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On some probabilistic estimates of heat kernel derivatives and applications

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Abstract

We describe how to obtain some probabilistic Bismut formulae for the derivatives of the heat kernel on a Riemannian manifold and give an application to the estimate of the energy in Euclidean Quantum Mechanics.

1. Introduction.

M shall denote a d-dimensional compact complete Riemannian manifold without boundary although generalizations (concerning compactness and boundary) are possible. With respect to the metric $ds^2 = \sum_{i,j} g_{i,j} dm^i dm^j$ the Laplace-Beltrami operator is defined by

$$\Delta = (detg)^{\frac{1}{2}} \frac{\partial}{\partial m^i} (g^{i,j} detg^{-\frac{1}{2}} \frac{\partial}{\partial m^j})$$

where $g^{i,j}$ denotes the inverse of the matrix $g_{i,j}$. Here again we could consider a more general operator by adding a first order term (a vector field) but we are more interested in explaining the ideas rather then consider full generality. There exists a huge number of works concerning estimates of the heat kernel associated with Δ, namely the function $p_t(m_0, m)$ satisfying the p.d.e.

$$\frac{\partial p}{\partial t} = \frac{1}{2}\Delta p \quad \text{with} \;\; p_t(m_0, m) \to \delta_{m_0}(m), t \to 0$$

A major insight on these problems is due to Kolmogorov ([10]), who associated with the Laplacian and, more generally, with an elliptic second order linear operator, a stochastic flow of diffeomorphisms, generalizing the well known fact that one can associate a deterministic flow with a vector field. The rôle of partial differential equations was since then made clear in the theory of Markov processes and, "reciprocally", stochastic processes turned out to be a central tool in the study of these equations.

We refer also to two works, that can be seen as landmarks on the subject: Varadhan's results ([17]) that essentially states the behaviour of the heat kernel for small times,

$$lim_{t\to 0}(-2tlog\ p_t(m_0, m)) = d^2(m_0, m)$$

and [11], where the authors prove (analytically) very precise estimates.

We are concerned here with estimates on the derivative of the heat kernel. Such estimates allow, in particular, to deduce the smoothness of the corresponding heat semigroup

$$(e^{\frac{t}{2}\Delta} f)(m_0) = \int_M f(m)p_t(m_0, m)dm$$

where dm denotes the Riemannian volume measure. Here again many authors have considered these type of problems, concerning ponctual or L^p estimates (cf., for example,[1],[7],[15],[16] and also [14], where large deviations arguments are used).

Bismut [1] showed that $t\nabla_{m_0} log\ p_t(m_0, m)$ can be expressed in terms of a conditional expectation of some stochastic process and used such an expression to study the small time assymptotics of the logarithmic derivative of the heat kernel. Other related formulae have been obtained since then (they are far from being unique).

The logarithmic derivative is quite a natural object to investigate. For example in (semiclassical) quantum physics, it has to do with the gradient of the action of the system under consideration.

The heat semigroup can be expressed as an expectation with respect to some stochastic process, in this case the M valued Brownian motion $\rho_w(t)$, starting at m_0 at time zero,

$$(e^{\frac{t}{2}\Delta} f)(m_0) = Ef(\rho_w(t))$$

Therefore it is natural to think that derivatives of the heat kernel can be transfered to some derivatives on the path space of the process. And, in order to accomplish such task, one should use the stochastic calculus of variations on the path space or Malliavin calculus ([13]).

This paper is organized as follows: in the next paragraph we recall some notions of Malliavin calculus (in the flat situation, namely on the Wiener space) and, in particular, its integration by parts formula. This one can also be interpreted a rigorous version of Feynman's integration by parts formula (c.f. [2], Part 2) in quantum physics. In paragraph 3 we describe a construction of the Brownian motion on a Riemannian manifold, we consider the Itô map and present an intertwinning formula that allows to transfer derivatives on the path space of a manifold to derivatives on the Wiener space. In paragraph 4 we show how to deduce Bismut formula for the heat kernel derivative and, finally, the last paragraph is devoted to an application: estimating the energy in Euclidean quantum mechanics.

