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par

Alexandre ENGOULATOV

LA GEOMETRIE ET LA THEORIE CONFORME DES CHAMPS

Soutenue le 11 décembre 2006 devant la commission d'examen :

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La géométrie et la théorie conforme des champs

Alexandre ENGOULATOV

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Chapter 1

Introduction

1.1 Le noyau de la chaleur

L'objet mathématique autour duquel est centré le présent travail est le noyau de l'opérateur de la chaleur. Cet objet très classique est source d'un vif intérêt scientifique actuel, ce qui s'explique par le fait qu'il intervient dans des domaines aussi variés que par exemple la géométrie riemannienne, l'analyse sur les variétés, le calcul stochastique sur les variétés et, plus récemment, ses contreparties discrètes.

Expliquons de façon intuitive de quoi il s'agit. Soit M une variété Riemannienne. Considérons une marche aléatoire sur M qui part d'un point $x \in M$ et qui, à chaque instant, choisit un point au hasard sur une petite sphère autour du point où elle se trouve pour s'y rendre à l'instant suivant. Cette construction conduit dans la limite d'échelle à un mouvement brownien X_t sur M qui est donc un processus continu qui se propage uniformément dans toutes les directions. De manière équivalente, le mouvement brownien est le processus de diffusion dont le générateur est $\frac{1}{2}\Delta$, où Δ est le laplacien sur M . On peut lui associer le semi-groupe de la chaleur qui s'écrit $(P_t f)(x) = \mathbb{E}_x f(X_t)$, si X_t n'explose pas en un temps fini. D'après la régularité des solutions des équations paraboliques non-dégénérées, P_t possède un noyau $H_t(x, y)$ qui est une fonction lisse sur $(0, \infty) \times M \times M$. C'est le *noyau de la chaleur* sur M .

Vue la définition du noyau de la chaleur, il est bien évident que son comportement est en liaison étroite avec les propriétés géométriques de la variété. Une grande partie de la recherche (citons par exemple [27, 9, 4, 13]) a eu pour but de dégager les quantités les plus pertinentes. Il s'avère qu'il s'agit de *la courbure de Ricci*, de la croissance des volumes des boules géodésiques et des profils isopérimétriques.

1.2 Résultats

Le résultat principal [14] de cette thèse s'inscrit logiquement dans ce cadre car il fournit une borne universelle pour le gradient de la fonction "logarithme du noyau de la chaleur" pour la classe des variétés à courbure de Ricci (Ric) minorée. La preuve fait apparaître l'opérateur Γ_2 du *carré du champ* introduit par D. Bakry [2]. Cet opérateur, à travers l'inégalité de *courbure-dimension* fournit une vision plus synthétique des diffusions, ce qui permet d'incorporer un champ de vecteurs B dans nos considérations et d'énoncer ainsi le

résultat principal pour les diffusions engendrées par $\Delta + B$. On montre le théorème suivant.

Théorème. *Soit M une variété riemannienne compacte. Soit $\mathcal{U}(t, x, y)$ la solution fondamentale de l'équation de la chaleur avec dérive:*

$$\left(\Delta_x + B - \frac{\partial}{\partial t} \right) \mathcal{U}(t, x, y) = 0,$$

où B est un champ de vecteurs de classe C^2 sur M . Supposons que l'opérateur $\Delta_B := \Delta + B$ vérifie la condition de courbure-dimension suivante:

$$\Gamma_2(f, f) \geq \frac{1}{m} (\Delta_B f)^2 - R\Gamma(f, f), \quad \text{pour toute } f \in C^\infty(M),$$

pour certains $m \geq 1$ et $R \geq 0$. Si $\text{diam}(M) \leq D$, il existe une constante $C(m)$ telle que

$$|\nabla \log \mathcal{U}(t, x, y)| \leq C(m) \left(\frac{D}{t} + \frac{1 + D\sqrt{R}}{\sqrt{t}} + R\sqrt{t} \right),$$

uniformément sur $(0, \infty) \times M \times M$.

Ceci n'est sûrement pas une borne optimale, surtout si $R > 0$, et une question ouverte est de l'améliorer.

Dans le cas où il n'y a pas de champ de vecteurs, l'hypothèse sur Γ_2 est impliquée par la minoration de la courbure de Ricci, $\text{Ric}(M) \geq -R$. S'il n'y a pas d'effondrement, c'est à dire, quand les volumes de boules ne sont pas trop petits, notre méthode permet alors de retrouver (partiellement) le résultat analogue de D. Stroock [36]. On obtient alors l'énoncé suivant. Soit M une variété riemannienne compacte de dimension n dont la courbure de Ricci est bornée inférieurement: $\text{Ric}(M) \geq -R$, pour une certaine constante $R \geq 0$. Supposons qu'il n'y ait pas d'effondrement, c'est à dire, qu'il existe $t_0, v_0 > 0$ tels que les volumes des boules géodésiques ne sont pas trop petits:

$$\text{Vol}(B_x(t_0)) \geq v_0, \quad \text{pour tout } x \in M.$$

Il existe alors une constante $C(R, n, v_0, t_0)$ telle que le gradient du logarithme du noyau de la chaleur $H_t(x, y)$ est contrôlé par

$$|\nabla \log H_t(x, y)| \leq C(R, n, v_0, t_0) \left(\frac{d(x, y)}{t} + \frac{1}{\sqrt{t}} \right),$$

uniformément sur $(0, 2t_0^2] \times M \times M$, où $d(x, y)$ est la distance riemannienne entre deux points.

C'est une borne optimale pour de petits temps. L'optimalité vient du fait que $d(x, y)/t$ est l'expression exacte pour le cas euclidien tandis que $1/\sqrt{t}$ est atteint pour le noyau de la chaleur du quotient de \mathbb{R}^n par l'involution $x \rightarrow -x$, pris sur la diagonale.

Il est conjecturé qu'une limite de variétés riemanniennes à courbure de Ricci minorée non effondrées est une variété riemannienne dont le lieu singulier est (conjecturalement) de codimension au moins 4, donc on n'est pas surpris que la contribution du lieu singulier soit petite (le terme en $1/\sqrt{t}$). En revanche, quand il y a effondrement, on sait très peu de choses de l'espace limite, donc la borne a priori sur le gradient est une forme de régularité.

La démonstration du théorème principal se fait en deux étapes. La première est largement inspirée par la méthode de E. P. Hsu [22, 21] qui a montré un résultat analogue au nôtre mais plus faible au sens que les constantes dans ses estimations dépendent de la variété de manière non-spécifiée. Cette méthode consiste à exploiter les propriétés du *pont brownien* $\mathbb{P}_{x,y,t}$ sur M , ou, en d'autres termes, de la mesure de Wiener conditionnée aux trajectoires partant de x et passant par y en temps t . Un fait notable est que, si l'on applique la formule d'Itô à une certaine fonction du pont brownien, cela fait apparaître l'opérateur Γ_2 .

La deuxième partie de la preuve utilise de manière cruciale la majoration de P. Li et S. T. Yau pour $H_t(x, y)$ lui-même qui se trouve dans [27] et les estimations de D. Bakry et Z. M. Qian [4] inspirées par [27].

La thèse est organisée de la manière suivante: dans le chapitre 2, on rappelle d'abord quelques définitions générales sur le laplacien et le noyau de la chaleur dans le contexte des variétés riemanniennes. La section 2.2 contient l'exposition détaillée des résultats fondamentaux de J. Cheeger, P. Li et S. T. Yau [9, 27] sur les estimations du noyau de la chaleur en fonction des bornes sur la courbure de Ricci. Nous y exposons aussi quelques généralisations proposées par D. Bakry et Z. M. Qian [4], F.-Y. Wang [40] et M. Arnaudon, A. Thalmaier et F.-Y. Wang [1]. Les majorations de P. Li et S. T. Yau et une inégalité de Harnack due à D. Bakry et Z. M. Qian serviront ultérieurement dans la preuve du résultat principal de la thèse.

Le chapitre 3 contient la preuve du résultat principal de la thèse. Il commence par un survol de quelques estimées gradients pour les semi-groupes de diffusion. Ensuite, on y trouve un bref aperçu de quelques éléments de calcul stochastique sur les variétés. Le chapitre se termine par la preuve, due à D. Stroock, de l'estimation gradient logarithmique pour le noyau de la chaleur. Il est à noter que D. Stroock utilise dans sa preuve une autre méthode s'appuyant sur la formule de J. M. Bismut qui, elle aussi, est rappelée vu son intérêt indépendant et son importance pour les questions considérées.

Le dernier chapitre (quelque peu spéculatif) est consacré aux applications. Dans un premier temps, on y démontre un théorème de convergence uniforme pour les noyaux de la chaleur pour les variétés à courbure de Ricci minorée et à diamètre borné qui convergent au sens de Gromov-Hausdorff mesuré. Ce résultat est une conséquence de la convergence des valeurs propres et des fonctions propres du laplacien pour de telles variétés, établie par J. Cheeger et T. H. Colding [8], d'une part, et des estimées sur le gradient des fonctions propres du laplacien dues à S. Y. Cheng et S. T. Yau [10], d'autre part. On montre donc la proposition suivante.

Proposition. *Soit (M_j^n) une suite de variétés riemanniennes de dimension n à courbure de Ricci uniformément minorée, i.e. $\text{Ric}(M_j^n) \geq -R$, où $R \geq 0$, et à diamètre uniformément borné, i.e. $\text{diam}(M_j^n) \leq D$, avec pour mesure les mesures riemanniennes normalisées : $\underline{\text{Vol}}_j(\cdot) = \text{Vol}_j^{-1}(M_j^n)\text{Vol}_j(\cdot)$. Supposons qu'il existe un espace limite (Z, d) avec la mesure μ tel qu'au sens de Gromov-Hausdorff mesuré,*

$$(M_j^n, d_j, \underline{\text{Vol}}_j) \rightarrow (Z, d, \mu),$$

quand $j \rightarrow \infty$. Soit $\psi_j: Z \rightarrow M_j$ une approximation de Gromov-Hausdorff. Alors pour chaque $t_0 > 0$, les noyaux de la chaleur H_t^j sur M_j^n , normalisés par le volume de M_j^n , convergent uniformément sur $[t_0, \infty) \times Z \times Z$ vers le noyau de la chaleur $H_t(x, y)$ sur Z , i.e.

$$\text{Vol}(M_j^n) H_t^j(\psi_j(x), \psi_j(y)) \rightarrow H_t(x, y).$$

Comme application, on montre une sorte de précompacité pour l'espace de modules de Théories de Champs sur Graphes (GFT) associées aux variétés de diamètre borné et de courbure de Ricci positive ou nulle. Cette question est motivée par un théorème récent de M. Kontsevich qui affirme que les GFTs apparaissent comme des limites des Théories Conformées de Champs (CFT) sous certaines dégénérescences quand l'énergie minimale tend vers 0 (cf. [24]). A chaque limite de ce type correspond une variété compacte $(X, \mathbb{R}_+^* \cdot g)$ à courbure de Ricci positive ou nulle dont la métrique g est définie à un scalaire positif près. La GFT sur (X, g) associe à chaque graphe métrique Γ avec k sommets "entrants" et l sommets "sortants", un opérateur intégral $\Phi_\Gamma: L^2(X, g)^{\otimes k} \rightarrow L^2(X, g)^{\otimes l}$ dont le noyau est produit du noyau de la chaleur sur X pris en des points et des temps différents.

Soit (M_j) une suite de variétés qui converge vers Z comme dans la proposition ci-dessus. D'après J. Cheeger et T. H. Colding [8], il y a un laplacien généralisé sur Z et, par conséquent, une GFT associée. Nous dirons qu'il y a une convergence de GFTs associées à M_j et Z , si pour chaque graphe métrique Γ avec k sommets entrants, chaque fonction lipschitzienne f sur $\underbrace{Z \times \cdots \times Z}_k$ et chaque suite de fonctions lipschitziennes (f_j) sur $\underbrace{M_j \times \cdots \times M_j}_k$ telle que $|f_j \circ \psi_j - f|_{L^\infty} \rightarrow 0$, on a

$$\Phi_\Gamma(f_j) \longrightarrow \Phi_\Gamma(f).$$

Théorème. *L'espace de GFTs associées aux variétés à courbure de Ricci positive ou nulle et à diamètre égal à 1, est précompact par rapport à la convergence définie ci-dessus.*

1.3 Perspectives

Il est utile de passer quelque temps sur les questions soulevées par la preuve de notre résultat. Premièrement, (et c'est ici, que l'on est contraint de supposer le diamètre borné uniformément) la loi de la distance $d(X_s^{x,y,t}, x)$ du pont brownien au point x intervient dans la preuve. Toute information sur cette loi permettrait de s'affranchir de la borne sur le diamètre et d'obtenir donc une estimation en temps grand même dans le cas effondré.

Il est probablement possible de se débarrasser de l'hypothèse de compacité dans la première assertion du théorème principal. Pour cela, il faudrait par exemple montrer la finitude d'une certaine intégrale sur $M \times [0, t]$ ou, sinon, appliquer le principe de localisation pour le pont brownien. Je remercie Michel Emery pour m'avoir indiqué que ces conditions ne sont pas automatiquement vérifiées si M est non-compacte.

P. Bougerol et Th. Jeulin montrent [6] pour un espace hyperbolique le résultat suivant. Soit $X_s^{x,x,t}$ le pont brownien qui revient à son point de départ. Le processus $\{1/\sqrt{t} d(x, X_{ts}^{x,x,t}), 0 \leq s \leq 1\}$ converge alors faiblement vers une excursion brownienne (l'excursion brownienne est la partie radiale du pont brownien sur \mathbb{R}^3). Donc, la distance maximale à laquelle s'éloigne $X^{x,x,t}$ est typiquement d'ordre \sqrt{t} . Comment démontrer une assertion analogue pour les variétés à courbure de Ricci minorée? La réponse à cette question rendrait le résultat de la thèse pour les grands temps t plus satisfaisant.

Une autre voie de recherche consiste (après s'être débarrassé de l'hypothèse de compacité) à affaiblir l'hypothèse sur la courbure de Ricci et à la supposer minorée par une fonction de la distance à un point marqué $p \in M$, i.e. $\text{Ric}(x) \geq f(d(x, p))$. Une borne inférieure pour $H_t(x, y)$ lui-même sous une telle hypothèse a été établie par J. Cheeger et S. T. Yau

dans [9] (leur preuve est résumée dans le chapitre 2.2 de la thèse). Il existe aussi des bornes supérieures sous une telle hypothèse [1].

Plus récemment, dans les travaux de A. Grigoryan, Th. Coulhon et L. Saloff-Coste, le comportement du noyau de la chaleur a été étudié sous des hypothèses plus robustes. Ce sont la croissance des volumes des boules géodesiques, l'inégalité de Poincaré et le profil isopérimétrique. A. Grigoryan [17] et L. Saloff-Coste [33] ont montré, que pour une variété riemannienne complète, il y a une estimation gaussienne

$$\frac{c}{\text{Vol}(B_x(\sqrt{t}))} \exp\left(-\frac{d^2(x, y)}{ct}\right) \leq H_t(x, y) \leq \frac{C}{\text{Vol}(B_x(\sqrt{t}))} \exp\left(-\frac{d^2(x, y)}{Ct}\right),$$

pour tous $x, y \in M$, $0 < t < c't_0$, où $t_0 \leq \infty$, si et seulement si la condition de doublement du volume et l'inégalité de Poincaré sont satisfaites jusqu'à l'échelle $\sqrt{t_0}$. Il serait intéressant de trouver des hypothèses similaires qui entraînent que

$$|\nabla \log H_t(x, y)| \leq C\left(\frac{d(x, y)}{t} + \frac{1}{\sqrt{t}}\right), \quad \text{quand } 0 < t < c't_0,$$

et de savoir si, de plus, une telle borne est invariante par quasi-isométries pour les grands temps. Notons que dans le cadre discret, i.e. pour les graphes, S. Ishiwata [23] a montré l'invariance par certaines quasi-isométries d'une borne similaire pour le gradient du noyau de la chaleur.

Signalons enfin que toutes les questions évoquées peuvent être posées dans le cadre discret, les graphes étant des espaces métriques mesurés. Récemment, dans les travaux de Lott et Villani, la notion de la courbure de Ricci et l'inégalité de courbure-dimension ont été formulées pour les graphes, quoique les hypothèses géométriques les plus naturelles dans ce contexte soient la croissance des volumes de boules ou, par exemple, l'inégalité de Faber-Krahn.

En outre, les invariants du pont brownien discret présentent leur intérêt propre, s'ouvrant vers les questions de la théorie géométrique des groupes. Signalons une telle question: trouver une minoration de l'aire de remplissage pour le pont brownien dans \mathbb{Z}^2 quand sa longueur tend vers l'infini. Dans le langage de la théorie géométrique des groupes il s'agit de la fonction de Dehn en moyenne sphérique $D_{sMean}(n)$. Avec les résultats de O. Bogopolski et E. Ventura [5], une telle borne donnerait une information précise sur le comportement de la fonction de Dehn en moyenne sphérique. Conjecturalement, on a $C_1 n \log n \leq D_{sMean}(n) \leq C_2 n \log^2 n$.

Dans l'application à la convergence des GFTs considérée ci-dessus, la précompacité des GFTs, associées aux variétés à courbure de Ricci non-négative et à diamètre borné, a été établie dans une topologie assez faible: on a montré qu'à transplantation ψ_j près, pour chaque f , $\Phi_{\Gamma, j}(f) \rightarrow \Phi_{\Gamma}(f)$ ponctuellement. Manifestement, l'équicontinuité des noyaux de la chaleur logarithmiques établie dans le théorème principal devrait impliquer une convergence plus forte des opérateurs Φ_{Γ} . Pour chaque opérateur Φ_{Γ} associé à un graphe métrique Γ avec k sommets entrants, tel que toutes les arêtes sont de longueur au moins égale à $2t$, et toutes fonctions lipschitziennes f_1^j, \dots, f_k^j sur M_j , uniformément proches de f_1, \dots, f_k sur Z , on devrait avoir quelque chose du type

$$\|\Phi_{\Gamma}(f_1, \dots, f_k) - \Phi_{\Gamma, j}(f_1^j, \dots, f_k^j) \circ \psi_j\|_{L^2} \leq \epsilon_j \|P_t f_1\|_{L^2} \cdots \|P_t f_k\|_{L^2},$$

où $\epsilon_j \rightarrow 0$ et P_t désigne l'action du semi-groupe de la chaleur sur f .

C'est une sorte de convergence en norme, où, pour comparer des espaces de Hilbert différents, on utilise les applications ψ_j qui ne sont pas des isomorphismes. Le complément orthogonal de l'image est serré par les $P_{t,j}$ quand j est grand et ce d'une manière uniforme, par tous les $\Phi_{\Gamma,j}$.

Chapter 2

Estimates of the heat kernel on manifolds

The heat propagation in different spaces is described by the heat equation, a parabolic PDE which equals the increment of temperature at a given point to the temperature function acted upon by the Laplace operator Δ . This model makes sense in different setups where the heat diffusion semigroup may be defined: first of all on Riemannian manifolds, and more generally, on weighted graphs, metric-measure-energy spaces...

2.1 Generalities about heat kernel on manifolds

The heat kernel $H_t(x, y)$ on a Riemannian manifold (M, g) is the smallest positive fundamental solution to the heat equation,

$$(\Delta_x - \partial_t)H_t(x, y) = 0, \tag{2.1}$$

with a source at y . Here the Laplacian is a natural second order operator associated with g , namely,

$$\Delta = \operatorname{div} \nabla$$

where ∇ and div are the Riemannian gradient and divergence, respectively. More generally, let μ be a Borel measure defined on M which possesses a smooth density m with respect to Vol_g . Such a couple (M, μ) is called a weighted manifold. The Laplacian associated to (M, μ) writes $\Delta_\mu = m^{-1} \operatorname{div} (m \nabla)$, ($\Delta = \Delta_{\operatorname{Vol}_g}$ is a particular case when $m = 1$). An energy form of Δ_μ is given by

$$\mathcal{E}_\mu(f) = \int_M |\nabla f|^2 d\mu.$$

By integration by parts formula it is equal to

$$\int_M f \Delta_\mu f d\mu$$

for a compactly supported function f .

Equivalently, the heat kernel may be defined as the transition density of the Brownian motion W_t on M , which is by definition a diffusion process generated by¹ Δ .

¹Probabilists prefer to add a 1/2 factor before Δ .

The most frequent question about the heat kernel is to estimate its behavior given some information about the geometry of the manifold. Various kinds of estimates are available by now such as uniform/pointwise, on/off-diagonal, upper/lower etc... The relevant geometric conditions are the metric-measure ones. They are essentially encoded in the geodesic balls' volume growth and isoperimetric profiles. However, historically the first result in this direction was the seminal paper by P. Li and S. T. Yau where they deduced upper and lower pointwise bounds on the heat kernel from the assumptions on the Ricci curvature of the manifold.

To study the heat kernel on general manifolds (or graphs) it is instructive to compare it with the simplest explicit example which is the Gaussian kernel in \mathbb{R}^n :

$$H_t(x, y) = \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{d^2(x, y)}{4t}\right).$$

Here $d(x, y)$ is the Riemannian distance between two points. Another explicit example is the hyperbolic 3-dimensional space \mathbb{H}^3 where

$$H_t(x, y) = \frac{1}{(4\pi t)^{3/2}} \exp\left(-t - \frac{d^2(x, y)}{4t}\right) \frac{d(x, y)}{\sinh d(x, y)}.$$

Note also that, if M is compact, then the operator Δ^{-1} is compact. Let $\{\phi_k\}_{k=0}^{\infty}$ be an orthonormal basis in $L^2(M, Vol)$ of eigenfunctions of Δ with eigenvalues

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots$$

Then the heat kernel $H_t(x, y)$ on M is determined by

$$H_t(x, y) = \sum_{k=0}^{\infty} e^{-\lambda_k t} \phi_k(x) \phi_k(y).$$

2.2 Heat kernel and curvature

The interplay between the heat kernel and the curvature of a manifold has been studied in the works of J. Cheeger, P. Li, S. T. Yau in 1980s [9, 27]. It relies heavily on the maximum principle for parabolic PDEs and its consequences. Some earlier results linking the heat kernel and the *sectional curvature* are to be found in [13].

