{L}(k)]\delta(x, x') = \delta(\hat{x}(1, p, \omega, x, x'), x')\,. \tag{6.272}$$

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

$$\hat{x}(1, \bar{p}, \omega, x, x') = x'\,. \tag{6.273}$$

Thus, eq. (6.273) 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,

$$\bar{p}(\omega, x, x') = p(1, \omega, \hat{x}, x, x')\Big|_{\hat{x}=x'}\,. \tag{6.274}$$

Then by making the change of variables $\hat{x} \mapsto p$ we obtain

$$\exp[\mathcal{L}(k)]\delta(x, x') = J(\omega, x, x')\delta[p - \bar{p}(\omega, x, x')]\,. \tag{6.275}$$

where

$$J(\omega, x, x') = g^{-1/2}(x')\det\left(\frac{\partial \hat{x}^i}{\partial p^a}\right)^{-1}\Big|_{p=\bar{p},\tau=1}\,. \tag{6.276}$$

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. Thus we need to compute the Jacobian $J(\omega, x, x')$.

Now, 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. (6.234) and (6.235) the equation (6.265) becomes

$$\frac{d\hat{y}^a}{d\tau} = \left(\sqrt{K(\hat{y})}\cot\sqrt{K(\hat{y})}\right)^a{}_b\, p^b - \omega^\mu D^a{}_{\mu b}\hat{y}^b\,, \tag{6.277}$$

with the initial condition

$$\hat{y}^a\big|_{\tau=0} = y^a\,. \tag{6.278}$$

The solution of this equation defines a function $\hat{y} = \hat{y}(\tau, p, \omega, y)$, which implicitly defines the function

$$p = p(\tau, \omega, \hat{y}, y)\,. \tag{6.279}$$

The function $\bar{p} = \bar{p}(\omega, y)$ is now defined by the equation

$$\hat{y}(1, \bar{p}, \omega, y) = 0\,, \tag{6.280}$$

or

$$\bar{p}(\omega, y) = p(1, \omega, 0, y)\,, \tag{6.281}$$

and the Jacobian $J(\omega, x, x')$ is now determined by

$$J(\omega, x, x') = \det\left(\frac{\partial\hat{y}^a}{\partial p^b}\right)^{-1}\Big|_{p=\bar{p},\tau=1}\,. \tag{6.282}$$

Next, we define the matrix $D(\omega)$ by

$$D(\omega) = \omega^\mu D_\mu\,. \tag{6.283}$$

Then the Taylor expansion of the function $\hat{y} = \hat{y}(\tau, p, \omega, y)$ in p and y reads

$$\hat{y}^a = (\exp[-\tau D(\omega)])^a{}_b y^b + \left(\frac{1-\exp[-\tau D(\omega)]}{D(\omega)}\right)^a{}_b p^b + O(y^2, p^2, py)\,. \tag{6.284}$$

Therefore, we find with the same accuracy the Taylor expansion of the function $\bar{p}(\omega, y)$ in y

$$\bar{p}^a = -\left(D(\omega)\frac{\exp[-D(\omega)]}{1-\exp[-D(\omega)]}\right)^a{}_b y^b + O(y^2)\,. \tag{6.285}$$

By using these equations we finally obtain the Jacobian

$$J(\omega, x, x') = \det\left(\frac{\sinh[\,D(\omega)/2]}{D(\omega)/2}\right)^{-1} + O(y)\,. \tag{6.286}$$

This should be enough to compute the heat kernel for small y (or x close to x'), in particular, the heat kernel diagonal when $x = x'$.

Remarks. We implicitly assumed above that there are no closed geodesics and that the equation of closed orbits of isometries

$$\hat{y}^a(1, \bar{p}, \omega, 0) = 0 \tag{6.287}$$

has a unique solution $\bar{p} = 0$. This is indeed true for non-compact symmetric spaces. However, on compact symmetric spaces this is not true: there are infinitely many closed geodesics and infinitely many closed orbits of isometries. This is reflected in the fact that the Jacobian $J(\omega, x, x')$ (6.282) can become singular for some values of ω^μ.

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. That is why we propose below to complexify the holonomy group (that is, let the coordinates ω^μ take complex values) in such a way that the equation (6.287) has a unique solution and the Jacobian is an analytic function. We will show below how this works in the case of the two-sphere, S^2.

In any case, these global solutions will not affect our local analysis. In particular, they do not affect the asymptotics of the heat kernel. That is why, we have neglected them here.

Heat Kernel

We define the matrix $F(\omega)$ by

$$F(\omega) = \omega^\mu F_\mu\,, \tag{6.288}$$

a scalar R_H by

$$R_H = -\frac{1}{4}\beta^{\alpha\beta}F^{\mu}{}_{\alpha\gamma}F^{\gamma}{}_{\beta\mu}\,, \tag{6.289}$$

and a matrix $B(\omega)$ by

$$B(\omega) = \left(\frac{\sinh\,[\,D(\omega)/2]}{D(\omega)/2}\right)^{-2}\,. \tag{6.290}$$

Then by using the above results one can compute the heat kernel of the scalar Laplacian Δ for x close to x'. We obtain

$$\begin{aligned} U(t;x,x') = (4\pi t)^{-n/2}\exp\left\{\left(\frac{1}{8}R+\frac{1}{6}R_H\right)t\right\} \\ \times\int\limits_{\mathbb{R}^n_{\rm reg}}\frac{d\omega}{(4\pi t)^{p/2}}\,|\beta|^{1/2}\exp\left\{-\frac{1}{4t}\left[\langle\omega,\beta\omega\rangle+\langle y,B(\omega)y\rangle\right]\right\} \\ \times\det\left(\frac{\sinh\,[\,F(\omega)/2]}{F(\omega)/2}\right)^{1/2}\det\left(\frac{\sinh\,[\,D(\omega)/2]}{D(\omega)/2}\right)^{-1/2} \\ +O(y)\,, \end{aligned} \tag{6.291}$$

where $|\beta| = \det\beta_{\mu\nu}$, $\langle\omega,\beta\omega\rangle = \beta_{\mu\nu}\omega^\mu\omega^\nu$ and $\langle y,B(\omega)y\rangle = y^aB_{ab}(\omega)y^b$.

Heat Kernel Diagonal

In particular, by setting $x = x'$, that is, $y = 0$, we obtain the heat kernel diagonal

$$\begin{aligned} U(t;x,x) &= (4\pi t)^{-n/2}\exp\left\{\left(\frac{1}{8}R+\frac{1}{6}R_H\right)t\right\} \\ &\times\int\limits_{\mathbb{R}^n_{\rm reg}}\frac{d\omega}{(4\pi t)^{p/2}}\,|\beta|^{1/2}\exp\left\{-\frac{1}{4t}\,\langle\omega,\beta\omega\rangle\right\} \\ &\times\det\left(\frac{\sinh\,[\,F(\omega)/2]}{F(\omega)/2}\right)^{1/2}\det\left(\frac{\sinh\,[\,D(\omega)/2]}{D(\omega)/2}\right)^{-1/2}\,. \end{aligned} \tag{6.292}$$

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

$$\langle f(\omega)\rangle = \int\limits_{\mathbb{R}^p_{\rm reg}}\frac{d\omega}{(4\pi)^{p/2}}\,|\beta|^{1/2}\exp\left(-\frac{1}{4}\,\langle\omega,\beta\omega\rangle\right)f(\omega) \tag{6.293}$$

Then we can write

$$U(t;x,x) = (4\pi t)^{-n/2} \exp\left\{\left(\frac{1}{8}R + \frac{1}{6}R_H\right)t\right\} \tag{6.294}$$

$$\times\left\langle \det\left(\frac{\sinh\left[\sqrt{t}\,F(\omega)/2\right]}{\sqrt{t}\,F(\omega)/2}\right)^{1/2} \det\left(\frac{\sinh\left[\sqrt{t}\,D(\omega)/2\right]}{\sqrt{t}\,D(\omega)/2}\right)^{-1/2}\right\rangle$$

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

$$\langle \omega_1^\mu \cdots \omega^{\mu_{2k+1}}\rangle = 0\,, \tag{6.295}$$

$$\langle \omega^{\mu_1} \cdots \omega^{\mu_{2k}}\rangle = \frac{(2k)!}{k!}\beta^{(\mu_1\mu_2}\cdots\beta^{\mu_{2k-1}\mu_{2k})}\,, \tag{6.296}$$

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

$$[a^\mu, a_\nu^*] = \delta^\mu{}_\nu\,, \tag{6.297}$$

$$[a^\mu, a^\nu] = [a_\mu^*, a_\nu^*] = 0\,. \tag{6.298}$$

Let $|0\rangle$ be a unit vector in the Hilbert space, called the *vacuum vector*, that satisfies the equations

$$\langle 0|0\rangle = 1\,, \tag{6.299}$$

$$a^\mu|0\rangle = \langle 0|a_\nu^* = 0\,. \tag{6.300}$$

Then the Gaussian average is nothing but the vacuum expectation value

$$\langle f(\omega)\rangle = \langle 0|f(a)\exp\langle a^*, \beta a^*\rangle|0\rangle\,, \tag{6.301}$$

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. (6.295), (6.296).

Regularization and Analytical Continuation

The above calculation was rather formal. In particular, we were not very careful with the range of the canonical coordinates k^A and ω^μ. As a result we obtained some integrals which have singularities if one extends the integration to the whole Euclidean space $\mathbb{R}^N$. That is why we need to regularize those integrals. In order to that we complexify the isometry group in the following sense. We extend the canonical coordinates $(k^A) = (p^a, \omega^\mu)$ to the whole complex Euclidean space $\mathbb{C}^N$. Then all group-theoretic functions introduced above become analytic functions of k^A possibly with some poles on the real section $\mathbb{R}^N$ for compact groups. In fact, we replace the actual real slice $\mathbb{R}^N$ of $\mathbb{C}^N$ with an N-dimensional subspace $\mathbb{R}^N_{\rm reg}$ in $\mathbb{C}^N$ obtained by rotating the real section $\mathbb{R}^N$ counterclockwise in $\mathbb{C}^N$ by $\pi/4$. That is, we replace each coordinate k^A by $e^{i\pi/4}k^A$. In the complex domain the group becomes non-compact. We call this procedure the *decompactification*. If the group is compact, or has a compact subgroup, then this plane will cover the original group infinitely many times.

Since the metric $(\gamma_{AB}) = \mathrm{diag}\,(\delta_{ab}, \beta_{\mu\nu})$ is not necessarily positive definite, (actually, only the metric of the holonomy group $\beta_{\mu\nu}$ is non-definite) we analytically continue the function $\Phi(t;k)$ in the complex plane of t with a cut along the negative imaginary axis so that $-\pi/2 < \arg t < 3\pi/2$. Thus, the function $\Phi(t;k)$ defines an analytic function of t and k^A. We also consider t to be *real negative*, $t < 0$. This is needed in order to make all integrals convergent and well defined and to be able to do the analytical continuation.

Note that the singularities occur only in the holonomy group. This means that there is no need to complexify the coordinates p^a. Thus, we assume the coordinates p^a to be real and the coordinates ω^μ to be complex, more precisely, to take values in the p-dimensional subspace $\mathbb{R}^p_{\rm reg}$ of $\mathbb{C}^p$ obtained by rotating $\mathbb{R}^p$ counterclockwise by $\pi/4$ in $\mathbb{C}^p$ That is, we have $\mathbb{R}^N_{\rm reg} = \mathbb{R}^n \times \mathbb{R}^p_{\rm reg}$.

This procedure (that we call a *regularization*) with the nonstandard contour of integration is necessary for the convergence of the integrals above since we are treating both the compact and the non-compact symmetric spaces simultaneously. Remember, that, in general, the nondegenerate diagonal matrix $\beta_{\mu\nu}$ is not positive definite. The space $\mathbb{R}^p_{\rm reg}$ is chosen in such a way to make the Gaussian exponent purely imaginary. Then the indefiniteness of the ma-

trix β does not cause any problems. Moreover, the integrand does not have any singularities on these contours. The convergence of the integral is guaranteed by the exponential growth of the sine for imaginary argument. These integrals can be computed then in the following way. The coordinates ω^μ corresponding to the compact directions are rotated further by another $\pi/4$ to imaginary axis and the coordinates ω^μ corresponding to the non-compact directions are rotated back to the real axis. Then, for $t < 0$ all the integrals above are well defined and convergent and define an analytic function of t in a complex plane with a cut along the negative imaginary axis.

6.5.6 Heat Kernel on S^2 and H^2

Two-sphere

Let us apply our result to a special case of a two-sphere S^2 of radius r, which is a compact symmetric space equal to the quotient of the isometry group, $SO(3)$, by the isotropy group, $SO(2)$,

$$S^2 = SO(3)/SO(2). \tag{6.302}$$

Let y^a be the normal coordinates defined above. On the 2-sphere of radius r they range over $-r\pi \le y^a \le r\pi$. We define the polar coordinates ρ and φ by

$$y^1 = \rho\cos\varphi, \qquad y^2 = \rho\sin\varphi\,, \tag{6.303}$$

so that $0 \le \rho \le r\pi$ and $0 \le \varphi \le 2\pi$.

