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### AN ESTIMATE ON THE HESSIAN OF THE HEAT KERNEL

DANIEL W. STROOCK

ABSTRACT. Let M be a compact, connected Riemannian manifold, and let  $p_t(x,y)$  denote the fundamental solution to Cauchy initial value problem for the heat equation  $\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u$ , where  $\Delta$  is the Levi-Civita Laplacian. The purpose of this note is to describe the behavior of the Hessian of  $\log p_T(\cdot, y)$  for small T > 0.

Emphasis is given to the difference between what happens outside, where the behavior is like  $\frac{1}{T}$ , as opposed to at the cut locus, where it is like  $\frac{1}{T^2}$ .

#### **§0:** INTRODUCTION

Let M be a compact, connected, d-dimensional Riemannian manifold, denote by  $\mathcal{O}(M)$  with fiber map  $\pi : \mathcal{O}(M) \longrightarrow M$  the associated bundle of orthonormal frames  $\mathfrak{e}$ , and use the Levi-Civita connection to determine the horizontal subspace  $H_{\mathfrak{e}}(\mathcal{O}(M))$  at each  $\mathfrak{f} \in \mathcal{O}(M)$ . Next, given  $\mathbf{v} \in \mathbb{R}^d$ , let  $\mathfrak{E}(\mathbf{v})$  be the *basic vector* field on  $\mathcal{O}(M)$  determined by properties that

$$\mathfrak{E}(\mathbf{v})_{\mathfrak{e}} \in H_{\mathfrak{e}}(\mathcal{O}(M))$$
 and  $d\pi \mathfrak{E}(\mathbf{v})_{\mathfrak{e}} = \mathfrak{e}\mathbf{v}$  for all  $\mathfrak{e} \in \mathcal{O}(M)$ .

(Here, and whenever convenient, we think of  $\mathfrak{e}$  as a isometry from  $\mathbb{R}^d$  onto  $T_{\pi(\mathfrak{e})}(M)$ .) In particular, if  $\{\mathbf{e}_1, \ldots, \mathbf{e}_d\}$  is the standard orthonormal basis in  $\mathbb{R}^d$ , then we set  $\mathfrak{E}_k(\mathfrak{e}) = \mathfrak{E}(\mathbf{e}_k)_{\mathfrak{e}}$ . If, for  $\mathcal{O} \in \mathcal{O}(d)$  (the orthogonal group on  $\mathbb{R}^d$ )  $R_{\mathcal{O}} : \mathcal{O}(M) \longrightarrow \mathcal{O}(M)$  is defined so that

$$R_{\mathcal{O}} \mathfrak{e} \mathbf{v} = \mathfrak{e} \mathcal{O} \mathbf{v}, \quad \mathfrak{e} \in \mathcal{O}(M) \text{ and } \mathbf{v} \in \mathbb{R}^d,$$

then it easy to check that

(0.1) 
$$dR_{\mathcal{O}}\mathfrak{E}(\mathbf{v})_{\mathfrak{e}} = \mathfrak{E}(\mathcal{O}^{\mathsf{T}}\mathbf{v})_{R_{\mathcal{O}}\mathfrak{e}}, \quad \mathfrak{e} \in \mathcal{O}(M) \text{ and } \mathbf{v} \in \mathbb{R}^{d}.$$

Given a smooth function F on  $\mathcal{O}(M)$ , we define  $\nabla F : \mathcal{O}(M) \longrightarrow \mathbb{R}^d$ ,  $\operatorname{Hess}(F) : \mathcal{O}(M) \longrightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ , and  $\Delta F : \mathcal{O}(M) \longrightarrow \mathbb{R}$  by

(0.2) 
$$\nabla F = \sum_{1}^{d} \mathfrak{E}_{k} F \mathbf{e}_{k}, \quad \text{Hess}\left(F\right) = \left(\left(\mathfrak{E}_{k} \circ \mathfrak{E}_{\ell} F\right)\right)_{1 \leq k, \ell \leq d}$$
$$\text{and} \quad \Delta F = \sum_{1}^{d} \mathfrak{E}_{k}^{2} F.$$