2.2.1 Comparison with model spaces (J. Cheeger-S. T. Yau)

Definition 2.1. A Riemannian manifold \mathfrak{M}^n is an open model if the following holds:

- (i) For some point $\mathfrak{x} \in \mathfrak{M}^n$ and $0 < R \leq \infty$, $\mathfrak{M}^n = B_R(\mathfrak{x})$ (the open ball of radius R around \mathfrak{x}) and $\exp_{\mathfrak{x}}|_{B_R(0)}$ is a diffeomorphism.
- (ii) For all $r < R$, the mean curvature of the distance sphere $S_r(\mathfrak{x})$ is constant on $S_r(\mathfrak{x})$.

A model \mathfrak{M}^n is an open Ricci model if its metric, when written in polar coordinates, is of the form

$$dr^2 + f^2(r)h,$$

where h is the standard metric on S^{n-1} . A compact Riemannian manifold \mathfrak{M}^n is a closed model (respectively, closed Ricci model) if, for some \mathfrak{x} , $\mathfrak{M}^n = \overline{B_R(\mathfrak{x})}$ and $B_R(\mathfrak{x})$ is an open model (respectively, Ricci model).

Let \mathfrak{M}^n be a model, and let $\mathfrak{m}(r)$ denote the mean curvature function for the distance sphere $S_r(\mathfrak{x})$ in the direction of the inward normal. It may be written as $\mathfrak{m}(r) = A'(r)/A(r)$, where $A(r)$ is the area element on $S_r(\mathfrak{x})$ (notice that $\mathfrak{m}(r) \sim \frac{n-1}{r}$). Given an open model, one can form the *associated Ricci model* by setting

$$f(r) = \left(\frac{A(1)}{\text{Vol } S^{n-1}} \right)^{\frac{1}{n-1}} \exp \left(\frac{1}{n-1} \int_1^r \mathfrak{m}(s) ds \right).$$

Since the mean curvature function of a Ricci model is given by

$$(n-1) \frac{f'}{f} = \mathfrak{m}(r),$$

the associated Ricci model has the same mean curvature function, $\mathfrak{m}(r)$.

To understand better the heat kernel on a model space, it will be instructive to write the heat equation in geodesic polar coordinates around some point x in a manifold M . If C is the *cut-locus* of x , the heat kernel H satisfies

$$\left(-\frac{\partial^2}{\partial r^2} - m(r, \theta) \frac{\partial}{\partial r} + \tilde{\Delta} + \frac{\partial}{\partial t} \right) H = 0, \quad (2.2)$$

on $M \setminus C$. Here $\tilde{\Delta}$ denotes the intrinsic Laplacian on $S_r(x)$ with its induced metric, and $m(r, \theta)$ stands for the mean curvature of the distance sphere $S_r(x)$ with $S_r(x) \cap C$ deleted.

Models can be characterized in terms of the behavior of the fundamental solution \mathfrak{H} to the heat equation on functions. Namely, we have the following statement.

Proposition 2.2 (J. Cheeger-S. T. Yau, [9]). (i) Let \mathfrak{M}^n be an open model (with Dirichlet or Neumann boundary conditions) or a closed model, centered at \mathfrak{x} . Then the heat kernel $\mathfrak{H}_t(\mathfrak{x}, \mathfrak{y}) = \mathfrak{H}_t(\overline{\mathfrak{x}}, \overline{\mathfrak{y}})$ depends only on the distance $\overline{\mathfrak{x}}, \overline{\mathfrak{y}} = r$ and t .

(ii) Conversely, let $\mathfrak{M}^n = B_R(\mathfrak{x})$ or $\overline{B_R(\mathfrak{x})}$, and assume that $\overline{B_R(\mathfrak{x})}$ is complete. Then if $\mathfrak{H}_t(\mathfrak{x}, \mathfrak{y})$ depends only on $\overline{\mathfrak{x}}, \overline{\mathfrak{y}} = r$, and t , it follows that \mathfrak{M}^n is a model.

Proposition 2.2 provides in particular a large family of mutually metrically distinct spaces, for which the heat kernels for some point are expressed by identical functions of r and t .

The following intuitively plausible property of models is crucial for the comparison theorem below.

Lemma 2.3. Let \mathfrak{M}^n be a model, and let $\mathfrak{H}_t(r)$ be the fundamental solution of the heat equation (with respect to Dirichlet or Neumann boundary conditions if \mathfrak{M}^n is open). Then for all $r, t > 0$,

$$\frac{\partial}{\partial r} \mathfrak{H}_t(r) < 0.$$

For small times and distances, the dominating term in the asymptotic expansion for $\partial\mathfrak{H}/\partial r$ is negative. Applying integration by parts and using the fact that $d\mathfrak{H} = (\partial\mathfrak{H}/\partial r)dr$ satisfies the heat equation corresponding to the Hodge Laplacian on one-forms, one then shows that $\partial\mathfrak{H}/\partial r \leq 0$ everywhere on $(0, \infty) \times \mathfrak{M}^n$. Note that the parabolic PDE for $(\partial/\partial r)\mathfrak{H}$ reads:

$$-\frac{\partial^2}{\partial r^2} \left(\frac{\partial\mathfrak{H}}{\partial r} \right) - m(r) \frac{\partial}{\partial r} \left(\frac{\partial\mathfrak{H}}{\partial r} \right) - m'(r) \left(\frac{\partial\mathfrak{H}}{\partial r} \right) + \frac{\partial}{\partial t} \left(\frac{\partial\mathfrak{H}}{\partial r} \right) = 0.$$

(It is the heat equation for one-forms which follows by differentiating (2.2) with respect to r .) Thus we conclude from the maximum principle that $(\partial/\partial r)\mathfrak{H} < 0$ for $r, t > 0$. \square

Let x be a point in a Riemannian manifold M^n . Fix an open ball $B_R(x)$. If $B_R(x)$ is not complete, let $\mathfrak{M}^n = B_R(\mathfrak{x})$ be an open model and fix the same choice of boundary conditions for $B_R(x)$, $B_R(\mathfrak{x})$. If $B_R(x)$ is complete (in which case $B_R(x) = M^n$), let $\mathfrak{M}^n = B_{R'}(\mathfrak{x})$ be an open model with Neumann boundary conditions and R' greater than or equal to the diameter of M^n ($R' = \infty$ if M^n is complete but not compact). In particular, $\overline{B_{R'}(\mathfrak{x})}$ might be a closed model. Should it happen, one can show that the restriction of its fundamental solution to $B_{R'}(\mathfrak{x})$ coincides with the Neumann fundamental solution on $B_{R'}(\mathfrak{x})$.

The heat kernel $\mathfrak{H}_t(\mathfrak{x}, \mathfrak{y}) = \mathfrak{H}_t(r)$ can be regarded as a function on $B_R(x)$, and we shall also denote this function by $\mathfrak{H}_t(r)$. So regarded, it is smooth on $B_R(x) \setminus C$, where C is the cut-locus of x . Let $m(r, \theta)$ denote the mean curvature function for the distance sphere $S_r(x)$, with $S_r(x) \cap C$ removed.

Theorem 2.4 (J. Cheeger-S. T. Yau, [9]). *Let $B_R(x)$ be a metric ball in a complete Riemannian manifold M^n , and let \mathfrak{M}^n be a model subject to conditions stated above. Suppose that $m(r, \theta) \leq m(r)$ on $B_R(x) \setminus C$. Then*

$$\mathfrak{H}_t(\overline{x, y}) \leq H_t(x, y),$$

and equality holds if and only if $\exp_x|_{B_R(0)}$ is a diffeomorphism and $m(r, \theta) = m(r)$. In case \mathfrak{M}^n is a Ricci model, denote its Ricci curvature by \mathfrak{Ric} . Then, by a comparison theory result, $\text{Ric}(\partial/\partial r, \partial/\partial r) \geq \mathfrak{Ric}(\partial/\partial r, \partial/\partial r)$ implies $m(r, \theta) \leq m(r)$ and hence, $\mathfrak{H}_t(\overline{x, y}) \leq H_t(x, y)$, and equality holds if and only if $B_R(x)$ is isometric to the ball of radius R in the model space.

Idea of proof. To prove the theorem, first, write

$$\begin{aligned} H_t(x, y) - \mathfrak{H}_t(\overline{x, y}) &= \int_0^t \int_{B_R(x)} \frac{d}{ds} \mathfrak{H}_{t-s}(\overline{x, w}) H_s(w, y) dw ds \\ &\quad + \int_0^t \int_{B_R(x)} \mathfrak{H}_{t-s}(\overline{x, w}) \frac{d}{ds} H_s(w, y) dw ds \\ &= \int_0^t \int_{B_R(x)} \frac{d}{ds} \mathfrak{H}_{t-s}(\overline{x, w}) H_s(w, y) dw ds \\ &\quad + \int_0^t \int_{B_R(x)} \mathfrak{H}_{t-s}(\overline{x, w}) \Delta H_s(w, y) dw ds. \end{aligned}$$

The idea is then to apply Lemma 2.3 to replace d/ds with Δ on the right-hand side of the last equation and use integration by parts. This should be done carefully, however, since $B_R(x) \setminus C$ is *not* a smooth manifold with boundary. \square

Remark 2.5. Theorem 2.4 generalizes a theorem from [13] where the authors consider a normal coordinate ball (with radius less than the *injectivity radius* at x , contrary to the above Theorem where no assumption is made on the injectivity radius) with Dirichlet boundary conditions. They use a lower bound on the sectional curvature to compare with a model space of constant curvature. It is also proved there that the *upper* sectional curvature bound implies a similar upper bound for the heat kernel. The proof in [13] goes through comparing the hitting times for the Brownian motions on M^n and on the model space of constant curvature.

2.2.2 Harnack inequalities and upper bounds for positive solutions of the heat equation

In this section we are going to discuss the paper [27] by P. Li and S. T. Yau where they study solutions to parabolic equations of the type

$$\left(\Delta - q(x, t) - \frac{\partial}{\partial t}\right) u(x, t) = 0 \quad (2.3)$$

on a general Riemannian manifold M . They established two-sided bounds for fundamental solutions of (2.3) and considered numerous applications of these estimates. We shall indicate, as well, some improvements due to D. Bakry and Z. M. Qian [4] which enable one to produce new Harnack inequalities.

Let us review the general line of reasoning in [27]. Consider the equation corresponding to (2.3), satisfied by $f = \log u$, where u is a positive solution to (2.3):

$$\left(\Delta - \frac{\partial}{\partial t}\right) f = -|\nabla f|^2 + q.$$

Applying the maximum principle to

$$F := t(|\nabla f|^2 - \alpha f_t - \alpha q),$$

where $\alpha > 1$ is a fixed constant, one can derive a gradient estimate for positive solutions which in the simplest case ($q = 0$) reads:

$$\frac{|\nabla u|^2}{u^2} - \frac{\alpha u_t}{u} \leq \frac{n\alpha^2}{2t} + \frac{n}{\sqrt{2}}\alpha^2(\alpha - 1)^{-1}R, \quad (2.4)$$

for an n -dimensional manifold whose Ricci curvature is greater than or equal to $-R$, for some non-negative constant R . It serves to establish a Harnack inequality for $u(x, t)$ by writing

$$\log u(x, t_1) - \log u(y, t_2) = \int_{\eta} d \log u.$$

Here $\eta: [0, 1] \rightarrow M \times [t_1, t_2]$ is a path defined by

$$\eta(s) = (\gamma(s), (1 - s)t_2 + st_1), \quad (2.5)$$

for any curve γ in M such that $\gamma(0) = y$ and $\gamma(1) = x$. Then upper and lower bounds for the fundamental solution of (2.3) are obtained by tricky integration using Harnack inequalities.

Let us consider in some detail the above issues for the case $q = 0$ (which is the most relevant for us since then the fundamental solution is nothing else than the heat kernel).

Gradient estimates

In the rest of the section, M is supposed to be an n -dimensional complete Riemannian manifold with (possibly empty) boundary, ∂M . Let $\partial/\partial\nu$ be the outward pointing unit normal vector to ∂M , and denote the second fundamental form of ∂M with respect to $\partial/\partial\nu$ by II .

Lemma 2.6. *Let $f(x, t)$ be a smooth function defined on $M \times [0, \infty)$ satisfying*

$$\left(\Delta - \frac{\partial}{\partial t}\right) f = -|\nabla f|^2.$$

For any given $\alpha \geq 1$, the function

$$F = t(|\nabla f|^2 - \alpha f_t)$$

satisfies the inequality

$$\left(\Delta - \frac{\partial}{\partial t}\right) F \geq -2\langle \nabla f, \nabla F \rangle - \frac{F}{t} - 2Rt|\nabla f|^2 + \frac{2t}{n}(|\nabla f|^2 - f_t)^2,$$

where $-R(x)$, with $R(x) \geq 0$, is a lower bound of the Ricci curvature on M at the point x .

To prove the Lemma, choose a local orthonormal frame field (e_i) on M and let the subscript i denote covariant differentiation in the direction e_i . Let us calculate $\Delta F = \sum_i F_{ii}$. This will give (adopting the convention to sum over repeated indices):

$$\begin{aligned} \Delta F &= t(2f_{ji}^2 + 2f_j f_{jii} - \alpha f_{tt}) \\ &\geq t \left(\frac{2}{n}(\Delta f)^2 + 2\langle \nabla f, \nabla \Delta f \rangle - 2R|\nabla f|^2 - \alpha(\Delta f)_t \right), \end{aligned}$$

where we have used the inequalities

$$\sum_{i,j} f_{ij}^2 \geq \frac{(f_{ii})^2}{n},$$

and

$$f_j f_{jii} = f_j f_{iij} + R_{ij} f_i f_j \geq \langle \nabla f, \nabla \Delta f \rangle - R|\nabla f|^2.$$

Recalling the definition of F , this suffices to conclude. \square

Applying the maximum principle to the function F from the Lemma gives the following gradient estimate.

Theorem 2.7 (P. Li-S. T. Yau, [27]). *Let M be a n -dimensional manifold with non-negative Ricci curvature. Suppose that M is either compact with convex boundary, i.e. $\text{II} \geq 0$, or complete without boundary. Let $u(x, t)$ be a non-negative solution of the heat equation on $M \times (0, \infty)$ with Neumann boundary conditions. Then u satisfies the estimate*

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leq \frac{n}{2t}$$

on $M \times (0, \infty)$.

Similar gradient estimates were obtained by D. Bakry and Z. M. Qian [4]. Their method consists in a smart choice of the test function F in Lemma 2.6. Suppose that $\text{Ric}(M) \geq -R$, $R \geq 0$. Let $C(t, Y)$ be the solution of the following differential equation on $(0, \infty)$ with a parameter $Y > -nR/4$:

$$\partial_t C + \frac{2}{n} C^2 - 2R(Y + C) = 0, \quad C(0) = \infty.$$

For each $Y_0 > -nR/4$, define $B(t, Y) := \partial_Y C(t, Y_0)(Y - Y_0) + C(t, Y_0)$ to be the linearization of C at Y_0 . Taking F in Lemma 2.6 to be $t(|\nabla f|^2 - f_t - B(t, f_t))$, the maximum principle yields

$$F \leq 0,$$

on $M \times (0, \infty)$. Therefore we arrive at the following theorem.

Theorem 2.8 (D. Bakry-Z. M. Qian [4]). *Let M be a complete manifold with $\text{Ric}(M) \geq -R$, $R \geq 0$. For a positive solution $u(x, t)$ of the heat equation,*

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leq \inf_{Y_0 > -nR/4} B\left(t, \frac{u_t}{u}\right). \quad \square$$

on $M \times (0, \infty)$.

Corollary 2.9. *Using the explicit formula for $B(t, Y)$ and letting $Y_0 \rightarrow -nR/4$, we get*

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leq \frac{2R}{3} t \left(\frac{u_t}{u} + \frac{Rn}{4} \right) + \frac{n}{2t} + \frac{Rn}{2}.$$

On the other hand, taking $Y_0 = u_t/u$, one has

$$\frac{|\nabla u|^2}{u^2} - \frac{u_t}{u} \leq \sqrt{Rn} \sqrt{\frac{u_t}{u} + \frac{Rn}{4}} + \frac{n}{2t} + \frac{Rn}{2}, \quad \text{on } \frac{u_t}{u} \geq -\frac{Rn}{4}. \quad \square$$

Motivated by the ideas of P. Li, S. T. Yau and Hamilton, P. Souplet and Q. S. Zhang [34] have discovered another type of gradient estimates for complete Riemannian manifolds. They have shown that after inserting a certain logarithmic correction term, an *elliptic (i.e. without derivatives with respect to time)* gradient estimate holds true for manifolds with Ricci curvature bounded from below. Their estimate is of local nature (to be compared with the localized *parabolic* version of P. Li-S. T. Yau estimate (2.4) (cf. [27, Theorem 1.2]) and with the elliptic estimate of S. Y. Cheng and S. T. Yau for harmonic functions (cf. Theorem 4.2 or [10, Theorem 6])). It reads as follows.

Theorem 2.10 (P. Souplet-Q. S. Zhang [34]). *Let M be a Riemannian manifold with $\text{Ric}(M) \geq -R$, for some $R \geq 0$. Suppose that u is any positive solution to the heat equation in $Q_{K,T} := B_{x_0}(K) \times [t_0 - T, t_0] \subset M \times \mathbb{R}$. Suppose also that $u \leq A$ in $Q_{K,T}$ for some constant A . Then there exists a dimensional constant c such that*

$$\frac{|\nabla u(x, t)|}{u(x, t)} \leq c \left(\frac{1}{K} + \frac{1}{T^{1/2}} + \sqrt{R} \right) \left(1 + \log \frac{A}{u(x, t)} \right)$$

in $Q_{K/2, T/2}$. Moreover, if M has non-negative Ricci curvature and u is any positive solution of the heat equation on $M \times (0, \infty)$, then there exists a dimensional constant c' such that

$$\frac{|\nabla u(x, t)|}{u(x, t)} \leq c' \frac{1}{t^{1/2}} \left(1 + \log \frac{u(x, 2t)}{u(x, t)} \right) \quad (2.6)$$

for all $(x, t) \in M \times (0, \infty)$.

In the last years, gradient estimates for solutions of the heat equation were generalized for time dependant metrics. Namely, the information about solutions of the conjugate heat equation and their W -entropy is of great importance in view of Perelman's work. Let us consider the conjugate heat equation under the Ricci flow:

$$\begin{cases} \Delta u - s u + \partial_t u = 0 \\ \partial_t g = -2\text{Ric}(g). \end{cases} \quad (2.7)$$

Here $u = u(x, t)$ and s stands for the scalar curvature. S. Kuang and Q. S. Zhang [25] generalized Perelman's estimate for the fundamental solution of (2.7) for *all positive* solutions. It is worth mentioning that they do not require any curvature assumption. Moreover, assuming only the lower bound on the Ricci curvature, their estimate has a local version which appears similar to the P. Li-S. T. Yau estimate for the linear heat equation.

Suppose that $g(t)$ evolves according to the Ricci flow, that is $\partial_t g = -2\text{Ric}(g)$ on a closed n -dimensional manifold M for $t \in [0, T)$, and $u: M \times [0, T) \rightarrow (0, \infty)$ is a positive solution to (2.7). Let $\tau = T - t$. Then if the scalar curvature $s \geq 0$, it is proved in [25] that

$$\frac{|\nabla u|^2}{u^2} - 2 \frac{u_\tau}{u} - s \leq \frac{2n}{\tau},$$

for all $x \in M$ and $t \in (0, T)$. Without assuming the non-negativity of s ,

$$\frac{|\nabla u|^2}{u^2} - 2 \frac{u_\tau}{u} - s \leq \frac{3n}{\tau},$$

for all $x \in M$ and $t \in [T/2, T)$.

The results of S. Kuang and Q. S. Zhang can be also adapted for the heat equation in the fixed metric case [25]. Specifically, let M be a closed manifold with the fixed metric g and non-negative Ricci curvature, u be the fundamental solution, and set $f := -\log u - \frac{n}{2} \log(4\pi t)$. Then for any constant $\alpha \geq 1$,

$$t(\alpha \Delta f - |\nabla f|^2) + f - \alpha \frac{n}{2} \leq 0.$$

Note that letting $\alpha \rightarrow \infty$, we recover the inequality in Theorem 2.7.