The orthonormal frame of 1-forms is

$$e^1 = d\rho\,, \qquad e^2 = r\sin\left(\frac{\rho}{r}\right) d\varphi\,, \tag{6.304}$$

which gives the curvature

$$R_{abcd} = \frac{1}{r^2}\varepsilon_{ab}\varepsilon_{cd} = \frac{1}{r^2}(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})\,, \tag{6.305}$$

with ε_{ab} being the antisymmetric Levi-Civita tensor, that is, $\varepsilon_{12} = -\varepsilon_{21} = 1$, the Ricci tensor

$$R_{ab} = \frac{1}{r^2}\delta_{ab}\,, \tag{6.306}$$

and the scalar curvature

$$R = \frac{2}{r^2}\,. \tag{6.307}$$

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 holonomy group $\beta_{\mu\nu}$ is now just a constant, $\beta = 1/r^2$. The only generator of the holonomy group in the vector representation is

$$D_{ab} = -\frac{1}{r^2} E_{ab} = -\frac{1}{r^2}\varepsilon_{ab}\,. \tag{6.308}$$

The Lie derivatives $\mathcal{L}_A$ are given by

$$\mathcal{L}_1 = \cos\varphi\partial_\rho - \frac{\sin\varphi}{r}\cot\left(\frac{\rho}{r}\right)\partial_\varphi\,, \tag{6.309}$$

$$\mathcal{L}_2 = \sin\varphi\partial_\rho + \frac{\cos\varphi}{r}\cot\left(\frac{\rho}{r}\right)\partial_\varphi\,, \tag{6.310}$$

$$\mathcal{L}_3 = \frac{1}{r^2}\partial_\varphi\,, \tag{6.311}$$

and form a representation of the $SO(3)$ algebra

$$[\mathcal{L}_1, \mathcal{L}_2] = -\mathcal{L}_3\,, \tag{6.312}$$

$$[\mathcal{L}_3, \mathcal{L}_1] = -\frac{1}{r^2}\mathcal{L}_2 \tag{6.313}$$

$$[\mathcal{L}_3, \mathcal{L}_2] = \frac{1}{r^2}\mathcal{L}_1\,. \tag{6.314}$$

The Laplacian is given by

$$\Delta = \partial_\rho^2 + \frac{1}{r}\cot\left(\frac{\rho}{r}\right)\partial_\rho + \frac{1}{r^2\sin^2(\rho/r)}\partial_\varphi^2\,. \tag{6.315}$$

The contour of integration over ω in (6.292) should be the real axis rotated counterclockwise by $\pi/4$. Since S^2 is compact, we rotate it further to the imaginary axis, compute the determinant

$$\det\left(\frac{\sinh[\omega D]}{\omega D}\right)^{-1/2} = \frac{\omega/(2r^2)]}{\sin[\omega/(2r^2)]}\,, \tag{6.316}$$

and rescale ω for $t < 0$ by $\omega \to r\sqrt{-t}\,\omega$ to obtain an analytic function

of t

$$\begin{aligned} U(t;x,x) &= \frac{1}{4\pi t}\exp\left(\frac{t}{4r^2}\right) \\ &\quad\times\int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{4\pi}}\exp\left(-\frac{\omega^2}{4}\right)\frac{\omega\sqrt{-t}/(2r)}{\sinh\left[\omega\sqrt{-t}/(2r)\right]}\,. \end{aligned} \tag{6.317}$$

If we would have rotated the contour to the real axis instead then we would have obtained after rescaling $\omega \to r\sqrt{t}\,\omega$ for $t > 0$,

$$\begin{aligned} U^{\rm diag}(t) &= \frac{1}{4\pi t}\exp\left(\frac{t}{4r^2}\right) \\ &\quad\times P\int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{4\pi}}\exp\left(-\frac{\omega^2}{4}\right)\frac{\omega\sqrt{t}/(2r)}{\sin\left[\omega\sqrt{t}/(2r)\right]}\,, \end{aligned} \tag{6.318}$$

where $P\int$ denotes the Cauchy principal value of the integral. This can also be written as

$$\begin{aligned} &U(t;x,x) = \frac{1}{4\pi t}\exp\left(\frac{t}{4r^2}\right) \\ &\times\sum_{k=-\infty}^{\infty}(-1)^k\int_0^{2\pi r/\sqrt{t}}\frac{d\omega}{\sqrt{4\pi}}\exp\left[-\frac{1}{4}\left(\omega+\frac{2\pi r}{\sqrt{t}}k\right)^2\right]\frac{\sqrt{t}}{2r}\frac{\left(\omega+\frac{2\pi r}{\sqrt{t}}k\right)}{\sin\left[\omega\sqrt{t}/(2r)\right]}\,. \end{aligned} \tag{6.319}$$

This is nothing but the sum over the closed geodesics of S^2.

Hyperbolic Plane

The non-compact symmetric space dual to the 2-sphere is the hyperbolic plane H^2. It is equal to the quotient of the isometry group, $SO(1,2)$, by the isotropy group, $SO(2)$,

$$H^2 = SO(1,2)/SO(2). \tag{6.320}$$

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

$$y^1 = u\cos\varphi, \qquad y^2 = u\sin\varphi\,, \tag{6.321}$$

so that $0 \le u \le \infty$ and $0 \le \varphi \le 2\pi$.

The orthonormal frame of 1-forms is

$$e^1 = du\,, \qquad e^2 = a\sinh\left(\frac{u}{a}\right)d\varphi\,, \tag{6.322}$$

where a is a real parameter, which gives the curvature

$$R_{abcd} = -\frac{1}{a^2}\varepsilon_{ab}\varepsilon_{cd} = -\frac{1}{a^2}(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})\,, \tag{6.323}$$

$$R_{ab} = -\frac{1}{a^2}\delta_{ab}\,, \tag{6.324}$$

$$R = -\frac{2}{a^2}\,. \tag{6.325}$$

The metric of the isotropy group $\beta_{\mu\nu}$ is just a constant, $\beta = -1/a^2$, and the only generator of the isotropy group in the vector representation is given by

$$D_{ab} = \frac{1}{a^2}E_{ab} = \frac{1}{a^2}\varepsilon_{ab}\,. \tag{6.326}$$

The Lie derivatives $\mathcal{L}_A$ are now

$$\mathcal{L}_1 = \cos\varphi\partial_u - \frac{\sin\varphi}{a}\coth\left(\frac{u}{a}\right)\partial_\varphi\,, \tag{6.327}$$

$$\mathcal{L}_2 = \sin\varphi\partial_u + \frac{\cos\varphi}{a}\coth\left(\frac{u}{a}\right)\partial_\varphi\,, \tag{6.328}$$

$$\mathcal{L}_3 = -\frac{1}{a^2}\partial_\varphi\,, \tag{6.329}$$

and form a representation of the $SO(1,2)$ algebra

$$[\mathcal{L}_1, \mathcal{L}_2] = -\mathcal{L}_3\,, \tag{6.330}$$

$$[\mathcal{L}_3, \mathcal{L}_1] = \frac{1}{a^2}\mathcal{L}_2 \tag{6.331}$$

$$[\mathcal{L}_3, \mathcal{L}_2] = -\frac{1}{a^2}\mathcal{L}_1\,. \tag{6.332}$$

The Laplacian is given by

$$\Delta = \partial_u^2 + \frac{1}{a}\coth\left(\frac{u}{a}\right)\partial_u + \frac{1}{a^2\sinh^2(u/a)}\partial_\varphi^2\,. \tag{6.333}$$

The contour of integration over ω in (6.292) 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

$$U(t;x,x) = \frac{1}{4\pi t}\exp\left(-\frac{t}{4a^2}\right) \times \int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{4\pi}}\exp\left(-\frac{\omega^2}{4}\right)\frac{\omega\sqrt{t}/(2a)}{\sinh\left[\omega\sqrt{t}/(2a)\right]}\,. \tag{6.334}$$

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, $a^2 \to -r^2$, or $a \to ir$, or, alternatively, by replacing $t \to -t$ (and $a = r$). One can go even further and compute the Plancherel (or Harish-Chandra) measure $\mu(\nu)$ in the case of H^2 and the spectrum in the case of S^2.

For H^2 we rescale the integration variable in (6.334) by $\omega \to \omega a/\sqrt{t}$, substitute

$$\frac{a}{\sqrt{4\pi t}}\exp\left(-\frac{a^2}{4t}\omega^2\right) = \int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\exp\left(-\frac{t}{a^2}\nu^2 + i\omega\nu\right)\,, \tag{6.335}$$

integrate by parts over ν, and use

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\,\frac{e^{i\omega\nu}}{\sinh\,(\omega/2)} = \tanh\,(\pi\nu) \tag{6.336}$$

to represent the heat kernel for H^2 in the form

$$U(t;x,x) = \frac{1}{4\pi a^2}\int_{-\infty}^{\infty} d\nu\;\mu(\nu)\exp\left\{-\left(\frac{1}{4}+\nu^2\right)\frac{t}{a^2}\right\}\,, \tag{6.337}$$

where

$$\mu(\nu) = \nu\tanh\nu\,. \tag{6.338}$$

For S^2 we proceed as follows. We cannot just substitute $a^2 \to -r^2$ in (6.337). Instead, first, we deform the contour of integration in (6.337) 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 $a^2 \to -r^2$, 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

$$d_k = k + \frac{1}{2}, \qquad k = 0, \pm 1 \pm 2, \dots , \tag{6.339}$$

Therefore, we can compute the integral by residue theory to get

$$U(t; x, x) = \frac{1}{4\pi r^2} \sum_{k=0}^{\infty} d_k \exp\left(-\lambda_k t\right) , \tag{6.340}$$

where

$$\lambda_k = \frac{1}{r^2} k(k+1) . \tag{6.341}$$

Thus, the analytic continuation from the hyperbolic plane allowed us to compute the spectrum for the sphere.

Chapter 7

Extensions and Applications in Finance

7.1 Heat Semi-group

7.1.1 Time-Independent Operators

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

$$U(t) = \exp(-tA) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} t^k A^k \tag{7.1}$$

is defined by the operator heat equation

$$(\partial_t + A)U(t) = 0 \tag{7.2}$$

with the initial condition

$$U(0) = I\,, \tag{7.3}$$

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

$$U(t_1 + t_2) = U(t_1)U(t_2)\,. \tag{7.4}$$

That is why, it is called the *heat semi-group*. 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 $t > 0$.

Duhamel Formula

We derive an integral equation for the heat semi-group. Let us decompose the operator A in two parts

$$A = A_0 + sA_1\,, \tag{7.5}$$

where s is a parameter. Let $U(t)$ be the heat semi-group of the operator A, and $U_0(t)$ be the semi-group of the operator A_0. Let

$$U(t) = U_0(t)K(t)\,. \tag{7.6}$$

Then the operator K satisfies the equation

$$\partial_t K(t) = -sU_0(-t)A_1U_0(t)K(t) \tag{7.7}$$

with initial condition

$$K(0) = 1\,. \tag{7.8}$$

By integrating this equation we obtain

$$K(t) = 1 - s\int_0^t d\tau\; U_0(-\tau)A_1U_0(\tau)K(\tau)\,, \tag{7.9}$$

and, therefore,

$$U(t) = U_0(t) - s\int_0^t d\tau\; U_0(t-\tau)A_1U(\tau)\,. \tag{7.10}$$

Similarly, we can obtain

$$U(t) = U_0(t) - s\int_0^t d\tau\; U(\tau)A_1U_0(t-\tau)\,. \tag{7.11}$$

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

$$\partial_s U(t) = -\int_0^t d\tau\; U(t-\tau)[\partial_s A]U(\tau)\,. \tag{7.12}$$

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.

Volterra Series

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

$$A(s) = A_0 + sA_1\,, \tag{7.13}$$

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

Then the Duhamel formula reads

$$\partial_s U(t) = -\int_0^t d\tau\; U(t-\tau)A_1U(\tau)\,. \tag{7.14}$$

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

$$\begin{aligned} U(t) &= U_0(t) + \sum_{k=1}^{\infty}(-1)^k s^k \int_0^t d\tau_k \int_0^{\tau_k} d\tau_{k-1}\cdots\int_0^{\tau_2} d\tau_1 \\ &\quad \times U_0(t-\tau_k)A_1U_0(\tau_k-\tau_{k-1})\cdots U_0(\tau_2-\tau_1)A_1U_0(\tau_1)\,. \end{aligned} \tag{7.15}$$

This expansion is called *Volterra series*.

Let us define an operator Ad_A that acts on operators as

$$Ad_A B = [A, B]\,. \tag{7.16}$$

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

$$(Ad_A)^k B = \underbrace{[A, [A, \cdots, [A, B]\cdots]]}_{k}\,. \tag{7.17}$$

Let us consider an operator-valued function

$$F(t) = e^{tA}Be^{-tA}\,. \tag{7.18}$$

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

$$\partial_t F = [A, F] = Ad_A F\,, \tag{7.19}$$

with an obvious initial condition

$$F(0) = B\,. \tag{7.20}$$

The solution of this equation is

$$F(t) = \exp[tAd_A]B\,. \tag{7.21}$$

Thus, we obtain a very useful expansion

$$\begin{aligned} e^{tA}Be^{-tA} &= \sum_{k=0}^{\infty}\frac{t^k}{k!}(Ad_A)^k B \\ &= B + t[A,B] + \frac{1}{2}t^2[A,[A,B]] + O(t^3)\,. \end{aligned} \tag{7.22}$$

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

$$\begin{aligned} V(t) &= e^{tA_0}A_1e^{-tA_0} = e^{tAd_{A_0}}A_1 \\ &= A_1 + t[A_0,A_1] + \frac{1}{2}t^2[A_0,[A_0,A_1]] + O(t^3)\,. \end{aligned} \tag{7.23}$$

Then Volterra series can be written in two equivalent forms

$$\begin{aligned} U(t) &= U_0(t)\Bigg\{I + \sum_{k=1}^{\infty}(-1)^k s^k \int_0^t d\tau_k \int_0^{\tau_k} d\tau_{k-1}\cdots\int_0^{\tau_2} d\tau_1 \\ &\qquad \times V(\tau_k)\cdots V(\tau_2)V(\tau_1)\Bigg\}\,, \end{aligned} \tag{7.24}$$

or

$$\begin{aligned} U(t) &= \Bigg\{I + \sum_{k=1}^{\infty}(-1)^k s^k \int_0^t d\tau_k \int_0^{\tau_k} d\tau_{k-1}\cdots\int_0^{\tau_2} d\tau_1 \\ &\qquad \times V(\tau_k - t)V(\tau_{k-1}-t)\cdots V(\tau_1 - t)\Bigg\}U_0(t)\,, \end{aligned} \tag{7.25}$$

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

$$U(t) = \left\{1 - stA_1 + \frac{t^2}{2}\left(s^2A_1^2 + s[A_0,A_1]\right) + O(t^3)\right\}U_0(t)\,. \tag{7.26}$$

Chronological Exponent

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

$$0 \le \tau_1 \le \tau_2 \le \tau_3 \le \cdots \le \tau_k \le t\,. \tag{7.27}$$

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

$$\begin{aligned} U(t) &= U_0(t)\left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} \int_0^t d\tau_k \cdots \int_0^t d\tau_2 \int_0^t d\tau_1\, V(\tau_k)\cdots V(\tau_1) \right\} \\ &= U_0(t)\left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} \left(\int_0^t d\tau\, V(\tau) \right)^k \right\} \\ &= U_0(t) \exp\left(-s \int_0^t d\tau\, V(\tau) \right)\,. \end{aligned} \tag{7.28}$$

Similar argument can be used to rewrite the perturbation series in general case 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,

$$T\left[V(\tau_2)V(\tau_1)\right] = \begin{cases} V(\tau_2)V(\tau_1) & \text{if } \tau_1 < \tau_2\,, \\ V(\tau_1)V(\tau_2) & \text{if } \tau_1 > \tau_2\,. \end{cases} \tag{7.29}$$

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,

$$T\left[V(\tau_{i_k})\cdots V(\tau_{i_1})\right] = V(\tau_k)\cdots V(\tau_1)\,. \tag{7.30}$$

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

in the following form

$$\begin{aligned} U(t) &= U_0(t)\left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} \int_0^t d\tau_k \cdots \int_0^t d\tau_2 \int_0^t d\tau_1 \, T\left[V(\tau_k)\cdots V(\tau_1)\right] \right\} \\ &= U_0(t)\left\{ I + \sum_{k=1}^{\infty} \frac{(-s)^k}{k!} T\left(\int_0^t d\tau \, V(\tau) \right)^k \right\} \\ &= U_0(t)\, T \exp\left(-s \int_0^t d\tau \, V(\tau) \right) . \end{aligned} \tag{7.31}$$

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

$$\exp[-t(A_0 + sA_1)] = e^{-tA_0} T \exp\left(-s \int_0^t d\tau \, e^{\tau A_0} A_1 e^{-\tau A_0} \right) \tag{7.32}$$

It will be convenient to rewrite this equation in another form. Let

$$B(\tau, t) = V(\tau - t) = e^{(\tau - t)A_0} A_1 e^{-(\tau - t)A_0} . \tag{7.33}$$

Then we have

$$U(t) = T \exp\left(-s \int_0^t d\tau \, B(\tau, t) \right) U_0(t) . \tag{7.34}$$

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. Then

$$V(\tau) = A_1 + \tau [A_0, A_1] , \tag{7.35}$$

and the chronological exponent becomes

$$U(t) \;=\; \exp\left(-stA_1 + s\frac{t^2}{2}[A_0, A_1]\right) U_0(t)\,, \tag{7.36}$$

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 $O(t^3)$.