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XXI.1

In particular, when f is a smooth function on M, we set

 $\nabla f \equiv \nabla (f \circ \pi), \quad \text{Hess} (f) \equiv \text{Hess} (f \circ \pi), \quad \text{and} \quad \Delta f \equiv \Delta (f \circ \pi).$ 

Starting from (0.1), it is an easy matter to check that

$$(\nabla f) \circ R_{\mathcal{O}} = \mathcal{O}^{\top} \nabla f, \quad (\text{Hess}(f)) \circ R_{\mathcal{O}} = \mathcal{O}^{\top} \text{Hess}(f) \mathcal{O},$$
  
and  $(\Delta f) \circ R_{\mathcal{O}} = \Delta f.$ 

Hence,  $|\nabla f|$ ,  $\|\text{Hess}(f)\|_{\text{H.S.}}$  (the Hilbert-Schmidt norm), and  $\Delta f$  are all well-defined on M. In fact,  $\Delta f$  is precisely the action of the Levi-Civita Laplacian on f.

Now consider Cauchy initial value for the heat equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u, \quad t \in (0,\infty) \quad \text{with} \quad \lim_{t \searrow 0} u(t,x) = f(x), \quad x \in M.$$

By standard elliptic regularity theory, one knows that there is a unique, smooth function  $(t, x, y) \in (0, \infty) \times M \times M \longmapsto p_t(x, y) \in (0, \infty)$  such that

$$u(t,x) = \int_M f(y) p_t(x,y) \lambda_M(dy), \quad (t,x) \in (0,\infty) \times M \text{ and } f \in C(M;\mathbb{R}),$$

where  $\lambda_M$  denotes the normalized Riemann measure on M. Moreover, because  $\Delta$  is essentially self-adjoint in  $L^2(\lambda_M)$ ,  $p_t(x, y) = p_t(y, x)$ .

### §1: THE RESULTS

We begin by considering the logarithmic gradient  $\nabla \log p_T(\cdot, y)$ , for which our initial result depends only on the dimension d and the lower bound

(1.1) 
$$\alpha \equiv \min_{\mathbf{e} \in \mathcal{O}(M)} \min_{\mathbf{v} \in S^{d-1}} \left( \mathbf{v}, \operatorname{Ric}(\mathbf{e}) \mathbf{v} \right)_{\mathbb{R}^d}$$

for the Ricci curvature. One (cf. [SZ]) can then show that there is a  $C(d, \alpha) < i\infty$  such that, for each  $\epsilon \in (0, 1)$ ,

(1.2)

$$\left|\nabla \log p_T(\cdot, y)\right|(x) \le \frac{\left((1+\epsilon)e^{\alpha T}\right)^{\frac{1}{2}}\rho(x, y)}{T} + \frac{C(d, \alpha)}{(\epsilon T)^{\frac{1}{2}}}, \quad (T, x, y) \in (0, 1] \times M^2,$$

where we have introduced  $\rho(x, y)$  to denote the Riemannian distance between x and y.

Notice that the preceding result does not feel the cut locus. To get a result which does, we look at what happens asymptoticly as  $T \searrow 0$ . What one finds (cf. the first part of Theorem 3.12 in [KS]) is that

(1.3) 
$$y \text{ ouside the cut locus of } x \equiv \pi(\mathfrak{e}) \Longrightarrow$$
$$\lim_{T \searrow 0} T[\nabla \log P_T(\cdot, y)](\geq) = \mathbf{v}(\mathfrak{e}, y),$$

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where  $\mathbf{v}(\mathbf{c}, y)$  is the element of  $\mathbb{R}^d$  which is determined by the requirement that the path  $\mathfrak{f} \in C^1([0, 1]; \mathcal{O}(M))$  satisfying

