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**Heat Kernel and  
Analysis on Manifolds**

**Alexander Grigor'yan**

# Heat Kernel and Analysis on Manifolds



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## Heat Kernel and Analysis on Manifolds

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To my wife Tatiana



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## Preface

The development of Mathematics in the past few decades has witnessed an unprecedented rise in the usage of the notion of heat kernel in the diverse and seemingly remote sections of Mathematics. In the paper [217], titled “*The ubiquitous heat kernel*”, Jay Jorgenson and Serge Lang called the heat kernel “... a universal gadget which is a dominant factor practically everywhere in mathematics, also in physics, and has very simple and powerful properties.”

Already in a first Analysis course, one sees a special role of the exponential function  $t \mapsto e^{at}$ . No wonder that a far reaching generalization of the exponential function – the *heat semigroup*  $\{e^{-tA}\}_{t \geq 0}$ , where  $A$  is a positive definite linear operator, plays similarly an indispensable role in Mathematics and Physics, not the least because it solves the associated *heat equation*  $\dot{u} + Au = 0$ . If the operator  $A$  acts in a function space then frequently the action of the semigroup  $e^{-tA}$  is given by an integral operator, whose kernel is called then *the heat kernel* of  $A$ .

Needless to say that any knowledge of the heat kernel, for example, upper and/or lower estimates, can help in solving various problems related to the operator  $A$  and its spectrum, the solutions to the heat equation, as well as to the properties of the underlying space. If in addition the operator  $A$  is Markovian, that is, generates a Markov process (for example, this is the case when  $A$  is a second order elliptic differential operator), then one can use information about the heat kernel to answer questions concerning the process itself.

This book is devoted to the study of the heat equation and the heat kernel of the Laplace operator on Riemannian manifolds. Over 140 years ago, in 1867, Eugenio Beltrami [29] introduced the Laplace operator for a Riemannian metric, which is also referred to as the Laplace-Beltrami operator. The next key step towards analysis of this operator was made in 1954 by Matthew Gaffney [126], who showed that on geodesically complete manifolds the Laplace operator is essentially self-adjoint in  $L^2$ . Gaffney also proved in [127] the first non-trivial sufficient condition for the stochastic completeness of the heat semigroup, that is, for the preservation of the  $L^1$ -norm by this semigroup. Nearly at the same time S. Minakshisundaram [275] constructed the heat kernel on compact Riemannian manifolds using the parametrix method.

However, it was not until the mid-1970s when the geometric analysis of the Laplace operator and the heat equation was revolutionized in the groundbreaking work of Shing-Tung Yau, which completely reshaped the area. The culmination of this work was the proof by Li and Yau [258] in 1986 of the parabolic Harnack inequality and the heat kernel two-sided estimates on complete manifolds of non-negative Ricci curvature, which stimulated further research on heat kernel estimates by many authors. Apart from the general wide influence on geometric analysis, the gradient estimates of Li and Yau motivated Richard Hamilton in his program on Ricci flow that eventually lead to the resolution of the Poincaré conjecture by Grigory Perel'man, which can be viewed as a most spectacular application of heat kernels in geometry<sup>1</sup>.

Another direction in heat kernel research was developed by Brian Davies [96] and Nick Varopoulos [353], [355], who used primarily function-analytic methods to relate heat kernel estimates to certain functional inequalities.

The purpose of this book is to provide an accessible for graduate students introduction to the geometric analysis of the Laplace operator and the heat equation, which would bridge the gap between the foundations of the subject and the current research. The book focuses on the following aspects of these notions, which form separate chapters or groups of chapters.

I. *Local geometric background.* A detailed introduction to Riemannian geometry is given, with emphasis on construction of the Riemannian measure and the Riemannian Laplace operator as an elliptic differential operator of second order, whose coefficients are determined by the Riemannian metric tensor.

II. *Spectral-theoretic properties.* It is a crucial observation that the Laplace operator can be extended to a self-adjoint operator in  $L^2$  space, which enables one to invoke the spectral theory and functional calculus of self-adjoint operator and, hence, to construct the associated heat semigroup. To treat properly the domains of the self-adjoint Laplacian and that of the associated energy form, one needs the Sobolev function spaces on manifolds. A detailed introduction to the theory of distributions and Sobolev spaces is given in the setting of  $\mathbb{R}^n$  and Riemannian manifolds.