7.1.2 Time Dependent Operators

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

$$[\partial_t + A(t)]U(t, t') = 0 \tag{7.37}$$

and the initial condition

$$U(t', t') = I\,. \tag{7.38}$$

It satisfies the semi-group property in the form

$$U(t, t') = U(t, t'')U(t'', t')\,. \tag{7.39}$$

In particular, this means that

$$U(t, t') = [U(t', t)]^{-1} \tag{7.40}$$

and

$$(\partial_\tau U(t, \tau))U(\tau, t') + U(t, \tau)\partial_\tau U(\tau, t') = 0\,. \tag{7.41}$$

Therefore,

$$\partial_\tau U(t, \tau) \;=\; -U(t, \tau)(\partial_\tau U(\tau, t'))U(t', \tau)\,. \tag{7.42}$$

Thus, the heat semi-group satisfies the equation

$$\partial_\tau U(t, \tau) = U(t, \tau)A(\tau)\,. \tag{7.43}$$

The differential equations are equivalent to the integral equations

$$U(t, t') = I - \int_{t'}^{t} d\tau\; A(\tau)U(\tau, t')\,, \tag{7.44}$$

and

$$U(t,t') = I + \int_{t'}^{t} d\tau\; U(t,\tau)A(\tau)\,. \tag{7.45}$$

Now we can solve this integral equation by the perturbation series

$$U(t,t') = I + \sum_{k=1}^{\infty}(-1)^k \int_{t'}^{t} d\tau_k \cdots \int_{t'}^{\tau_3} d\tau_2 \int_{t'}^{\tau_2} d\tau_1\; A(\tau_k)\cdots A(\tau_1)\,, \tag{7.46}$$

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

$$t' \le \tau_1 \le \tau_2 \le \tau_3 \le \cdots \le \tau_k \le t\,. \tag{7.47}$$

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

$$U(t,t') = \exp\left(-\int_{t'}^{t} d\tau\; A(\tau)\right)\,. \tag{7.48}$$

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

$$U(t,t') = \exp[-(t-t')A]\,. \tag{7.49}$$

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

$$U(t,t') = T\exp\left(-\int_{t'}^{t} d\tau\; A(\tau)\right)\,. \tag{7.50}$$

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.

Duhamel Formula and Volterra Series

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

$$A(t,s) = A_0(t) + sA_1(t)\,, \tag{7.51}$$

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

$$U(t,t') = U_0(t,t') - s\int_{t'}^{t} d\tau\; U_0(t,\tau)A_1(\tau)U(\tau,t')\,, \tag{7.52}$$

and

$$U(t,t') = U_0(t,t') - s\int_{t'}^{t} d\tau\; U(t,\tau)A_1(\tau)U_0(\tau,t')\,. \tag{7.53}$$

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

$$\partial_s U(t,t') = -\int_{t'}^{t} d\tau\; U(t,\tau)[\partial_s A(\tau)]U(\tau,t')\,. \tag{7.54}$$

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

$$A(t,s) = A_0(t) + sA_1(t)\,, \tag{7.55}$$

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

$$\begin{aligned} U(t,t') = U_0(t,t') + \sum_{k=1}^{\infty}(-1)^k s^k \int_{t'}^{t} d\tau_k \int_{t'}^{\tau_k} d\tau_{k-1}\cdots\int_{t'}^{\tau_2} d\tau_1 \\ \times U_0(t,\tau_k)A_1(\tau_k)U_0(\tau_k,\tau_{k-1})\cdots A_1(\tau_2)U_0(\tau_2,\tau_1)A_1(\tau_1)U_0(\tau_1,t')\,. \end{aligned} \tag{7.56}$$

Now, let us define the operator

$$B(\tau,t) = U_0(t,\tau)A_1(\tau)U_0(\tau,t)\,. \tag{7.57}$$

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

$$\begin{aligned} B(\tau,t) &= A_1(\tau) - \int_\tau^t d\tau\ [A_0(\tau_1), A_1(\tau)] \\ &\quad + \int_\tau^t d\tau_2 \int_\tau^{\tau_2} d\tau_1\ [A_0(\tau_2), [A_0(\tau_1), A_1(\tau)]] + O[(t-\tau)^3]\,. \end{aligned} \tag{7.58}$$

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

$$\begin{aligned} U(t,t') = \Bigg\{ I + \sum_{k=1}^{\infty} (-1)^k s^k \int_{t'}^t d\tau_k \int_{t'}^{\tau_k} d\tau_{k-1} \cdots \int_{t'}^{\tau_2} d\tau_1 \\ \times B(\tau_k,t) B(\tau_{k-1},t) \cdots B(\tau_2,t) B(\tau_1,t) \Bigg\} U_0(t,t')\,. \end{aligned} \tag{7.59}$$

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

$$\begin{aligned} U(t,t') &= \Bigg\{ I - s \int_{t'}^t d\tau\ A_1(\tau) \\ &\quad + \int_{t'}^t d\tau_2 \int_{t'}^{\tau_2} d\tau_1\ \left\{ s^2 A_1(\tau_2) A_1(\tau_1) + s[A_0(\tau_2), A_1(\tau_1)] \right\} \\ &\quad + O[(t-t')^3] \Bigg\} U_0(t,t')\,. \end{aligned}$$

Of course, in the case of time-independent operators this coincides with our previous results.

7.2 Heat Kernel Asymptotics by Fourier Transform

Here we derive a very simple alternative derivation of the asymptotic expansion of the heat kernel by using semi-group perturbation theory. Let L be an elliptic second-order partial differential operator of

the form

$$L(x,\partial) = -\sum_{i,j=1}^{n} \alpha^{ij}(x)\partial_i\partial_j + \sum_{i=1}^{n} \beta^i(x)\partial_i + \gamma(x)\,. \tag{7.60}$$

The heat kernel of the operator L is given by

$$U(t;x,x') = \exp(-tL)\delta(x-x')\,. \tag{7.61}$$

By using Fourier representation for the delta-function we obtain

$$\begin{aligned} U(t;x,x') &= \int\limits_{\mathbb{R}^n} \frac{d\omega}{(2\pi)^n} e^{-i\langle p,x'\rangle} \exp[-tL(x,\partial)] e^{i\langle p,x\rangle} \\ &= \int\limits_{\mathbb{R}^n} \frac{d\omega}{(2\pi)^n} e^{i\langle p,(x-x')\rangle} \exp[-t(H+K+L)]\cdot 1\,, \end{aligned} \tag{7.62}$$

where H is the leading symbol of the operator L

$$H(x,p) = \sum_{i,j=1}^{n} \alpha^{ij}(x) p_i p_j\,, \tag{7.63}$$

and K is a first-order differential operator defined by

$$K = ip_j \left[\beta^j(x) - 2i\sum_{j,k=1}^{n} \alpha^{jk}(x)\partial_k\right]\,. \tag{7.64}$$

Here the operators in the exponent act on 1 from the left.

Now, by rescaling $p \to t^{-1/2}p$ we obtain

$$U(t;x,x') = (4\pi t)^{-n/2} \int\limits_{\mathbb{R}^n} \frac{dp}{\pi^{n/2}} e^{it^{-1/2}\langle p,(x-x')\rangle} \exp[-H - \sqrt{t}\,K - tL)]\cdot 1\,. \tag{7.65}$$

Now, by expanding in a power series in t one gets the asymptotic expansion of the heat kernel. All integrals over p are standard Gaussian integral 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 to get the expansion.

7.3 Time-dependent Heat Equation

7.3.1 Solutions of the Heat Equation

Let L be an elliptic positive operator acting on functions on $\mathbb{R}^n$, $u_0(x)$ be a function on $\mathbb{R}^n$ and $f(t,x)$ be a function on $[0,\infty)\times\mathbb{R}^n$. Then the solution of the non-homogeneous heat equation

$$(\partial_t + L)u = f(t) \tag{7.66}$$

with the initial condition

$$u(0,x) = u_0(x) \tag{7.67}$$

is given by

$$u(t) = e^{-tL}u_0 + \int_0^t d\tau\; e^{-(t-\tau)L} f(\tau)\,. \tag{7.68}$$

Now, let us consider an operator $L = L(t)$ which depends on t as a parameter. Then the solution of the non-homogeneous heat equation

$$(\partial_t + L(t))u = f(t) \tag{7.69}$$

with the initial condition

$$u(0,x) = u_0(x) \tag{7.70}$$

is given by

$$u(t) = U(t,0)u_0 + \int_0^t d\tau\; U(t,\tau) f(\tau)\,. \tag{7.71}$$

7.3.2 Perturbation Theory for Heat Kernel

The heat kernel for a time dependent operator $L(t)$ is defined by the chronological exponent defined above. To be able to use that formula we have to develop some perturbation series. There are at least two kinds of perturbation theory.

The simplest one is based on Volterra series. We separate a time-independent operator L_0 and treat the time-dependent part as a perturbation, that is,

$$L(t) = L_0 + \varepsilon L_1(t)\,. \tag{7.72}$$

By using the expansion of the semi-groups described above we obtain the heat kernel up to the second order in ε and $(t-t')$,

$$\begin{aligned} U(t,x|t',x') &= \Big\{1-\varepsilon\int_{t'}^{t} d\tau\ L_1(\tau) \\ &\quad +\int_{t'}^{t} d\tau_2 \int_{t'}^{\tau_2} d\tau_1\ \left\{\varepsilon^2 L_1(\tau_2)L_1(\tau_1)+\varepsilon[L_0,L_1(\tau_1)]\right\} \\ &\quad +O[(t-t')^3,\varepsilon^3]\Big\}U_0(t-t';x,x')\,. \end{aligned}$$

Here $U_0(t;x,x')$ is the heat kernel of time-independent operator L_0 and 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

$$[L(\tau_1),L(\tau_2)] \tag{7.73}$$

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

$$L_0=\frac{1}{(t-t')}\int_{t'}^{t} d\tau L(\tau)\,, \tag{7.74}$$

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

$$L_1(\tau;t,t')=L(\tau)-L_0(t,t')\,, \tag{7.75}$$

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

$$L(\tau)=L_0+L_1(\tau)\,, \tag{7.76}$$

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. In the zero order of this approximation the following formula

$$U_0(t,x|t',x')=U_0(\tau;x,x')\Big|_{\tau=t-t'}\,, \tag{7.77}$$

where $U_0(\tau; x, x')$ is the heat kernel of the operator L_0 computed with both t and t' being fixed. 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.

7.3.3 Asymptotics of Singularly Perturbed Heat Equation

Another method consists in generalizing the singular perturbation method described in the previous lectures. To be specific, let us consider the operator

$$\begin{aligned} L &= -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q, \qquad (7.78)\\ &= -g^{-1/2}(t,x)[\partial_i + \mathcal{A}_i(t,x)]g^{1/2}(t,x)g^{ij}(t,x)[\partial_j + \mathcal{A}_j(t,x)] + Q(t,x)\,, \end{aligned}$$

where now all coefficients are functions of both t and x.

Let $\varepsilon > 0$ be a small parameter and let us scale the operator L,

$$L_\varepsilon = \varepsilon^2 L \qquad (7.79)$$

Note that we introduce the small parameter ε for the whole operator L rather than the partial derivatives. This is done to simplify the method and to establish a connection with a previous method for time-independent operators described in a previous lecture. We consider the following singularly perturbed heat equation

$$[\varepsilon\partial_t + L_\varepsilon]\, U(t,x|t',x') = 0\,, \qquad (7.80)$$

with the initial conditions

$$U(t',x|t',x') = \delta(x,x')\,. \qquad (7.81)$$

Then we look for a solution in form of an asymptotic series

$$U(t,x|t',x') \sim \exp\left[-\frac{1}{\varepsilon}S(t,x|t',x')\right]\sum_{k=0}^{\infty}\varepsilon^k b_k(t,x|t',x')\,. \qquad (7.82)$$

The leading asymptotics of the heat kernel is

$$U(t,x|t',x') \sim \exp\left[-\frac{1}{\varepsilon}S(t,x|t',x')\right] b_0(t,x|t',x')\,. \qquad (7.83)$$

The functions S and b_0 as $t \to t'$ are normalized as follows. We require that there must exist well-defined limits

$$\Phi(t', x, x') = \lim_{t \to t'} 4(t - t') S(t, x' | t', x') \,, \tag{7.84}$$

$$\psi(t', x, x') = \lim_{t \to t'} [4\pi(t - t')]^{n/2} b_0(t, x | t', x') \,, \tag{7.85}$$

and that the function $\Phi(t', x, x')$ has non-degenerate Hessian, that is, the matrix of mixed derivatives,

$$\det \left[\partial_i \partial_{j'} \Phi(t', x, x') \right] \neq 0 \,, \tag{7.86}$$

at least for x close to x'. Then

$$\psi(t', x, x') = g^{-1/4}(t', x') g^{-1/4}(t', x) \left(\det \left[\partial_i \partial_{j'} \Phi(x, x') \right] \right)^{1/2} . \tag{7.87}$$

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 (t, x) and (t', x').