Harnack inequalities

With (2.4) at hand, let us take a positive solution $u(x, t)$ of the heat equation and integrate $d \log u$ along the path η defined by (2.5). This yields

$$\begin{aligned} \log u(x, t_1) - \log u(y, t_2) &= \int_0^1 \left(\frac{d}{ds} \log u \right) ds \\ &= \int_0^1 [\langle \dot{\gamma}, \nabla(\log u) \rangle - (t_2 - t_1)(\log u)_t] ds, \end{aligned}$$

where $t_1 < t_2$. Applying (2.4) to $-(\log u)_t$, we get

$$\log \left(\frac{u(x, t_1)}{u(y, t_2)} \right) \leq \int_0^1 \left\{ |\dot{\gamma}| |\nabla \log u| + (t_2 - t_1) \left[\frac{n}{\sqrt{2}} \alpha (\alpha - 1)^{-1} R + \frac{n}{2} \alpha t^{-1} \right] - (t_2 - t_1) \alpha^{-1} |\nabla \log u|^2 \right\} ds. \quad (2.8)$$

Viewing $|\nabla \log u|$ as a variable and the integrand as a quadratic in $|\nabla \log u|$, we observe that it can be dominated from above by

$$\frac{\alpha |\dot{\gamma}|^2}{4(t_2 - t_1)} + (t_2 - t_1) \left[\frac{n}{\sqrt{2}} \alpha (\alpha - 1)^{-1} R + \frac{n}{2} \alpha t^{-1} \right].$$

Since $t = (1 - s)t_2 + st_1$, (2.8) gives

$$\log \left(\frac{u(x, t_1)}{u(y, t_2)} \right) \leq \frac{\alpha}{4(t_2 - t_1)} \int_0^1 |\dot{\gamma}|^2 ds + \frac{n\alpha}{2} \log \left(\frac{t_2}{t_1} \right) + \frac{n}{\sqrt{2}} \alpha (\alpha - 1)^{-1} R (t_2 - t_1),$$

which yields the following theorem.

Theorem 2.11 (P. Li-S. T. Yau [27]). *Let M be a n -dimensional manifold with Ricci curvature bounded from below by $-R$ for some constant $R \geq 0$. We assume that M is either compact with convex boundary, i.e. $\Pi \geq 0$, or complete without boundary. Let $u(x, t)$ be a positive solution on $M \times (0, \infty)$ of the heat equation*

$$\left(\Delta - \frac{\partial}{\partial t} \right) u(x, t) = 0,$$

with Neumann boundary condition

$$\frac{\partial u}{\partial \nu} = 0$$

on $\partial M \times [0, \infty)$. Then for any $\alpha > 1$, $x, y \in M$, and $0 < t_1 < t_2$, we have

$$u(x, t_1) \leq u(y, t_2) \left(\frac{t_2}{t_1} \right)^{n\alpha/2} \exp \left(\frac{n\alpha}{\sqrt{2}} (\alpha - 1)^{-1} R (t_2 - t_1) + \frac{\alpha d^2(x, y)}{4(t_2 - t_1)} \right), \quad (2.9)$$

where $d(x, y)$ is the distance between x and y . \square

The same line of reasoning which has led to Theorem 2.11 can be applied to the inequalities from Corollary 2.9. to obtain

Theorem 2.12 (D. Bakry-Z. M. Qian [4]). *Let $\text{Ric}(M) \geq -R$, for some $R \geq 0$. For a positive solution $u(x, t)$ of the heat equation, one has*

$$u(x, t_1) \leq u(y, t_2) \left(\frac{t_2}{t_1} \right)^{n/2} \exp \left(\frac{(d(x, y) + \sqrt{Rn}(t_2 - t_1))^2}{4(t_2 - t_1)} + \frac{\sqrt{Rn}}{2} \min \left\{ (\sqrt{2} - 1)d(x, y), \frac{\sqrt{Rn}}{2}(t_2 - t_1) \right\} \right), \quad (2.10)$$

where $0 < t_1 < t_2$, $x, y \in M$ and $d(x, y)$ is the distance between them.

The advantage of (2.10) as opposed to (2.9) is that it extends to diffusions of the form $\Delta + B$, with a C^2 -vector field B . This fact will be taken advantage of in the proof of Theorem 3.5 in Chapter 3.

A mean value type inequality can be easily derived by averaging the function over any set in either the x -variable or the y -variable. In fact, this will be the form most utilized in what follows. For example, a corresponding mean value inequality of Theorem 2.11 reads

$$u(x, t_1) \leq \left(\int_{B_x(r)} u^p(y, t_2) \right)^{1/p} \left(\frac{t_2}{t_1} \right)^{n\alpha/2} \exp \left(\frac{n\alpha}{\sqrt{2}} (\alpha - 1)^{-1} R(t_2 - t_1) + \frac{\alpha r^2}{4(t_2 - t_1)} \right),$$

where $p \geq 1$.

Corollary 2.13. *Let M be a compact manifold with non-negative Ricci curvature. If $\partial M \neq \emptyset$, we assume that it must be convex. The Neumann heat kernel on M must satisfy*

$$H_t(x, y) \geq \frac{1}{(4\pi t)^{n/2}} \exp \left(-\frac{d^2(x, y)}{4t} \right).$$

In particular, the Neumann eigenvalues μ_i of M satisfy

$$\sum_{i=0}^{\infty} e^{-\mu_i t} \geq (4\pi t)^{-n/2} \text{Vol}(M).$$

For complete manifolds this follows directly from Theorem 2.4.

Proof. Applying Theorem 2.11 to the function $u(y, t) = H_t(x, y)$ gives

$$H_{t_1}(x, x) \leq H_{t_2}(x, y) \left(\frac{t_2}{t_1} \right)^{n/2} \exp \left(\frac{r^2(x, y)}{4(t_2 - t_1)} \right).$$

Since

$$H_{t_1}(x, x) \sim (4\pi t)^{-n/2}$$

(cf. the asymptotic expansion in Chapter 3) as $t_1 \rightarrow 0$ the estimate for $H_t(x, y)$ follows. For the second estimate, integrate over M . \square

The Harnack inequalities considered so far are formulated with a time shift. Another possibility is to seek for Hölder type inequalities with an exponent strictly bigger than 1. A dimension-free Harnack inequality (with an exponent bigger than 1) was established by F.-Y. Wang in [40] for diffusion semigroups with generators having curvature bounded from below. Let M be a (possibly non-compact) manifold with boundary either empty or convex. Fix $f \in C_b(M)$, and $\alpha > 1$. Let $L = \Delta + \nabla V$, for some $V \in C^2(M)$ such that $\int_M e^V dx < \infty$, be a diffusion satisfying

$$\text{Ric} - \text{Hess}(V) \geq -R, \quad \text{for some } R \in \mathbb{R},$$

and P_t be its semigroup. One has (see [38]) $|\nabla P_s F| \leq e^{Rs} P_s |\nabla F|$, for $s \geq 0$, $F \in C_b^1(M)$. By integrating the function

$$\log P_s(P_{t-s} f)^\alpha$$

along the geodesic segment joining x and $y \in M$, F.-Y. Wang showed that

$$|P_t f(x)|^\alpha \leq P_t |f|^\alpha(y) \exp \left[\frac{\alpha d^2(x, y) \int_0^t g^2(s) ds}{4(\alpha - 1) \left(\int_0^t g(s) e^{-Rs} ds \right)^2} \right], \quad (2.11)$$

for any positive function $g \in C[0, t]$. In particular,

$$|P_t f(x)|^\alpha \leq P_t |f|^\alpha(y) \exp \left[\frac{\alpha d^2(x, y)}{4(\alpha - 1)t} \frac{(Rt)^2}{(1 - e^{-Rt})^2} \right].$$

This inequality entails a *dimension free* lower bound for the logarithmic Sobolev constant on compact manifolds and enables one to prove the existence of a logarithmic Sobolev inequality on non-compact manifolds.

M. Arnaudon, A. Thalmaier and F.-Y. Wang [1] have further generalized (2.11) for diffusions with curvature unbounded from below. Let M be a complete n -dimensional manifold (possibly with convex boundary) whose Ricci curvature is controlled by the distance to a fixed point $p \in M$:

$$\text{Ric}(x) \geq -c(1 + d^2(p, x)), \quad (2.12)$$

for some constant $c > 0$. Consider the (reflecting) Brownian motion on M and assume that it is non-explosive. Under these assumptions, for any $\epsilon \in (0, 1]$ there exists a constant $c(\epsilon) > 0$ such that

$$|P_t f|^\alpha(y) \leq P_t |f|^\alpha(x) \exp \left\{ \frac{\alpha(\epsilon\alpha + 1)d^2(x, y)}{2(2 - \epsilon)(\alpha - 1)t} + \frac{c(\epsilon)\alpha^2(\alpha + 1)^2}{(\alpha - 1)^3} (1 + d^2(x, y)) d^2(x, y) + \frac{\alpha - 1}{2} (1 + d^2(p, x)) \right\} \quad (2.13)$$

holds for all $\alpha > 1$, $t > 0$, $x, y \in M$ and any bounded measurable function f on M . The proof, unlike those considered above, is probabilistic and goes through a coupling by parallel translation along with Girsanov's theorem. The bound (2.13) can be generalized for diffusions generated by $\Delta + B$ for a C^1 -vector field B satisfying some mild growing conditions with respect to $d(p, x)$.

Upper bounds

Lemma 2.14. *Let M be a complete manifold, possibly with convex boundary, ∂M . Suppose $H_t(x, y)$ is the fundamental solution of the heat equation on $M \times M \times (0, \infty)$, satisfying either Dirichlet or Neumann boundary conditions if $\partial M \neq \emptyset$. Let*

$$F(y, t) = \int_{S_1} H_t(y, z) H_T(x, z) dz$$

for $x \in M$, $S_1 \subseteq M$, and $0 \leq t \leq \tau < (1 + 2\delta)T$. Then for any subset $S_2 \subseteq M$, we have

$$\int_{S_2} F^2(z, \tau) dz \leq \int_{S_1} H_T^2(x, z) dz \exp \left(-\frac{d^2(x, S_1)}{2(1 + 2\delta)T} \right) \sup_{z \in S_2} \exp \left(\frac{d^2(x, z)}{2(1 + 2\delta)T - 2\tau} \right).$$

Idea of proof. Suppose to simplify that M is compact, (otherwise one should introduce a cut-off function of the distance balls around x into the integrals below). Let

$$g(x, y, t) = -\frac{d^2(x, y)}{2(1 + 2\delta)T - 2t}.$$

Then

$$1/2|\nabla_y g|^2 + g_t = 0. \quad (2.14)$$

Since F satisfies $(\Delta_y - \partial_t)F = 0$, we consider

$$0 = 2 \int_0^T \int_M \exp(g(x, y, t)) F(y, t) \left(\Delta_y - \frac{\partial}{\partial t} \right) F(y, t) dy dt. \quad (2.15)$$

Integrating the right-hand side of (2.15) by parts and applying Minkowski's inequality to $\int_0^T \int_M e^g F \langle \nabla g, \nabla F \rangle$, together with (2.14), gives

$$\int_{S_2} \exp(g(x, y, \tau)) F^2(y, \tau) dy \leq \int_M \exp(g(x, y, \tau)) F^2(y, \tau) dy \leq \int_M \exp(g(x, y, 0)) F^2(y, 0) dy.$$

Recalling the definition of $F(y, t)$ suffices to conclude. \square

The following theorem will be used in the proof of the main result of this thesis (cf. (3.32)).

Theorem 2.15 (P. Li-S. T. Yau [27]). *Let M be either a complete manifold without boundary or a compact manifold with convex boundary whenever $\partial M \neq \emptyset$. Assume the Ricci curvature of M is bounded from below by $-R$, for some constant $R \geq 0$. Then the fundamental solution $H_t(x, y)$ of the heat equation (with Neumann boundary conditions if $\partial M \neq \emptyset$) must satisfy*

$$H_t(x, y) \leq C(n, \varepsilon)^\alpha \text{Vol}^{-1/2}(B_x(\sqrt{t})) \text{Vol}^{-1/2}(B_y(\sqrt{t})) \exp \left[C' \varepsilon (\alpha - 1)^{-1} R t - \frac{d^2(x, y)}{(4 + \varepsilon)t} \right]$$

for all $1 < \alpha < 2$ and $0 < \varepsilon < 1$, where the constant $C(n, \varepsilon) \rightarrow \infty$ as $\varepsilon \rightarrow 0$ and the constant C' depends only on the dimension of M . When $R = 0$, after letting $\alpha \rightarrow 1$, this estimate can be written as

$$H_t(x, y) \leq C(n, \varepsilon) \text{Vol}^{-1}(B_x(\sqrt{t})) \exp \left(-\frac{d^2(x, y)}{(4 + \varepsilon)t} \right).$$

Idea of proof. Fix $\delta > 0$. Let us apply Theorem 2.11 to the function $F(y, t)$ of Lemma 2.14. This yields

$$\begin{aligned} \left(\int_{S_1} H_T^2(x, z) dz \right)^2 &= F^2(x, T) \\ &\leq (1 + \delta)^{n\alpha} \exp \left(n\alpha\sqrt{2}(\alpha - 1)^{-1} R(\delta T) + \sup_{z \in S_2} \frac{\alpha d^2(x, z)}{2(\delta T)} \right. \\ &\quad \left. + \sup_{z \in S_2} \frac{d^2(x, z)}{2(\delta T)} - \inf_{z \in S_1} \frac{d^2(x, z)}{2(1 + 2\delta)T} \right) \text{Vol}^{-1}(S_2) \int_{S_1} H_T^2(x, z) dz, \end{aligned}$$

by setting $\tau = (1 + \delta)T$ in Lemma 2.14. Applying Theorem 2.11 to the function $H_T(x, z)$ and setting $T = (1 + \delta)t$, we obtain

$$\begin{aligned}
H_t^2(x, y) \leq (1 + \delta)^{2n\alpha} \exp \left(n\alpha\sqrt{2}(\alpha - 1)^{-1}R\delta(2 + \delta)t \right. \\
\left. + \sup_{z \in S_1} \frac{\alpha d^2(y, z)}{2(\delta t)} + \frac{1}{2}(\alpha + 1) \sup_{z \in S_2} \frac{d^2(x, z)}{\delta(1 + \delta)t} \right. \\
\left. - \inf_{z \in S_1} \frac{d^2(x, z)}{2(1 + 2\delta)(1 + \delta)t} \right) Vol^{-1}(S_2)Vol^{-1}(S_1). \tag{2.16}
\end{aligned}$$

Put $S_1 = B_y(\sqrt{t})$, $S_2 = B_x(\sqrt{t})$. Estimating the terms in (2.16) when $1 < \alpha < 2$, one gets the first estimate of the Theorem as claimed.

For the second estimate distinguish two cases: $\sqrt{t} > 2d(x, y)$ and $\sqrt{t} \leq 2d(x, y)$. With the relative volume comparison theorem, it is possible to estimate $Vol(B_x(\sqrt{t}))$ from above by $Vol(B_y(\sqrt{t}))$ and $d(x, y)/\sqrt{t}$ in either case. This suffices to derive the second estimate of the Theorem. \square

The remarkable results obtained by P. Li and S. T. Yau – by far, the sharpest available at the time – set up a cornerstone for the heat kernel bounds relying upon the Ricci curvature assumptions. They were subject to further improvements and modifications carried out later on by different authors. A new boost to the study of the heat kernel was given in 90s, when the problem was tackled from a different viewpoint involving the metric-measure assumptions on the underlying manifold, such as e.g. the doubling condition or the Poincaré inequality.

To close this section, let us mention two more heat kernel upper bounds. D. Bakry, M. Ledoux et Z. M. Qian [3] starting with (2.11) established a *dimension-free* upper bound for the heat kernel under the conditions stated before (2.11): for any $\delta > 2$,

$$H_t(x, y) \leq \frac{\exp \left(\frac{2\delta(Rt)^2}{(\delta-2)(1-e^{-Rt})^2} + \frac{2(\delta+2)}{\delta(\delta-2)} \right)}{\sqrt{Vol B_x(\sqrt{t}) Vol B_y(\sqrt{t})}} \exp \left(-\frac{d^2(x, y)}{2\delta t} \right),$$

$(t, x, y) \in (0, \infty) \times M \times M$. Similarly, the Harnack inequality (2.13) leads to the following heat kernel upper bound. Assume that (2.12) holds. For any $\delta > 2$ there exists a constant $c(\delta) > 0$ such that for any $t > 0$,

$$H_t(x, y) \leq \frac{\exp \left\{ -\frac{d^2(x, y)}{2\delta t} + c(\delta)(1 + t + t^2 + d^2(p, x) + d^2(p, y)) \right\}}{\sqrt{Vol B_x(\sqrt{2t}) Vol B_y(\sqrt{2t})}}, \quad x, y \in M.$$

Chapter 3

Probability techniques and gradient estimates

This chapter is devoted to the study of the gradient of the heat kernel. A great deal of it will be concerned with the short time behavior. The reason for this is that one has an asymptotic expansion of $H_t(x, y)$ as a product of the Euclidean kernel and an integer power series in t for $t \searrow 0$. Namely, let C_y denote the *cut-locus* of y in M , M being an n -dimensional manifold. As is known, $x \in C_y \iff y \in C_x$. Define

$$C_M = \{(x, y) \in M \times M \mid x \in C_y\}.$$

Then there are smooth functions $G_i(x, y)$ defined on $M \times M \setminus C_M$ with the properties $G_0(x, y) > 0$ and $G_0(x, x) = 1$ such that

$$H_t(x, y) \sim \left(\frac{1}{4\pi t}\right)^{n/2} e^{-d^2(x, y)/4t} \sum_{i=0}^{\infty} G_i(x, y) t^i. \quad (3.1)$$

This expansion holds uniformly as $t \searrow 0$ on any compact subset of $M \times M \setminus C_M$. (3.1) implies the following formula, known as *Varadhan's asymptotic relation*:

$$\lim_{t \searrow 0} t \log H_t(x, y) = -\frac{1}{4} d^2(x, y). \quad (3.2)$$

Moreover, contrary to the asymptotic expansion above, Varadhan's relation holds for any pair of points on a complete Riemannian manifold, uniformly on compact subsets of $M \times M$.

Since the heat kernel is the transition density for the Brownian motion, many problems related to it lend themselves to a probabilistic interpretation and thus can be investigated via stochastic analysis techniques. This is the case for example for the logarithmic gradient of $H_t(x, y)$. Let us give an idea of why it is so. Let (Z_t) be a Markov process on \mathbb{R}^+ with values in M and with generator L , starting from $x \in M$. For $t \geq 0$, let $p_t(\bar{x}, \bar{y})$ be the associated heat kernel, i.e. the density (with respect to the Riemannian measure) of the distribution of Z_{t+s} when $Z_s = \bar{x}$. For any $T > 0$ consider the bridge $\{Z_t^{(T)}, 0 \leq t \leq T\}$ of length T starting from x and ending at y at time T . Intuitively, this is the process (Z_t) conditioned by $Z_T = y$. But since $\mathbb{P}(Z_T = y) = 0$, some care has to be taken in this formulation. For instance, $Z_t^{(T)}$ can be rigorously defined as the *non-homogeneous* Markov process on \mathbb{R}^+ with

transition probabilities of density

$$p_{s,t}(\bar{x}, \bar{y}) = \frac{p_{t-s}(\bar{x}, \bar{y})p_{T-t}(\bar{y}, y)}{p_{T-s}(\bar{x}, y)},$$

with respect to the Riemannian measure. Then the generator for $Z_t^{(T)}$ acts on a function f as

$$L f + 2\langle \nabla \log p_{T-t}(\cdot, y), \nabla f \rangle,$$

the expression which involves the logarithmic gradient of p_t . This is the starting point for the gradient estimates derived by E. P. Hsu [22] who showed that on a compact Riemannian manifold, for all $(T, x, y) \in (0, 1] \times M \times M$,

$$|\nabla^N \log H_T(x, y)| \leq C_N \left\{ \frac{d(x, y)}{T} + \frac{1}{\sqrt{T}} \right\}^N, \quad (3.3)$$

where C_N is a constant depending on M and N . The same result was obtained in a work of D. Stroock and J. Turetsky [35] by a different method using *J. M. Bismut's formula* (see also [36], especially chapters 6 and 10 therein).

If $N = 1$, i.e. in the case of the first logarithmic derivative, the above result has been further improved in [14] for compact manifolds with bounded Ricci curvature. Specifically, it has been shown there that the constant in (3.3) can be chosen to be universal, i.e. depending only on the lower bound of Ricci curvature, dimension and diameter of the manifold. Also, the estimate has been generalized there for diffusions generated by $\Delta + B$, where B is a C^2 -vector field on the manifold.

3.1 An overview of some gradient estimates for diffusion semigroups

Let us emphasize that the gradient estimates for solutions of PDEs are a topic of lively scientific interest. For instance, there is a number of papers that aim at estimating the gradient of a solution to some parabolic PDE with the help of the initial value function. Thus, in [15] the authors consider a parabolic Dirichlet problem in an unbounded domain $\Omega \ni x$ in the Euclidean space \mathbb{R}^n :

$$(\partial_t - \mathcal{L})u(t, x) = 0, \quad (t, x) \in (0, T) \times \Omega, \quad (*)$$

with the initial value $u(0, x) = f(x)$. Here \mathcal{L} is a second-order elliptic operator with (possibly) unbounded regular coefficients. Under some regularity assumptions on the boundary $\partial\Omega$ and the coefficients of \mathcal{L} , for any continuous bounded function $f \in C_b(\Omega)$ there exists a unique bounded classical solution $u(t, x)$ of (*) which satisfies

$$\|\nabla u(t, \cdot)\|_\infty \leq \frac{C}{\sqrt{t}} \|f\|_\infty, \quad t \in (0, T).$$

Hypoelliptic case

There are similar results in the manifold setting as well. Specifically, let

$$\mathcal{L} := \Xi_0 + \sum_1^n \Xi_i^2/2$$

be a diffusion generator on a compact Riemannian manifold M with C^∞ vector fields Ξ_i and P_t be the corresponding semigroup. Suppose that \mathcal{L} is *hypoelliptic* and such that the tangent space $T_x M$ is generated by Ξ_i and their brackets $[\Xi_i, \Xi_j]$ for any point $x \in M$. J. Picard [31] has shown that then there exists a $C > 0$ such that

$$|\nabla(P_t f)(x)| \leq \frac{C}{t \wedge 1} \|f\|_\infty, \quad (3.4)$$

for any $t > 0$ and any bounded Borel function f (the wedge stands for the minimum of two numbers). His method relates the gradient estimates to the estimation of the quadratic variation of some martingale. With the help of Burkholder and Doob inequalities, the latter can be controlled by the final value of the martingale.