III. *Markovian properties and maximum principles.* The above spectral-theoretic aspect of the Laplace operator exploits its ellipticity and symmetry. The fact that its order is 2 leads to the so-called Markovian properties, that is, to maximum and minimum principles for solutions to the Laplace equation and the heat equation. Various versions of maximum/minimum principles are presented in different parts of the book, in the weak, normal, and strong forms. The Markovian properties are tightly related to the diffusion Markov process associated with the Laplacian, where is reflected in

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<sup>1</sup>Another striking application of heat kernels is the heat equation approach to the Atiyah-Singer index theorem – see [12], [132], [317].

the terminology. However, we do not treat stochastic processes here, leaving this topic for a prospective second volume.

IV. *Smoothness properties.* As it is well-known, elliptic and parabolic equations feature an added regularity phenomenon, when the degree of smoothness of solutions is higher than a priori necessary. A detailed account of the local regularity theory in  $\mathbb{R}^n$  (and consequently on manifolds) is given for elliptic and parabolic operators with smooth coefficients. This includes the study of the smoothness of solutions in the scale of Sobolev spaces of positive and negative orders, as well as the embedding theorems of Sobolev spaces into  $C^k$ . The local estimates of solutions are used, in particular, to prove the existence of the heat kernel on an arbitrary manifold.

V. *Global geometric aspects.* These are those properties of solutions which depend on the geometry of the manifold in the large, such as the essential self-adjointness of the Laplace operator (that is, the uniqueness of the self-adjoint extension), the stochastic completeness of the heat kernel, the uniqueness in the bounded Cauchy problem for the heat equation, and the quantitative estimates of solutions, in particular, of the heat kernel. A special attention is given to upper bounds of the heat kernel, especially the on-diagonal upper bounds with the long-time dependence, and the Gaussian upper bounds reflecting the long-distance behavior. The lower bounds as well as the related uniform Harnack inequalities and gradient estimates are omitted and will be included in the second volume.

The prerequisites for reading of this books are Analysis in  $\mathbb{R}^n$  and the basics of Functional Analysis, including Measure Theory, Hilbert spaces, and Spectral Theorem for self-adjoint operators (the necessary material from Functional Analysis is briefly surveyed in Appendix). The book can be used as a source for a number of graduate lecture courses on the following topics: Riemannian Geometry, Analysis on Manifolds, Sobolev Spaces, Partial Differential Equations, Heat Semigroups, Heat Kernel Estimates, and others. In fact, it grew up from a graduate course “Analysis on Manifolds” that was taught by the author in 1995-2005 at Imperial College London and in 2002, 2005 at Chinese University of Hong Kong.

The book is equipped with over 400 exercises whose level of difficulty ranges from “general nonsense” to quite involved. The exercises extend and illustrate the main text, some of them are used in the main text as lemmas. The detailed solutions of the exercises (about 200 pages) as well as their  $\text{\LaTeX}$  sources are available on the web page of the AMS

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where also additional material on the subject of the book will be posted.

The book has little intersection with the existing monographs on the subject. The above mentioned upper bounds of heat kernels, which were obtained mostly by the author in 1990s, are presented for the first time in a book format. However, the background material is also significantly different from the previous accounts. The main distinctive feature of the foundation

part of this book is a new method of construction of the heat kernel on an arbitrary Riemannian manifold. Since the above mentioned work by Minakshisundaram, the traditional method of constructing the heat kernel was by using the parametrix method (see, for example, [36], [37], [51], [317], [326]). However, a recent development of analysis on metric spaces, including fractals (see [22], [186], [187], [224]), has led to emergence of other methods that are not linked so much to the local Euclidean structure of the underlying space.

Although singular spaces are not treated here, we still employ whenever possible those methods that could be applied also on such spaces. This desire has resulted in the abandonment of the parametrix method as well as the tools using smooth hypersurfaces such as the coarea formula and the boundary regularity of solutions, sometimes at expense of more technical arguments. Consequently, many proofs in this book are entirely new, even for the old well-known properties of the heat kernel and the Green function. A number of key theorems are presented with more than one proof, which should provide enough flexibility for building lecture courses for audiences with diverse background.