We have the commutation formula

$$\exp\left(\frac{1}{\varepsilon} S\right) \left[\varepsilon \partial_t + L_\varepsilon\right] \exp\left(-\frac{1}{\varepsilon} S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 T_2 \,, \tag{7.88}$$

where T_0 is a function,

$$T_0 = -\partial_t S - g^{ij} S_{;i} S_{;j} \,, \tag{7.89}$$

T_1 is a first order partial differential operator

$$T_1 = \partial_t + 2 g^{ij} S_{;j} \nabla_i^{\mathcal{A}} + g^{ij} S_{;ij} \,, \tag{7.90}$$

and T_2 is a second-order differential operator

$$T_2 = L \,. \tag{7.91}$$

Recall that $S_{;i} = \nabla_i S$ and $S_{;ij} = \nabla_i \nabla_j S$.

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) for the function S, that we call the *action*,

$$\partial_t S + g^{ij}(t, x) S_{;i} S_{;j} = 0 \,, \tag{7.92}$$

and the recurrence relations (transport equations) for the coefficients b_k for $k = 0, 1, \ldots,$

$$T_1 b_0 = 0 \tag{7.93}$$

$$T_1 b_{k+1} = -T_2 b_k\,, \qquad k = 1, 2, \ldots\,. \tag{7.94}$$

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 world function

$$S(t, x|, t', x') = \frac{1}{2(t-t')}\sigma(x, x')\,. \tag{7.95}$$

Recall that $\sigma(x, x')$ is equal to one half the square of the geodesic distance between x and x' and satisfies the equation

$$\sigma = \frac{1}{2} g^{ij}\sigma_{;i}\sigma_{;j}\,. \tag{7.96}$$

Indeed, by using this equation we see that $S = \sigma/[2(t-t')]$ solves the Hamilton-Jacobi equation. That is, S is nothing but a generalization of the world function.

The solution of Hamilton-Jacobi equation can be obtained as follows. Let us introduce the corresponding Hamiltonian system

$$\frac{dx^i}{d\tau} = 2g^{ij}(\tau, x)p_j\,, \tag{7.97}$$

$$\frac{dp_k}{d\tau} = -\partial_k g^{ij}(\tau, x)p_i p_j\,. \tag{7.98}$$

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.

Let $[x(\tau), p(\tau)]$ be the solution of this system with the following boundary conditions

$$x(t') = x'\,, \qquad x(t) = x\,. \tag{7.99}$$

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

$$S(t, x|t', x') = \int_{t'}^{t} d\tau\, \frac{1}{4} g_{ij}(\tau, x(\tau))\frac{dx^i(\tau)}{d\tau}\frac{dx^j(\tau)}{d\tau}\,, \tag{7.100}$$

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.

Then one can show that

$$\frac{\partial S(t,x|t',x')}{\partial x^i} = p_i(t)\,, \tag{7.101}$$

$$\frac{\partial S(t,x|t',x')}{\partial x'^i} = -p_i(t')\,, \tag{7.102}$$

and that $S(t,x|t',x')$ satisfies Hamilton-Jacobi equation.

Next, we define the total derivative d/dt (along the trajectories of the Hamiltonian system) of a function that depends on t and x, that is,

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{dx^i}{dt}\frac{\partial}{\partial x^i}\,. \tag{7.103}$$

Then, it should be clear that the differential operator T_1 has the form

$$T_1 = \frac{d}{dt} + 2g^{ij}S_{;i}\mathcal{A}_j + g^{ij}S_{;ij}\,, \tag{7.104}$$

The action S has another important property. Let us define the determinant

$$Z(t,x|t',x') = g^{-1/2}(t,x)\det\left[-\partial_i\partial_{j'}S(t,x|t',x')\right]g^{-1/2}(t',x')\,. \tag{7.105}$$

Then one can show that the function Z satisfies the equation

$$\left(\partial_t + 2g^{ij}S_{;j}\nabla_i + g^{ij}S_{;ij}\right)Z^{1/2} = 0\,, \tag{7.106}$$

or

$$\left(\frac{d}{dt} + g^{ij}S_{;ij}\right)Z^{1/2} = 0\,. \tag{7.107}$$

Notice that for time-independent metric the function Z is determined by the Van-Vleck determinant

$$Z(t,x|t',x') = \frac{1}{[2(t-t')]^n}\Delta(x,x') \tag{7.108}$$

and the above equation follows from the equation for Van Vleck determinant

$$\sigma^i\nabla_i\Delta^{1/2} = \frac{1}{2}\left(n - g^{ij}\sigma_{;ij}\right)\Delta^{1/2}\,. \tag{7.109}$$

Therefore, the operator T_1 can be written as

$$T_1 = Z^{1/2}\left(\frac{d}{dt} + 2g^{ij}S_{;i}\mathcal{A}_j\right)Z^{-1/2}\,. \tag{7.110}$$

Thus, by integrating the transport equation we get the coefficient b_0

$$b_0(t,x|t',x') = (2\pi)^{-n/2}\mathcal{W}(t,x|t',x')Z^{1/2}(t,x|t',x')\,, \tag{7.111}$$

where

$$\mathcal{W}(t,x|t',x') = \exp\left\{-\int_{t'}^{t} d\tau\ \frac{dx^i(\tau)}{d\tau}\mathcal{A}_i(\tau,x(\tau))\right\}\,. \tag{7.112}$$

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 W is nothing bu the function $\mathcal{P}(x,x')$ introduced in previous lectures.

Finally, the leading asymptotics of the singularly perturbed heat kernel as $\varepsilon \to 0$ has the form

$$U(t,x|t',x') \sim (2\pi)^{-n/2}Z^{1/2}(t,x|t',x')\mathcal{W}(t,x|t',x')\exp\left\{-\frac{1}{\varepsilon}S(t,x,x')\right\}\,. \tag{7.113}$$

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 lecture.

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 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

$$L_\varepsilon = -\varepsilon^2 g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}} + Q\,. \tag{7.114}$$

Note that we introduce the small parameter ε for the covariant derivatives rather than the partial derivatives. This is done to have a covariant method. We consider the singularly perturbed heat equation

$$[\varepsilon\partial_t + L_\varepsilon]\,U(t,x|t',x') = 0\,, \tag{7.115}$$

with the initial conditions

$$U(t', x|t', x') = \delta(x, x')\,, \tag{7.116}$$

and look for a solution in the form of an asymptotic series

$$U(t, x|t', x') \sim \exp\left[-\frac{1}{\varepsilon}S(t, x|t', x')\right] \sum_{k=0}^{\infty} \varepsilon^k b_k(t, x|t', x')\,. \tag{7.117}$$

Since the initial condition is the same the functions S and b_0 as $t \to t'$ are normalized exactly as before.

Again, we have a commutation formula

$$\exp\left(\frac{1}{\varepsilon}S\right)[\varepsilon\partial_t + L_\varepsilon]\exp\left(-\frac{1}{\varepsilon}S\right) = T_0 + \varepsilon T_1 + \varepsilon^2 T_2\,, \tag{7.118}$$

where now

$$T_0 = -\partial_t S - g^{ij}S_{;i}S_{;j} + Q\,, \tag{7.119}$$

$$T_1 = \partial_t + 2g^{ij}S_{;j}\nabla_i^{\mathcal{A}} + g^{ij}S_{;ij}\,, \tag{7.120}$$

and

$$T_2 = -g^{ij}\nabla_i^{\mathcal{A}}\nabla_j^{\mathcal{A}}\,. \tag{7.121}$$

Note that the potential form Q appears now in T_0 and not T_2.

Now, the Hamilton-Jacobi equation for the action has the form

$$\partial_t S + g^{ij}(t, x)S_{;i}S_{;j} - Q = 0\,, \tag{7.122}$$

and the recurrence relations (transport equations) for the coefficients b_k for $k = 0, 1, \ldots$, are formally the same,

$$T_1 b_0 = 0 \tag{7.123}$$

$$T_1 b_{k+1} = -T_2 b_k\,, \qquad k = 1, 2, \ldots\,. \tag{7.124}$$

The corresponding Hamiltonian system reads now

$$\frac{dx^i}{d\tau} = 2g^{ij}(\tau, x)p_j\,, \tag{7.125}$$

$$\frac{dp_k}{d\tau} = -\partial_k g^{ij}(\tau, x)p_i p_j + \partial_k Q\,. \tag{7.126}$$

This system describes a particle on a curved manifold in a time-dependent metric and in a time-dependent potential $(-Q)$.

Let $[x(\tau), p(\tau)]$ be the solution of this system with the following boundary conditions

$$x(t') = x' \,, \qquad x(t) = x \,. \tag{7.127}$$

Let

$$S(t, x|t', x') = \int_{t'}^{t} d\tau \, \left\{ \frac{1}{4} g_{ij}(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} \frac{dx^j(\tau)}{d\tau} + Q(\tau, x(\tau)) \right\} \,, \tag{7.128}$$

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 anymore. 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.

7.4 Path Integrals

7.4.1 Discretization

Finding heat semi-group for finite t is equivalent to solving the heat equation. However, for small t it can be obtained by perturbation theory

$$U(t) = e^{-tA} = I - tA + O(t^2) \,. \tag{7.129}$$

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

$$U(t) = \lim_{N \to \infty} \left[U\left(\frac{t}{N}\right) \right]^N \,. \tag{7.130}$$

A similar representation exists even in the case when the operator $A = A(t)$ is time-dependent. As we have seen above the heat

semi-group $U(t,t')$ for t close to t' is given by

$$\begin{aligned} U(t,t') &= I - \int_{t'}^{t} d\tau\ A(\tau) + O[(t-t')^2] \\ &= = \exp\left[- \int_{t'}^{t} d\tau\ A(\tau) \right] + O[(t-t')^2]\,. \end{aligned} \tag{7.131}$$

Let us partition the interval (t',t), (we assume that $t > t'$) in N equal subintervals of length $(t-t')/N$ and let

$$t_k = t' + k\frac{(t-t')}{N}\,. \qquad k = 0, 1, \ldots, N, \tag{7.132}$$

and τ_k be some arbitrary points in the subintervals $[t_{k-1}, t_k]$. Then by using the semi-group property we have

$$U(t,t') = U(t,t_{N-1})U(t_{N-1},t_{N-2})\cdots U(t_2,t_1)U(t_1,t')\,. \tag{7.133}$$

By taking the limit as $N \to \infty$ we can replace each heat semi-group by the approximate exponential form to get

$$U(t,t') = \lim_{N\to\infty} \exp\left[- \int_{t_{N-1}}^{t} d\tau_N A(\tau_N) \right] \cdots \exp\left[- \int_{t'}^{t_1} d\tau_1 A(\tau_1) \right]\,. \tag{7.134}$$

Such representation of the heat semi-group is the basis for the Feynmann path integral representation of the heat kernel. Indeed, let us consider an elliptic second-order partial differential operator L of the form

$$L = -\sum_{i,j=1}^{n} \alpha^{ij}(x,t)\partial_i\partial_j + \sum_{j=1}^{n} \beta^j(x,t)\partial_j + \gamma(x,t)\,. \tag{7.135}$$

Then by using the above formulas we obtain for the heat kernel of the operator L

$$\begin{aligned} U(t,x|t',x') = \lim_{N\to\infty} \int_{\mathbb{R}^{Nn}} dx_1 \ldots dx_N\ U(t,x|t_{N-1},x_{N-1}) \\ \times U(t_{N-1},x_{N-1}|t_{N-2},x_{N-2})\cdots U(t_2,x_2|t_1,x_1)U(t_1,x_1|t',x')\,. \end{aligned} \tag{7.136}$$

7.4.2 Formal Expression

We know that as $t \to t'$ the heat kernel looks like

$$\begin{aligned} U(t,x|t',x') \;\sim\; & [4\pi(t-t')]^{-n/2}[\det A]^{-1/2} \\ & \times \exp\left\{-\frac{\left\langle (x-x'), A^{-1}(x-x')\right\rangle}{4(t-t')}\right\} \\ & \times \exp\left\{\frac{1}{2}\left\langle (x-x'), A^{-1}\beta\right\rangle - (t-t')\left[\gamma + \frac{1}{4}\left\langle \beta, A^{-1}\beta\right\rangle\right]\right\}, \end{aligned} \tag{7.137}$$

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

$$U(t,x|t',x') = \int\limits_{\mathcal{M}} \mathcal{D}x(\tau)\exp[-S(t,x|t',x'))]\,. \tag{7.138}$$

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,

$$x(t') = x'\,, \qquad x(t) = x\,, \tag{7.139}$$

and $S(t,x|t',x')$ is the following function called the *action functional*

$$\begin{aligned} S(t,x|t',x') \;=\; & \int\limits_{t'}^{t} d\tau \left\{\frac{1}{4}\left\langle \frac{dx}{d\tau}, A^{-1}(x,\tau)\frac{dx}{d\tau}\right\rangle + \frac{1}{2}\left\langle \frac{dx}{d\tau}, A^{-1}(x,\tau)\beta(x,\tau)\right\rangle \right. \\ & \left. +\gamma(x,\tau) + \frac{1}{4}\left\langle \beta(x,\tau), A^{-1}(x,\tau)\beta(x,\tau)\right\rangle\right\}. \end{aligned} \tag{7.140}$$

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

$$L = -g^{ij}\nabla_i^A\nabla_j^A + Q\,, \tag{7.141}$$

where $g^{ij} = \alpha^{ij}$ and $\mathcal{A}_i$ and Q are related to β^i and γ by obvious relations. Then the short time heat kernel is

$$\begin{aligned} U(t,x|t',x') &\sim (2\pi)^{-n/2} Z^{1/2}(t,x|t',x') \\ &\quad \times \exp\left\{ -\int_{t'}^{t} d\tau \left[\frac{1}{4} g_{ij}(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} \frac{dx^j(\tau)}{d\tau} \right.\right. \\ &\quad \left.\left. + \mathcal{A}_i(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} + Q(\tau, x(\tau)) \right] \right\}. \end{aligned} \tag{7.142}$$

For t close to t' and x close to x' the function Z has the following form

$$Z^{1/2}(t,x|t',x') \sim [2(t-t')]^{-n} \exp\left\{ (t-t') \int_{t'}^{t} d\tau \, \frac{1}{12} R_{ij}(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} \frac{dx^j(\tau)}{d\tau} \right\}. \tag{7.143}$$

Because of the extra factor $(t-t')$ in the exponent this term does not contribute to the action. By substituting this form in the discretized heat kernel we obtain the path integral with the action in the form

$$\begin{aligned} S(t,x|t',x') &= \int_{t'}^{t} d\tau \left\{ \frac{1}{4} g_{ij}(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} \frac{dx^j(\tau)}{d\tau} + \mathcal{A}_i(\tau, x(\tau)) \frac{dx^i(\tau)}{d\tau} \right. \\ &\quad \left. + Q(\tau, x(\tau)) \right\}. \end{aligned} \tag{7.144}$$

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.