A related result for *nilpotent Lie groups* was obtained by T. Melcher [29]. Let G be an d -dimensional Lie group with Lie algebra \mathfrak{g} . Suppose that $\{X_1, \dots, X_k\}$ is a Lie generating set in \mathfrak{g} , that is \mathfrak{g} is spanned by (X_i) and their iterated brackets. Define a scalar product $\langle \cdot, \cdot \rangle$ on \mathfrak{g} such that $\{X_i\}$, $i = 1, \dots, k$ is an orthonormal set and extend it to a right invariant metric on G by

$$\langle v, w \rangle_g := \langle R_{g^{-1}*} v, R_{g^{-1}*} w \rangle, \quad \text{for all } v, w \in T_g G.$$

Given an element $X \in \mathfrak{g}$, let \tilde{X} (respectively, \hat{X}) denote the left (respectively, the right) invariant vector field on G such that it equals X at the identity $e \in G$. The left gradient on G is the operator on $C^1(G)$ defined by $\tilde{\nabla} := (\tilde{X}_1, \dots, \tilde{X}_k)$. Let

$$\mathcal{L} := \sum_1^k \tilde{X}_i^2/2$$

be the associated hypoelliptic operator with the semigroup P_t . Let $K_p(t)$ be the best function such that

$$|\tilde{\nabla} P_t f|^p \leq K_p(t) P_t |\tilde{\nabla} f|^p, \quad p \in [1, \infty), \quad (3.5)$$

for all $f \in C_0^\infty(G)$ and $t > 0$. T. Melcher's theorem [29] states that for all $p \in (1, \infty)$, $K_p(t) < \infty$ for a general Lie group G and, moreover, if G is a nilpotent Lie group, then there exists a constant $K_p < \infty$ such that $K_p(t) < K_p$ for all $t > 0$. By the left invariance of $\tilde{\nabla}$ and P_t , it suffices to check (3.5) at the identity, i.e. to verify that $|\tilde{\nabla} P_t f|^p(e) \leq K_p(t) P_t |\tilde{\nabla} f|^p(e)$. To this end, one should pass the gradient through P_t . But it is the right gradient, not the left one, which commutes with P_t . However they coincide at e . Thus the task amounts to express the right invariant vector fields \hat{X}_i with the help of (\tilde{X}_j) . One can show that the right gradient is the sum of iterated left gradients with coefficients $c_\alpha(g)$ which are smooth functions on G . Representing P_t as the expectation of a function on Wiener space transforms the finite dimensional problem to a problem on Wiener space. After applying Hölder's inequality, it remains to control $\mathbb{E} |\mathbf{X}^{i_1} \dots \mathbf{X}^{i_k} c_\alpha(W_t)|^q$, where \mathbf{X}^i are the adjoints of the vector fields on Wiener space obtained by "lifting" of X_i , W_t is a Brownian motion on

G starting from e , and $1/p + 1/q = 1$. It is shown that these expectations are finite. The finiteness of the constant $K_p(t)$ is then proved first for nilpotent *stratified* Lie groups by a scaling dilation argument. The general case comes by covering G with a *free* nilpotent group of an appropriate rank and number of generators.

If the Hörmander set $\{X_i\}_{i=1}^k$ spans the whole Lie algebra \mathfrak{g} , then it is well known that

$$|\nabla P_t f|^p \leq e^{Rpt/2} P_t |\nabla f|^p,$$

where $-R$ is the lower bound on the Ricci curvature. Thus, T. Melcher's theorem improves this result for large t . As a consequence, one has the following Poincaré inequality for nilpotent Lie groups. Let $p_t(g)$ be the hypoelliptic heat kernel. Then

$$\int_G f^2(g) p_t(g) dg - \left(\int_G f(g) p_t(g) dg \right)^2 \leq K_2 t \int_G |\tilde{\nabla} f|^2(g) p_t(g) dg,$$

for all $f \in C_0^\infty(G)$ and $t > 0$.

In the case of an *elliptic* diffusion, J. Picard's estimate (3.4) may be refined as follows [31]: for any $q > 1$,

$$|\nabla P_t f(x)| \leq \frac{C}{\sqrt{t} \wedge 1} P_t(|f|^q)(x)^{1/q}, \quad \text{for } (t, x) \in (0, \infty) \times M, \quad (3.6)$$

where f is a bounded Borel function. This may be also generalized [31] for some manifold-valued diffusions. Let us note that the logarithmic gradient estimates for the heat kernel in Theorem 3.5 below provide, by applying the Hölder inequality, universal bounds similar to (3.6) but with a worse order in t .

J. Picard's estimate (3.6) is analogous for small times to a related bound due to F.-Y. Wang [39]. Let M be a compact manifold with boundary either convex or empty with the diffusion $L = \Delta + Z$ where Z is a C^1 -vector field and $R = -\inf_M(\text{Ric} - \nabla Z)$. Using a J. M. Bismut type formula (cf. below for an account of J. M. Bismut's formula) F.-Y. Wang obtained a (universal) upper bound for a C^1 -function f which reads:

$$|\nabla P_t f(x)| \leq \frac{((2n-1)!)^{1/2n}}{2t} \sqrt{\frac{\exp(2Rt) - 1}{R}} (P_t |f|^{2n/(2n-1)}(x))^{(2n-1)/2n}, \quad n \in \mathbb{N}.$$

Note that this estimate is dimension free.

Let us also note that for $q \geq 2$, a variant of (3.6) can be drawn from the P. Li-S. T. Yau gradient inequality. Indeed, since

$$\int_M -\frac{\partial}{\partial t} H_t(x, z) dz = \int_M -\Delta_z H_t(x, z) dz = 0,$$

(2.4) implies that

$$\begin{aligned} \int_M \frac{|\nabla_x H_t(x, z)|^2}{H_t(x, z)} dz &\leq \left(\frac{n\alpha^2}{2t} + \frac{n}{\sqrt{2}} \left(\frac{\alpha^2}{\alpha-1} \right) R \right) \int_M H_t(x, z) dz \\ &= \frac{n\alpha^2}{2t} + \frac{n}{\sqrt{2}} \left(\frac{\alpha^2}{\alpha-1} \right) R, \end{aligned}$$

on a manifold whose Ricci curvature is greater than or equal to $-R$. Therefore,

$$\begin{aligned}
|\nabla P_t f(x)| &\leq \int_M |\nabla_x H_t(x, z)| |f(z)| dz \\
&\leq \left(\int_M \frac{|\nabla_x H_t(x, z)|^2}{H_t(x, z)} dz \right)^{1/2} \left(\int_M H_t(x, z) f^2(z) dz \right)^{1/2} \\
&\leq \left(\int_M \frac{|\nabla_x H_t(x, z)|^2}{H_t(x, z)} dz \right)^{1/2} \left(\int_M H_t(x, z) f^q(z) dz \right)^{1/q} \\
&\leq \left(\frac{n\alpha^2}{2t} + \frac{n}{\sqrt{2}} \left(\frac{\alpha^2}{\alpha-1} \right) R \right)^{1/2} P_t(|f|^q)(x)^{1/q}.
\end{aligned}$$

Now, let (x_t, y_t) be a coupling of the L -diffusion process by reflection (see [21, Chapter 6]) on a (possibly non-compact) manifold M . We suppose it with reflecting boundary whenever $\partial M \neq \emptyset$. Let $T := \inf\{t \geq 0 \mid x_t = y_t\}$ be the coupling time. One has

$$\begin{aligned}
\frac{|P_t f(x) - P_t f(y)|}{d(x, y)} &= \frac{|P_s P_{t-s} f(x) - P_s P_{t-s} f(y)|}{d(x, y)} \\
&\leq \mathbb{E} \frac{|P_{t-s} f(x_s) - P_{t-s} f(y_s)|}{d(x, y)} \leq 2 \|P_{t-s} f\|_\infty \frac{\mathbb{P}(T > s)}{d(x, y)}, \quad t > s > 0.
\end{aligned}$$

Hence, one needs to control the distribution of the coupling time $\mathbb{P}(T > s)$ to obtain a gradient estimate. As a result, there exists a function $C_{R, \dim M, Z}(s)$, with R , $\dim M$, and the vector field Z as the parameters, such that

$$\|\nabla P_t f\|_\infty \leq C_{R, \dim M, Z}(s) \|P_{t-s} f\|_\infty,$$

for all $t > s > 0$. Moreover, under some additional assumption, $C_{R, \dim M, Z}(s)$ decreases exponentially in s .

Similar arguments involving the P. Li-S. T. Yau inequality (2.4) – exactly the same way as above – may help obtain the last inequality if there is no vector field ($Z = 0$). I am grateful to S. Gallot for these observations.

Short time behavior for distant points

The physical intuition behind the Varadhan's relation (3.2) comes from the Feynman-type path integral representation

$$H_T(x, y) = C(T) \int_{p(0)=x, p(1)=y} \exp\left(-\frac{1}{2T} \int_0^1 |\dot{p}(t)|^2 dt\right) \mathcal{D}p,$$

where the right-hand side conveys the idea of integrating over all continuous paths in M which run from x to y , and one attributes a weight to a path according to its energy. P. Malliavin and D. Stroock [28] have investigated the validity of (3.2) after taking derivatives. They showed that, on a compact manifold M , as long as x stays outside the cut-locus of y , (3.2) holds even after taking derivatives up to the second order, i.e.

$$\begin{aligned}
\lim_{T \searrow 0} [T \nabla \log H_T(\cdot, y)] &= -\frac{1}{4} \nabla d^2(\cdot, y), \\
\lim_{T \searrow 0} [T \text{Hess} \log H_T(\cdot, y)] &= -\frac{1}{4} \text{Hess} d^2(\cdot, y),
\end{aligned} \tag{3.7}$$

uniformly on compact subsets of $M \setminus C_y$. The first two spatial derivatives of $\log H_T(x, y)$ are represented by certain integrals with respect to Wiener's measure. This above result is obtained as an application of the theory of large deviations to the asymptotic analysis of these integrals.

On the other hand, (3.7) may break down if there are more than one minimizing geodesic (or even a non-trivial Jacobi field) from x to y . Namely, the integral with respect to Wiener's measure corresponding to the logarithmic Hessian $\text{Hess} \log H_T(x, y)$ contains terms of order $1/T^2$ which may not cancel out in the limit $T \searrow 0$. These terms can be interpreted as a variance of a certain function.

We need a couple of definitions to state the theorem which elucidates the behavior of the logarithmic derivatives of the heat kernel for points in each other's cut-locus. Set

$$M(x, y) = \{X \in T_x M : y = \exp_x(X) \text{ and } d(x, y) = |X|\}$$

and

$$\widetilde{M}(x, y) = \left\{ (X, W) \in M(x, y) \times (T_x M \setminus \{0\}) : \frac{d}{ds} \exp_x(X + sW)|_{s=0} = 0 \right\}.$$

Clearly, $x \in C_y$ if and only if either $M(x, y)$ contains more than one element or $\widetilde{M}(x, y)$ is non-empty.

Theorem 3.1 (P. Malliavin-D. Stroock [28]). *Assume that $M(x, y)$ contains more than one element and that there exists a submanifold $\widetilde{M}(x, y) \supset M(x, y)$ of $T_x M$ with the property that*

$$(X, W) \in \widetilde{M}(x, y) \implies W \perp T_X(\widetilde{M}(x, y)).$$

Further, assume that $M(x, y)$ has positive measure in $\widetilde{M}(x, y)$ when $\widetilde{M}(x, y)$ is given the measure determined by the Riemannian structure it inherits as a submanifold. There exists a non-degenerate (i.e. not concentrated at a single point) Borel probability measure $\lambda_{x,y}$ on $T_x M$ which is supported on $M(x, y)$ and for which

$$\lim_{T \searrow 0} T [V \cdot \log H_T(\cdot, y)] = - \int (V, \theta) \lambda_{x,y}(d\theta), \quad V \in T_x M,$$

and

$$\lim_{T \searrow 0} T^2 [V \circ V \log H_T(\cdot, y)] = \int (V, \theta)^2 \lambda_{x,y}(d\theta) - \left(\int (V, \theta) \lambda_{x,y}(d\theta) \right)^2, \quad V \in T_x M.$$

In particular, $\lim_{T \searrow 0} T |\nabla \log H_T(\cdot, y)| < d(x, y)$ and $\lim_{T \searrow 0} T^2 [\text{Hess} \log H_T(\cdot, y)] > 0$.

Noncompact case

In the case where M is noncompact, one still has a bound for the logarithmic gradient of the heat kernel which is not optimal, however. Suppose that $\text{Ric}(M) \geq 0$. By combining the two-sided P. Li-S. T. Yau heat kernel estimates, volume comparison theorem and the elliptic gradient estimate (2.6), P. Souplet and Q. S. Zhang [34] showed that there is a universal dimensional constant C such that

$$\frac{|\nabla H_t(x, y)|}{H_t(x, y)} \leq C \frac{1}{\sqrt{t}} \left(1 + \frac{d^2(x, y)}{t} \right),$$

uniformly on $M \times (0, \infty)$.

3.2 Stochastic analysis on manifolds: general framework

In this section we review some facts concerning diffusion processes on manifolds which we will need in what follows. Details can be found in [21].

Frame bundle

Let $\pi : \mathcal{O}M \rightarrow M$ be the orthonormal frame bundle over a complete n -dimensional Riemannian manifold M . The orthogonal group $O(n)$ acts isometrically on the fibers of this bundle inducing for each $u \in \mathcal{O}M$ a tangent isomorphism from $\mathfrak{o}(n)$ to $V_u\mathcal{O}M$, the vertical (i.e. tangent to the fibres) subspace of $T_u\mathcal{O}M$. The Levi-Civita connection on M gives rise to an $O(n)$ -invariant connection on $\mathcal{O}M$, that is, at each point $u \in \mathcal{O}M$ there is a horizontal subspace $H_u\mathcal{O}M$ such that $T_u\mathcal{O}M$ is decomposed into a direct sum:

$$T_u\mathcal{O}M = V_u\mathcal{O}M \oplus H_u\mathcal{O}M.$$

Thus, $T_u\pi$ restricted to $H_u\mathcal{O}M$ induces an isomorphism from $H_u\mathcal{O}M$ to $T_{\pi u}M$ for each frame u at $\pi u = x \in M$.

If $e \in \mathbb{R}^n$, denote by ue the contraction of u and e which is a vector in $T_{\pi u}M$. By virtue of the above isomorphism, ue possesses a unique lift $H_e(u)$ to $H_u\mathcal{O}M \subset T_u\mathcal{O}M$. In particular, taking $e = e_i$, the vectors of the canonical basis of \mathbb{R}^n , one gets n horizontal vector fields $H_i = H_{e_i}$ on $\mathcal{O}M$. These are called the fundamental (canonical) vector fields. The fields H_e are $O(n)$ -equivariant in the following sense: for each $g \in O(n)$ and $u \in \mathcal{O}M$,

$$g_*H_e(u) = H_{ge}(gu).$$

Lemma 3.2. *Let θ be a differential one-form on M and let $X \in T_xM$. If to each $u \in \mathcal{O}M$ one assigns the coordinates of θ in the dual basis u^* , one gets a map $\tilde{\theta} : \mathcal{O}M \rightarrow \mathbb{R}^n$ which satisfies the following property:*

$$\widetilde{\nabla_X \theta} = \tilde{X} \tilde{\theta},$$

where \tilde{X} is the horizontal lift of X to $\mathcal{O}M$.

Next consider how the Laplacian is transformed under the lift to $\mathcal{O}M$. Let us define the Bochner horizontal Laplacian to be the following second order operator on $\mathcal{O}M$:

$$\Delta_{\mathcal{O}M} = \sum_{i=1}^n H_i^2.$$

Lemma 3.3. *Let $f \in C^\infty(M)$ and $\tilde{f} = f \circ \pi$ its lift to $\mathcal{O}M$. Then for any $u \in \mathcal{O}M$,*

$$\Delta f(x) = \Delta_{\mathcal{O}M} \tilde{f}(u), \tag{3.8}$$

where $x = \pi u$.

Proof. These facts are standard and can be proved by a computation in a parallel frame [21]. \square

Let $\mathcal{U}(t, x, y)$ be the fundamental solution of the perturbed heat equation

$$(\Delta_B - \partial_t)\mathcal{U}(t, x, y) = 0, \quad (3.9)$$

where $\Delta_B := \Delta + B$ for a C^2 -vector field B on M . Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and X_t a diffusion process on M generated by Δ_B . Suppose that X_t does not blow up in finite time. As is known, $\mathcal{U}(t, x, y)$ is the transition density function for X_t , i.e., if \mathbb{P}_x denotes the law of X_t starting from x ,

$$\mathbb{E}_x(f(X_t)) = \int_M \mathcal{U}(t, x, y) f(y) dy,$$

for any continuous function f on M .¹

Lifting diffusions to the orthonormal frame bundle

Recall that in the stochastic calculus framework, a stochastic differential equation (SDE) on M is defined by k vector fields and a driving semimartingale W with values in \mathbb{R}^k . A semimartingale U_t on $\mathcal{O}M$ is said to be horizontal if it is a solution of the SDE which can be written symbolically as

$$dU_t = \sum_i H_i(U_t) \circ dW_t^i,$$

where H_i are the canonical horizontal vector fields on $\mathcal{O}M$. This means that for any $f \in C^\infty(\mathcal{O}M)$,

$$f(U_t) = f(U_0) + \sum_i \int_0^t H_i f(U_s) \circ dW_s^i,$$

where the integral is understood in Stratonovich sense. Converting it into equivalent Itô integral we obtain Itô's formula:

$$df(U_s) = \sum_i H_i f(U_s) dW_s^i + \frac{1}{2} \sum_{i,j} H_i H_j f(U_s) d\langle W^i, W^j \rangle_s. \quad (3.10)$$

Furthermore, if X_t is a semimartingale on M (with respect to its proper filtration) and U_0 is an \mathcal{F}_0^X -measurable random variable with values in $\mathcal{O}M$ such that $\pi U_0 = X_0$, then there exists a unique horizontal semimartingale U_t on $\mathcal{O}M$ starting from U_0 which satisfies $\pi U = X$. It is referred to as the horizontal lift of X . In the case when X_t is the Δ_B -diffusion, the driving SDE for U_t reads

$$dU_t = \sum_i H_i(U_t) \sqrt{2} \circ dW_t^i + \tilde{B}(U_t) dt, \quad (3.11)$$

where \tilde{B} is the horizontal lift of B and W is the standard Brownian motion.

¹Throughout the discussion we adopt the convention to omit the $1/2$ factor in the expression for Laplacian, hence we retrieve the standard Brownian motion process times $\sqrt{2}$ as the Δ -diffusion.

The logarithm of the heat kernel

Let us fix the point $y \in M$ and the terminal time T (that will be dropped from the notations henceforth if there is no confusion). We will work with the function

$$J(t, u) \stackrel{\text{def}}{=} \log \mathcal{U}(T - t, \pi u, y) \quad (3.12)$$

defined on the orthonormal frame bundle $\mathcal{O}M$. Note the reversal of time on the right side. Define its horizontal gradient as an n -tuple:

$$\nabla^H J = (H_1 J, \dots, H_n J), \quad (3.13)$$

(it is always taken with respect to the first spatial variable). The horizontal hessian $\text{Hess}^H J$ is defined similarly. From (3.8), (3.9) and the definition of J it is readily seen that the heat equation for J becomes

$$\frac{\partial J}{\partial t} + \Delta_{\mathcal{O}M} J + \partial_{\bar{B}} J = -|\nabla^H J|^2. \quad (3.14)$$

The diffusion bridge

Finally, we need to define the Δ_B -diffusion bridge measure $\mathbb{P}_{x,y,T}$ between two points on a stochastically complete manifold M . Roughly speaking, it is a probability on the path space of M concentrated on the trajectories which start from x and pass through y at time T , obtained by conditioning the Δ_B -diffusion process:

$$\mathbb{P}_{x,y,T}(\cdot) = \mathbb{P}_x(\cdot | X_T = y).$$

If $\mathcal{U}(T, x, y)$ is the Δ_B -transition density on M , one can verify that under $\mathbb{P}_{x,y,T}$ the joint density of X_{s_1}, \dots, X_{s_l} , $0 = s_0 < s_1 < \dots < s_l < s_{l+1} = T$, is equal to

$$\mathcal{U}(T, x, y)^{-1} \prod_{i=0}^l \mathcal{U}(s_{i+1} - s_i, x_i, x_{i+1}),$$

where $x_0 = x$, $x_{l+1} = y$. The measure $\mathbb{P}_{x,y,T}$ is absolutely continuous with respect to \mathbb{P}_x on the σ -field \mathcal{B}_s generated by coordinate functions up to time s for any $s < T$ and its Radon-Nikodym derivative is given by

$$\left. \frac{d\mathbb{P}_{x,y,T}}{d\mathbb{P}_x} \right|_{\mathcal{B}_s} = \frac{\mathcal{U}(T - s, X_s, y)}{\mathcal{U}(T, x, y)} = \exp(J(s, U_s) - J(0, U_0)),$$

where U_s is the horizontal lift of X_s . Taking stochastic differential $dJ(t, U_t)$ with the help of Itô's formula (3.10) implies

$$dJ(t, U_t) = \frac{\partial J(t, U_t)}{\partial t} dt + \langle \sqrt{2} \nabla^H J(t, U_t), dW_t \rangle + \partial_{\bar{B}} J(t, U_t) dt + \Delta_{\mathcal{O}M} J(t, U_t) dt, \quad (3.15)$$

which yields, using (3.14),

$$\left. \frac{d\mathbb{P}_{x,y,T}}{d\mathbb{P}_x} \right|_{\mathcal{B}_s} = \exp \left[\int_0^s \langle \sqrt{2} \nabla^H J(\tau, U_\tau), dW_\tau \rangle - \int_0^s |\nabla^H J(\tau, U_\tau)|^2 d\tau \right].$$

It follows, by Girsanov's theorem, that the process

$$b_s = W_s - \sqrt{2} \int_0^s \nabla^H J(\tau, U_\tau) d\tau, \quad 0 \leq s < T, \quad (3.16)$$

is a Brownian motion under $\mathbb{P}_{x,y,T}$. Summarizing the above considerations, we derive from (3.11)

Lemma 3.4. *The horizontal lift U_s of a Δ_B -diffusion bridge on M from x to y during the time T is the solution of the following SDE:*

$$dU_s = \sum_i H_i(U_s) \circ \{ \sqrt{2} db_s^i + 2H_i \log \mathcal{U}(T-s, \pi U_s, y) ds \} + \tilde{B}(U_s) ds,$$

where b_s is a standard Brownian motion under $\mathbb{P}_{x,y,T}$. □

3.3 Estimates of logarithmic derivatives of the heat kernel via carré du champ operators

Let M be a compact Riemannian manifold with Ricci curvature bounded from below by a non-positive constant, $\text{Ric}(M) \geq -R$, $R \geq 0$. The aim of this section is to derive a universal bound on the gradient of logarithm of the heat kernel which depends on R and some other parameters. This can be viewed as an improvement of the result of E. P. Hsu [22] who obtained a similar bound but with a constant depending on the manifold in an unspecified way. His method involving probabilistic techniques is essentially used here.