The material of Chapters 1 - 10, the first part of Chapter 11, and Chapter 13, belongs to the foundation of the subject. The rest of the book – the second part of Chapter 11, Chapters 12 and 14 - 16, contains more advanced results, obtained in the 1980s -1990s.

Let us briefly describe the contents of the individual chapters.

Chapters 1, 2, 6 contain the necessary material on the analysis in  $\mathbb{R}^n$  and the regularity theory of elliptic and parabolic equations in  $\mathbb{R}^n$ . They do not depend on the other chapters and can be either read independently or used as a reference source on the subject.

Chapter 3 contains a rather elementary introduction to Riemannian geometry, which focuses on the Laplace-Beltrami operator and the Green formula.

Chapter 4 introduces the Dirichlet Laplace operator as a self-adjoint operator in  $L^2$ , which allows then to define the associated heat semigroup and to prove its basic properties. The spectral theorem is the main tool in this part.

Chapter 5 treats the Markovian properties of the heat semigroup, which amounts to the chain rule for the weak gradient, and the weak maximum principle for elliptic and parabolic problems. The account here does not use the smoothness of solutions; hence, the main tools are the Sobolev spaces.

Chapter 7 introduces the heat kernel on an arbitrary manifold as the integral kernel of the heat semigroup. The main tool is the regularity theory of Chapter 6, transplanted to manifolds. The existence of the heat kernel is derived from a local  $L^2 \rightarrow L^\infty$  estimate of the heat semigroup, which in turn is a consequence of the Sobolev embedding theorem and the regularity theory. The latter implies also the smoothness of the heat kernel.

Chapter 8 deals with a number of issues related to the positivity or boundedness of solutions to the heat equation, which can be regarded as an extension of Chapter 5 using the smoothness of the solutions. It contains the results on the minimality of the heat semigroup and resolvent, the strong minimum principle for positive supersolutions, and some basic criteria for the stochastic completeness.

Chapter 9 treats the heat kernel as a fundamental solution. Based on that, some useful tools are introduced for verifying that a given function is the heat kernel, and some examples of heat kernels are given.

Chapter 10 deals with basic spectral properties of the Dirichlet Laplacian. It contains the variational principle for the bottom of the spectrum  $\lambda_1$ , the positivity of the bottom eigenfunction, the discreteness of the spectrum and the positivity of  $\lambda_1$  in relatively compact domains, and the characterization of the long time behavior of the heat kernel in terms of  $\lambda_1$ .

Chapter 11 contains the material related to the use of the geodesic distance. It starts with the properties of Lipschitz functions, in particular, their weak differentiability, which allows then to use Lipschitz functions as test functions in various proofs. The following results are proved using the distance function: the essential self-adjointness of the Dirichlet Laplacian on geodesically complete manifolds, the volume tests for the stochastic completeness and parabolicity, and the estimates of the bottom of the spectrum.

Chapter 12 is the first of the four chapters dealing with upper bounds of the heat kernel. It contains the results on the integrated Gaussian estimates that are valid on an arbitrary manifold: the integrated maximum principle, the Davies-Gaffney inequality, Takeda's inequality, and some consequences. The proofs use the carefully chosen test functions based on the geodesic distance.

Chapter 13 is devoted to the Green function of the Laplace operator, which is constructed by integrating the heat kernel in time. Using the Green function together with the strong minimum principle allows to prove the local Harnack inequality for  $\alpha$ -harmonic functions and its consequences – convergence theorems. As an example of application, the existence of the ground state on an arbitrary manifold is proved. Logically this Chapter belongs to the foundations of the subject and should have been placed much earlier in the sequence of the chapters. However, the proof of the local Harnack inequality requires one of the results of Chapter 12, which has necessitated the present order.