7.4.3 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. 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 semiclassical approximation discussed below.

The classical trajectories are given by the critical points of the action functional determined by the variational (functional) derivative

$$\frac{\delta S}{\delta x} = 0\,. \tag{7.145}$$

By varying the action functional with respect to the path $x(\tau)$ with fixed endpoints, $x(t') = x'$ and $x(t) = x$, we get the equations for classical trajectories

$$\frac{d^2x^m}{dt^2} + \sum_{j,k=1}^{n} B^m{}_{jk}(x,t)\frac{dx^j}{dt}\frac{dx^k}{dt} + \sum_{j=1}^{n} C^m{}_j(x,t)\frac{dx^j}{dt} + D^m(x,t) = 0\,, \tag{7.146}$$

where $B^m{}_{jk}(x,t)$, $C^m{}_j(x,t)$ and $D(x,t)$ are some functions defined as follows. Let α_{ij} be the entries of the matrix $A^{-1} = (\alpha_{ij})$ inverse to the matrix $A = (\alpha^{ij})$. Then

$$B^m{}_{jk} = \frac{1}{2}\sum_{i=1}^{n} \alpha^{im}\left(\partial_k\alpha_{ij} + \partial_j\alpha_{ik} - \partial_i\alpha_{kj}\right)\,, \tag{7.147}$$

$$C^m{}_j = \partial_j\beta^m + \sum_{i,k=1}^{n} \beta^k\alpha^{im}\partial_j\alpha_{ik} - \sum_{i,k=1}^{n} \alpha^{im}\partial_i(\alpha_{kj}\beta^k) + \sum_{i=1}^{n} \alpha^{im}\partial_t\alpha_{ij}\,, \tag{7.148}$$

$$D^m = -2\sum_{i=1}^{n} \alpha^{im}\partial_i\gamma - \frac{1}{2}\sum_{i,k,j=1}^{n} \alpha^{im}\partial_i(\alpha_{kj}\beta^k\beta^j) + \partial_t\beta^m + \sum_{i,j=1}^{n} \alpha^{im}\beta^j\partial_t\alpha_{ij}\,. \tag{7.149}$$

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

$$\frac{d^2x^m}{d\tau^2} + \Gamma^m{}_{kj}\frac{dx^k}{d\tau}\frac{dx^j}{d\tau} + \left[g^{im}(\partial_t g_{ik}) - 2g^{im}\mathcal{R}_{ik}\right]\frac{dx^k}{d\tau} + 2g^{im}\partial_t\mathcal{A}_i - 2g^{im}\partial_i Q = 0\,, \tag{7.150}$$

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

$$x(\tau) = x_0(\tau) + y(\tau)\,, \tag{7.151}$$

where $y(\tau)$ is a continuous path with zero boundary conditions, that is,

$$y(t') = y(t) = 0\,, \tag{7.152}$$

and expand the action in a functional Taylor series in powers of y and separate the quadratic terms

$$S(x(\tau)) = S(x_0(\tau)) + \frac{1}{2}\int_{t'}^{t} d\tau\ \langle y(\tau), H(\tau)y(\tau)\rangle + V(y(\tau))\,, \tag{7.153}$$

where H is a second-order ordinary differential operator determined by the second variational derivative of the action at the critical point

$$H_{ij} = \left.\frac{\delta^2 S(x(\tau))}{\delta x^i(\tau)\delta x^j(\tau')}\right|_{x(\tau)=x_0(\tau)}\,, \tag{7.154}$$

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.

Gaussian Path Integrals

By expanding the $\exp(-V)$ in a powers series we get a perturbation theory with only *Gaussian path integrals* of the form

$$G^{i_1\cdots i_k}(\tau_1,\ldots,\tau_k) = \tag{7.155}$$
$$\times \int\limits_{\mathcal{M}_y} \mathcal{D}y(\tau) \exp\left[-\frac{1}{2}\int\limits_{t'}^{t} d\tau \ \langle y(\tau), H(\tau)y(\tau)\rangle\right] y^{i_1}(\tau_1)\cdots y^{i_k}(\tau_k)\,.$$

Such integrals can be evaluated exactly in the same way as Gaussian integrals in finite dimensions. Let $G^{ij}(\tau,\tau')$ be the Green function of the operator H_{ij} defined by

$$\sum_{j=1}^{n} H_{ij}(\tau)G^{jk}(\tau,\tau') = \delta^k{}_i\delta(\tau-\tau')\,. \tag{7.156}$$

We obtain

$$G^{i_1\cdots i_{2k+1}}(\tau_1,\ldots,\tau_{2k+1}) = 0 \tag{7.157}$$

$$G^{i_1\cdots i_{2k}}(\tau_1,\ldots,\tau_{2k}) \tag{7.158}$$
$$= (\operatorname{Det} H)^{-1/2}\,\frac{(2k)!}{2^k k!}\operatorname{Sym} G^{i_1\,i_2}(\tau_1,\tau_2)\cdots G^{i_{2k-1}\,i_{2k}}(\tau_{2k-1},\tau_{2k})\,.$$

Here the operator Sym denotes the complete symmetrization over the arguments of the Green function including the discrete indices. For example,

$$\operatorname{Sym} G^{i_1\,i_2}(\tau_1,\tau_2)G^{i_3\,i_4}(\tau_3,\tau_4) = \frac{1}{3}\Big\{G^{i_1\,i_2}(\tau_1,\tau_2)G^{i_3\,i_4}(\tau_3,\tau_4)$$
$$+G^{i_1\,i_3}(\tau_1,\tau_3)G^{i_2\,i_4}(\tau_2,\tau_4) + G^{i_1\,i_4}(\tau_1,\tau_4)G^{i_2\,i_3}(\tau_2,\tau_3)\Big\}\,. \tag{7.159}$$

Further, in the above formula $\operatorname{Det} H$ denotes so-called functional determinant of the operator H. It can be defined in terms of the zeta function $\zeta(s)$ of the operator H introduced in a previous section as follows

$$\operatorname{Det} H = \exp\left(-\zeta'(0)\right)\,. \tag{7.160}$$

However, this is not needed here since it can be absorbed in the definition of the measure 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.

Example

Let us consider the (trivial) case when α_{ij} is constant and $\beta = \gamma = 0$. Then the classical trajectories are the straight lines

$$x_0^i(\tau) = x'^i + \frac{\tau - t'}{t - t'}(x - x')^i \,, \tag{7.161}$$

and the classical action is

$$S_0(t, x|t', x') = S(x_0(\tau)) = \frac{1}{4(t - t')} \left\langle (x - x'), A^{-1}(x - x') \right\rangle \,. \tag{7.162}$$

The operator H has the form

$$H_{ij} = -\frac{1}{4}\alpha_{ij}\frac{d^2}{d\tau^2} \,, \tag{7.163}$$

and $V(y) = 0$. Therefore, the path integral gives the correct heat kernel provided we normalize the Gaussian path integral measure by

$$\int\limits_{\mathcal{M}_y} \mathcal{D}y(\tau) \exp\left[-\frac{1}{2}\int\limits_{t'}^{t} d\tau \;\; \langle y(\tau), H(\tau)y(\tau)\rangle\right] = [4\pi(t - t')]^{-n/2}(\det A)^{-1/2} \,. \tag{7.164}$$

7.5 Spectral Expansions and Long Time Behavior of the Heat Kernel

Let L be a Laplace type operator,

$$L = -g^{ij}\nabla_i^A\nabla_j^A + Q \tag{7.165}$$

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,

$$\lambda_1 \leq \lambda_2 \leq \cdots , \tag{7.166}$$

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

$$U(t; x, x') = \sum_{k=1}^{\infty} \exp(-t\lambda_k)\varphi_k(x)\varphi_k(x') \, . \tag{7.167}$$

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,

$$U(t; x, x') = \exp(-t\lambda_1)\varphi_1(x)\varphi_1(x') + \cdots . \tag{7.168}$$

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, 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. There exist even an encyclopedia of exactly solvable problems. In all such cases the spectrum is know 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 little more subtle issue then.

7.6 Boundary Value Problems

7.6.1 Geometry of the Boundary

In this section we briefly describe the construction of the heat kernel asymptotics for a Laplace type operator on manifolds with boundary. Let M be a n-dimensional Riemannian manifold 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 the Latin indices will label the components of tensors on the manifold and the Greek indices will label the components of tensors on the boundary. In a sufficiently small neighborhood of the boundary one can connect each point x with a point $\hat{x}$ on the boundary by a unique geodesics. The length of this geodesics determines the normal geodesic distance r from the point x to the boundary. Therefore, there exists a local diffeomorphism

$$r = r(x) \qquad \hat{x}^\mu = \hat{x}^\mu(x)\,, \tag{7.169}$$

and the inverse diffeomorphism

$$x^i = x^\mu(r, \hat{x})\,, \tag{7.170}$$

such that for any point on the boundary

$$r(x) = 0\,, \tag{7.171}$$

and for any point in the interior

$$r(x) > 0\,. \tag{7.172}$$

Then the whole manifold can be split 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.

We define the vectors

$$e_\mu{}^i = \frac{\partial x^i}{\partial \hat{x}^\mu} \tag{7.173}$$

$$N^i = \frac{\partial x^i}{\partial r}\,. \tag{7.174}$$

Then, for $r = 0$, that is, on the boundary the vectors $e_\mu{}^i$ are tangent to the boundary and form a basis in the tangent space and the vector N^i is an *inward pointing normal* to the boundary, in particular,

$$g_{ij} e_\mu{}^i N^j = 0\,. \tag{7.175}$$

We also define the covector

$$N_i = \frac{1}{J}\frac{\partial r}{\partial x^i}\,, \tag{7.176}$$

where J is the Jacobian of the above diffeomorphism,

$$J = \frac{\partial(x^1, x^2, \ldots, x^n)}{\partial(r, \hat{x}^1, \ldots, \hat{x}^{n-1})} = \det\left(N^i, e_1{}^i, \ldots, e_{n-1}{}^i\right)\,. \tag{7.177}$$

One can show that N_i is the normal covector to the boundary, that is,

$$N_i = g_{ij} N^j\,, \tag{7.178}$$

and

$$N_i e_\mu{}^i = 0\,. \tag{7.179}$$

We fix the orientation of the boundary by requiring the Jacobian J to be positive, that is, $J > 0$.

Let g_{ij} be the metric on the manifold M. Then there is a naturally *induced Riemannian metric* $\hat{g}_{\mu\nu}$ on the boundary defined by

$$\hat{g}_{\mu\nu} = g_{ij} e_\mu{}^i e_\nu{}^j\,. \tag{7.180}$$

The induced metric allows one to define the induced tangential covariant derivatives $\hat{\nabla}_\mu$ on the boundary as well. The Riemannian volume element on M takes the form in these coordinates

$$g^{1/2} dx = J\, \hat{g}^{1/2} dr\, d\hat{x}\,, \tag{7.181}$$

where $\hat{g} = \det \hat{g}_{\mu\nu}$. Then Stokes' theorem enables one to integrate by parts; for any vector field K^i and a scalar field φ we have

$$\int\limits_M dx\; g^{1/2} \varphi \nabla_i K^i = -\int\limits_M dx\; g^{1/2} (\nabla_i \varphi) K^i + \int\limits_{\partial M} d\hat{x}\; \hat{g}^{1/2} \varphi N_i K^i\,. \tag{7.182}$$

7.6.2 Boundary Conditions

Let L be a Laplace type operator acting on real-valued scalar functions of M

$$L(x,\partial_x) = -\Delta + Q\,, \tag{7.183}$$

with some smooth function Q.

The operator L is *formally self-adjoint*. Indeed, for any two smooth functions, φ and ψ, with compact support in the interior of the manifold (that is, functions that vanish in the boundary part) by integrating by parts twice we see that

$$\int\limits_M dx\; g^{1/2}\varphi L\psi = \int\limits_M dx\; g^{1/2}(L\varphi)\psi\,. \tag{7.184}$$

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. 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

$$\nabla_N f\big|_{\partial M} = \partial_r f\big|_{\partial M}\,. \tag{7.185}$$

at the boundary. The boundary conditions are some conditions on the boundary data, that is,

$$Bf\big|_{\partial M} = [B_1\nabla_N + B_2]\, f\big|_{\partial M} = 0\,, \tag{7.186}$$

where B is the *boundary operator*, usually a first-order (or zero-order) differential operator. The classical boundary conditions are: Dirichlet

$$f\big|_{\partial M} = 0\,, \tag{7.187}$$

and Neumann

$$\nabla_N f\big|_{\partial M} = 0\,. \tag{7.188}$$

There is also a slight modification of Neumann boundary conditions called Robin boundary conditions,

$$(\nabla_N + h)\, f\big|_{\partial M} = 0 \tag{7.189}$$

where $h(\hat{x})$ 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, 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 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, co-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.

