HEAT KERNEL ASYMPTOTICS AND THE DISTANCE FUNCTION IN LIPSCHITZ RIEMANNIAN MANIFOLDS

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Abstract. We establish a characterization of the distance function d in a Lipschitz Riemannian manifold in terms of paths of least action. We extend to this context Varadhan's theorems on the small time asymptotics of the heat kernel

$$t \log p(t,x,y) \to -d(x,y)^2/4$$

and on the principle of not feeling the boundary.

1. Introduction

In a solid medium, heat flow is governed by two characteristics, conductivity and capacity, which may vary over the medium, sometimes in an irregular way. A general mathematical model is provided by a manifold M, in which the conductivity, or rather its inverse, the resistance, corresponds to a Riemannian metric, and the capacity corresponds to a Borel measure m. We shall be concerned with the heat flow on M associated to the Dirichlet form

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

In particular, we shall consider the Dirichlet heat kernel $p_0(t,x,y)$ and the Neumann heat kernel $p(t,x,y)$. Physically, these express the rise in temperature at y after time t, due to unit heat input at x, when, respectively, the boundary is maintained at a fixed temperature or is perfectly insulated. Our main aim will be to relate, under minimal hypotheses, the small time asymptotics of these heat kernels to distance functions derived from the metric. We shall show that the basic asymptotic formula of Varadhan [V1] remains valid without smoothness assumptions on the metric or measure, and indeed without any sort of completeness or curvature bound on the underlying space.

We work throughout in the context of a Lipschitz Riemannian manifold M, of dimension n, on which is given a Borel measure m. See for example [DP1],[T],[Z].

We thus have a maximal atlas of charts, the transition functions between which are locally Lipschitz homeomorphisms in $\mathbb{R}^n$. Henceforth we shall write Lipschitz to mean locally Lipschitz. We systematically refer to a chart by its domain U, which is moreover then identified with its image, an open set in $\mathbb{R}^n$. We assume that in each chart U the measure m is absolutely continuous with respect to Lebesgue measure l in $\mathbb{R}^n$. In each chart U the metric and measure are given by measurable functions

$$a : U \to \mathbb{R}^n \otimes \mathbb{R}^n, \quad \mu : U \to [0, \infty)$$

where

$$a^{ij}(x) = \langle dx^i, dx^j \rangle = a^{ji}(x), \quad \mu(x) = dm/dl.$$

Our basic assumption is that for some atlas $\mathcal{U}$ of charts U, there are constants $\lambda = \lambda(U) < \infty$ such that, for all $x \in U$ and $\xi \in (\mathbb{R}^n)^*$

$$\lambda^{-1}|\xi|^2 \leq \sum_{i,j=1}^{n} a^{ij}(x)\xi_i\xi_j \leq \lambda|\xi|^2, \quad \lambda^{-1} \leq \mu(x) \leq \lambda. \tag{$*$}$$

We do not assume that the constants $\lambda(U), U \in \mathcal{U}$, are uniformly bounded. Note that, since the transition functions are Lipschitz, once bounds of the type $(*)$ hold for some atlas $\mathcal{U}$, they also hold for all charts with relatively compact domain. Given a chart U with $\lambda(U) < \infty$, we shall write C for a finite positive constant depending only on λ and n. Further dependence will be made explicit in the notation: thus $C(\varepsilon)$ will denote a finite positive constant depending on ε, λ and n. The value of these constants may be adjusted from line to line.

For measurable functions $f : M \to \mathbb{R}$ having a weak derivative ∇f we set

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

We define

$$\mathcal{D} = W^{1,2}(M) = \{f : \mathcal{E}(f) + \|f\|_2^2 < \infty\}.$$

Recall that every Lipschitz function has a weak derivative. The set of Lipschitz functions in $\mathcal{D}$ is dense in $\mathcal{D}$. The closure in $\mathcal{D}$ of the set of Lipschitz functions of compact support will be denoted $\mathcal{D}_0 = W_0^{1,2}(M)$. Given a non-empty closed set $K \subseteq M$, the closure in $\mathcal{D}$ of the set of Lipschitz functions vanishing on K will be denoted $\mathcal{D}_K$.