Chapter 14 deals with the on-diagonal upper bounds of the heat kernel, which requires additional hypothesis on the manifold in question. Normally such hypotheses are stated in terms of some isoperimetric or functional inequalities. We use here the approach based on the Faber-Krahn inequality for the bottom eigenvalue, which creates useful links with the spectral properties. The main result is that, to a certain extent, the on-diagonal upper bounds of the heat kernel are equivalent to the Faber-Krahn inequalities.



Chapter 15 continues the topic of the Gaussian estimates. The main technical result is Moser's mean-value inequality for solutions of the heat equation, which together with the integrated maximum principle allows to obtain pointwise Gaussian upper bounds of the heat kernel. We consider such estimates in the following three settings: arbitrary manifolds, the manifolds with the global Faber-Krahn inequality, and the manifolds with the relative Faber-Krahn inequality that leads to the Li-Yau estimates of the heat kernel.

Chapter 16 introduces alternative tools to deal with the Gaussian estimates. The main point is that the Gaussian upper bounds can be deduced directly from the on-diagonal upper bounds, although in a quite elaborate manner. As an application of these techniques, some on-diagonal lower estimates are proved.

Finally, Appendix A contains some reference material as was already mentioned above.

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## Some notation

- $\mathbb{R}_+ \equiv (0, +\infty)$
- $\text{esup}$  – the essential supremum
- $\text{einf}$  – the essential infimum
- $f_+ \equiv \frac{1}{2}(|f| + f)$  - the positive part
- $f_- \equiv \frac{1}{2}(|f| - f)$  - the negative part
- $[f]_a^b \equiv f(b) - f(a)$
- $\log_+ x \equiv (\log x)_+$
- $\simeq$  “comparable to”; namely,  $f(x) \simeq g(x)$  if there exists a constant  $C > 0$  such that  $C^{-1}g(x) \leq f(x) \leq Cg(x)$  for all  $x$  from a specified domain.
- $B_r(x)$  – a ball in  $\mathbb{R}^n$ , that is,  $B_r(x) = \{y \in \mathbb{R}^n : |x - y| < r\}$
- $B_r \equiv B_r(0) = \{y \in \mathbb{R}^n : |y| < r\}$ .
- $\omega_n$  – the area of the unit  $(n - 1)$ -sphere in  $\mathbb{R}^n$ .
- $1_A$  – the indicator function of a set  $A$ , that is,  $1_A(x) = 1$  if  $x \in A$  and  $1_A(x) = 0$  otherwise.
- $\Subset$  “compact inclusion”;  $A \Subset B$  means that the closure  $\overline{A}$  of the set  $A$  is compact and  $\overline{A} \subset B$ .
- $\mathcal{H}$  – a Hilbert space
- $\rightharpoonup$  the sign of the weak convergence (in a Hilbert space)
- $M$  – a Riemannian manifold
- $x \rightarrow \infty$  – a sequence of points on a manifold eventually leaving any compact set.
- $\mathbf{g}$  – the Riemannian metric on  $M$
- $\mu$  – a reference measure on  $M$
- $\Delta_\mu$  – the weighted Laplace operator on  $M$
- $\mathcal{L}$  – the Dirichlet Laplace operator on  $M$
- $L^p(M, \mu)$  – the Lebesgue function space
- $\|\cdot\|_p \equiv \|\cdot\|_{L^p}$
- $u \leq v \text{ mod } W_0^1$  means that  $u \leq v + w$  where  $w \in W_0^1$ .
- $d$  – the geodesic distance on  $M$
- $B(x, r)$  – a geodesic ball on  $M$  with respect to the geodesic distance  $d(x, y)$ .

*Conventions.*

- Summation is assumed over repeated indices. For example,

$$\xi_i x^i = \sum_{i=1}^n \xi_i x^i, \quad a^{ij} u_j = \sum_{j=1}^n a^{ij} u_j, \quad g_{ij} v^i v^j = \sum_{i,j=1}^n g_{ij} v^i v^j,$$

etc.

- Letters  $c, C, c', C'$ , etc denote positive constants (depending on specified parameters) whose value may change at each occurrence.
- positive  $\equiv$  strictly positive, negative  $\equiv$  strictly negative, decreasing  $\equiv$  non-increasing, increasing  $\equiv$  non-decreasing



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