7.6.3 Interior Heat Kernel

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 $U^{\text{int}}(t;x,x')$ 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 ε 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^{int}, choosing the normal coordinates at this point (with $g_{ij}(x') = \delta_{ij}$), scaling

$$x \mapsto x' + \varepsilon(x - x'), \qquad t \mapsto \varepsilon^2 t, \tag{7.190}$$

and expanding in a power series in ε. Of course, the derivatives are scaled by

$$\partial_i \mapsto \frac{1}{\varepsilon}\partial_i\,, \qquad \partial_t \mapsto \frac{1}{\varepsilon^2}\partial_t\,. \tag{7.191}$$

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 power (asymptotic) 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

$$L_\varepsilon \;=\; \sum_{k=0}^{\infty} \varepsilon^{k-2} L_k = \frac{1}{\varepsilon^2}L_0 + \frac{1}{\varepsilon}L_1 + L_2 + \cdots\,, \tag{7.192}$$

where L_k are second-order differential operators. By expanding the interior heat kernel in the power series in ε

$$U_\varepsilon^{\rm int} = \sum_{k=0}^{\infty} \varepsilon^{k-n} U_k\,, \tag{7.193}$$

we get the following recursion for $k \geq 1$

$$(\partial_t + L_0)U_k = -\sum_{m=1}^{k} L_m U_{k-m}\,. \tag{7.194}$$

The initial conditions for the coefficients U_k are

$$U_0(t; x, x') = \delta(x, x')\,, \tag{7.195}$$

and

$$U_k(0; x, x') = 0\,, \qquad \text{for } k \geq 1\,. \tag{7.196}$$

Note that the leading order operator,

$$L_0 = -\delta^{ij}\partial_i\partial_j\,, \tag{7.197}$$

has constant coefficients, and, therefore, is easy to handle. The leading order interior heat kernel is

$$U_0^{\rm int}(t; x, x') = (4\pi t)^{-m/2} \exp\left(-\frac{|x - x'|^2}{4t}\right)\,, \tag{7.198}$$

where $|x-x'|^2 = \delta_{ij}(x-x')^i(x-x')^j$. This enables one to solve the recursion system.

Of course, for the interior heat kernel there is a much better covariant approach described in previous lectures.

7.6.4 Heat Kernel Near Boundary

For an elliptic boundary-value problem the diagonal of the heat kernel $U^{\rm bnd}(t;x,x)$ in $M_1^{\rm bnd}$ 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, $x_0 \in \partial M$, 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

$$\hat{x} \mapsto \hat{x}_0 + \varepsilon(\hat{x}-\hat{x}_0), \qquad \hat{x}' \mapsto \hat{x}_0 + \varepsilon(\hat{x}'-\hat{x}_0) \tag{7.199}$$

$$r \mapsto \varepsilon r, \qquad r' \mapsto \varepsilon r', \qquad t \mapsto \varepsilon^2 t\,. \tag{7.200}$$

The corresponding differential operators are scaled by

$$\hat{\partial}_\mu \mapsto \frac{1}{\varepsilon}\hat{\partial}_\mu, \qquad \partial_r \mapsto \frac{1}{\varepsilon}\partial_r, \qquad \partial_t \mapsto \frac{1}{\varepsilon^2}\partial_t\,. \tag{7.201}$$

Then, we expand the scaled operator L_ε in the power series in ε, i.e.

$$L_\varepsilon = \sum_{k=0}^{\infty} \varepsilon^{k-2} L_k, \tag{7.202}$$

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

$$U_\varepsilon^{\rm bnd} \sim \sum_{n=0}^{\infty} \varepsilon^{2-m+n} U_n^{\rm bnd}, \tag{7.203}$$

and substitute into the scaled version of the heat equation and the Dirichlet boundary condition. Then, by equating the like powers in ε one gets an infinite set of recursive differential equations

$$(\partial_t + L_0) U_k^{\rm bnd} = -\sum_{n=1}^{k} L_n U_{k-n}^{\rm bnd}\,. \tag{7.204}$$

The initial conditions are

$$U_0^{\rm bnd}(0; r, \hat{x}; r', \hat{x}') = \delta(r - r')\delta(\hat{x}, \hat{x}') \tag{7.205}$$

and for $k \geq 1$

$$U_k^{\rm bnd}(0; r, \hat{x}; r', \hat{x}') = 0\,. \tag{7.206}$$

The boundary conditions read

$$U_k^{\rm bnd}(t; 0, \hat{x}; r', \hat{x}') = U_k^{\rm bnd}(t; r, \hat{x}; 0, \hat{x}') = 0 \tag{7.207}$$

for Dirichlet boundary value problem and

$$\partial_r U_k^{\rm bnd}(t; r, \hat{x}; r', \hat{x}')\Big|_{r=0} = \partial_{r'} U_k^{\rm bnd}(t; r, \hat{x}; r', \hat{x}')\Big|_{r'=0} = 0,\ . \tag{7.208}$$

for Neumann boundary value problem. Moreover, e should impose asymptotic conditions

$$\lim_{r\to\infty} U_k^{\rm bnd}(t; r, \hat{x}; r', \hat{x}') = \lim_{r'\to\infty} U_k^{\rm bnd}(t; r, \hat{x}; r', \hat{x}') = 0\,. \tag{7.209}$$

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 x_0 is *one-dimensional*. The leading order term $U_0^{\rm bnd}$ is defined by the heat equation

$$(\partial_t + L_0) U_0^{\rm bnd} = 0, \tag{7.210}$$

where

$$L_0 = -\partial_r^2 - \delta^{\mu\nu}\hat{\partial}_\mu \hat{\partial}_\nu\,, \tag{7.211}$$

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. 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

$$U_0^{\rm bnd}(t; r, \hat{x}; r', \hat{x}') = (4\pi t)^{-n/2} \exp\left(-|\hat{x} - \hat{x}'|^2\right) K(t; r, r')\,, \qquad (7.212)$$

where $|\hat{x} - \hat{x}'|^2 = \delta_{\mu\nu}(\hat{x} - \hat{x}')^\mu(\hat{x} - \hat{x}')^\nu$ and the function $K(t; r, r')$ has the form

$$K_D(t; r, r') = \exp\left(-\frac{(r - r')^2}{4t}\right) - \exp\left(-\frac{(r + r')^2}{4t}\right) \qquad (7.213)$$

for Dirichlet problem, and

$$K_N(t; r, r') = \exp\left(-\frac{(r - r')^2}{4t}\right) + \exp\left(-\frac{(r + r')^2}{4t}\right) \qquad (7.214)$$

for Neumann problem. This enables us, in principle, to solve the recursion system.

7.6.5 Method of Geodesics Reflected from the Boundary

Let us describe briefly another, more geometrical, method for calculation of the heat kernel $U(t; x, x')$ near boundary for small t and x close to x' . Let us fix the Dirichlet boundary conditions.

This method is based on the following semi-classical ansatz

$$U(t; x, x') = (4\pi t)^{-n/2} \Delta^{1/2}(x, x') \exp\left[-\frac{\sigma(x, x')}{2t}\right] \Omega(t; x, x') \qquad (7.215)$$

As we already know from a previous lecture, 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 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 boundaries of the manifold one or more times.

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. We want to construct an asymptotics as $t \to 0$. In this case 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 near the boundary, that is, $\delta(r)$ 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. Thus, we have an ansatz

$$\begin{aligned} U(t;x,x') &= (4\pi t)^{-n/2}\Bigg\{\exp\left[-\frac{\sigma(x,x')}{2t}\right]\Delta^{1/2}(x,x')\Omega(t;x,x') \\ &\quad + \exp\left[-\frac{\phi(x,x')}{2t}\right]\Psi(t;x,x')\Bigg\} \end{aligned} \tag{7.216}$$

where $\phi(x,x')$ is the geodesic interval (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 functions ϕ and Ψ satisfy equations similar to the equations for the functions σ and Ω,

$$\phi = \frac{1}{2}g^{ij}\phi_{;i}\phi_{;j} = \frac{1}{2}g^{i'j'}\phi_{;i'}\phi_{j'}\,, \tag{7.217}$$

and

$$F\Psi = 0 \tag{7.218}$$

where

$$F = \frac{\partial}{\partial t} + \frac{1}{t}\left(\phi^{;i}\nabla_i + \frac{1}{2}\left(\phi^{;i}{}_{;i} - n\right)\right) - L \tag{7.219}$$

The part due to the direct geodesic was analyzed before. It has exactly the same form here. What we need to do now is to compute the function Ψ. For the Dirichlet problem the boundary conditions for the function Ψ have the form

$$\Psi\big|_{x\in\partial M} = -\Delta^{1/2}\Omega\big|_{x\in\partial M}\,. \tag{7.220}$$

Now, we choose the coordinate system $(r, \hat{x}^\mu)$, 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 neighbourhood of the boundary, that is, at $r = 0$.

The further strategy is rather simple. We scale the coordinates as described above (7.199)-(7.201). We expand the transport operator F and the transport function Ψ in formal series in the small parameter ε

$$F_\varepsilon = \sum_{k=0}^{\infty} \varepsilon^{k-2} F_k \tag{7.221}$$

$$\Psi = \sum_{k=0}^{\infty} \varepsilon^k \Psi_k\,, \tag{7.222}$$

and obtain the following differential recursion relations

$$L_0\Psi_0 = 0\,, \tag{7.223}$$

and

$$L_0\Psi_k = -\sum_{m=1}^{k} L_k\Psi_{k-m}\,. \tag{7.224}$$

We list below the solution for Dirichlet boundary conditions. First of all, we have

$$\Psi_0 = -1 \tag{7.225}$$

The calculation of next orders is considerably more difficult though it offers no particular problems. To present the result we introduce the following notation. Let $h(z)$ be a function defined by

$$h(z) = \int_0^\infty dx \exp(-x^2 - 2zx) = \exp(z^2)\mathrm{Erfc}\,(z) \tag{7.226}$$

where $\mathrm{Erfc}\,(z)$ is the complimentary error function. Let $f_1(z)$ and $f_2(z)$ be the functions defined by

$$f_1(z) = \frac{1}{6} + \frac{z^2}{6}\left(2 + \frac{1}{2}z^2 - z(z^2+6)h(z)\right), \tag{7.227}$$

$$f_2(z) = -\frac{1}{6} + \frac{1}{12}z^2\left(-4 + \frac{1}{2}z^2 - 4z^3 h(z)\right). \tag{7.228}$$

Let $K_{\mu\nu}$ be the extrinsic curvature of the boundary defined by

$$K_{\mu\nu} = -\frac{1}{2}\frac{\partial}{\partial r} g_{\mu\nu}\bigg|_{r=0}, \tag{7.229}$$

and

$$K = \hat{g}^{\mu\nu} K_{\mu\nu}\,. \tag{7.230}$$

Further, let $\hat{R}$ be the scalar curvature of the boundary and

$$R^0_{NN} = N^i N^j R_{ij}\bigg|_{r=0}. \tag{7.231}$$

Then the coincidence limit of the first two correction terms is

$$[\Psi_1] = \sqrt{t}\left\{-\frac{r^2}{t}h\left(\frac{r}{\sqrt{t}}\right)K\right\} \tag{7.232}$$

$$[\Psi_2] = t\Bigg\{\left(Q - \frac{1}{6}\hat{R}\right) - \frac{1}{3}\left(1 + \frac{r^2}{t}\right)R^0_{nn} \tag{7.233}$$

$$+ f_1\left(\frac{r}{\sqrt{t}}\right)K^2 + f_2\left(\frac{r}{\sqrt{t}}\right)K_{\mu\nu}K^{\mu\nu}\Bigg\} \tag{7.234}$$

where all tensor quantities are calculated on the boundary.

7.7 Applications to Stochastic Volatility Problems

7.7.1 Hagan Formula

Let us apply now the methods described in previous lectures to the SABR model. Let us consider a European option on a forward asset expiring T years from today. Let $G(t, f, \sigma; T, F, \Sigma)$ be the price of

Arrow-Debreu securitiy whose payoff at time T is given by Dirac delta-function. For time $0 < t < T$ it satisfies the partial differential equation

$$\left(\frac{\partial}{\partial t} + L\right) G = 0\,, \tag{7.235}$$

where

$$L = \frac{1}{2}\sigma^2 \left(C(f)^2 \frac{\partial^2}{\partial f^2} + 2v\rho C(f) \frac{\partial^2}{\partial f \partial \sigma} + v^2 \frac{\partial^2}{\partial \sigma^2} \right)\,, \tag{7.236}$$

with the terminal condition

$$G(T, f, \sigma; T, F, \Sigma) = \delta(f - F)\delta(\sigma - \Sigma)\,. \tag{7.237}$$

Here v is a constant parameter (volatility of volatility) and it is assumed that $v^2 T$ is small, ρ is the correlation coefficient between two Winer processes. The function $C(f)$ is supposed to be positive monotone non-decreasing and smooth. It is extended to negative values of the argument by

$$C(-f) = -C(f)\,. \tag{7.238}$$

Actually, it has to be smooth at zero as well, more precisely,

$$\partial_f C(f)\Big|_{f=0} = 0\,. \tag{7.239}$$

It this is not so then the first derivative has a jump at zero and the problem becomes non-smooth.