Write L for the symmetric divergence form operator in $L^2(M)$ given formally in a chart U by

$$Lf = \mu(x)^{-1} \sum_{i,j=1}^{n} \frac{\partial}{\partial x^i} \left(\mu(x) a^{ij}(x) \frac{\partial f}{\partial x^i} \right).$$

We say that a continuous map $t \mapsto u_t : [0, \infty) \to L^2(M)$ is a solution of the heat equation

$$\partial u / \partial t = Lu$$

with Neumann boundary conditions if $u \in L^2([0, t] \times \mathcal{D})$ for all $t > 0$ and for all $\phi \in \mathcal{D}$ we have

$$\int_M \phi u_t dm - \int_M \phi u_0 dm = -\int_0^t \int_M \langle \nabla \phi, \nabla u_s \rangle dm ds.$$

When $\mathcal{D}$ is replaced by $\mathcal{D}_0$ we get the notion of a solution with Dirichlet boundary conditions. When $\mathcal{D}$ is replaced by $\mathcal{D}_K$ we say u has Dirichlet boundary conditions on K and Neumann boundary conditions at infinity. It is well known that, for a given initial function $u_0 \in L^2(M)$, there exist unique solutions, in all three cases. Moreover these solutions may be expressed in terms of fundamental solutions or heat kernels which we denote, respectively, p, p_0 and p_K. See for example [LM],[S2]. Thus, for example, in the Neumann case we have

$$u(t,x) = \int_M p(t,x,y)u_0(y)m(dy).$$

Of course we have $p_0 \leq p$ and $p_K \leq p$.

The distance function for M is defined by

$$d(x,y) = \sup\{w(y) - w(x)\}$$

where the supremum is taken over all Lipschitz functions $w : M \to \mathbb{R}$ such that $|\nabla w| \leq 1$ almost everywhere. We emphasize that we do not assume M is complete.

Before stating our results, we shall review briefly the history of the problem we consider. The early results concern the case where $M = \mathbb{R}^n$ and $\lambda(\mathbb{R}^n) < \infty$, where, in particular, $p = p_0$. In 1968, Varadhan [V1],[V2] considered the case of the non-divergence form operator

$$Lf = \sum_{i,j=1}^{n} a^{ij}(x)\frac{\partial^2 f}{\partial x^i \partial x^j}.$$

He proved, under the assumption that the metric a is uniformly Hölder continuous, the fundamental asymptotic result, as $t \to 0$

$$t \log p(t,x,y) \to -d(x,y)^2/4.$$

Soon afterwards, Aronson obtained, in the divergence form case, and without any hypothesis of continuity on the metric, global Gaussian estimates on the heat kernel, from which follow immediately the asymptotic estimates

$$-Cd(x,y)^2 \leq \liminf_{t\to 0} t\log p(t,x,y) \leq \limsup_{t\to 0} t\log p(t,x,y) \leq -d(x,y)^2/C.$$

Aronson's Gaussian estimates are of fundamental importance in the study of linear and non-linear heat equations – in particular, the absence of regularity assumptions is relevant in the modelling of many physical systems, as well as in more theoretical developments. The question whether one can take $C = 1$ in the asymptotic estimates, and so recover Varadhan's formula, without regularity assumptions, has since remained open.