2. Malliavin calculus.

Let X denote the Wiener space, namely the space of continuous paths $\gamma : [0,1] \to \mathbb{R}^d, \gamma(0) = x_0$ endowed with the Wiener measure μ. This measure is the law of the $\mathbb{R}^d$ valued Brownian motion and is associated to the Laplacian in the sense that the corresponding heat semigroup has the representation

$$(e^{\frac{t}{2}\Delta} f)(x_0) = E_\mu(f(\gamma(t)))$$

Let H be the (Hilbert) subspace of X, named after Cameron and Martin, of the paths which are absolutely continuous and whose derivative satisfy $\int_0^1 |\dot\gamma(\tau)|^2 d\tau < \infty$. Although dense in X, the (μ) measure of H is zero.

For a cylindrical functional $F = f(\gamma(\tau_1), \ ..., \gamma(\tau_m))$ the Malliavin derivative ([13]) is defined by

$$D_\tau F(\gamma) = \sum_{k=1}^m \mathbf{1}_{\tau<\tau_k} \partial_k f(\gamma(\tau_1), \ ..., \gamma(\tau_m))$$

The operator D is closed on the completion of the space of cylindrical functionals with respect to the norm $||F||^2 = E_\mu(|F|^2 + \int_0^1 |D_\tau F|^2 d\tau)$ and can therefore be extended to this space. For a "vector field" $z : X \to H$, we define the directional derivatives

$$D_z F = \int_0 < D_\tau F, \dot z(\tau) > d\tau$$

where $<,>$ denotes the scalar product in $\mathbb{R}^d$. They coincide with the more familiar limit (taken in the a.e.-μ sense) of $\frac{1}{\epsilon}(F(\gamma + \epsilon z) - F(\gamma))$ when $\epsilon \to 0$.

Girsanov-Cameron-Martin theorem states that, when z is adapted to the increasing filtration $\mathcal{P}_\tau$ generated by the events before time τ (the Itô filtration), then a shift $\gamma \to \gamma + z$ induces a transformation of the Wiener measure to a measure which is absolutely continuous with respect to μ and we have an explicit formula for the Radon-Nikodym density (c.f. [18]):

$$E_\mu F(\gamma+z) = E_\mu\big(F(\gamma)exp\{\int_0^1 <\dot z, d\gamma(\tau)> -\frac{1}{2}\int_0^1 |\dot z|^2 d\tau\}\big)$$

The integral in $d\gamma$ is the Itô integral with respect to Brownian motion.

In the case of deterministic z, Cameron and Martin actually proved that belonging to H is a necessary and sufficient condition for the shifted measure to be absolutely continuous with respect to μ. It is therefore natural to consider variations with respect to H valued functionals and therefore consider this space as a tangent space (which explains the terminology "vector fields" used before).

The dual of the derivative with respect to the measure μ is called the divergence operator. For adapted vector fields z such that $E_\mu \int_0^1 |\dot z(\tau)|^2 d\tau < \infty$ it follows from Girsanov-Cameron-Martin theorem that the divergence coincides with the Itô integral and we have the following integration by parts formula:

$$E_\mu(D_z F) = E_\mu\big(F\int_0^1 <\dot z(\tau), d\gamma(\tau)>\big)$$

More generally the divergence coincides with an extension of this integral, the so-called Skorohod integral (c.f.[13] and references therein).