This equation should be also supplemented by appropriate boundary conditions at zero and at infinity. In particular, it is assumed that

$$\lim_{F,\Sigma\to\infty} G(t, f, \sigma; T, F, \Sigma) = 0\,. \tag{7.240}$$

We change variables to convert this problem to the usual heat equation setting

$$\tau = T - t, \qquad x^1 = x = f\,, \qquad x^2 = y = \frac{\sigma}{v}\,. \tag{7.241}$$

Then the equation becomes

$$(\partial_\tau + L)U(\tau; x, x') = 0\,, \tag{7.242}$$

where

$$L = -\frac{v^2}{2} y^2 \left[C^2(x)\partial_x^2 + 2\rho C(x)\partial_x\partial_y + \partial_y^2 \right] . \tag{7.243}$$

This operator defines a Riemannian metric g^{ij} with components

$$g^{11} = \frac{v^2}{2} y^2 C^2 , \tag{7.244}$$

$$g^{12} = \frac{v^2}{2} \rho y^2 C , \tag{7.245}$$

$$g^{22} = \frac{v^2}{2} y^2 . \tag{7.246}$$

The covariant components of the metric are obtained by inverting the matrix (g^{ij})

$$g_{11} = \frac{2}{v^2(1-\rho^2)} \frac{1}{y^2 C^2} , \tag{7.247}$$

$$g_{12} = -\frac{2\rho}{v^2(1-\rho^2)} \frac{1}{y^2 C} , \tag{7.248}$$

$$g_{22} = \frac{2}{v^2(1-\rho^2)} \frac{1}{y^2} . \tag{7.249}$$

The Riemannian volume element is determined now by the determinant of the metric g_{ij}

$$g = \det g_{ij} = \frac{4}{v^4(1-\rho^2)} \frac{1}{y^4 C^2} . \tag{7.250}$$

We also note the following useful combination

$$g^{1/2} g^{11} = \frac{1}{\sqrt{1-\rho^2}} C , \tag{7.251}$$

$$g^{1/2} g^{12} = \frac{\rho}{\sqrt{1-\rho^2}} , \tag{7.252}$$

$$g^{1/2} g^{22} = \frac{1}{\sqrt{1-\rho^2}} \frac{1}{C} . \tag{7.253}$$

The intrinsic properties of the metric are characterized by the curvature. Let us compute the curvature of this metric. Omitting lengthy but straightforward calculations we list the result. Christofel

symbols are

$$\Gamma^1{}_{11} = -\frac{C'}{C} + \frac{\rho}{1-\rho^2}\frac{1}{yC} \tag{7.254}$$

$$\Gamma^2{}_{11} = \frac{1}{1-\rho^2}\frac{1}{yC^2} \tag{7.255}$$

$$\Gamma^1{}_{22} = \frac{\rho}{1-\rho^2}\frac{C}{y} \tag{7.256}$$

$$\Gamma^2{}_{22} = -\frac{1-2\rho^2}{1-\rho^2}\frac{1}{y} \tag{7.257}$$

$$\Gamma^1{}_{12} = -\frac{1}{1-\rho^2}\frac{1}{y} \tag{7.258}$$

$$\Gamma^2{}_{12} = -\frac{\rho}{1-\rho^2}\frac{1}{yC}\,. \tag{7.259}$$

By using these equations one can show that the Riemann tensor (which has only one nontrivial component in two dimensions) takes the form

$$R^{12}{}_{12} = -\frac{v^2}{2}\,. \tag{7.260}$$

This is nothing but Gaussian curvature. The scalar curvature is

$$R = -v^2\,. \tag{7.261}$$

Note that the curvature does not depend on the function $C(x)$ at all. This means that the arbitrariness of the function C just reflects the possibility to make an arbitrary change of coordinates (diffeomorphism). It does not change the geometry, which remains the geometry of the hyperbolic plane, a space of constant negative curvature.

Therefore, our metric has constant curvature and is nothing but hyperbolic plane H^2 in some non-trivial coordinates. By solving the equations of geodesics one can find the relation of these coordinates to the standard geodesic coordinates. We assume that this has been already done.

Now, we rewrite the operator in the form

$$L = L_0 + L_1 \tag{7.262}$$

where L_0 is the scalar Laplacian,

$$L_0 = -g^{-1/2}\partial_i g^{1/2} g^{ij}\partial_j\,, \tag{7.263}$$

and L_1 is a first order operator,

$$L_1 = \frac{v^2}{2} y^2 C(x) C'(x) \partial_x \,. \tag{7.264}$$

We have already found the heat kernel of the operator L_0 in the hyperbolic plane in a previous lecture, at least at the limit $t \to 0$. Let r be the geodesic distance between x and x'. Then the heat kernel of the operator L_0 reads

$$\begin{aligned} U_0(t; x, x') &= \frac{1}{4\pi t} \sqrt{\frac{\rho r}{\sinh(\rho r)}} \exp\left(-\frac{r^2}{4t}\right) \\ &\quad \times \left\{ 1 - \frac{t}{4r^2} \left[\rho^2 r^2 + \rho r \coth(\rho r) - 1 \right] + O(t^2) \right\}, \end{aligned} \tag{7.265}$$

where

$$\rho = \frac{v}{\sqrt{2}} \,. \tag{7.266}$$

By treating the operator L_1 as a perturbation, we get

$$U(t; x, x') = \left\{ 1 - t L_1 + \frac{t^2}{2} \left(L_1^2 + [L_0, L_1] \right) + O(t^3) \right\} U_0(t; x, x') \,. \tag{7.267}$$

If we restrict ourselves to the linear order in L_1 and substitutes here an expression for the geodesic distance as a function of coordinates x and y, then this equation reduces to *Hagan formula*.

7.7.2 Heston Formula

In this section we show how to solve the parabolic equation for the Heston model. It is described by the equation

$$\left(-\frac{\partial}{\partial t} + L \right) V = 0 \,, \tag{7.268}$$

where L is the operator defined by

$$L = -\frac{1}{2} v S^2 \frac{\partial^2}{\partial S^2} - \rho \eta v S \frac{\partial^2}{\partial S \partial v} - \frac{1}{2} \eta^2 v \frac{\partial^2}{\partial v^2} - r S \frac{\partial}{\partial S} + \lambda (v - \bar{v}) \frac{\partial}{\partial v} + r \,. \tag{7.269}$$

Here S is the stock price, v is its variance, η is the volatility of volatility, r is the risk-free interest rate, and ρ, λ and $\bar{v}$ are some real parameters. The range of the variables S and v is

$$0 \le S < \infty \,, \qquad \text{and } 0 \le v < \infty \,. \tag{7.270}$$

We impose some terminal condition at $t = T$

$$V(T, S, v) = V_0(S, v)\,. \tag{7.271}$$

We also need some boundary conditions for the variables S and v. It is easy to see that the points $S = 0$ and $v = 0$ are singular. The issue of the boundary condition at a singular point is actually a subtle one. One cannot impose an arbitrary boundary condition at a singular point; the boundary condition has to be compatible with the equation. It turns out that the conditions that the function V vanishes at the boundary is compatible. So, we choose

$$V(t, 0, v) = V(t, S, 0) = 0\,. \tag{7.272}$$

Of course, there is always the regularity condition at infinity, as $S \to \infty$ and $v \to \infty$.

Since the operator L is homogeneous in the variable S we could apply Mellin transform in the variable S and Laplace transform in the time variable. We prefer to make the following change of variables first

$$x = \log S\,, \qquad u = \frac{v}{\eta}\,, \qquad \tau = \frac{\eta}{2}(T - t)\,. \tag{7.273}$$

The equation takes the following form in new variables

$$(\partial_\tau + \tilde{L})V = 0\,, \tag{7.274}$$

where

$$\tilde{L} = -u\left(\partial_x^2 + 2\rho\partial_x\partial_u + \partial_u^2\right) + \left(u - 2\frac{r}{\eta}\right)\partial_x + 2\frac{\lambda}{\eta}\left(u - \frac{\bar{v}}{\eta}\right)\partial_u + 2\frac{r}{\eta}\,. \tag{7.275}$$

The heat kernel $U(\tau; x, u,', u')$ of the operator $\tilde{L}$ is now defined by the equation

$$(\partial_\tau + \tilde{L})U = 0\,, \tag{7.276}$$

with the initial condition

$$U(0; x, u, x', u') = \delta(x - x')\delta(u - u')\,, \tag{7.277}$$

and the appropriate boundary conditions.

The operator $\tilde{L}$ defines a Riemannian metric

$$(g^{ij}) = u\begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\,. \tag{7.278}$$

The inverse metric is

$$(g_{ij}) = \frac{1}{u}\frac{1}{1-\rho^2}\begin{pmatrix} 1 & -\rho \\ -\rho & 1 \end{pmatrix}. \tag{7.279}$$

Therefore, the Riemannian volume element is

$$g^{1/2}dx\,du = \frac{1}{\sqrt{1-\rho^2}}\frac{dx\,du}{u}. \tag{7.280}$$

First of all, we note that for the operator to be elliptic the parameter ρ should satisfy the inequality

$$\rho < 1. \tag{7.281}$$

Second, omitting a lengthy (but straightforward) calculation we obtain the Gaussian curvature

$$K = -\frac{1}{2u}. \tag{7.282}$$

Thus, the manifold is that of negative curvature with *true singularity* at the boundary $u = 0$. This poses serious problems in dealing with this equation. The corresponding manifold is actually not a smooth manifold; the whole geometric picture breaks down at the singularity. Thus one needs some other methods to explore the region close to boundary.

Now, since the coefficients of the operator do not depend on x we can apply Fourier transform in x. By using

$$U(\tau; x, u, x', u') = \int_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} e^{ip(x-x')}\hat{U}(\tau, p; u, u'), \tag{7.283}$$

where a is a real constant that must be chosen in such a way that the integral converges, we obtain an equation for $\hat{U}$

$$\left[\partial_\tau - u\partial_u^2 + (2\beta_1 u + \beta_0)\partial_u + \gamma_1 u + \gamma_0\right]\hat{U} = 0, \tag{7.284}$$

where

$$\beta_1 = \frac{\lambda}{\eta} - i\rho p, \tag{7.285}$$

$$\beta_0 = -2\frac{\lambda}{\eta^2}\bar{v}, \tag{7.286}$$

$$\gamma_1 = p^2 + ip, \tag{7.287}$$

$$\gamma_0 = 2\frac{r}{\eta}(1 - ip), \tag{7.288}$$

with the initial condition

$$\hat{U}(0,p;u,u') = \delta(u-u')\,. \tag{7.289}$$

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 variables S with a contour of integration in the strip of analyticity. That is why Fourier integral in the variables 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.

Further, since the coefficients of the operator L are linear in u we can apply Laplace transform in the variable u. Thus we represent the heat kernel in the form

$$U(\tau;x,u,x',u') = \int\limits_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} \int\limits_{b-i\infty}^{b+i\infty} \frac{dq}{2\pi i} e^{ip(x-x')+qu} F(\tau,p,q;u')\,, \tag{7.290}$$

where b is a sufficiently large positive constant.

Substituting this form of the heat kernel into the equation we obtain a *first-order* differential equation

$$\left[\partial_\tau + f(q)\partial_q + \varphi(q)\right] F = 0\,, \tag{7.291}$$

where

$$f(q) = q^2 - 2\beta_1 q - \gamma_1 \tag{7.292}$$

$$\varphi(q) = (\beta_0+2)q + \gamma_0 - 2\beta_1\,. \tag{7.293}$$

The initial condition for the function F has the form

$$F(0,p,q;u') = e^{-qu'}\,. \tag{7.294}$$

This equation is of the Hamilton-Jacobi type; it can be solved by the method described in the third lecture. We write

$$F = e^{\Psi}\,. \tag{7.295}$$

Then the initial condition for the function Ψ is

$$\Psi(0,p,q;u') = -qu'\,. \tag{7.296}$$

Then the above equation can be written in the form

$$\left[\partial_\tau + f(q)\partial_q\right]\Psi = -\varphi(q)\,, \tag{7.297}$$

Now, we consider the characteristic Hamiltonian system

$$\frac{d\hat{q}}{d\tau} = f(\hat{q})\,, \tag{7.298}$$

$$\frac{d\hat{\Psi}}{d\tau} = -\varphi(\hat{q})\,. \tag{7.299}$$

These equations are separable and can be easily integrated. We obtain

$$\tau = \int_{q_0}^{q} \frac{d\hat{q}}{f(\hat{q})} \tag{7.300}$$

and

$$\Psi(\tau, p, q; u') = -q_0 u' - \int_{q_0}^{q} d\hat{q}\, \frac{\varphi(\hat{q})}{f(\hat{q})}\,, \tag{7.301}$$

where $q_0 = q_0(\tau, q)$ is a function of τ and q that is implicitly defined by the first equation.

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

$$f(q) = q^2 - 2\beta_1 q - \gamma_1 = 0\,. \tag{7.302}$$

We have

$$q_{1,2} = \beta_1 \pm D\,, \tag{7.303}$$

where

$$D = \sqrt{\beta_1^2 + \gamma_1}\,. \tag{7.304}$$

Then

$$\frac{1}{q^2 - 2\beta_1 q - \gamma_1} = \frac{1}{2D}\left(\frac{1}{q - q_1} - \frac{1}{q - q_2}\right) \tag{7.305}$$

and we compute

$$\int dq \frac{1}{q^2 - 2\beta_1 q - \gamma_1} = \frac{1}{2D} \log \frac{q - q_1}{q - q_2} \tag{7.306}$$

and

$$\int dq \frac{q}{q^2 - 2\beta_1 q - \gamma_1} = \frac{1}{2D}\left[q_1 \log(q - q_1) - q_2 \log(q - q_2)\right]\,. \tag{7.307}$$

By using these integrals we obtain

$$\tau = \frac{1}{2D} \log \left[\frac{(q-q_1)(q_0-q_2)}{(q_0-q_1)(q-q_2)} \right] \tag{7.308}$$

and

$$\Psi = -q_0 u' - a_1 \log \frac{q-q_1}{q_0-q_1} - a_2 \log \frac{q-q_2}{q_0-q_2}\,, \tag{7.309}$$

where

$$a_1 = \frac{1}{2D}\left[(\beta_0+2)D + \gamma_0 + \beta_0\beta_1\right] \tag{7.310}$$

$$a_2 = \frac{1}{2D}\left[(\beta_0+2)D - \gamma_0 - \beta_0\beta_1\right] \tag{7.311}$$

Now, let us introduce a function

$$\begin{aligned} R = R(\tau, q) &= \frac{q-q_1}{q-q_2} e^{-2D\tau} \\ &= \frac{q-\beta_1-D}{q-\beta_1+D} e^{-2D\tau}\,. \end{aligned} \tag{7.312}$$

Then from the equation for τ we obtain

$$\begin{aligned} q_0 &= \frac{q_1 - R q_2}{1-R} \\ &= \beta_1 + D\frac{1+R}{1-R}\,. \end{aligned} \tag{7.313}$$

Thus, the function Ψ can be expressed in terms of the function R

$$\begin{aligned} \Psi &= -\left(\beta_1 + D\frac{1+R}{1-R}\right) u' \\ &\quad -a_1 \log \frac{(q-\beta_1-D)(1-R)}{2DR} \\ &\quad -a_2 \log \frac{(q-\beta_1+D)(1-R)}{2D}\,. \end{aligned} \tag{7.314}$$

Finally, let us write down the heat kernel

$$U(\tau; x, u, x', u') = \int\limits_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} \int\limits_{b-i\infty}^{b+i\infty} \frac{dq}{2\pi i} e^{ip(x-x')+qu-q_0u'} \left(\frac{q_0-q_1}{q-q_1}\right)^{a_1} \left(\frac{q_0-q_2}{q-q_2}\right)^{a_2}\,. \tag{7.315}$$

This formula gives a complete solution for the heat kernel it is pretty complicated since it involves two complex integrals. Recall that all parameters here depend on p as well.