Theorem 3.5. *Let M be a compact Riemannian manifold of dimension n with Ricci curvature bounded from below, $\text{Ric}(M) \geq -R$, $R \geq 0$.*

- (1.) *Suppose a non-collapsing condition is satisfied on M , namely, there exist $t_0 > 0$ and $v_0 > 0$ such that for any $x \in M$, the volume of the geodesic ball of radius t_0 centered at x is not too small,*

$$\text{Vol}(B_x(t_0)) \geq v_0. \quad (3.17)$$

Then there exists a constant $C(R, n, v_0, t_0)$ such that the gradient of logarithm of the heat kernel $H_t(x, y)$ is controlled by

$$|\nabla \log H_t(x, y)| \leq C(R, n, v_0, t_0) \left(\frac{d(x, y)}{t} + \frac{1}{\sqrt{t}} \right), \quad (3.18)$$

uniformly on $(0, 2t_0^2] \times M \times M$, where $d(x, y)$ is the Riemannian distance between two points.

- (2.) *Suppose that $\text{diam}(M) \leq D$. Then there exists a constant $C(n)$ such that*

$$|\nabla \log H_t(x, y)| \leq C(n) \left(\frac{D}{t} + \frac{1 + D\sqrt{R}}{\sqrt{t}} + R\sqrt{t} \right), \quad (3.19)$$

uniformly on $(0, \infty) \times M \times M$.

I am grateful to S. Gallot for the following remark and Proposition 3.7 below.

Remark 3.6. It is clear that (3.19) is invariant under rescaling of the Riemannian metric g on M . Indeed, if we set $h_g(t, x, y) = |\nabla \log H_t(x, y)|$, where the heat kernel, the gradient and the norm are taken with respect to g , it is clearly seen that

$$h_{\lambda^2 g}(t, x, y) = \frac{1}{\lambda} h_g(t/\lambda^2, x, y),$$

where λ^2 is the scaling factor. Thus it is of interest to write also (3.18) in a scaling-invariant form. Let us introduce the quantity

$$\tilde{v}_0 = \sup_{x \in M} \frac{Vol^{\{-R\}}(\frac{t_0}{\sqrt{R}})}{Vol(B_x(\frac{t_0}{\sqrt{R}}))}, \quad (3.20)$$

where $Vol^{\{-R\}}(t)$ stands for the volume of a ball of radius t in the space of constant curvature $-R/(n-1)$. Since $B_x^g(t/\sqrt{R^g}) = B_x^{\lambda^2 g}(t/\sqrt{R^{\lambda^2 g}})$, \tilde{v}_0 is invariant under rescaling of g . With this notation at hand, we will show in course of the proof that it is possible to rewrite the first statement of Theorem 3.5 in a scaling-invariant form:

$$|\nabla \log H_t(x, y)| \leq C_2(n, \tilde{v}_0, t_0) \left(\frac{d(x, y)}{t} + \frac{1}{\sqrt{t}} + \sqrt{R} \right),$$

uniformly on $(0, 2t_0^2/R] \times M \times M$. Notice that there is now an additional term \sqrt{R} on the right-hand side.

Proposition 3.7 (S. Gallot). *Let M be a compact n -dimensional Riemannian manifold with Ricci curvature bounded from below, $\text{Ric}(M) \geq -R$, $R \geq 0$. With the above notations, for each $\delta \in (0, 1)$,*

$$\begin{aligned} |\nabla \log H_t(x, y)| \leq & \left(1 + \frac{\delta}{2}\right) \left[\frac{d(x, y)}{2t} + \frac{1}{\sqrt{t}} \left(\frac{d(x, y)\sqrt{R}}{\sqrt{2}} + \left(\frac{1}{\delta} + C'(n) + \log \tilde{v}_0 \right)^{1/2} \right) \right. \\ & \left. + \sqrt{2R} \left(\tilde{C}'\sqrt{n} + \left(\frac{1}{\delta} + C'(n) + \log \tilde{v}_0 \right)^{1/2} \right) + \sqrt{t} \tilde{C}' R\sqrt{n} \right], \end{aligned}$$

uniformly on $(0, 2t_0^2/R] \times M \times M$. ($C'(n)$ and \tilde{C}' are constants with indicated dependencies.)

Because of Varadhan's asymptotic relation, the coefficient near the principle term is almost optimal, δ being arbitrarily close to 0.

Remark 3.8. The proof of Theorem 3.5 relies on some formal properties of the Ricci curvature which are best seen in the so-called curvature-dimension inequality. In fact, we will prove a stronger version of part 2 of Theorem 3.5. In order to formulate the assumption in a more general setting, we need to introduce some additional notations. The vocabulary introduced below was developed by D. Bakry [2] to study the theory of elliptic diffusion generators in their relation to geometry. Given a C^2 -vector field B , let $\Delta_B = \Delta + \partial_B$ be an elliptic operator on M . For $f, g \in C^\infty(M)$ define two bilinear operators:

$$\Gamma(f, g) = \frac{1}{2}(\Delta_B(fg) - f\Delta_B g - g\Delta_B f) = \langle \nabla f, \nabla g \rangle,$$

and iterating this definition:

$$\Gamma_2(f, g) = \frac{1}{2}(\Delta_B \Gamma(f, g) - \Gamma(f, \Delta_B g) - \Gamma(g, \Delta_B f)).$$

These are called the *carré du champ* operators, they first appeared in the work of D. Bakry [2]. Morally, Γ measures how far Δ_B is from a differentiation. Γ_2 is related to the Ricci curvature via the classical Bochner identity:

$$\Gamma_2(f, g) = \langle \text{Hess } f, \text{Hess } g \rangle + \text{Ric}(\nabla f, \nabla g) - \nabla^{\text{sym}} B(\nabla f, \nabla g), \quad (3.21)$$

where $\nabla^{\text{sym}} B$ stands for the symmetrized gradient of B . In the case of $B = 0$, since $|\text{Hess } f|^2 \geq (\Delta f)^2/n$, the assumption on Ricci curvature translates into the following *curvature-dimension* inequality:

$$\Gamma_2(f, f) \geq \frac{1}{n}(\Delta f)^2 - R\Gamma(f, f), \quad \text{for all } f \in C^\infty(M).$$

This is the only form in which the Ricci curvature will be exploited in what follows. Moreover, the geometric dimension of M is relevant only for the proof of the first assertion in Theorem 3.5 to the extent that it appears in the estimates for the geodesic balls' volume growth provided by the Bishop-Gromov theorem. Thus the second assertion in Theorem 3.5 can be generalized as follows:

(2'.) Consider the heat equation (2.1) with Δ replaced by Δ_B introduced above and let $\mathcal{U}(t, x, y)$ be its fundamental solution. Suppose that Δ_B satisfies the $CD(m, -R)$ curvature-dimension inequality, that is, by definition:

$$\Gamma_2(f, f) \geq \frac{1}{m}(\Delta_B f)^2 - R\Gamma(f, f), \quad \text{for all } f \in C^\infty(M). \quad (3.22)$$

Then, if $\text{diam}(M) \leq D$, (3.19) holds for $\nabla \log \mathcal{U}(t, x, y)$ with the constant replaced by $C(m)$:

$$|\nabla \log \mathcal{U}(t, x, y)| \leq C(m) \left(\frac{D}{t} + \frac{1 + D\sqrt{R}}{\sqrt{t}} + R\sqrt{t} \right), \quad (3.23)$$

uniformly on $(0, \infty) \times M \times M$.

Remark 3.9. A careful examination of constants entering the proof of Theorem 3.5 shows that

$$|\nabla \log \mathcal{U}(t, x, y)| \leq \frac{D}{t} + \frac{2\sqrt{m} + D\sqrt{R}}{\sqrt{t}} + 2\sqrt{t}\sqrt{m}R$$

actually holds in (3.23).

The proof of Theorem 3.5 is divided into two steps which we now outline. First, we apply Itô's formula to the square of $\nabla \log H_{t-s}(X_s, y)$ process where X_s is the Brownian bridge on M from x to y during the time t (in the case of $B = 0$), or, in other words, the Wiener measure conditioned to trajectories leaving from x and passing through y at time t . This enables $\nabla \log H_t(x, y)$ to be controlled by the expectation of the difference of $\log H_{t-s}(X_s, y)$ taken at times $t/2$ and 0. To avoid technical difficulties all the processes are considered as

horizontal lifts to the orthonormal frame bundle $\mathcal{O}M$ over M . This is a convenient stochastic calculus formalism due to the existence of n canonical horizontal vector fields on $\mathcal{O}M$.

Second, we make use of Harnack inequalities and fundamental estimates on the heat kernel derived by P. Li and S. T. Yau from the maximum principle in their paper [27] of 1986 and of some of their modifications obtained by D. Bakry and Z. M. Qian [4]. The first part of Theorem 3.5 relies on P. Li-S. T. Yau upper bound on $H_t(x, y)$ which involves volumes of geodesic balls, while the second part is a straightforward application of a Harnack inequality.

The first term on the right hand side of (3.18) is expected due to Varadhan's asymptotic relation (3.2). We now give an argument that justifies the presence of the second term on the right hand side of (3.18).

Example. Let X be the quotient space of \mathbb{R}^n under the involution $x \rightarrow -x$. Then the heat kernel on X evaluated at two points, say \bar{x} and \bar{y} , equals to the sum

$$H_t^{\mathbb{R}^n}(x, y) + H_t^{\mathbb{R}^n}(x, -y),$$

x (respectively, y) being (any) pre-images of \bar{x} (respectively, \bar{y}) under the quotient map. Since $H_t^{\mathbb{R}^n}(x, y) = (4\pi t)^{-\frac{n}{2}} \exp\left(-\frac{|x-y|^2}{4t}\right)$, it is easily seen that

$$\sup_{\bar{x}} |\nabla \log H_t^X(\bar{x}, \bar{x})| = \frac{1}{\sqrt{t}} \max_{z \in \mathbb{R}^+} \frac{z}{e^{z^2} + 1}.$$

X has $K \geq 0$ in Alexandrov's sense. If $n = 4$, X can be approximated by smooth Ricci flat manifolds, the Eguchi-Hanson metrics on $T\mathbb{C}P^1$ [30].

Proof of Theorem 3.5

From now on, the probability measure will be $\mathbb{P}_{x,y,T}$ (in particular, \mathbb{E} and U_t will be associated to this measure). Let J be the function defined by (3.12) and let $\nabla^H J$ be its horizontal gradient defined by (3.13). The first step in the proof of Theorem 3.5 consists in applying Itô's formula to the square of $\nabla^H J$. This is the purpose of

Proposition 3.10. *Let M be a complete Riemannian manifold and let B be a C^2 -vector field on M . Consider a Δ_B -diffusion bridge X_t from x to y during the time T introduced in Section 3.2 and its horizontal lift U_t . Suppose that X_t does not blow up in finite time. If $\mathcal{U}(T, x, y)$ is the fundamental solution of (3.9) then*

$$|\nabla^H J(t, U_t)|^2 - |\nabla^H J(0, U_0)|^2 = \sqrt{2} \int_0^t \langle \nabla^H |\nabla^H J(s, U_s)|^2, db_s \rangle + 2 \int_0^t \Gamma_2(J(s, U_s), J(s, U_s)) ds \quad (3.24)$$

for $0 < t < T$, where b_s is a standard Brownian motion.

Remark 3.11. The following proof amounts to compute the action of the Δ_B -diffusion bridge generator, $L_t := \Delta + B + 2\nabla \log \mathcal{U}(T-t, \cdot, y)$, upon the function $|\nabla \log \mathcal{U}(T-t, \cdot, y)|^2$.

Proof. Take the Δ_B -diffusion bridge process X_t from x to y during the time T and apply Itô's formula to the square of $\nabla^H J(t, U_t)$, where U_t is the horizontal lift of X_t to $\mathcal{O}M$. This yields, using Lemma 3.4,

$$d\langle \nabla^H J(t, U_t), \nabla^H J(t, U_t) \rangle = \langle \nabla^H |\nabla^H J|^2, \sqrt{2} db_t + 2\nabla^H J dt + \bar{B}(U_t) dt \rangle + (\partial_t + \Delta_{\mathcal{O}M}) |\nabla^H J|^2 dt. \quad (3.25)$$

The action of $\Delta_{\mathcal{O}M}$ on $|\nabla^H J|^2$ is given by

$$\begin{aligned}\Delta_{\mathcal{O}M}\langle \nabla^H J, \nabla^H J \rangle &= \sum_{i,j} H_i^2 (H_j J)^2 = 2 \sum_{i,j} H_i (H_i H_j J H_j J) \\ &= 2 \sum_{i,j} (H_i^2 H_j J) (H_j J) + (H_i H_j J)^2 \\ &= 2\langle \Delta_{\mathcal{O}M} \nabla^H J, \nabla^H J \rangle + 2|\text{Hess}^H J|^2.\end{aligned}$$

On the other hand, applying ∇^H to (3.14) yields

$$\partial_t |\nabla^H J|^2 = -2\langle \nabla^H \Delta_{\mathcal{O}M} J, \nabla^H J \rangle - 2\langle \nabla^H \partial_{\bar{B}} J, \nabla^H J \rangle - 2\langle \nabla^H |\nabla^H J|^2, \nabla^H J \rangle.$$

Finally, inserting this stuff into (3.25) we obtain

$$\begin{aligned}d|\nabla^H J|^2 &= \langle \sqrt{2} \nabla^H |\nabla^H J|^2, db_t \rangle \\ &\quad + 2 \left(\langle [\Delta_{\mathcal{O}M}, \nabla^H] J, \nabla^H J \rangle + |\text{Hess}^H J|^2 - \widetilde{\nabla B}(\nabla^H J, \nabla^H J) \right) dt,\end{aligned}\tag{3.26}$$

(like in Lemma 3.2, ∇B gives rise to a map $\widetilde{\nabla B}: \mathcal{O}M \rightarrow \mathbb{R}^n \otimes \mathbb{R}^n$). The bracket $[\Delta_{\mathcal{O}M}, \nabla^H]$ in the above expression involves Ricci curvature. Indeed, as in Section 3.2, let for $u \in \mathcal{O}M$ and $e \in \mathbb{R}^n$, u^*e denote their contraction in $T_{\pi u}^*M$. Then Lemma 3.2 implies

$$\begin{aligned}u^*(\Delta_{\mathcal{O}M} \nabla^H J) &= u^* \left(\sum_i H_i^2 \nabla^H J \right) = \sum_i \nabla_{ue_i} \nabla_{ue_i} d \log \mathcal{U}(T-t, \cdot, y) \\ &= -\nabla^* \nabla d \log \mathcal{U}(T-t, \cdot, y).\end{aligned}$$

Recall that the Hodge-de Rham Laplacian is an order two differential operator on forms defined by $\Delta_{HdR} = d^*d + dd^*$, where d^* is the formal adjoint of d . Hence it commutes with the exterior derivative. Using the Bochner formula, $-\Delta_{HdR} = \nabla^* \nabla + \text{Ric}$, for the Hodge-de Rham Laplacian on the 1-forms, we infer that

$$\begin{aligned}u^*([\Delta_{\mathcal{O}M}, \nabla^H] J) &= (\Delta_{HdR} d - d \Delta) \log \mathcal{U}(T-t, \cdot, y) + \text{Ric}(d \log \mathcal{U}(T-t, \cdot, y)) \\ &= \text{Ric}(d \log \mathcal{U}(T-t, \cdot, y)).\end{aligned}$$

Thus, recalling the formula (3.21) for the carré du champ operator, imply (3.24). \square

Remark 3.12. If M is compact the integral with respect to Brownian motion is actually a martingale, thus taking expectation gives

$$\mathbb{E}|\nabla^H J(t, U_t)|^2 - |\nabla^H J(0, U_0)|^2 = 2\mathbb{E} \int_0^t \Gamma_2(J, J) ds.\tag{3.27}$$

In general,

$$\mathbb{E} \int_0^t |\nabla^H |\nabla^H J|^2|^2 ds < \infty$$

or even

$$\mathbb{E} \sqrt{\int_0^t |\nabla^H |\nabla^H J|^2|^2 ds} < \infty$$

is enough to ensure that $\int_0^t \langle \nabla^H |\nabla^H J|^2, db_s \rangle$ be a martingale and, thence, (3.27) hold. Let $\zeta_K := \inf\{t \mid d(x, X_t) = K\}$ be the hitting time of the ball of radius K around x for the Δ_B -diffusion bridge. When restricted to $B_K(x)$, all the functions are bounded, and we can write:

$$\mathbb{E} |\nabla^H J(t \wedge \zeta_K, U_{t \wedge \zeta_K})|^2 - |\nabla^H J(0, U_0)|^2 = 2\mathbb{E} \int_0^{t \wedge \zeta_K} \Gamma_2(J, J) ds,$$

for any M (compact or not).

Corollary 3.13. *Suppose that M is compact and the curvature-dimension $CD(\infty, -R)$ inequality (3.22) is satisfied on M , i.e.,*

$$\Gamma_2(f, f) \geq -R|\nabla f|^2.$$

Then for any $T > 0$,

$$|\nabla \log \mathcal{U}(T, x, y)|^2 \leq 2 \left(\frac{1}{T} + R \right) \mathbb{E} \log \frac{\mathcal{U}(T/2, X_{T/2}, y)}{\mathcal{U}(T, x, y)}, \quad (3.28)$$

where X_t is a Δ_B -diffusion bridge from x to y during the time T . In particular,

$$|\nabla \log \mathcal{U}(T, x, y)|^2 \leq 2 \left(\frac{1}{T} + R \right) \log \frac{\|\mathcal{U}(T/2, \cdot, y)\|_\infty}{\mathcal{U}(T, x, y)}, \quad (3.29)$$

Proof. In view of (3.27),

$$\mathbb{E} |\nabla^H J(s, U_s)|^2 - |\nabla^H J(0, U_0)|^2 \geq -2R \mathbb{E} \int_0^s |\nabla^H J(t, U_t)|^2 dt.$$

Integrating once more with respect to s gives

$$\frac{T}{2} |\nabla^H J(0, U_0)|^2 \leq (1 + RT) \mathbb{E} \int_0^{T/2} |\nabla^H J|^2 ds. \quad (3.30)$$

The latter integral is calculated with the help of Itô's formula applied to $J(t, U_t)$ (3.15), (3.16):

$$dJ = \left(\frac{\partial J}{\partial t} + \partial_{\bar{B}} J + \Delta_{OM} J \right) dt + \langle \sqrt{2} \nabla^H J, db_t + \sqrt{2} \nabla^H J dt \rangle,$$

and the heat equation (3.14):

$$dJ = -|\nabla^H J|^2 dt + \langle \sqrt{2} \nabla^H J, db_t \rangle + 2|\nabla^H J|^2 dt.$$

Thus,

$$\mathbb{E} \int_0^{T/2} |\nabla^H J|^2 ds = \mathbb{E} J(T/2, U_{T/2}) - J(0, U_0). \quad (3.31)$$

Now Corollary follows from (3.30) and (3.31). \square

Remark 3.14. Suppose that the non-collapsing condition of part 1 of Theorem 3.5 holds on M . If M is non-compact, the preceding arguments together with the dominated convergence theorem imply that

$$\begin{aligned} \frac{T}{2} |\nabla^H J(0, U_0)|^2 &\leq (1 + RT) \left(\mathbb{E} J(T/2, U_{T/2}) - J(0, U_0) \right) \\ &\quad + \liminf_{K \rightarrow \infty} \mathbb{E} \left((T/2 - \zeta_K)_+ |\nabla^H J(\zeta_K, U_{\zeta_K})|^2 \right). \end{aligned}$$

We are now in position to prove Theorem 3.5. First let us restate, in the form adapted to our needs, the results from [27] and [4] which we will make use of.