Two major advances, relevant to this question, were made around 1986. Firstly, in the smooth case, and for a complete Riemannian manifold with Ricci curvature bounded below, Li and Yau [LY] obtained upper and lower Gaussian estimates on the heat kernel, from which Varadhan's asymptotic result follows immediately. Secondly, Davies [D1] succeeded in sharpening Aronson's upper estimate in $\mathbb{R}^n$ enough to give the upper estimate that would be needed to generalize Varadhan's formula. Later, Davies [D3] also gave an adequate upper estimate for Riemannian manifolds, without smoothness or curvature bounds. In collaboration with Dan Stroock [NS], we obtained a Gaussian lower bound, which complements Davies' upper bound in $\mathbb{R}^n$ and allows one to deduce small time asmptotics when the metric is only continuous but the measure is still Lipschitz. Zheng [Z] recently proved Varadhan's formula in $\mathbb{R}^n$, by a probabilistic method, in the case where the metric a is constant, but allowing a general measure m.

There remain important open problems in the investigation small time asymptotics in the absence of local ellipticity or symmetry of the operator, and in spaces that are not locally approximately Euclidean. We mention some significant results in these directions. Léandre [L1],[L2] has proved a version of Varadhan's formula for subelliptic operators of Hörmander type. Sturm [S2] has a very general form of Davies' upper bound, which applies to a general class of Dirichlet spaces. Hsu [H] has proved a version of Varadhan's formula in the non-symmetric case, involving a extra geometric condition, which he shows to be necessary.

Here is the main result of this paper.

Theorem 1.1. *Uniformly on compact sets in $M \times M$, as $t \to 0$*

$$t \log p(t,x,y) \to -d(x,y)^2/4,$$
$$t \log p_0(t,x,y) \to -d(x,y)^2/4.$$

Note, in particular, that the limit does not depend on the measure m. In fact we prove a more general result concerning the heat which passes through a given closed set K. Define

$$p(t,x,K,y) = p(t,x,y) - p_K(t,x,y),$$
$$p_0(t,x,K,y) = p_0(t,x,y) - p_0^{M \setminus K}(t,x,y).$$

Here we have used the superscript $M \setminus K$ to indicate that we consider the given notion, here the Dirichlet heat kernel, relative to the open submanifold $M \setminus K$. We will do this systematically. Define also

$$d(x,K,y) = \inf\{d(x,z) + d(z,y) : z \in K\}.$$

Theorem 1.2. *Assume that K is the closure of its interior. Uniformly on compact sets in $M \times M$, as $t \to 0$*

$$t \log p(t,x,K,y) \to -d(x,K,y)^2/4,$$
$$t \log p_0(t,x,K,y) \to -d(x,K,y)^2/4.$$

The fact that the Dirichlet and Neumann limits are the same in these theorems is a manifestation of the "principle of not feeling the boundary". We also prove the following result which expresses the same principle in a stronger form, but subject to an additional hypothesis. Given an open set $U \subseteq M$, define a neighbourhood of the diagonal in $U \times U$

$$\Delta_M(U) = \{(x,y) \in U \times U : d(x,y) < d(x, M \setminus U, y)\}.$$

Theorem 1.3. *Uniformly on compact sets in $\Delta_M(U)$, as $t \to 0$*

$$p_{M\setminus U}(t,x,y)/p(t,x,y) \to 1,$$
$$p_0^U(t,x,y)/p_0(t,x,y) \to 1.$$

Here is the plan of the paper. In §2 we prove a global upper bound on the heat kernel $p(t,x,K,y)$ for an arbitrary closed set K, which immediately gives the upper estimates needed for Theorems 1.1 and 1.2. In §3 we introduce a second distance function $d_0(x,y)$, defined in terms of paths of least action, and show that $d = d_0$. Then in §4 we obtain the asymptotic lower bounds needed to complete the proofs of Theorems 1.1 and 1.2. A key step in the argument for the lower bound of Theorem 1.1 and also the proof of Theorem 1.3, involves the upper bound of Theorem 1.2. The following facts will be needed in §2 and §4. The first is easy and well known; see [S2], so we omit the proof.