We notice that there is, in particular, a class of adapted transformations preserving the Wiener measure: these are the rotations (Levy's theorem). So, if $d\xi^i(\tau) = \sum_j a_{i,j} d\gamma(\tau)$ where $a \equiv a_{i,j}$ is an antisymmetric matrix, $a(0) = 0$, and if $D_\xi F = \int_0^1 D_\tau F d\xi(\tau)$, we have

$$E_\mu(D_\xi(F)) = 0$$

The tangent space to the Wiener space can therefore be extended to include processes ξ satisfying a stochastic differential equation of the form

$$d\xi^i(\tau) = \sum_j a_{i,j} d\gamma^j(\tau) + z^i d\tau$$

with a as above (the so-called tangent processes, c.f. [3]).

3. Brownian motion on a Riemannian manifold.

If M is a d-dimensional Riemannian manifold, let $O(M)$ denote the bundle of orthonormal frames over M, namely

$$O(M) = \{(m,r) : m \in M, r : \mathbb{R}^d \to T_m(M) \text{ is an Euclidean isometry}\}$$

and $\pi : O(M) \to M$, $\pi(r) = m$ the canonical projection. Let $m_k(t)$ denote the (unique) geodesic starting at m at time zero and having initial velocity $r(e_k)$ with e_k,$k = 1, ..., d$, a vector in the canonical basis of $\mathbb{R}^d$. The parallel transport of

r along m_k defined by the equation $\frac{dr_k}{dt} + \Gamma_{\dot{m}_k} r_k = 0, \quad r_k(0) = Id$, where Γ are the Christoffel symbols of the Levi-Civita connection, determines a vector field on $O(M)$: $A_k(m,r) = \frac{d}{dt}_{|t=0} r_k(t)$. We consider the horizontal Laplacian on $O(M)$, namely the second order differential operator

$$\Delta_{O(M)} = \sum_{k=1}^{d} A_k^2$$

Then

$$\Delta_{O(M)}(fo\pi) = (\Delta f)o\pi$$

where Δ is the Laplace-Beltrami operator on M. These two Laplacians induce two probability measures or two stochastic flows, defined in the path spaces of $O(M)$ and of M, respectively; and π realizes an isomorphism between these probability spaces. The measure in

$$\mathbb{P}_{m_0}(M) = \{\rho : [0,1] \to M, \rho \text{ continuous}, \ \rho(0) = m_0\}$$

that we shall denote by ν, is the Wiener measure, or the law of the Brownian motion on M and satisfies $(e^{\frac{t}{2}\Delta_M} f)(m_0) = E_\nu(f(\rho(t)))$. The measure in $\mathbb{P}_{m_0}(O(M))$ corresponds to the law of $r(\tau)$, the (Itô stochastic) parallel displacement along the curve $\rho(\tau)$ with respect to the Levi-Civita connection. This lifted curve satisfies an stochastic differential equation of the form $dr_\gamma(\tau) = \sum_k A_k(r_\gamma(\tau) d\gamma^k(\tau), \quad r_\gamma(0) = r_0$, with $\pi(r_0) = m_0$ (c.f., for example, [9]).

In [12] Malliavin defined the Itô map $I : X \to \mathbb{P}_{m_0}(M)$,

$$I(\gamma)(\tau) = \pi(r_\gamma(\tau))$$

and proved that I is a.s. bijective and provides an isomorphism of measures.

A vector field along the path ρ is a section process of the tangent bundle of M, namely a measurable map $Z_\rho(\tau) \in T_{\rho(\tau)}(M)$. We denote by z the image of Z through the parallel transport,

$$z(\tau) = r_0 o[r_\gamma(\tau)]^{-1}(Z(\tau))$$

and assume that z belongs to the Cameron-Martin space H.

The derivative of a cylindrical functional $F = f(\rho(\tau_1), \ ..., \rho(\tau_m))$ along a vector field is given by

$$D_Z F(\rho) = \sum_{k=1}^{m} < r_0 o[r_\gamma(\tau_k)]^{-1} \partial_k f, Z(\tau_k) >$$

This derivative can be extended by closure to a suitable Sobolev space of functionals.