Let M be a complete manifold without boundary. If the Ricci curvature of M is bounded below by $-R$, for some constant $R \geq 0$, then the heat kernel satisfies the upper bound:

$$H_T(x, y) \leq C(n) \text{Vol}^{-1/2}(B_x(\sqrt{T})) \text{Vol}^{-1/2}(B_y(\sqrt{T})) \exp \left[\tilde{C} n R T - \frac{2d^2(x, y)}{9T} \right], \quad (3.32)$$

for all $(T, x, y) \in (0, \infty) \times M \times M$, where \tilde{C} is a universal constant and $C(n)$ depends only on the dimension of M [27, Corollary 3.1] (cf. Theorem 2.15).

Let M be a complete manifold and Δ_B the elliptic operator introduced in Section 3.2. Assume that Δ_B satisfies the curvature-dimension $CD(m, -R)$ inequality (3.22) for some constants $m > 0$ and $R \geq 0$. If \mathcal{U} is a positive solution of the heat equation (3.9) on $[0, \infty) \times M$, then the following Harnack inequality holds on M :

$$\frac{\mathcal{U}(t, x)}{\mathcal{U}(t+s, y)} \leq \left(\frac{t+s}{t} \right)^{m/2} \times \exp \left[\frac{(d(x, y) + \sqrt{Rms})^2}{4s} + \frac{\sqrt{Rm}}{4} \min\{d(x, y), \sqrt{Rms}\} \right], \quad (3.33)$$

for all $s > 0$, $t \geq 0$, x and $y \in M$ ([4, Theorem 10], see also p. 175). In particular, if there is no vector field, i. e., $B = 0$ and the Ricci curvature of M is bounded from below by $-R$, $R \geq 0$, (3.33) holds for m replaced with the dimension n of M . Hence, passing to the limit $t \rightarrow 0$ and using the heat kernel asymptotics $H_t(x, x) \sim (4\pi t)^{-n/2}$ for small times yield a lower bound estimate for the heat kernel,

$$H_T(x, y) \geq (4\pi T)^{-n/2} \times \exp \left[-\frac{(d(x, y) + \sqrt{RnT})^2}{4T} - \frac{\sqrt{Rn}}{4} \min\{d(x, y), \sqrt{RnT}\} \right], \quad (3.34)$$

for all $(T, x, y) \in (0, \infty) \times M \times M$.

Proof of Theorem 3.5. We will first prove part 2 of the theorem. Since M is compact, the Δ_B -diffusion does not blow up in finite time. Setting $t = s = T/2$ in (3.33), we infer that

$$\mathbb{E} \log \frac{\mathcal{U}(T/2, X_{T/2}, y)}{\mathcal{U}(T, x, y)} \leq C(m) \mathbb{E} \left(\frac{d^2(X_{T/2}, x)}{T} + 1 + RT \right).$$

If $\text{diam}(M) \leq D$, combining this with (3.28) gives

$$|\nabla \log \mathcal{U}(T, x, y)|^2 \leq C(m) \left(\frac{1}{T} + R \right) \left(\frac{D^2}{T} + 1 + RT \right),$$

from which (3.23) follows.

In order to prove part 1 of the theorem (thus in the case where $\mathcal{U}(t, \cdot, \cdot) = H_t$), we will first apply the Bishop-Gromov theorem. Set

$$\tilde{v}_0(R, t_0, M) := \sup_{x \in M} \frac{\text{Vol}^{\{-R\}}(t_0)}{\text{Vol}(B_x(t_0))},$$

where $\text{Vol}^{\{-R\}}(t)$ stands for the volume of a ball of radius t in the space of constant curvature $-R/(n-1)$. Anyway, it is greater than the volume of the corresponding ball in Euclidean space which is proportional to t^n . Then

$$\frac{1}{\text{Vol}(B_x(t))} \leq \tilde{v}_0(R, t_0, M) \frac{1}{\text{Vol}^{\{-R\}}(t)} \quad (3.35)$$

for $t \leq t_0$. Now suppose that $T \leq 2t_0^2$, then (3.35) and (3.32) imply

$$\mathbb{E}J(T/2, U_{T/2}) \leq C(n) + \log \tilde{v}_0(R, t_0, M) - \frac{n}{2} \log T + \tilde{C}(n) RT,$$

and (3.34) implies

$$J(0, U_0) \geq -C(n) - \frac{n}{2} \log T - \frac{2d^2(x, y)}{3T} - \tilde{C}(n) RT.$$

Inserting two last inequalities into (3.28) yields

$$|\nabla \log H_T(x, y)|^2 = |\nabla^H J(0, U_0)|^2 \leq C(n, \tilde{v}_0(R, t_0, M)) (1 + Rt_0^2) \left(\frac{d^2(x, y)}{T^2} + \frac{1}{T} + R \right),$$

on $(0, 2t_0^2] \times M \times M$. In view of (3.20), replacing t_0 with t_0/\sqrt{R} provides a scaling-invariant estimate. Taking the square root of both sides in the last inequality completes the proof of the theorem (and the statement in the Remark 3.6). \square

Proof of Proposition 3.7. With the notations of Proposition 3.10, let us introduce the following functions:

$$g(t, x, y) = \mathbb{E}|\nabla^H J(t, U_t)|^2, \quad h(t, x, y) = \mathbb{E}J(t, U_t).$$

We know from (3.31) that $g(t, x, y) = \partial_t h(t, x, y)$. Recall that Corollary 3.13 implies

$$\frac{\partial g}{\partial t}(t, x, y) \geq -2R g(t, x, y),$$

whence for each $t \in (0, T]$ and each $\delta \in (0, 1)$,

$$\begin{aligned} \frac{d}{dt} [(T-t)^{1+\delta} g(t, x, y)] &\geq -(1+\delta)(T-t)^\delta g(t, x, y) - 2R(T-t)^{1+\delta} g(t, x, y) \\ &\geq -(1+\delta+2RT)(T-t)^\delta \frac{\partial h}{\partial t}(t, x, y). \end{aligned}$$

Integrating by parts from 0 to $T-s$, one has

$$\begin{aligned} s^{1+\delta} g(T-s, x, y) - T^{1+\delta} g(0, x, y) &\geq - \left[(1+\delta+2RT)(T-t)^\delta h(t, x, y) \right]_0^{T-s} \\ &\quad - \int_0^{T-s} \delta(1+\delta+2RT)(T-t)^{\delta-1} h(t, x, y) dt. \end{aligned}$$

Thus,

$$\begin{aligned}
T^{1+\delta}g(0, x, y) &\leq s^{1+\delta}g(T-s, x, y) + (1 + \delta + 2RT)s^\delta h(T-s, x, y) \\
&\quad + \delta(1 + \delta + 2RT) \int_s^T t^{\delta-1} \left[h(T-t, x, y) - h(0, x, y) \right] dt \\
&\quad - (1 + \delta + 2RT)s^\delta h(0, x, y).
\end{aligned} \tag{3.36}$$

Let us calculate the limit of each term in this formula as $s \rightarrow 0_+$. Since the manifold M is compact and fixed, the asymptotic expansion of the heat kernel gives:

$$\log H_s(z, y) = -\frac{n}{2} \log(4\pi s) - \frac{d^2(y, z)}{4s} + \log \left[u_0(y, z) + su_1(y, z) + \dots \right].$$

It follows that

$$\log H_s(z, y) \leq -\frac{d^2(y, z)}{4s} - \frac{n}{2} \log s + C_1,$$

when $s \rightarrow 0_+$. Similarly,

$$|\nabla_z \log H_s(z, y)|^2 \leq \frac{d^2(y, z)}{4s^2} + C_2.$$

Let us denote by $dP_{t,x,y}(z)$ the probability distribution of the time- T -Brownian bridge between x and y at time t . Then

$$\begin{aligned}
&s^{1+\delta}g(T-s, x, y) + (1 + \delta + 2RT)s^\delta h(T-s, x, y) \\
&= s^{1+\delta} \int_M |\nabla_z \log H_s(z, y)|^2 dP_{T-s,x,y}(z) + (1 + \delta + 2RT)s^\delta \int_M \log H_s(z, y) dP_{T-s,x,y}(z).
\end{aligned}$$

It follows that

$$\begin{aligned}
&s^{1+\delta}g(T-s, x, y) + (1 + \delta + 2RT)s^\delta h(T-s, x, y) \leq C_2 s^{1+\delta} \\
&\quad - \frac{n}{2}(1 + \delta + 2RT)s^\delta \log s + C_1(1 + \delta + 2RT)s^\delta - \int_M \frac{d^2(y, z)}{4s^{1-\delta}} (\delta + 2RT) dP_{T-s,x,y}(z).
\end{aligned}$$

Clearly, the limit of the last expression as $s \rightarrow 0_+$ is non-positive. (Actually, it is equal to 0 since $\int_M \frac{d^2(y, z)}{4s^{1-\delta}} dP_{T-s,x,y}(z) = O(s^\delta)$.) Inserting this stuff into (3.36) entails

$$T^{1+\delta} |\nabla_x \log H_T(x, y)|^2 \leq \delta(1 + \delta + 2RT) \lim_{s \rightarrow 0_+} \int_s^T t^{\delta-1} \int_M \log \left(\frac{H_t(z, y)}{H_T(x, y)} \right) dP_{T-t,x,y}(z) dt.$$

It is not difficult to see that the last integral converges because, when $s \rightarrow 0_+$,

$$\begin{aligned}
&\int_0^s t^{\delta-1} \int_M \log H_t(z, y) dP_{T-t,x,y}(z) dt \\
&\leq C_1 \int_0^s t^{\delta-1} \left(|\log t| + C_2 + \int_M \frac{d^2(y, z)}{t} \frac{e^{-\frac{d^2(y, z)}{4t}}}{(4\pi t)^{n/2}} dv_g(z) \right) dt \\
&\leq C_1 \int_0^s t^{\delta-1} \left(|\log t| + C'_2 \right) dt \xrightarrow{s \rightarrow 0_+} 0.
\end{aligned}$$

Thus, we have

$$T^{1+\delta} |\nabla_x \log H_T(x, y)|^2 \leq (1+\delta+2RT) \int_0^T \delta t^{\delta-1} \int_M \log \left(\frac{H_t(z, y)}{H_T(x, y)} \right) dP_{T-t, x, y}(z) dt. \quad (3.37)$$

Using (3.34), we infer that

$$\begin{aligned} \log H_T(x, y) &\geq -\frac{n}{2} \log T - \frac{n}{2} \log(4\pi) \\ &\quad - \frac{1}{4T} \left([d(x, y) + \sqrt{nR}T]^2 + \min\{\sqrt{nR}d(x, y)T, nRT^2\} \right) \\ &\geq -\frac{n}{2} \log T - \frac{n}{2} \log(4\pi) - \frac{1}{4T} \left[d^2(x, y) + nRT^2 \right. \\ &\quad \left. + 2\sqrt{nR}d(x, y)T + 2(\sqrt{5}-2)\sqrt{nR}d(x, y)T + (5-2\sqrt{5})nRT^2 \right], \end{aligned}$$

and hence,

$$-\log H_T(x, y) \leq \frac{n}{2} \log T + \frac{n}{2} \log(4\pi) + \frac{1}{4T} \left[d(x, y) + (\sqrt{5}-1)\sqrt{nR}T \right]^2.$$

On the other hand, (3.32) implies

$$\log H_t(z, y) \leq \log(C(n)\tilde{v}_0) - \frac{n}{2} \log t + \tilde{C}nRt - \frac{2d^2(y, z)}{9t}.$$

Adding two last inequalities gives:

$$\log \left(\frac{H_t(z, y)}{H_T(x, y)} \right) \leq \frac{n}{2} \log \left(\frac{T}{t} \right) + C'(n) + \log \tilde{v}_0 + \tilde{C}nRt + \frac{1}{4T} [d(x, y) + (\sqrt{5}-1)\sqrt{nR}T]^2.$$

Performing integration in (3.37) and using the fact that $\int_M dP_{T-t, x, y} = 1$, we obtain that

$$\begin{aligned} \int_0^T \delta t^{\delta-1} \int_M \log \left(\frac{H_t(z, y)}{H_T(x, y)} \right) dP_{T-t, x, y}(z) dt &\leq \frac{n}{2} T^\delta \log T - \frac{n}{2} T^\delta \log T + \frac{1}{\delta} T^\delta \\ &\quad + (C'(n) + \log \tilde{v}_0) T^\delta + \tilde{C}' nRT^{1+\delta} + \frac{T^\delta}{4T} [d(x, y) + (\sqrt{5}-1)\sqrt{nR}T]^2. \end{aligned}$$

This gives, together with (3.37),

$$\begin{aligned} |\nabla_x \log H_T(x, y)|^2 &\leq (1+\delta+2RT) \left[\frac{1}{4T^2} \left(d(x, y) + (\sqrt{5}-1)\sqrt{nR}T \right)^2 \right. \\ &\quad \left. + \frac{1}{T} \left(\frac{1}{\delta} + C'(n) + \log \tilde{v}_0 \right) + \tilde{C}' nR \right]. \end{aligned}$$

To finish the proof, take the square root of both sides and arrange the coefficients near the powers of T . \square

Remark 3.15. As it is clear from the proof of the main theorem,

$$|\nabla \log \mathcal{U}(T, x, y)|^2 \leq C(m) \left(\frac{1}{T} + R \right) \left(\frac{\mathbb{E} d^2(X_{T/2}, x)}{T} + 1 + RT \right).$$

Hence, any information about the expectation of the squared distance of the Brownian bridge to its starting point would make the statement more precise. For instance, in the Euclidean case $M = \mathbb{R}^n$,

$$\mathbb{E} d^2(X_s, x) = 2n \frac{s(T-s)}{T} + \frac{s^2|x-y|^2}{T^2},$$

for the Brownian bridge from x to y during the time T , and Theorem 3.5 amounts to

$$\frac{|x-y|^2}{4T^2} = |\nabla \log H_T(x, y)|^2 \leq \frac{C(n)}{T} + \frac{|x-y|^2}{4T^2}.$$

Higher derivatives

To finish the discussion, let us give a comment on higher derivatives' estimates for the logarithmic heat kernel. In [22] the author applies repeatedly Itô's formula in order to express $\nabla^N \log H_t(x, y)$ in terms of lower derivatives. His argument uses essentially commutation relations for the canonical horizontal vector fields H_i , $1 \leq i \leq n$, and the canonical vertical vector fields which arise from the action of $O(n)$ on the fibers of $\pi : \mathcal{O}M \rightarrow M$ (the latter ones correspond simply to the canonical basis of $\mathfrak{o}(n)$). By the structure equations, the coefficients of the decomposition of the Lie brackets of these fields are either components of the Riemannian curvature tensor Ω or universal constants. Hence, following the argument in [22] it is readily seen that the claim therein may be refined as follows. Let M be an n -dimensional manifold of diameter D . For each $N \geq 2$ there exists a constant C depending on N , n and the L_∞ -norms of the covariant derivatives of Ω up to the order $N-1$,

$$C = C(N, n, \|\Omega\|_{L_\infty}, \|\nabla \Omega\|_{L_\infty}, \dots, \|\nabla^{N-1} \Omega\|_{L_\infty}),$$

such that

$$|\nabla^N \log H_t(x, y)| \leq C \left(\frac{D}{t} + \frac{1}{\sqrt{t}} \right)^N,$$

uniformly on $(0, 1] \times M \times M$.

3.4 Estimates of logarithmic derivatives of the heat kernel via J. M. Bismut's formula

This section is included for the sake of completeness. We present here another approach to gradient estimates of the logarithmic heat kernel which is due to D. Stroock [36]. As above, the manifold M under consideration is supposed stochastically complete (so that the Brownian motion on M does not blow up in finite time).

3.4.1 J. M. Bismut's formula

Here we derive *J. M. Bismut's* formula for the logarithmic gradient of the heat kernel. The interest of having such a representation is that it avoids differentiation on the right-hand side.

Recall that the heat equation can be written for differential forms, provided the Laplacian on functions is replaced with the Hodge-de Rham Laplacian, $\Delta_{HdR} := d^*d + dd^*$ where d is the exterior derivative and d^* is its formal adjoint. Hence, Δ_{HdR} commutes with d . The heat equation on forms then reads:

$$\begin{cases} \frac{\partial \theta}{\partial t} + \frac{1}{2} \Delta_{HdR} \theta = 0, & (t, x) \in (0, \infty) \times M; \\ \theta(0, x) = \theta_0(x), & x \in M. \end{cases} \quad (3.38)$$

The difference

$$\Delta_{HdR} - \nabla^* \nabla =: D^*(\Omega)$$

is a fibre-wise linear operator, $D^*(\Omega)$ being a linear functional of the curvature tensor Ω specified by the *Weitzenböck* formula. We will be concerned with the case of one-forms, when it equals Ric, according to the Bochner formula. As above, we denote by U_t the horizontal lift to $\mathcal{O}M$ of the Brownian motion X_t on M . Let M_t be the $\text{End}(\wedge^* \mathbb{R}^n)$ -valued multiplicative functional determined by

$$\frac{dM_t}{dt} = -\frac{1}{2} M_t \widetilde{D^*(\Omega)}(U_t), \quad M_0 = I_n \text{ (the identity matrix).}$$

The solution to the initial problem (3.38) is given by the Feynman-Kac formula. One gets

$$\theta(t, x) = \mathbb{E}_x(U_0 M_t U_t^{-1} \theta_0(X_t)). \quad (3.39)$$

When there is no confusion, we will drop U_0 from the notation, keeping in mind the identification between $T_x M$ and \mathbb{R}^n , realized by U_0 .

Let us define the action of the heat semi-group on differential forms as $P_t = e^{-\Delta_{HdR} t/2}$. Then $P_t(df)(x)$ is the solution of (3.38) with the initial condition $\theta(0, x) = df(x)$. Since P_t commutes with d , we arrive at the following theorem (a particular case of (3.39)):

Theorem 3.16. *Let X be the Brownian motion on M starting from x and U be its horizontal lift starting from U_0 . Define a multiplicative functional M by*

$$\frac{dM_s}{ds} + \frac{1}{2} M_s \text{Ric}_{U_s} = 0, \quad M_0 = I, \quad (3.40)$$

where $\text{Ric}_u \in \text{End}(\mathbb{R}^n)$ is the Ricci transform at $u \in \mathcal{O}M$. For $f \in C^\infty(M)$ we have

$$\nabla P_T f(x) = \mathbb{E}_x(M_T U_T^{-1} \nabla f(X_T)).$$

The statement of this theorem results essentially from the fact that

$$N_s := M_s \nabla^H P_{T-s} f(\pi U_s) = M_s U_s^{-1} \nabla P_{T-s} f(\pi U_s)$$

is a martingale on $\{0 \leq s \leq T\}$.

Now consider the *Cameron-Martin* space \mathcal{H} . It consists of absolutely continuous paths $[0, T] \rightarrow \mathbb{R}^n$ which start at the origin, such that \dot{h} is square-integrable, and is equipped with the norm

$$|h|_{\mathcal{H}} = \left(\int_0^T |\dot{h}_s|^2 ds \right)^{1/2}.$$

Theorem 3.17. *Let M be a compact Riemannian manifold and let X , U and W be a Brownian motion on M , its horizontal lift and its anti-development, respectively. Let $\{h_s\}$ be an adapted process with sample paths in \mathcal{H} such that $\mathbb{E}|h|_{\mathcal{H}}^2 < \infty$. Then for any $f \in C^\infty(M)$ we have*

$$\mathbb{E}\langle \nabla f(X_T), U_T h_T \rangle = \mathbb{E} \left[f(X_T) \int_0^T \left\langle \dot{h}_s + \frac{1}{2} \text{Ric}_{U_s} h_s, dW_s \right\rangle \right].$$

For a smooth path $\theta \in C^\infty([0, \infty), \mathbb{R}^n)$ take $h_s = M_s^\dagger \theta_s$ where M_s^\dagger is the transpose of M_s defined by (3.40). Applying successively Theorem 3.16 to pass the gradient through the heat kernel and Theorem 3.17 with $h_s = M_s^\dagger \theta_s$ to get rid of the gradient on the right-hand side, one gets *J. M. Bismut's formula*:

$$U_0 \theta_T \cdot P_T f(x) - U_0 \theta_0 \cdot P_T f(x) = \mathbb{E}_x \left\{ f(X_T) \int_0^T \left\langle M_s^\dagger \dot{\theta}_s, dW_s \right\rangle \right\}. \quad (3.41)$$

In particular, if $\theta_s = (s/T)e$, for some element $e \in \mathbb{R}^n$, (3.41) becomes

$$\nabla P_T f(x) = \frac{1}{T} \mathbb{E}_x \left\{ f(X_T) \int_0^T M_s dW_s \right\}.$$

This equality can be rewritten as

$$\int_M \nabla_x H_T(x, y) f(y) dy = \int_M \left[\frac{1}{T} \mathbb{E}_{x, y, T} \int_0^T M_s dW_s \right] H_T(x, y) f(y) dy,$$

where $\mathbb{E}_{x, y, T}$ stands for the expectation under the Brownian bridge law. The latter equality entails another version of J. M. Bismut's formula:

$$\nabla_x \log H_T(x, y) = \frac{1}{T} \mathbb{E}_{x, y, T} \int_0^T M_s dW_s.$$

3.4.2 D. Stroock's proof of the logarithmic gradient estimate

The idea is to apply J. M. Bismut's formula to get a bound on $|\nabla \log P_T f|$ and then take $f(x) = H_T(x, y)$.