Proposition 1.4. *Let u be a solution of $\partial u/\partial t = Lu$ on $[0,\infty)\times M$ with Neumann boundary conditions. Let ϕ be a Lipschitz function on M, bounded with bounded derivative. Then*

$$\begin{aligned}&\int_M \phi u_t^2 dm - \int_M \phi u_0^2 dm\\ &\quad = -2\int_0^t\int_M \phi|\nabla u_s|^2 dmds - 2\int_0^t\int_M u_s\langle\nabla\phi,\nabla u_s\rangle dmds.\end{aligned}$$

Proposition 1.5. *Let u be a bounded solution of $\partial u/\partial t = Lu$ on $[0,\infty)\times M$ with Dirichlet boundary conditions. Let $\phi : [0,\infty)\times M \to \mathbb{R}$ be Lipschitz and of compact support. Then for all $f \in C^2(\mathbb{R})$*

$$\begin{aligned}&\int_M \phi_t f(u_t) dm - \int_M \phi_0 f(u_0) dm\\ &\quad = \int_0^t\int_M \frac{\partial\phi}{\partial s} f(u_s) dmds - \int_0^t\int_M \phi_s f''(u_s)|\nabla u_s|^2 dmds\\ &\qquad - \int_0^t\int_M \phi_s f'(u_s)\langle\nabla\phi_s,\nabla u_s\rangle dmds.\end{aligned}$$

Proof. Consider
$$u_t^{(n)} = n^{-1}\int_t^{t+n^{-1}} u_s ds.$$
Then $u_t^{(n)} \to u_t$ in $L^2(M)$ and $u^{(n)} \to u$ in $L^2([0,t],W^{1,2}(M))$ for all t, as $n\to\infty$. So it suffices to prove the identity for $u^{(n)}$. In addition to being a solution, $u^{(n)}$ has the property that $t \mapsto u_t^{(n)} : [0,\infty) \to W^{1,2}(M)$ is continuous. Let us assume then that u has this property.

We deal first with the case where ϕ is independent of t. Denote by $\mathcal{A}$ the set of those $f \in C^2(\mathbb{R})$ such that the identity holds whenever $\phi \in L^\infty(M)\cap W^{1,2}(M)$ and ϕ has compact support. Obviously $\mathcal{A}$ is a vector space, which contains the constants. By dominated convergence, $\mathcal{A}$ is closed in $C^2(\mathbb{R})$. The fact that u is a solution says that $f(u) = u$ belongs to $\mathcal{A}$. So by the density of polynomials in $C^2(\mathbb{R})$, it suffices to show that $\mathcal{A}$ is an algebra.

Let $f, g \in \mathcal{A}$ and let $\phi \in L^\infty(M) \cap W^{1,2}(M)$ of compact support. Then $\phi f(u_t), \phi g(u_t) \in L^\infty(M) \cap W^{1,2}(M)$ for all t. Fix n and set $\underline{s} = n^{-1}\lfloor ns/t \rfloor, \bar{s} = n^{-1}\lceil ns/t \rceil$. Then by splitting the interval $[0,t]$ into n subintervals, we deduce from the identities for f and g that

$$\begin{aligned}
&\int_M \phi f(u_t) g(u_t) dm - \int_M \phi f(u_0) g(u_0) dm \\
&= - \int_0^t \int_M \phi \{ f(u_{\bar{s}}) g''(u_s) + f''(u_s) g(u_{\underline{s}}) \} |\nabla u_s|^2 dm ds \\
&\quad - \int_0^t \int_M \phi f'(u_{\bar{s}}) g'(u_s) \langle \nabla u_{\bar{s}}, \nabla u_s \rangle dm ds \\
&\quad - \int_0^t \int_M \phi f'(u_s) g'(u_{\underline{s}}) \langle \nabla u_{\underline{s}}, \nabla u_s \rangle dm ds \\
&\quad - \int_0^t \int_M \{ f(u_{\bar{s}}) g'(u_s) + f'(u_s) g(u_{\underline{s}}) \} \langle \nabla \phi, \nabla u_s \rangle dm ds.
\end{aligned}$$

This yields the desired identity for the product fg on letting $n \to \infty$.