The theorem that follows expresses how derivatives in the path space can be transfered to derivatives in the Wiener space. We shall not be precise, here, in the assumptions, namely in the regularity needed for the functionals and the vector fields.

The result is a consequence of the formula for the derivative of the Itô map. Since a (stochastic) parallel transport along the Brownian motion is differentiated, the variation is given in terms of the integral of the curvature tensor along this curve.

Theorem (Intertwinning formula [3], [4], [6], [8])
A functional F is differentialble along a vector field Z in $\mathcal{P}_{m_0}(M)$ iff FoI is differentiable in X along the process

$$d\xi(\tau) = [\dot{z} + \frac{1}{2}Ricc(z)]d\tau - (\int_0^\tau \Omega(z, od\gamma))d\gamma(\tau)$$

where $d\gamma$, $od\gamma$ denote, resp., Itô and Stratonovich stochastic differentiation (c.f.[9]), Ω and Ricci the curvature and the Ricci tensors in M. Furthermore we have:

$$(D_Z F)oI = D_\xi(FoI)$$

From this theorem we can deduce, in particular, Bismut integration by parts formula:

$$E_\nu(D_Z F) = E_\mu\big((FoI)\int_0^1 [\dot{z}(\tau) + \frac{1}{2}\mathcal{R}_\tau(z(\tau))]d\gamma(\tau)\big)$$

with $\mathcal{R}_\tau$ the Ricci tensor read in the frame bundle. This result follows from the integration by parts formula on the Wiener space and from the fact that Ω is antisymmetric, the corresponding term in the intertwinning formula having therefore zero divergence.

4. Heat kernel derivatives.

Given the probabilistic representation of the heat kernel, we differentiate this function by derivating the Brownian motion on M in a convenient direction. Then we apply the intertwinning theorem to tranfer this derivative to the Wiener space (c.f. [5]). The following result can be obtained:

Theorem (Bismut formula) *Let f be a smooth function on M and v a vector in the tangent space $T_{m_0}(M)$. For fixed $t > 0$ and denoting $P_t f = e^{\frac{t}{2}\Delta} f$, we have:*

$$< \nabla P_t f, v >_{T_{m_0}(M)} = \frac{1}{t} E_\mu\big(f(\rho_\gamma(t))\int_0^t [v + \frac{1}{2}(\tau - t)\mathcal{R}_\tau v]d\gamma(\tau)\big)$$

Idea of the proof:
Let U be the solution of the o.d.e.

$$\frac{dU(\tau)}{d\tau} = -\frac{1}{2}\mathcal{R}_\tau U(\tau), \quad U(0) = Id_{T_{m_0}(M)}$$

Consider $y(\tau) = U(\tau)v - \frac{1}{t}(t - \tau \wedge t)v$, which is a Cameron-Martin vector field. From the intertwinning formula we derive

$$\begin{aligned}
< \nabla P_t f, v >_{T_{m_0}(M)} &= E < r_\gamma(t) r_0^{-1} \nabla f, U(t)v >_{T_{m_0}(M)} \\
&= E < r_\gamma(t) r_0^{-1} \nabla f, y(t) >_{T_{m_0}(M)} \\
&= E(D_Y f(\gamma(t)))
\end{aligned}$$

where Y denotes the parallel transport of the vector y. The result follows from the integration by parts on the path space.

Remark 1. From this result we may, in particular, obtain L^p estimates for the derivative of the heat semigroup. For example, in the situation where

$$||Ricc||_{L^p(dm)} = C_p < \infty$$

for every $p > 1$, we obtain

$$||\nabla P_t f||_{L^p(dm)} \leq (\frac{2}{t} + \frac{t}{6} C^2_{\frac{pq}{q-p}})^{\frac{1}{2}} ||f||^{\frac{p}{q}}_{L^q(dm)}$$

Remark 2.