As above, M is assumed compact with $\text{Ric}(M) \geq -R$, $R \geq 0$. To start with, we will separate the stochastic integral involved into J. M. Bismut's formula (3.41),

$$\int_0^T \left\langle M_s^\dagger \dot{\theta}_s, dW_s \right\rangle,$$

and $f(X_T)$, under the expectation. Let us take θ_s such that $\theta_0 = 0$ and $\theta_T = \theta$. By Jensen's inequality, for each $\alpha \in \mathbb{R}$ and a positive function f ,

$$\alpha(U_0 \theta \cdot \log P_T f(x)) \leq \mathbb{E}_x \left[\frac{f(X_T)}{P_T f(x)} \log \frac{f(X_T)}{P_T f(x)} \right] + \log \mathbb{E}_x \left[\exp \left(\alpha \int_0^T \left\langle M_s^\dagger \dot{\theta}_s, dW_s \right\rangle \right) \right] \quad (3.42)$$

The second term on the right-hand side can be dealt with as follows. Consider the exponential local martingale, associated with $\int \langle M_s^\dagger \dot{\theta}_s, dW_s \rangle$:

$$\exp \left(\alpha \int_0^T \langle M_s^\dagger \dot{\theta}_s, dW_s \rangle - \frac{\alpha^2}{2} \int_0^T |M_s^\dagger \dot{\theta}_s|^2 ds \right).$$

Under the assumption on $\text{Ric}(M)$ we can apply Gronwall's lemma to M_s and thereby obtain

$$\log \mathbb{E}_x \left[\exp \left(\alpha \int_0^T \langle M_s^\dagger \dot{\theta}_s, dW_s \rangle \right) \right] \leq \frac{\alpha^2}{2} \int_0^T e^{Rs} |\dot{\theta}_s|^2 ds. \quad (3.43)$$

Now plug (3.43) into (3.42) and minimize first with respect to $(\theta_s)_{0 \leq s \leq T}$ subject to boundary conditions, and then with respect to $\alpha > 0$. Thus we arrive at the following estimate.

Theorem 3.18 (D. Stroock, [36]). *Let M be a compact manifold with $\text{Ric}(M) \geq -R$, $R \geq 0$. Set*

$$\beta(s) = \frac{s}{e^s - 1} (\equiv 1 \text{ when } s = 0).$$

Then, for each $f \in C^1(M, \mathbb{R}_+^*)$,

$$|\nabla \log P_T f|^2(x) \leq \frac{2\beta(-RT)^2}{T} \log \frac{\|f\|_\infty}{P_T f(x)}. \quad (3.44)$$

It is instructive to compare (3.44) with (3.29). There we have obtained an estimate on the logarithmic gradient of the heat kernel in terms of the expectation of the logarithmic ratio on the right-hand side. Here we have, for an arbitrary function, the L_∞ -norm on the right-hand side. So, for the heat kernel, the estimate in (3.28) is sharper (modulo the factors which are functions of T). However, further this sharpness is not taken advantage of. So, morally, for the purpose of estimating the logarithmic derivatives, both estimates are equivalent. As we will see now, D. Stroock treats his estimate in a more keen manner that avoids imposing the additional non-collapsing condition.

Thus, he aims at proving the gradient estimate for $\log H_T(x, y)$, i.e. he wants to show (very much like what we have done in the previous section) that *there exists a constant $C = C(R, n)$ such that*

$$|\nabla \log H_T(x, y)| \leq C(R, n) \left(\frac{d(x, y)}{T} + \frac{1}{\sqrt{T}} \right),$$

uniformly on $(0, 1] \times M \times M$. To this end, take $f(x) = H_T(x, y)$ and write

$$\frac{H_T(z, y)}{H_{2T}(x, y)} = \frac{H_T(z, y)}{H_T(y, y)} \frac{H_T(y, y)}{H_{2T}(x, y)}.$$

By Theorem 2.11, for each $\alpha > 1$,

$$\frac{H_T(y, y)}{H_{2T}(x, y)} \leq C(R, n, \alpha) \exp \left(\frac{\alpha d^2(x, y)}{4T} \right), \quad (T, x, y) \in (0, 1] \times M \times M,$$

where $C(R, n, \alpha)$ is a constant with indicated dependencies. Thus, given Theorem 3.18, all it remains to show, is that $H_T(z, y)/H_T(y, y)$ is uniformly bounded by a constant with required dependencies. By Theorem 2.15, for each $0 < \varepsilon < 1$,

$$H_T(z, y) \leq C(R, n, \varepsilon) \text{Vol}^{-1/2}(B_z(\sqrt{T})) \text{Vol}^{-1/2}(B_y(\sqrt{T})) \exp\left(-\frac{d^2(z, y)}{(4 + \varepsilon)T}\right)$$

on $(0, 1] \times M \times M$. It remains to estimate $H_T(y, y)$ from below. We will need the following lemma [36, Theorem 8.62].

Lemma 3.19. *Let M be a connected, complete, n -dimensional manifold with $\text{Ric}(M) \geq -R$ for some $R \in \mathbb{R}$. Let X be a Brownian motion on M starting at x . Then for every $\varepsilon \in (0, 1)$, $(T, x) \in (0, \infty) \times M$, and $K > 0$,*

$$\mathbb{P}_x\left(\sup_{t \in [0, T]} d(x, X_t) \geq K\right) \leq 2(1 - \varepsilon)^{-1/2} \exp\left[\varepsilon\left(-\frac{K^2}{2T} + \frac{4n + \max\{R, 0\}n^2T}{2(1 - \varepsilon)}\right)\right].$$

Using this Lemma, choose $\beta \in [1, \infty)$, depending only on R and n , so that

$$\mathbb{P}_y\left(d(X_{T/2}, y) \geq \beta\sqrt{T}\right) \leq \frac{1}{2}, \quad \text{for all } (T, y) \in (0, 1] \times M.$$

In particular, with this choice of β , we have

$$\begin{aligned} H_T(y, y) &= \int_M H_{T/2}(y, z) H_{T/2}(z, y) dz \geq \int_{B_y(\beta\sqrt{T})} H_{T/2}(y, z)^2 dz \\ &\geq \frac{1}{\text{Vol}(B_y(\beta\sqrt{T}))} \left(\int_{B_y(\beta\sqrt{T})} H_{T/2}(y, z) dz \right)^2 \geq \frac{1}{4\text{Vol}(B_y(\beta\sqrt{T}))}. \end{aligned}$$

Now, the required universal bound for $H_T(z, y)/H_T(y, y)$ follows using the Bishop-Gromov volume comparison theorem. Summarizing, we have proved the following theorem, of which the gradient estimate for the logarithmic heat kernel is an immediate consequence.

Theorem 3.20 (D. Stroock, [36]). *Let M be a compact manifold with $\text{Ric}(M) \geq -R$, $R \geq 0$. Then*

$$\log \frac{\|H_T(\cdot, y)\|_\infty}{H_{2T}(x, y)} \leq C(R, n) \left(1 + \frac{d^2(x, y)}{T}\right), \quad \text{for all } (T, x, y) \in (0, 1] \times M \times M.$$

The case of higher derivatives is treated in [35] by a method of *backward* and *forward* perturbations of Brownian paths on a manifold.

Chapter 4

Convergence under measured Gromov-Hausdorff limits

This not so long chapter deals with the heat kernel convergence under the measured Gromov-Hausdorff limits for manifolds with bounded Ricci curvature and diameter. A heuristic evidence of why it should seem plausible stems from the results of Chapter 3 where it has been shown that the gradient of the (renormalized¹) heat kernel on such a manifold is uniformly bounded for $t \geq t_0 > 0$. Thus, an Arzela-Ascoli argument should enable one to extract of each sequence of manifolds, with uniformly bounded Ricci curvature and diameter, a subsequence with uniformly convergent heat kernels.

There are however two major obstacles for the implementation of this program: first, the limit space is not necessarily a manifold and therefore it's not quite clear at a first glance what the heat kernel on it is. Second, we are forced to compare functions defined a priori on different spaces.

Fortunately it turns out that these difficulties may be successfully surmounted, and (less fortunately) even more so: the gradient estimates derived in the previous Chapter are *not* indispensable to conclude on the convergence of heat kernels.

The existence of the Laplacian on the limit space is guaranteed by the results of J. Cheeger and T. H. Colding on the structure of limit spaces of manifolds with bounded Ricci curvature [8]. As far as the comparison of Lipschitz functions on different spaces is concerned, an appropriate procedure of transplantation was developed by J. Cheeger in [7] (cf. especially Lemma 10.7 therein). Putting together this stuff with the gradient estimates from [10] for the Laplacian eigenfunctions provides a concise and economic way to prove the heat kernel convergence claimed for above.

As a consequence, we consider an application to the convergence of Graph Field Theories associated with the underlying manifolds.

¹One should beware of the situation which occurs as the volume of a manifold shrinks to 0, since in that case $H_t(x, y)$ becomes arbitrarily big in order to satisfy the heat conservation property, that is $\int_M H_t(x, y) dy = 1$. Such a possibility is excluded by considering the renormalized heat kernel which is a heat kernel times $Vol(M)$.

4.1 Heat kernel convergence under measured Gromov-Hausdorff limits for manifolds with bounded Ricci curvature and diameter

Consider a sequence of compact n -dimensional Riemannian manifolds (M_i) endowed with their Riemannian measures $Vol_i(\cdot)$; from now on, we shall consider them as endowed with the renormalized probability measures, defined as:

$$\underline{Vol}_i(\cdot) := Vol_i^{-1}(M_i)Vol_i(\cdot),$$

We assume that M_i have definite bounds on Ricci curvature which will be greater (after rescaling) than $-(n-1)$. The Bishop-Gromov relative volume comparison theorem implies then that Riemannian volume measures $\mu = Vol_i$ satisfy the doubling condition, i.e., for each $z \in M_i$,

$$\mu(B_{2r}(z)) \leq 2^\kappa \mu(B_r(z)), \quad (4.1)$$

which holds for all $0 < r \leq R$ with $\kappa = \kappa(R, n)$ uniformly in i . Thus, by [7, Th. 9.1], there exists a limit space, (Z, d, μ) , with μ a Radon measure satisfying (4.1) with the same κ , such that for some subsequence,

$$(M_j, d_j, \underline{Vol}_j) \xrightarrow{mGH} (Z, d, \mu). \quad (4.2)$$

Here d_j is the Riemannian distance and mGH stands for the measured Gromov-Hausdorff convergence in the following sense: it is the usual GH convergence with an additional requirement that for all $M_j \ni \bar{m}_j \rightarrow \bar{z} \in Z$ and all $r > 0$,

$$\underline{Vol}_j(B_r(\bar{m}_j)) \rightarrow \mu(B_r(\bar{z})).$$

Let us note that when the limit space (Z, d, μ) is a Riemannian manifold of the same dimension, n , the volume convergence had been previously established by T. H. Colding.

On the limit space, consider the following bilinear form on Lipschitz functions:

$$\int_Z \langle df_1, df_2 \rangle d\mu. \quad (4.3)$$

It is a Dirichlet form in the sense of Kato. The unique positive self-adjoint operator associated to its minimal closure is referred to as a (generalized) Laplacian [8], and will be denoted by Δ .

If $\text{diam}(Z) < \infty$, (we always suppose Z complete), $(I + \Delta)^{-1}$ is a compact operator. Hence, the spectrum of Δ is a discrete subset in \mathbb{R}_+ ,

$$\{0 \leq \lambda_1 \leq \lambda_2 \leq \dots\},$$

where the eigenvalues are counted according to their multiplicities.

Let us fix a Gromov-Hausdorff approximation $\psi_j : Z \rightarrow M_j$ for each j , i.e.,

$$\text{dis}(\psi_j) := \sup |d(\psi_j(x), \psi_j(y)) - d(x, y)| < \epsilon_j$$

and M_j is contained in the ϵ_j -neighborhood of $\psi_j(Z)$, with $\epsilon_j \rightarrow 0$. From now on, these maps will be implicitly understood without special mention. Thus, if $x \in M_j$, $y \in Z$, we will write \bar{x}, \bar{y} for $d(x, \psi_j(y))$ and \bar{f}, \bar{g} for $|f \circ \psi_j - g|_{L^\infty}$, where f and g are continuous functions on M_j and Z .

Theorem 4.1 (J. Cheeger-T. H. Colding). *It is proved in [8] that under the above conditions, that is, if*

$$\text{Ric}(M_j^n) \geq -(n-1), \quad (4.4)$$

and

$$\text{diam}(Z) < \infty,$$

the Laplacian spectrum as well as the eigenfunctions is continuous under the measured Gromov-Hausdorff convergence. Specifically, let $\{\lambda_{k,j}\}$ be the eigenvalues of Δ^{M_j} arranged in nondecreasing order. Then

$$\lambda_{k,j} \xrightarrow{j \rightarrow \infty} \lambda_k.$$

Furthermore, given an orthonormal basis $\{f_k\}$ of eigenfunctions on Z , there exist orthonormal bases $\{f_{k,j}\}$ of eigenfunctions on M_j such that $\overline{f_{k,j}, f_k} \xrightarrow{j \rightarrow \infty} 0$.

Although the limit spaces are not smooth manifolds in general, their structure is "nice" enough to enable a good portion of calculus. Let us briefly outline the notions in terms of which (Z, μ) can be described. It is shown in [8] that under the assumption (4.4), the limit space (Z, μ) is in fact μ -rectifiable. It means, by definition, that there exists an integer m , a countable collection of Borel sets, $C_{k,i} \subset Z$, where $k \leq m$ and bi-Lipschitz maps, $\phi_{k,i} : C_{k,i} \rightarrow \phi_{k,i}(C_{k,i}) \subset \mathbb{R}^k$, such that

$$(i) \quad \mu(Z \setminus \cup_{k,i} C_{k,i}) = 0,$$

$$(ii) \quad \mu \text{ is Ahlfors } k\text{-regular at } x, \text{ for all } x \in C_{k,i}, \text{ i.e., there exists a constant } K = K(x), \text{ such that for } r \leq 1,$$

$$K^{-1}r^k \leq \mu(B_r(x)) \leq Kr^k.$$

Moreover, the covering subsets $C_{k,i}$ can be chosen so that the Lipschitz constant of the atlas maps $\phi_{k,i}$ be arbitrarily close to 1:

$$(iii) \quad \text{For all } x \in \cup_{k,i} C_{k,i} \text{ and all } \lambda > 0, \text{ there exists } C_{k,i} \text{ such that } x \in C_{k,i} \text{ and the map } \phi_{k,i} : C_{k,i} \rightarrow \phi_{k,i}(C_{k,i}) \subset \mathbb{R}^k \text{ is } e^{\pm\lambda}\text{-bi-Lipschitz.}$$

The existence of the Laplacian on the limit space follows from the closability of the bilinear form (4.3). By the condition (iii) above, (4.3) is correctly defined. The conditions which guarantee its closability on a μ -rectifiable space are the doubling measure condition (4.1) and the Poincaré inequality [8, Thms 6.7, 6.25]. As for the first one, it passes to the measured Gromov-Hausdorff limit of Ricci-bounded manifolds. The Poincaré inequality is the consequence of the segment inequality [8, p. 45]. The latter is verified on Ricci-bounded manifolds and is stable under Gromov-Hausdorff limits.

Consider the renormalized heat kernel on M_j :

$$H_t^j(x, y) = \sum_k e^{-\lambda_{k,j}t} f_{k,j}(x) f_{k,j}(y),$$

where $|f_{k,j}|_{L_2(M_j, \text{Vol}_j)} = 1$. From the Harnack inequality for manifolds with bounded Ricci curvature [27, 4], H^j are uniformly bounded for $t \geq t_0$. For a fixed t , Theorem 3.5 implies that $\log H^j$ are equicontinuous in spacial variables.

We will use the S. Y. Cheng-S. T. Yau [10, Th. 6] gradient estimate², a variant of which can be formulated as follows:

Theorem 4.2 (S. Y. Cheng-S. T. Yau). *Let $\text{Ric}(M^n) \geq -R$, $R \geq 0$ and $\text{diam}(M^n) \leq D$. There exists a constant α_n depending only on n such that if $\Delta f = \lambda f$,*

$$|\nabla f(x)| \leq \alpha_n (f(x) + |f|_{L_\infty}) \max\{\sqrt{\lambda}, \sqrt{R} + D^{-1}\}.$$

From now on, $\alpha_n(R, D)$ will denote a constant depending on n, R, D , the explicit value of which may vary from time to time. The subscript L_2 refers to the $L_2(M^n, \text{Vol})$ space.

Lemma 4.3. *Let f be an eigenfunction of Δ with $\Delta f = \lambda f$. Then there exists a constant $\alpha_n(R, D)$ such that $|f|_{L_\infty} \leq \alpha_n(R, D) \left(\max\{\sqrt{\lambda}, \sqrt{R} + D^{-1}\}\right)^{n/2} |f|_{L_2}$. (Recall that the L_2 -norm is taken with respect to renormalized measure.)*

Remark 4.4. This fact, as well as the first inequality in the forthcoming corollary, had been independently proved by S. Gallot.

Proof. Suppose that $R > 0$. Choose x , where $|f(x)| = |f|_{L_\infty}$. Then, by Cheng-Yau's Theorem, $|\nabla f(x)| \leq C|f|_{L_\infty}$ with $C = 2\alpha_n \max\{\sqrt{\lambda}, \sqrt{R} + D^{-1}\}$. Hence, $f(x) \geq \frac{|f|_{L_\infty}}{2}$ on $B_{\frac{1}{2C}}(x)$. Integrating, we get

$$|f|_{L_2}^2 \geq \frac{|f|_{L_\infty}^2 \text{Vol}\left(B_{\frac{1}{2C}}(x)\right)}{4}.$$

By the relative volume comparison theorem, the latter volume is greater than $\alpha_n C^{-n} R^n \times \exp(-\sqrt{R}(n-1)D)$. Hence

$$|f|_{L_\infty} \leq \alpha_n e^{\sqrt{R}(n-1)D/2} R^{-n/2} \left(\max\{\sqrt{\lambda}, \sqrt{R} + D^{-1}\}\right)^{n/2} |f|_{L_2},$$

which suffices to conclude. In the case $R = 0$, the volumes of balls in M are compared with the volumes of Euclidean balls. Correspondingly, $e^{\sqrt{R}(n-1)D} R^{-n}$ should be replaced with D^n . \square

Corollary 4.5. *For k_0 large enough, the remainder term for the renormalized heat kernel H may be controlled as follows:*

$$\left| \sum_{k \geq k_0} e^{-\lambda_k t} f_k(x) f_k(y) \right| \leq \alpha_n(R, D) \sum_{k \geq k_0} e^{-\lambda_k t} \lambda_k^{n/2}, \quad (4.5)$$

and a similar estimate holds for the gradient of H :

$$\left| \nabla_x \left(\sum_{k \geq k_0} e^{-\lambda_k t} f_k(x) f_k(y) \right) \right| \leq \alpha_n(R, D) \sum_{k \geq k_0} e^{-\lambda_k t} \lambda_k^{(n+1)/2}. \quad (4.6)$$

²the inequality in the statement of Theorem 6 in [10] is not quite correct, since non-homogeneous, it is rectified below for the case we need.

The Weyl asymptotic formula shows that λ_k 's grow like $k^{2/n}$. The lower bound for λ_k is due to P. Li and S. T. Yau [26] (cf. also [20, Appendix 3] and [27, Theorem 5.3]), where the authors also found upper bounds for the gradient of the Laplacian eigenfunctions as optimal powers of the corresponding eigenvalues:

$$\lambda_k \geq D^{-2} \alpha_n^{1+D} \sqrt{\frac{R}{n-1}} k^{2/n}. \quad (4.7)$$

Thus, the right-hand sides in (4.5),(4.6) are bounded by some $\varphi(k_0, t) \xrightarrow{k_0 \rightarrow \infty} 0$ uniformly in $t \geq t_0 > 0$, n , D , R being fixed.

Proposition 4.6. *Under measured Gromov-Hausdorff convergence (4.2) for manifolds with bounded Ricci curvature and diameter, their renormalized heat kernels converge uniformly in $[t_0, \infty) \times Z \times Z$ to the generalized Δ -kernel $H_t(x, y)$, i.e.,*

$$\overline{H^j, H} := \sup_{(t,x,y) \in [t_0, \infty) \times Z \times Z} |H_t^j(\psi_j(x), \psi_j(y)) - H_t(x, y)| \rightarrow 0.$$

Proof. We will use the notations from J. Cheeger and T. H. Colding's theorem. Since $\overline{f_{k,j}, f_k} \xrightarrow{j \rightarrow \infty} 0$ and $\lambda_{k,j} \xrightarrow{j \rightarrow \infty} \lambda_k$, the inequality in Lemma 4.3 passes to the limit when $j \rightarrow \infty$. Also, (4.7) holds for the eigenvalues of the generalized Laplacian Δ on Z . Fix an arbitrary small $\epsilon > 0$. Take k_0 such that the right hand side in (4.5) is smaller than $\epsilon/3$ for $t \geq t_0$. Then take j_0 such that when $j \geq j_0$

$$\sum_{k < k_0} \overline{e^{-\lambda_{k,j}t} f_{k,j}(x) f_{k,j}(y), e^{-\lambda_k t} f_k(x) f_k(y)} \leq \epsilon/3,$$

by J. Cheeger-T. H. Colding Theorem. Thus, for $j \geq j_0$, we have

$$\overline{H^j, H} \leq \epsilon.$$

□

4.2 Compactness of the moduli space of Graph Field Theories

This somewhat speculative section aims at establishing the (pre)-compactness of the moduli space of Graph Field Theories associated with manifolds of bounded Ricci curvature and diameter and their measured Gromov-Hausdorff limits.