We extend to the case where ϕ depends on t by a similar argument, first reducing to the case where $t \mapsto \phi_t : [0,\infty) \to W^{1,2}(M)$ is continuous, and then letting $n \to \infty$ in the identity

$$\begin{aligned}
&\int_M \phi_t f(u_t) dm - \int_M \phi_0 f(u_0) dm \\
&= \int_0^t \int_M \frac{\partial \phi}{\partial s} f(u_{\bar{s}}) dm ds - \int_0^t \int_M \phi_{\underline{s}} f''(u_s) |\nabla u_s|^2 dm ds \\
&\quad - \int_0^t \int_M \phi_{\underline{s}} f'(u_s) \langle \nabla \phi_{\underline{s}}, \nabla u_s \rangle dm ds. \qquad \square
\end{aligned}$$

Certain of the results of this paper have been announced in [N2]. I would like to thank Weian Zheng for posing the question which led to this work and to thank Brian Davies for some helpful remarks.

2. Upper bounds

In this section we prove an upper bound on the heat kernel $p(t,x,K,y)$, giving the temperature at y due to unit heat starting from x and passing through a closed set K. The basic argument, which deals with the case $K = M$, is well known: see [D3],[S2]. Here we combine that argument with a reflection principle to deal with the general case.

We recall an argument of Gaffney [G]. Let $A, B \subseteq M$ be Borel sets and let $w : M \to \mathbb{R}$ be a bounded Lipschitz function, constant on A and B, such that

$|\nabla w| \leq 1$ almost everywhere. Denote by u_t, v_t solutions to the heat equation with Neumann boundary conditions, with, respectively, $u_0 = 1_A, v_0 = 1_B$. Fix $\alpha \in \mathbb{R}$ and set

$$g(t) = \int_M (e^{\alpha w} u_t)^2 dm.$$

By Proposition 1.4, g is differentiable almost everywhere with

$$\begin{aligned} g'(t) &= -2 \int_M e^{2\alpha w} |\nabla u_t|^2 dm - 4\alpha \int_M e^{2\alpha w} \langle \nabla u_t, u_t \nabla w \rangle dm \\ &\leq 2\alpha^2 \int_M e^{2\alpha w} u_t^2 |\nabla w|^2 dm \leq 2\alpha^2 g(t). \end{aligned}$$

So, by Gronwall's Lemma, $g(t) \leq e^{2\alpha^2 t} g(0)$. Thus

$$\|e^{\alpha w} u_t\|_2 \leq e^{\alpha^2 t} \|e^{\alpha w} u_0\|_2 = m(A)^{1/2} e^{\alpha w(A) + \alpha^2 t}$$

and by the same argument

$$\|e^{-\alpha w} v_t\|_2 \leq m(B)^{1/2} e^{-\alpha w(B) + \alpha^2 t}.$$

Hence for the heat kernel we obtain

$$\begin{aligned} \int_A \int_B p(t,x,y) m(dy) m(dx) &= \int_M u_{t/2} v_{t/2} dm \\ &= \int_M (e^{\alpha w} u_{t/2})(e^{-\alpha w} v_{t/2}) dm \\ &\leq m(A)^{1/2} m(B)^{1/2} e^{\alpha(w(A) - w(B)) + \alpha^2 t} \end{aligned}$$

and, on optimizing over α and w,

$$\int_A \int_B p(t,x,y) m(dy) m(dx) \leq m(A)^{1/2} m(B)^{1/2} e^{-d(A,B)^2/4t}$$

where

$$d(A,B) = \sup\{w(B) - w(A)\}.$$

Fix now a closed set $K \subseteq M$. Recall that

$$p(t,x,K,y) = p(t,x,y) - p_K(t,x,y)$$

where p_K is the heat kernel in $M \setminus K$ with Dirichlet conditions on K and Neumann conditions at infinity. We propose to combine a mild generalization of Gaffney's argument with a general form of the reflection principle, in order to deduce an upper bound on $p(t,x,K,y)$. In fact, Gaffney's argument can be expressed in terms of the Dirichlet space structure alone: see for example [S2].