Bismut formula appears sometimes as a probabilistic espression for the logarithmic derivative $\nabla log p_t(m_0, m)$ (c.f. [1]). Such expressions can be obtained from the one in last theorem by taking conditional expectations on the underlying stochastic processes.

Remark 3.

Formulae for derivatives of the heat kernel with respect to the second variable written in terms of stochastic integrals can also be deduced by similar methods.

5. An application.

In Euclidean Quantum Mechanics (c.f. [2] and [18]) a family of stochastic processes is associated to the self-adjoint Hamiltonian observable $\mathcal{H} = -\frac{1}{2}\Delta + V$, where V denotes a bounded below scalar potential. These processes solve stochastic differential equations of the form (in local coordinates):

$$dz^i(t) = \hbar^{\frac{1}{2}} \sigma_{i,k}(z(t)) d\gamma^k(t) - \frac{\hbar}{2} g^{j,k} \Gamma^i_{j,k}(z(t)) dt + \hbar \partial_i log \eta_t(z(t)) dt$$

where $\sigma = \sqrt{g}$ and with respect to the (usual) past Itô filtration and

$$d_* z^i(t) = \hbar^{\frac{1}{2}} \sigma_{i,k} d_* \gamma^k_*(t) - \frac{\hbar}{2} g^{j,k} \Gamma^i_{j,k} dt - \hbar \partial_i log \eta^*_t dt$$

with respect to the future filtratio. Here η and η^* are, respectively, positive solutions of final and initial value problems for the heat equation with potential V. Considering time running in the interval $[0, T]$,

$$\eta_t(x) = e^{\frac{1}{\hbar}(t-T)\mathcal{H}}\eta_T$$

$$\eta_t^*(x) = e^{-\frac{1}{\hbar}t\mathcal{H}}\eta_0^*$$

The law of z at time t is absolutely continuous with respect to the volume measure and its density is $\eta_t\eta_t^*$.

In this framework the energy is defined (following Feynman) by

$$\mathcal{E} = -\frac{1}{2}|\hbar\nabla log\eta_t|^2 - \frac{\hbar^2}{2}div\nabla log\eta_t + V$$

or, in the other filtration, by

$$\mathcal{E}^* = -\frac{1}{2}|\hbar\nabla log\eta_t^*|^2 - \frac{\hbar^2}{2}div\nabla log\eta_t^* + V$$

We want to estimate the mean value of the energy along the trajectories of the process $z(t)$, namely the quantity

$$e(t) = E(\mathcal{E}(z(t)) = \int_M \mathcal{E}\eta_t\eta_t^* dm$$

which is also equal to $E(\mathcal{E}^*(z(t))$, and correspond to the path space counterparts of $< \psi|\mathcal{H}\psi >_{L^2(dm)}$ in quantum mechanics, for a state ψ. Since

$$\int_M (div\nabla log\eta_t^*)\eta_t\eta_t^* dm = -\int_M < \nabla log\eta_t^*, \nabla(\eta_t\eta_t^*) > dm$$

we have

$$e(t) = \frac{\hbar^2}{2}\int_M < \nabla\eta_t, \nabla\eta_t^* > dm + \int_M V\eta_t\eta_t^* dm$$

We observe that the energy (say, its L^p norm) in this framework can be entirely estimated in terms of the heat kernel and its derivatives, together with the initial and final conditions and the assumptions on the potential V.

In the absence of the potential (if V is different from zero we should introduce a Feynman-Kac representation for the corresponding semigroups) and in the situation of Remark 2. of the last paragraph, we can obtain, for example, the following estimation:

$$|e(t)|^4 \leq \frac{\hbar^8}{2^4}\Big(\frac{2\hbar}{T-t} + \frac{T-t}{6\hbar}C_2\Big)\Big(\frac{2\hbar}{t} + \frac{t}{2\hbar}C_2\Big)||\eta_T||^2_{L^2(dm)}||\eta_0^*||^2_{L^2(dm)}$$

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