Now, let us consider a solution of the heat equation $P_n(\tau; x, u)$ with the initial conditions that do not depend on u and have the form

$$P_n(0; x, u) = e^{nx}\theta(x)\,, \tag{7.316}$$

where $\theta(x)$ is the step-function

$$\theta(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{if } x < 0\,. \end{cases} \tag{7.317}$$

Then the solution is given by

$$P_n(\tau; x, u) = \int_0^\infty dx' \int_0^\infty du'\, U(\tau; x, u, x', u') e^{nx'}\,. \tag{7.318}$$

Now, by using the above heat kernel we obtain

$$P_n(\tau; x, u) = \int_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} \int_{b-i\infty}^{b+i\infty} \frac{dq}{2\pi i} e^{ipx+qu} \frac{1}{q_0(n-ip)} \left(\frac{q_0-q_1}{q-q_1}\right)^{a_1} \left(\frac{q_0-q_2}{q-q_2}\right)^{a_2}\,. \tag{7.319}$$

This integral can be computed by residue theory. However, it is much easier to solve the equation directly without Laplace transform. We write

$$P_n(\tau; x, u) = \int_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} e^{ipx} \hat{P}_n(\tau, p; u)\,, \tag{7.320}$$

where a is a sufficiently large negative real constant, so that $a < -n$.

The Fourier transformed function $\hat{P}_n(\tau, p; u)$ satisfies the equation

$$\left[\partial_\tau - u\partial_u^2 + (2\beta_1 u + \beta_0)\partial_u + \gamma_1 u + \gamma_0\right] \hat{P}_n = 0\,, \tag{7.321}$$

and the initial condition

$$\hat{P}_n(0, p; u) = \frac{1}{ip - n}\,. \tag{7.322}$$

Now, we use the singular perturbation technique. We rescale all derivatives

$$\left[\varepsilon\partial_\tau - \varepsilon^2 u\partial_u^2 + (2\beta_1 u + \beta_0)\varepsilon\partial_u + \gamma_1 u + \gamma_0\right]\hat{P}_n = 0\,, \tag{7.323}$$

and look for a solution in the form

$$P_n = \exp\left(\frac{\Phi}{\varepsilon}\right)\Omega\,, \tag{7.324}$$

where

$$\Omega = \sum_{k=0}^{\infty}\varepsilon^k\Omega_k\,. \tag{7.325}$$

These functions satisfy the initial conditions

$$\Phi(0,p;u) = 0 \tag{7.326}$$

and

$$\Omega(0,p;u) = \frac{1}{ip-n}\,. \tag{7.327}$$

Substituting this ansatz into the equation we obtain the Hamilton-Jacobi equation for Φ, the action,

$$\partial_\tau\Phi - u(\partial_u\Phi)^2 + (2\beta_1 u + \beta_0)\partial_u\Phi + \gamma_1 u + \gamma_0 = 0 \tag{7.328}$$

and a recursive system for the coefficients Ω_k

$$\left\{\partial_\tau + \left[2\beta_1 u + \beta_0 - 2u(\partial_u\Phi)\right]\partial_u - u(\partial_u^2\Phi)\right\}\Omega_k = u\partial_u^2\Omega_{k-1}\,. \tag{7.329}$$

The first equation is solved by the ansatz

$$\Phi(\tau,p,u) = uA(\tau,p) + B(\tau,p)\,. \tag{7.330}$$

Substituting this into the Hamilton-Jacobi equation we obtain equations for functions A and B

$$\partial_\tau A = A^2 - 2\beta_1 A - \gamma_1\,, \tag{7.331}$$

$$\partial_\tau B = -\beta_0 A - \gamma_0\,. \tag{7.332}$$

This system is almost identical to the system for functions $\hat{q}$ and Ψ. The solution of this system with the initial conditions

$$A(0) = B(0) = 0 \tag{7.333}$$

reads

$$\tau = \frac{1}{2D} \log \left[\frac{(A - q_1)q_2}{q_1(A - q_2)} \right] , \tag{7.334}$$

so that

$$\begin{aligned} A &= \frac{q_1 q_2 (1 - e^{-2D\tau})}{q_1 - q_2 e^{-2D\tau}} \\ &= -\gamma_1 \frac{\sinh(D\tau)}{\beta_1 \sinh(D\tau) + D\cosh(D\tau)} , \end{aligned} \tag{7.335}$$

and

$$B = -(\gamma_0 + \beta_0\beta_1)\tau + \beta_0 \log \left[\cosh(D\tau) + \beta_1 \frac{\sinh(D\tau)}{D} \right] . \tag{7.336}$$

Next, the equation for Ω_0 is

$$\{\partial_\tau + [2\beta_1 u + \beta_0 - 2uA]\,\partial_u\}\,\Omega_0 = 0\,. \tag{7.337}$$

Since the initial value is constant the solution of this equation is constant

$$\Omega_0 = \frac{1}{ip - n}\,. \tag{7.338}$$

Once this is established then from the recursion system it follows that all higher-order coefficients are zero. Thus the solution of the initial value problem is

$$\begin{aligned} P_n(\tau; x, u) &= \int_{ia-\infty}^{ia+\infty} \frac{dp}{2\pi} \frac{1}{(ip - n)} e^{ipx - (\gamma_0 + \beta_0\beta_1)\tau} \\ &\quad \times \exp\left(-\frac{u\gamma_1 \sinh(D\tau)}{\beta_1 \sinh(D\tau) + D\cosh(D\tau)} \right) \\ &\quad \times \left(\cosh(D\tau) + \beta_1 \frac{\sinh(D\tau)}{D} \right)^{\beta_0} , \end{aligned} \tag{7.339}$$

This is the basis of the well-known Heston formula.

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Bibliography

[1] K. Andersson, *Stochastic volatility*, UUDM Project Report 2003:18, Uppsala University

[2] S. Albeverio, F. Gesztesy, R. Hoegh-Krohn, and H. Holden, *Solvable Models in Quantum Mechanics*, AMS Chelsea Publishing, 2004

[3] I. G. Avramidi, *Covariant Methods for the Calculation of the Effective Action in Quantum Field Theory and Investigation of Higher-Derivative Quantum Gravity*, PhD Thesis, Moscow State University (1986), arXiv:hep-th/9510140, 159 pp.

[4] I. G. Avramidi, *The covariant technique for calculation of the heat kernel asymptotic expansion*, Physics Letters B, **238** (1990) 92–97.

[5] I. G. Avramidi, *The nonlocal structure of one-loop effective action via partial summation of asymptotic expansion*, Physics Letters B, **236** (1990) 443–449.

[6] I. G. Avramidi, *A covariant technique for the calculation of the one-loop effective action*, Nuclear Physics B, **355** (1991) 712–754; Erratum: Nuclear Physics B, **509** (1998) 557–558.

[7] I. G. Avramidi, *A method for calculating the heat kernel for manifolds with boundary*, Yadernaya Fizika, 56 (1993) 245-252, [in Russian]; Physics of Atomic Nuclei, 56 (1993), [in English]; available at arXiv:hep-th/9509078

[8] I. G. Avramidi, *A new algebraic approach for calculating the heat kernel in gauge theories*, Physics Letters B, **305** (1993) 27–34.

[9] I. G. Avramidi, *Covariant methods for calculating the low-energy effective action in quantum field theory and quantum gravity*, University of Greifswald (March, 1994), arXiv:gr-qc/9403036, 48 pp.

[10] I. G. Avramidi, *The heat kernel on symmetric spaces via integrating over the group of isometries*, Physics Letters B, **336** (1994) 171–177.

[11] I. G. Avramidi, *Covariant algebraic method for calculation of the low-energy heat kernel*, Journal of Mathematical Physics, **36** (1995) 5055–5070.

[12] I. G. Avramidi, *New algebraic methods for calculating the heat kernel and the effective action in quantum gravity and gauge theories*, in: *Heat Kernel Techniques and Quantum Gravity*, Ed. S. A. Fulling, Discourses in Mathematics and Its Applications, (College Station: Texas A&M University, 1995), pp. 115–140; arXiv:gr-qc/9408028.

[13] I. G. Avramidi, *A new algebraic approach for calculating the heat kernel in quantum gravity*, Journal of Mathematical Physics, **37** (1996) 374–394.

[14] I. G. Avramidi, *Covariant approximation schemes for calculation of the heat kernel in quantum field theory*, in: *Quantum Gravity*, Eds. V. A. Berezin, V. A. Rubakov and D. V. Semikoz, (Singapore: World Scientific, 1997), pp. 61–78; arXiv:hep-th/9509075.

[15] I. G. Avramidi, *Nonperturbative methods for calculating the heat kernel*, in: *Global Analysis, Differential Geometry and Lie Algebras*, Ed. G. Tsagas, (Bucharest: Geometry Balcan Press, 1998), pp. 7–21; arXiv:hep-th/9602169.

[16] I. G. Avramidi, *Covariant techniques for computation of the heat kernel*, Reviews in Mathematical Physics, **11** (1999) 947–980.

[17] I. G. Avramidi, *Heat Kernel and Quantum Gravity*, Lecture Notes in Physics, New Series m: Monographs, LNP:m64 (Berlin-New York: Springer-Verlag 2000).

[18] I. G. Avramidi, *Heat kernel in quantum field theory*, Nuclear Physics Proc. Suppl., **104** (2002) 3–32.

[19] I. G. Avramidi, *Heat kernel asymptotics of Zaremba boundary value problem*, Mathematical Physics, Analysis and Geometry, **7** (2004) 9–46.

[20] I. G. Avramidi, *Non-Laplace type operators on manifolds with boundary*, in: *Analysis, Geometry and Topology of Elliptic Operators*, Papers in Honor of Krzysztof P. Wojciechowski, Eds. B. Booss-Bavnbek, S. Klimek, M. Lesch and W. Zhang (Singapore: World Scientific, 2006), pp. 119-152.

[21] I. G. Avramidi, *Heat kernel asymptotics on symmetric spaces*, International Journal of Geometry and Topology, (2007) (to appear) arXiv:math.DG/0605762, 20 pp.

[22] I. G. Avramidi, *Heat kernel on homogeneous bundles over symmetric spaces*, New Mexico Tech (January 2007), arXiv:math.AP/0701489, 56 pp.

[23] I. G. Avramidi and T. Branson, *Heat kernel asymptotics of operators with non-Laplace principal part*, Reviews in Mathematical Physics, **6** (2001) 1–44.

[24] I. G. Avramidi and G. Esposito, *Gauge theories on manifolds with boundary*, Communications in Mathematical Physics, **200** (1999) 495–543.

[25] I. G. Avramidi and R. Schimming, *Algorithms for the calculation of the heat kernel coefficients*, in: '*Quantum Field Theory under the Influence of External Conditions*', Ed. M. Bordag, Teubner-Texte zur Physik, Band 30, (Stuttgart: Teubner, 1996), pp. 150–162; arXiv:hep-th/9510206

[26] I. G. Avramidi and R. Schimming, *Heat kernel coefficients to the matrix Schrödinger operator*, Journal of Mathematical Physics, **36** (1995) 5042–5054.

[27] I. G. Avramidi and R. Schimming, *A new explicit expression for the Korteweg-De Vries hierarchy*, Mathematische Nachrichten, **219** (2000) 45–64.

[28] M. Baxter and A. Rennie, *Financial Calculus: An Introduction to Derivative Pricing*, Cambridge University Press, 1996

[29] H. Berestycki, J. Busca and I. Florent, *Computing the implied volatility in stochastic volatility models*, Communications on Pure and Applied Mathematics, **LVII** (2004) 0001-0022

[30] P. Bourgade and O. Croissant, *Heat kernel expansion for a family of stochastic volatility models:* δ*-geometry*, arXiv:cs.CE/0511024

[31] Y. H. Choi and T. P. Branson, *Option pricing on multiple assets*, Acta Applicandae Mathematicae, **94** (2006) 137–162

[32] A. Dragulescu and V. M. Yakovenko, *Probability distribution of returns in the Heston model with stochastic volatility*, Quantitative Finance, **2** (2002) 443–453.

[33] D. Duffie, D. Filipović and W. Schachermayer, *Affine processes and applications in finance*, Preprint

[34] L. Evans, An Introduction to Stochastic Differential Equations, Lecture Notes, UC Berkeley

[35] S. Flügge, *Practical Quantum Mechanics*, Springer, 1974.

[36] J. Gatheral and M. Lynch, *Lecture 1: Stochastic Volatility and Local Volatility*, Preprint

[37] P. Hagan, A. Lesniewski and D. Woodward, *Probability distribution in the SABR model of stochastic volatility*, Preprint

[38] P. S. Hagan, D. Kumar, A. S. Lesniewski and D. E. Woodward, *Managing smile risk*, Preprint

[39] P. S. Hagan and D. E. Woodward, *Equivalent Black volatilities*, Applied Mathematical Finance, **6** (1999) 147–157.

[40] J. Hull, Introduction to Futures and Options Markets, Simon & Schuster, 1991

[41] J. Hull, *Options, Futures and Other Derivatives*, Prentice Hall, 1999

[42] P. Henry-Labordére, *Unifying the BGM and SABR models: a short ride in hyperbolic geometry*, arXiv:ccsd-00015510

[43] P. Henry-Labordére, *A general asymptotic implied volatility for stochastic volatility models*, arXiv:cond-mat/0504317

[44] E. Lieb and D. Mattis, *Mathematical physics in one dimension*, Academic Press, 1965.

[45] V. Linetsky, *The spectral decomposition of the option value*, Preprint

[46] D. Mattis, *Encyclopedia of exactly solved models in one dimension: many-body problem*, World Scientific, 1993.

[47] V. V. Piterbarg, *A stochastic volatility forward libor model with a term structure of volatility smiles*, Preprint

[48] A. Sepp, *Pricing European style options under jump diffusion processes with stochastic volatility: applications of Fourier transform*, Preprint

[49] M. E. Taylor, *Partial Differential Equations*, vol. I, II, Springer, New York, 1991

[50] P. Wilmott, *Derivatives. The Theory and Practice of Financial Engineering*, Wiley, Chichester, 1998

[51] P. Willmott, S. Howison and J. Dewynne, *The Mathematics of Financial Derivatives*, Cambridge University Press, 1995