Consider the Dirichlet space $\tilde{M} = K \cup (M \setminus K)^+ \cup (M \setminus K)^-$ obtained by glueing together two copies of M over the set K. Then $\tilde{M}$ inherits a metric from M, defined almost everywhere, and we have a measure $\tilde{m}$ on $\tilde{M}$ given by

$$\tilde{m}(A) = \begin{cases} 2m(A) & \text{if } A \subseteq K \\ m(A) & \text{if } A \cap K = \emptyset. \end{cases}$$

On $W^{1,2}(\tilde{M})$ there is a Dirichlet form given by

$$\tilde{\mathcal{E}}(\tilde{f}) = \int_{\tilde{M}} |\nabla \tilde{f}|^2 d\tilde{m}.$$

Given any function $\tilde{f}$ on $\tilde{M}$ we obtain two functions f^+, f^- on M by restricting $\tilde{f}$ to $K \cup (M \setminus K)^+$ or to $K \cup (M \setminus K)^-$. Set $f = f^+ + f^-, f_K = f^+ - f^-$. Then it is easy to check that $\tilde{f} \mapsto (f, f_K)/\sqrt{2}$ gives an isometry

$$W^{1,2}(\tilde{M}) \to W^{1,2}(M) \oplus W^{1,2}_K(M).$$

Let $\tilde{u}$ be a solution of the heat equation for $\tilde{\mathcal{E}}$, with Neumann boundary conditions. Thus $t \mapsto \tilde{u}_t : [0, \infty) \to L^2(\tilde{M})$ is continuous, $\tilde{u}_t \in W^{1,2}(\tilde{M})$ for all t and, for all $\tilde{\phi} \in W^{1,2}(\tilde{M})$

$$\int_{\tilde{M}} \tilde{\phi}\tilde{u}_t d\tilde{m} - \int_{\tilde{M}} \tilde{\phi}\tilde{u}_0 d\tilde{m} = -\int_0^t \int_{\tilde{M}} \langle \nabla\tilde{\phi}, \nabla\tilde{u}_s \rangle d\tilde{m} ds.$$

By suitable choice of test functions $\tilde{\phi}$, we deduce that $u = u^+ + u^-$ satisfies the heat equation for $(\mathcal{E}, \mathcal{D})$, and $u_K = u^+ - u^-$ satisfies the heat equation for $(\mathcal{E}, \mathcal{D}_K)$. Hence the heat kernel for $\tilde{\mathcal{E}}$ is given by

$$\tilde{p}(t,x,y) = \begin{cases} \frac{1}{2}p(t,x,y) & \text{for } x \in K \text{ or } y \in K, \\ \frac{1}{2}(p + p_K)(t,x,y) & \text{for } x, y \in (M \setminus K)^+, \\ \frac{1}{2}(p - p_K)(t,x,y) & \text{for } x \in (M \setminus K)^+, y \in (M \setminus K)^-. \end{cases}$$

For Borel sets $A, B \subseteq M \setminus K$ we define

$$d(A, K, B) = \sup\{w^+(B) - w^-(A)\}$$

where $w^+, w^- : M \to \mathbb{R}$ are Lipschitz functions, w^+ constant on B, w^- constant on A, such that $|\nabla w^+|, |\nabla w^-| \leq 1$ almost everywhere and $w^+ = w^-$ on K. It follows that

$$d(A, K, B) = \tilde{d}(\tilde{A}, \tilde{B})$$

where $\tilde{A}$ is the lifting of A in $(M \setminus K)^-$, $\tilde{B}$ is the lifting of B in $(M \setminus K)^+$, and

$$\tilde{d}(\tilde{A}, \tilde{B}) = \sup\{\tilde{w}(\tilde{B}) - \tilde{w}(\tilde{A})\}$$

the supremum taken over Lipschitz functions $\tilde{w} : \tilde{M} \to \mathbb{R}$, constant on $\tilde{A}$ and $\tilde{B}$, such that $|\nabla \tilde{w}| \leq 1$ almost everywhere.