A Graph Field Theory (GFT) is defined in the spirit common for all Field Theories, that is, as a functor from a suitable category of metric graphs to the category of tensor powers of a certain Hilbert space \mathcal{H} . Consider a metric graph Γ , i.e. a graph whose edges are labelled with (non-negative) lengths t_i . Suppose further that there is a number of *entering*, say $\{in_1, \dots, in_k\}$, and a number of *exiting*, say $\{out_1, \dots, out_l\}$, vertices (these subsets are disjoint and generally do not cover the set of all vertices, the rest of them being denoted by $(x_t)_t$). To Γ is associated an operator Φ_Γ :

$$\Phi_\Gamma: \mathcal{H}^{\otimes k} \longrightarrow \mathcal{H}^{\otimes l},$$

which is assumed to be trace class, in such a way that

- if Γ is a disjoint union of Γ' et Γ'' , then

$$\Phi_\Gamma = \Phi_{\Gamma'} \otimes \Phi_{\Gamma''};$$

- if Γ is obtained from Γ' by gluing of an entering and an exiting vertex, in_i and out_j , then

$$\Phi_\Gamma = tr_{i,j} \Phi_{\Gamma'},$$

where $tr_{i,j}$ denotes the partial trace in the \mathcal{H} factors corresponding to i and j .

To each compact Riemannian manifold (M, g) corresponds a GFT with operators Φ_Γ defined in terms of the renormalized heat kernel of M . Specifically, let $\mathcal{H} = L^2(M, g)$, $H_t(x, y)$ be the renormalized heat kernel (i.e. the heat kernel times $Vol(M)$) on M and define for each Γ as above,

$$(\Phi_\Gamma f)(out_1, \dots, out_l) = \int_M f(in_1, \dots, in_k) \prod_{\substack{\text{over all} \\ \text{edges } t_i \text{ of } \Gamma}} H_{t_i}(x_{i_1}, x_{i_2}) \prod_r d in_r \prod_t d x_t,$$

where in_r stand for the entering vertices, x_t for the inner (neither entering nor exiting) vertices (cf. above), and for each edge t_i , x_{i_1} and x_{i_2} denote its ends. In the trivial case of a one-edged graph Φ is given merely by the action of the heat semigroup.

It was suggested by M. Kontsevich [24] that GFT can be considered as boundary points of the moduli spaces of Conformal Field Theories (CFT) under certain degenerations. In order to give a hint of the qualitative picture of this convergence, let us briefly sketch some definitions setting a CFT and reproduce some (however far from being rigorous) arguments from [24].

There is an axiomatic approach to the definition of CFT [16] proposed by Segal. Let (Σ, γ) be a Riemann surface (connected or disconnected) with the boundary composed of the connected components \mathcal{C}_i , $i \in I$. Each \mathcal{C}_i will be parameterized in a real analytic way by the standard unit circle $S^1 \subset \mathbb{C}$. The components \mathcal{C}_i may be divided into "in" and "out" ones, depending on whether the parametrization disagrees or agrees with the orientation of \mathcal{C}_i inherited from Σ . This induces a splitting $I = I_{in} \cup I_{out}$ of the set of indices.

To Σ with parameterized boundary, we may uniquely assign a compact surface $\hat{\Sigma}$ without a boundary by gluing a copy of the disc $D = \{|z| \leq 1\} \subset \mathbb{C}P^1$ to each "in" boundary component and a copy of the disc $D' = \{|z| \geq 1\} \subset \mathbb{C}P^1$ to each "out" boundary component. Conversely, given a closed Riemann surface $\hat{\Sigma}$ with holomorphically embedded disjoint discs D and D' , by removing their interiors we obtain the surface Σ with boundary parameterized by the standard circles $\{|z| = 1\}$. We shall always assume the metric γ flat at the boundary, i.e. of the form $|z|^{-2}|dz|^2$ in the local holomorphic coordinate around \mathcal{C}_i extending its parametrization. With this convention, the metrics on D and D' glue smoothly with γ to the metric on $\hat{\Sigma}$.

We shall postulate that to each (Σ, γ) is associated an operator $A_{\Sigma, \gamma}$ mapping the tensor products of the CFT Hilbert spaces associated to the boundary components of Σ . $A_{\Sigma, \gamma}$ satisfies, in particular, the following axioms (cf. the axioms for GFT):

- For each compact Riemann surface (Σ, γ) (with parameterized boundary or without boundary, connected or disconnected) the operator³

$$A_{\Sigma, \gamma}: \bigotimes_{i \in I_{in}} \mathcal{H} \longrightarrow \bigotimes_{i \in I_{out}} \mathcal{H},$$

is assumed trace class. The operators $A_{\Sigma, \gamma}$ encode the information contained in the operator product expansion (OPE).

- If Σ is a disjoint union of Σ' and Σ'' , then

$$A_{\Sigma, \gamma} = A_{\Sigma', \gamma} \otimes A_{\Sigma'', \gamma}.$$

- If Σ' is obtained from Σ by gluing of the \mathcal{C}_{i_0} and \mathcal{C}_{i_1} boundary components then

$$A_{\Sigma', \gamma} = tr_{i_0, i_1} A_{\Sigma, \gamma},$$

where tr_{i_0, i_1} denotes the partial trace in the \mathcal{H} factors corresponding to \mathcal{C}_{i_0} and \mathcal{C}_{i_1} .

- For any function σ on Σ vanishing around the boundary

$$A_{\Sigma, e^{\sigma} \gamma} = e^{\frac{c}{96\pi} (|\partial\sigma|_{L^2}^2 + 4 \int_{\Sigma} \sigma r dv)} A_{\Sigma, \gamma},$$

where r is the *scalar curvature* and c is a non-negative constant called *central charge* (cf. the definition of the Virasoro algebra below).

Alternatively, a (unitary two-dimensional) Conformal Field Theory (CFT) is specified, in particular, by the following data:

- A bi-graded complex pre-Hilbert space of states $\mathcal{H} = \bigoplus_{\substack{p, q \in \mathbb{R}_+ \\ p - q \in \mathbb{Z}}} \mathcal{H}^{p, q}$ with an action of two

commuting copies of the *Virasoro algebra* $Vir \times \overline{Vir}$ such that $\mathcal{H}^{p, q}$ is the eigenspace of the L_0 (resp. \overline{L}_0) generator with the eigenvalue p (resp. q). Recall that the Virasoro algebra is generated by L_i , $i \in \mathbb{Z}$ and has the following commutation relations:

$$[L_m, L_n] = (m - n)L_{m+n} + \frac{c}{12}(m^3 - m)\delta_{m+n, 0},$$

where c is the central charge. It is a central extension of the Lie algebra of vector fields on a circle.

- An anti-linear involution $*$ on \mathcal{H} , often called *charge conjugation*, which commutes with the action of Vir and \overline{Vir} .
- L_n is adjoint to L_{-n} , i.e. $\forall \phi, \psi \in \mathcal{H}$, $\langle \phi, L_n \psi \rangle = \langle L_{-n} \phi, \psi \rangle$, and similarly for \overline{L}_n .
- A *growth condition* on the dimension of eigenspaces $\mathcal{H}^{p, q}$: there exist $\nu \in \mathbb{R}_+$ and $V \in \mathbb{R}_+$ such that

$$\infty > \dim \left(\bigoplus_{(p+q)^\nu \leq E} \mathcal{H}^{p, q} \right) \stackrel{E \rightarrow \infty}{\sim} \exp(V\sqrt{E}).$$

³the empty tensor product should be interpreted as \mathbb{C}

- The space \mathcal{H} carries some additional structures derived from the operator product expansion (OPE). They satisfy a list of axioms which we will not discuss here.

A CFT is called *irreducible* if $\mathcal{H}^{0,0}$ is one-dimensional. Let $\phi \in \mathcal{H}^{p,q}$. Then the number $p+q$ is called the *energy* (or the *conformal dimension*) of ϕ , and $p-q$ is called the *spin* of ϕ . Notice that, since the spin is an integer number, the condition $p+q < 1$ implies $p=q$. Let us fix $c_0 \geq 0$ and $E > 0$, and consider the moduli space $\mathcal{M}_{c \leq c_0}^E$ of all irreducible CFTs with central charge $c \leq c_0$ and

$$E_{min} := \min\{p+q > 0 \mid \mathcal{H}^{p,q} \neq 0\} \geq E.$$

It is expected that $\mathcal{M}_{c \leq c_0}^E$ is a *compact* real analytic stack of finite local dimension. Define

$$\mathcal{M}_{c \leq c_0} = \bigcup_{E>0} \mathcal{M}_{c \leq c_0}^E.$$

One would like to compactify this space by adding boundary components corresponding to certain asymptotic degenerations of the theories with $E \rightarrow 0$. This presumes the definition of topological data on the families of CFTs under consideration. The following definition is proposed in [32]. A CFT-space is given by the following data: a sheaf \mathcal{S} over a topological Hausdorff space \mathcal{M} , such that for each $p \in \mathcal{M}$, \mathcal{C}_p is a CFT with associated pre-Hilbert space $\mathcal{H}_p := \mathcal{S}_p$. Furthermore, all CFT-structures as e.g. OPE-coefficients, evaluated on local sections of \mathcal{S} , are continuous.

Since $(L_1)^* = L_{-1}$, the relation $2L_0 = [(L_1)^*, L_1]$ shows that L_0 is positive semi-definite, and similarly for \bar{L}_0 . Thus $H := L_0 + \bar{L}_0$ is a self-adjoint positive semi-definite operator.

The information contained in the definition of a CFT can be partially reformulated in the language of non-commutative geometry à la Connes [32]. Namely, given a CFT, say \mathcal{C} , one can associate with it a triple $(\tilde{\mathbb{H}}, H, \tilde{\mathcal{A}})$, where $\tilde{\mathbb{H}} \subset \mathcal{H}$ is a complex pre-Hilbert space that should be thought of as a space of square integrable functions over some Riemannian manifold M , $H := L_0 + \bar{L}_0$ is the self-adjoint positive semi-definite Hamiltonian on $\tilde{\mathbb{H}}$ and $\tilde{\mathcal{A}}$ is an algebra of operators acting on $\tilde{\mathbb{H}}$ that should be thought of as an algebra of smooth functions on M . Moreover, the eigenspaces of H have the following growth behavior: if ν is the constant in the growth condition from the definition of CFT,

$$N(E) := \dim_{\mathbb{C}} \left(\bigoplus_{\lambda \leq E} \{\phi \in \tilde{\mathbb{H}} \mid H\phi = \lambda\phi\} \right) \stackrel{E \rightarrow \infty}{\simeq} V E^{\nu/2},$$

for some $V \in \mathbb{R}$.

Generally speaking, $\tilde{\mathcal{A}}$ is non-commutative. Let c be the central charge of the CFT \mathcal{C} . Suppose there is a subspace $\mathbb{H} \subset \tilde{\mathbb{H}}$, such that the restriction $\mathcal{A} := \tilde{\mathcal{A}}|_{\mathbb{H}}$ is commutative. If there are appropriate completions $\bar{\mathbb{H}}, \bar{\mathcal{A}}$ of \mathbb{H}, \mathcal{A} such that $\bar{\mathbb{H}} = L^2(M, Vol_g)$, $H = \frac{1}{2}\Delta_{\bar{g}}$, $\bar{\mathcal{A}} = C^\infty(M)$ for some Riemannian manifold (M, g) of dimension c and $Vol_g = e^{2\Psi} Vol_{\bar{g}}$, $\Psi \in C^\infty(M)$, then $(\mathbb{H}, H, \mathcal{A})$ is called a *geometric interpretation* of \mathcal{C} .

It is argued that $\mathcal{H}^{0,0} \simeq \mathbb{C}$ (i.e. \mathcal{C} is irreducible) if and only if M is connected and that the minimal energy E_{min} is proportional to $\text{diam}(M)^{-2}$.

In order to compactify $\mathcal{M}_{c \leq c_0}$ consider degenerations of CFTs as $E_{min} \rightarrow 0$. A degeneration is given by a one-parameter (discrete or continuous) family \mathcal{H}_ε , $\varepsilon \rightarrow 0$ of bi-graded spaces

as above, where $(p, q) = (p(\varepsilon), q(\varepsilon))$. These spaces are equipped with OPEs. The subspace of fields with conformal dimension vanishing as $\varepsilon \rightarrow 0$ gives rise to a commutative algebra $\mathcal{H}^{small} = \bigoplus_{p(\varepsilon) \ll 1} \mathcal{H}_\varepsilon^{p(\varepsilon), p(\varepsilon)}$ (the algebra structure is given by the leading terms in OPEs). The spectrum X of \mathcal{H}^{small} is expected to be a compact space (manifold with singularities) such that $\dim X \leq c_0$. It follows from the conformal invariance and the OPE, that there is a second order differential operator defined on the smooth part of X with positive eigenvalues which is determined up to multiplication by a scalar. This implies that the smooth part of X carries a metric g_X , which is also defined up to a multiplication by a scalar. Other terms in OPEs give rise to additional differential-geometric structures on X .

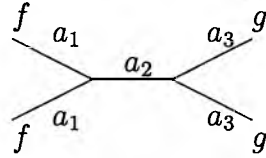
Thus, the degeneration of the family of CFTs is described by a boundary point of $\overline{\mathcal{M}}_{c \leq c_0}$ which is a triple $(X, \mathbb{R}_+^* \cdot g_X, \phi_X)$, where the metric g_X is defined up to a positive scalar factor, and $\phi_X: X \rightarrow \mathcal{M}_{c \leq c_0 - \dim X}$ is a map. Purely bosonic sigma-models correspond to the case when $c_0 = \dim X$ and the residual theories (those lying in the image of ϕ_X) are trivial.

Theorem 4.7 (M. Kontsevich). *Let $\mathcal{C}_n \in \mathcal{M}_{c \leq c_0}$ be a converging sequence of CFTs with $E_{min} \rightarrow 0$ such that*

$$\left(\mathcal{H}_n, \frac{L_0 + \bar{L}_0}{E_{min}} \right) \xrightarrow{E_{min} \rightarrow 0} (\mathcal{H}_\infty, L).$$

Let $(X, \mathbb{R}_+^ \cdot g_X, \phi_X)$ be the triple corresponding to the limit point of this sequence. Then the Segal operators $A_{\Sigma, \gamma}$ corresponding to \mathcal{C}_n converge to the GFT on X (the convergence is formulated in terms of the convergence of the correlation functions which information is encoded in the OPE). Moreover, $\text{Ric}(X) \geq 0$.*

Idea of proof. Consider the following graph $\Gamma(a_1, a_2, a_3)$ with four "in" vertices:



Let Φ_{a_1, a_2, a_3} be the Graph Field Theory operator corresponding to $\Gamma(a_1, a_2, a_3)$. Fix positive a_1, a_2, a_3 and define for any $f, g \in L^2(X, \text{vol}_{g_X})$ the function

$$\varphi(\lambda) := \Phi_{a_1 + \lambda, a_2 - \lambda, a_3}(f \otimes f \otimes g \otimes g) = \int_X (e^{\Delta a_3} g)^2 e^{\Delta(a_2 - \lambda)} ((e^{\Delta(a_1 + \lambda)} f)^2),$$

which is obtained by "unzipping" the graph. Using the *physical (Osterwalder-Schrader) positivity*, one can show that φ is convex at $\lambda = 0$, i.e., $\varphi''(0) \geq 0$. Since $a_i, i = 1, 2, 3$ and f, g are arbitrary, the latter condition is equivalent to

$$\left. \frac{\partial^2}{\partial \lambda^2} \right|_{\lambda=0} e^{-\Delta \lambda} (e^{\Delta \lambda} h)^2 \equiv \Gamma_2(h, h) \geq 0, \quad \forall h \in C^\infty(X),$$

with Γ_2 standing for the second carré du champ operator, which holds in turn if and only if $\text{Ric}(X) \geq 0$ [2, 37]. \square

A natural question which arises is whether the space of GFTs associated to compact manifolds with metric defined up to a scalar factor, with non-negative Ricci curvature, is

compact or not. Since the metric is defined up to a scalar factor, we can always suppose the diameter equal to 1. Let (M_j) be a sequence of manifolds converging to Z as in (4.2). From [8] (cf. the discussion before Theorem 4.1), there is a generalized Laplacian on the limit space Z and, hence, a GFT associated to Z .

Definition 4.8. *We will say that there is a convergence of Graph Field Theories corresponding to M_j and Z , and write $GFT(M_j) \longrightarrow GFT(Z)$, if for any metric graph Γ with k "in" vertices, any Lipschitz function f on $\underbrace{Z \times \cdots \times Z}_k$ and any sequence of Lipschitz functions (f_j) on $\underbrace{M_j \times \cdots \times M_j}_k$ such that $\overline{f_j}, f \rightarrow 0$ (in the sense explained in the preceding section),*

$$\Phi_\Gamma(f_j) \longrightarrow \Phi_\Gamma(f).$$

Theorem 4.9. *The space of GFTs associated with Ricci non-negative manifolds of diameter 1 is precompact.*

Proof. Take a sequence (M_j) with $\text{diam}(M_j) = 1$, $\text{Ric}(M_j) \geq 0$. From the results of the preceding section we know that there exists a space (Z, z, d, μ) with doubling measure μ such that, passing to a subsequence,

$$(M_j, m_j, d_j, \text{Vol}_j) \rightarrow (Z, z, d, \mu)$$

in the measured Gromov-Hausdorff sense. From Proposition 4.6, $\overline{H^j}, \overline{H} \rightarrow 0$ for the renormalized heat kernels on M_j and Z . Take a metric graph Γ with k "in" vertices, a sequence (f_j) , and a function f as in the above Definition. Let $\psi_j: Z \rightarrow M_j$ be the Gromov-Hausdorff approximations. Then

$$\left| \Phi_\Gamma(f) - \int_{Z \times \cdots \times Z} f_j(\psi_j(in_1), \dots, \psi_j(in_k)) \prod_{\substack{\text{over all} \\ \text{edges } t_i \text{ of } \Gamma}} H_{t_i}^j(\psi_j(x_{i_1}), \psi_j(x_{i_2})) \prod_r d in_r \prod_t d x_t \right| \rightarrow 0,$$

by dominated convergence theorem. But, since the volumes of balls in M_j converge to those in Z , the second summand in the above formula is close to

$$\Phi_\Gamma(f_j) := \int_{M_j \times \cdots \times M_j} f_j(in_1, \dots, in_k) \prod_{\substack{\text{over all} \\ \text{edges } t_i \text{ of } \Gamma}} H_{t_i}^j(x_{i_1}, x_{i_2}) \prod_r d in_r \prod_t d x_t.$$

Thus, $GFT(M_j) \longrightarrow GFT(Z)$ which establishes the Theorem. □

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La géométrie et la théorie conforme des champs

Cette thèse porte sur une question de géométrie riemannienne motivée par l'étude de la compactification de l'espace de modules de théories de champs conformes.

M. Kontsevich associe à une suite de théories de champs conformes qui dégénère un objet limite qui comporte une variété riemannienne M à courbure de Ricci positive ou nulle, et sa théorie de champs sur graphes. Il s'agit d'une famille d'opérateurs sur les puissances tensorielles de l'espace de Hilbert $L^2(M)$, indexés par des graphes métriques. Le prototype est le semi-groupe de la chaleur P_t , associé au graphe à deux sommets et une arête de longueur t .

Le résultat principal de la thèse est une estimation de la norme du gradient du logarithme du noyau de la chaleur sur une variété riemannienne compacte, en temps petit, en fonction de la borne inférieure de la courbure de Ricci et du diamètre seulement. La preuve, qui utilise le calcul stochastique, s'étend à certains semi-groupes satisfaisant une inégalité de courbure-dimension à la D. Bakry-M. Emery.

A l'aide de résultats de J. Cheeger et T. H. Colding sur la structure des espaces limites (au sens de Gromov-Hausdorff mesuré) de telles variétés riemanniennes, on montre que l'estimation s'étend à ces espaces singuliers, et on en déduit un théorème de compacité pour l'espace de modules de théories de champs sur graphes associées à des variétés riemanniennes compactes à courbure de Ricci uniformément minorée.

Mots-clés: Equation de la chaleur, Courbure de Ricci, Pont brownien, Espace métrique mesuré, Géométrie riemannienne, Probabilités, Calcul stochastique, Convergence de Gromov-Hausdorff, Singularité.

Code matière AMS: 58J35; 32Q10; 58J60; 58J65; 60H07; 81T20.

Geometry and Conformal Field Theory

This thesis deals with a Riemannian geometric question which is motivated by the problem of compactifying the moduli space of Conformal Field Theories (CFT).

M. Kontsevich associates to a degenerating sequence of CFT's a limiting object which contains a Riemannian manifold M with nonnegative Ricci curvature, and its graph field theory. This amounts to a family of operators on tensor powers of the Hilbert space $L^2(M)$, indexed by metric graphs. For instance, the operator attached to the graph with two vertices and one edge of length t is the heat semigroup P_t .

The main result in the thesis is an a priori estimate of the norm of the gradient of the logarithm of the heat kernel on a compact Riemannian manifold, for short times, depending on the lower bound on Ricci curvature and on diameter only. The proof, which uses stochastic calculus, extends to certain semigroups satisfying curvature-dimension inequalities, in the sense of D. Bakry and M. Emery.

Using J. Cheeger and T. H. Colding's structure results on limit spaces of such Riemannian manifolds, it is shown that the a priori estimate extends to these singular limit spaces. A compactness theorem for graph field theories associated with compact Riemannian manifolds satisfying a uniform lower bound on Ricci curvature follows.

Keywords: Heat equation, Ricci curvature, Brownian bridge, Metric measure space, Riemannian geometry, Probability, Stochastic calculus, Gromov-Hausdorff convergence, Singularity.

AMS MSC: 58J35; 32Q10; 58J60; 58J65; 60H07; 81T20.