(1.4) 
$$\mathfrak{f}(0) = \mathfrak{e} \text{ and } \mathfrak{f}(t) = \mathfrak{E}\big(\mathbf{v}(\mathfrak{e}, y)\big)_{\mathfrak{e}(t)}$$

is the horizontal lift to  $\mathfrak{e}$  of the (unique) minimal geodesic going from x to y. When y is at the cut locus of x, one should not expect (1.3) to hold. In fact, take S(x, y) in  $T_x(M)$  to be the set of initial directions in which minimal geodesics from x to y can proceed. When S(x, y) forms a non-trivial differentiable submanifold, then one can use the second part of Theorem 3.12 in [KS] to see that the limit on the left side of (1.3) exists and is a non-trivial convex combination of elements of  $\mathfrak{e}^{-1}(S(x, y))$ . In particular, since all elements of have the same length, this limit has length strictly less than  $\rho(x, y)$  in this case. For example, when M is the circle centered at the origin in  $\mathbb{R}^2$  with unit circumference,

(1.5) 
$$p_T\left(\theta, \frac{1}{2}\right) = (2\pi T)^{-\frac{1}{2}} \sum_{m \in \mathbb{Z}} \exp\left(-\frac{\left(\theta - \frac{1}{2} - m\right)^2}{2T}\right),$$

and so it is clear that

$$\lim_{T\searrow 0} T\left[\nabla \log p_T\left(\cdot, \frac{1}{2}\right)\right](0) = 0.$$

The analysis of the Hessian of  $\log p_T(\cdot, y)$  is more challenging. What it leads to is a general estimate (cf. [S]) of the form

(1.6) 
$$-\frac{C}{T} \leq \left[\operatorname{Hess}\log p_T(\cdot, y)\right](\mathfrak{e}) \leq C\left(\frac{1}{T} + \frac{\rho(x, y)^2}{T^2}\right)$$
for  $\mathfrak{e} \in \pi^{-1}(x)$  and  $(T, x, y) \in (0, 1] \times M^2$ .

Unlike the constant in (1.2), the C in (1.6) depends on more than the lower bound  $\alpha$  in (1.2). In fact, asymptotic analysis based on [KS] gives

y outside the cut locus of  $\implies$ 

(1.7) 
$$\lim_{T\searrow 0} T \big[ \operatorname{Hess} \log p_T(\cdot, y) \big](\mathfrak{e}) = -\mathbf{I} + \int_0^1 (1-t)^2 \operatorname{Sec}\big(\mathfrak{f}(t), \mathbf{v}(\mathfrak{e}, y)\big) \, dt,$$

where  $\mathbf{v}(\boldsymbol{\epsilon}, y) \in \mathbb{R}^d$  and  $\mathbf{f} \in C^1([0, 1]; \mathcal{O}(M))$  are defined as above (cf. (1.4)) and Sec:  $\mathcal{O}(M) \times \mathbb{R}^d \mapsto \mathbb{R}^d \otimes \mathbb{R}^d$  is the (unnormalized) sectional curvature given by

$$(\xi, \operatorname{Sec}(\mathfrak{g}, \mathbf{v})\eta)_{\mathbb{R}^d} = (\operatorname{Riem}_{\mathfrak{g}}(\xi, \mathbf{v})\eta, \mathbf{v})_{\mathbb{R}^d}.$$

On the other hand, when y is at the cut locus of x and the set S(x, y)

has the sort of structure described in the preceding paragraph, then one can show that

 $\lim_{T\searrow 0} T^2 \big[ \operatorname{Hess} \log p_T(\,\cdot\,,y) \big](\mathfrak{e}) \text{ exists and is strictly positive definite.}$ 

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For example, in the case of the circle considered above,

$$\lim_{T\searrow 0} T^2 \left[ \operatorname{Hess} \log p_T \left( \cdot, \frac{1}{2} \right) \right] (0) = \frac{1}{4}.$$

The proofs of these results are based on probabilistic representations of  $p_T(\cdot, y)$  and its derivatives in terms of the Brownian motion on M (cf. (2.2) and (2.12) in [S]).

Remark: Because, by an old result of Varadhan's, one knows that

$$\lim_{T\searrow 0} T\log p_T(x,y) = \frac{\rho(x,y)^2}{2} \text{ for all } x, y \in M,$$

the expression on the right hand side of (1.7) must equal the Hessian of  $\frac{1}{2}\rho(\cdot, y)^2$ . However, to date, the author has found no corroboration in differential geometry texts.

#### References

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