Now Gaffney's argument applies without alteration in $\tilde{M}$, so we have

$$\int_{\tilde{A}} \int_{\tilde{B}} \tilde{p}(t,x,y)\tilde{m}(dy)\tilde{m}(dx) \leq \tilde{m}(\tilde{A})^{1/2}\tilde{m}(\tilde{B})^{1/2}e^{-\tilde{d}(\tilde{A},\tilde{B})^2/4t}.$$

Hence we deduce

$$\int_A \int_B p(t,x,K,y)m(dy)m(dx) \leq 2m(A)^{1/2}m(B)^{1/2}e^{-d(A,K,B)^2/4t}.$$

Note that the same estimate remains valid when either A or B intersect K, because, in that case, $d(A, K, B) = d(A, B)$, and the original argument may be used.

Moreover there is a well established way to deduce, from Gaffney's integrated estimate, a pointwise estimate on the heat kernel, using Moser's parabolic Harnack inequality [M1],[M2]. In the generality we require here, this procedure is found in [S2], to which we refer for the details. We deduce from [S2], Theorem 2.6, applied to $\tilde{p}$, the following pointwise estimate. Given an open set $U \subseteq \mathbb{R}^n$ and $\delta > 0$, set

$$U(\delta) = \{x \in U : |x - x'| \leq \delta \text{ implies } x' \in U\}.$$

Theorem 2.1. *Let K be a closed set in M. Let U, V be charts such that $\lambda = \max\{\lambda(U), \lambda(V)\} < \infty$. There is a constant $C(\lambda, n) < \infty$ such that, for all $\delta > 0$, all $t > 0$, all $x \in U(\delta)$ and all $y \in V(\delta)$*

$$p(t, x, K, y) \leq C \max\{t^{-n/2}, \delta^{-n}\}(1 + d(x, K, y)^2/t)^{n/2} e^{-d(x,K,y)^2/4t}.$$

This estimate shows in particular that, for all $\varepsilon, \delta > 0$, all $t < \delta^2$, all $x \in U(\delta)$ and all $y \in V(\delta)$

$$t \log p(t, x, K, y) \leq -(1 - \varepsilon) d(x, K, y)^2/4 + (n/2) t \log(C/\varepsilon t),$$

which certainly implies the upper estimate in Theorem 1.2.

3 The distance function

Recall that for $x, y \in M$ we define

$$d(x, y) = \sup\{w(y) - w(x)\}$$

where the supremum is taken over all Lipschitz functions $w : M \to \mathbb{R}$ with $|\nabla w| \leq 1$ almost everywhere. The main purpose of this section is to give an alternative characterization of this distance function d in terms of paths of least action. Two features of the context make this difficult: first, for a measurable Riemannian structure, some local regularization is necessary in order to define the action of a path; second, the lack of completeness allows a minimizing sequence of paths to leave all compact sets.

We begin by considering the case where $M = \mathbb{R}^n$ with $\lambda = \lambda(\mathbb{R}^n) < \infty$. Thus, for all $x \in \mathbb{R}^n$ and $\xi \in (\mathbb{R}^n)^*$

$$\lambda^{-1}|\xi|^2 \leq \sum_{i,j=1}^{n} a^{ij}(x)\xi_i\xi_j \leq \lambda|\xi|^2.$$

In this case, only the problem of local regularization remains. When, as now, M is identified as having a global chart, we will always make the metric explicit to avoid confusion with the standard metric in $\mathbb{R}^n$. Thus, for a Lipschitz path $\gamma : [0, 1] \to \mathbb{R}^n$, we write

$$|\dot{\gamma}_s|^2_{a^{-1}} = \sum_{i,j=1}^{n} (a^{-1})_{ij}(\gamma_s)\dot{\gamma}^i_s\dot{\gamma}^j_s.$$

When a is continuous, it is easy to show that

$$d(x, y)^2 = \inf_{\gamma} \int_0^1 |\dot{\gamma}_s|^2_{a^{-1}} ds$$

where the infimum is taken over Lipschitz paths with $\gamma_0 = x, \gamma_1 = y$. However it is clear that this identity must fail in general, because the right hand side may depend on the values taken by a on a set of measure zero, which the left hand side does not.

Motivated by the lower bound in [NS], let us instead define a family of distance functions, one for each continuous probability density function ϕ on $\mathbb{R}^n$, of finite variance $\sigma^2(\phi)$. Set

$$d_\phi(x,y) = \left(\inf_\gamma \int_0^1 |\dot\gamma_s|^2_{a^{-1}*\phi} ds\right)^{1/2}.$$

Thus d_ϕ is the distance function corresponding to the regularized inner product $a^{-1} * \phi$. We will show that

$$d_\phi(x,y) \to d_0(x,y) \qquad \text{as } \sigma(\phi) \to 0$$

for some distance function d_0, and then that $d_0 = d$.

The following properties are obvious:

(i) $d_\phi(x,y) \le d_\phi(x,z) + d_\phi(z,y)$,
(ii) $d_{\psi*\phi}(x,y) \to d_\phi(x,y)$ as $\sigma(\psi) \to 0$,
(iii) $(\sqrt{\lambda})^{-1}|x-y| \le d_\phi(x,y) \le \sqrt{\lambda}|x-y|$.

Proposition 3.1. *We have*

$$d_\phi(x,y) + 2\sqrt{\lambda}\sigma(\phi) \ge d(x,y).$$

Proof. Let $w : \mathbb{R}^n \to \mathbb{R}$ be a Lipschitz function with $|\nabla w|_a \le 1$ almost everywhere. Let $\gamma : [0,1] \to \mathbb{R}^n$ be a Lipschitz path with $\gamma(0) = x, \gamma(1) = y$. Then

$$\begin{aligned} w(y) - w(x) &\le (w * \phi)(y) - (w * \phi)(x) + 2\sqrt{\lambda}\sigma(\phi) \\ &= \int_0^1 \int_{\mathbb{R}^n} \langle \nabla w(z), \dot\gamma_s \rangle \phi(\gamma_s - z) dz ds + 2\sqrt{\lambda}\sigma(\phi) \\ &\le \left(\int_0^1 |\dot\gamma_s|^2_{a^{-1}*\phi} ds\right)^{1/2} + 2\sqrt{\lambda}\sigma(\phi). \end{aligned}$$

The claim follows on optimizing over w and γ. □

Proposition 3.2. *We have*

$$d_{\psi*\phi}(x,y) + 2\sqrt{\lambda}\sigma(\phi) \ge d_\psi(x,y).$$

Proof. Note the inequality

$$d_\psi(x-z, y-z) + 2\sqrt{\lambda}|z| \ge d_\psi(x,y).$$

We have

$$\begin{aligned} d_{\psi*\phi}(x,y)^2 &= \inf_\gamma \int_0^1 |\dot\gamma_s|^2_{(a^{-1}*\psi)*\phi} ds \\ &= \inf_\gamma \int_{\mathbb{R}^n} \phi(z) \int_0^1 |\dot\gamma_s|^2_{(a^{-1}*\psi)(\gamma_s - z)} ds dz \\ &\ge \int_{\mathbb{R}^n} \phi(z) d_\psi(x-z, y-z)^2 dz \end{aligned}$$

so

$$d_{\psi*\phi}(x,y) \geq d_\psi(x,y) - 2\sqrt{\lambda}\sigma(\phi). \qquad \square$$

We deduce from Proposition 3.2 that

$$\limsup_{\sigma(\psi)\to 0} d_\psi(x,y) \leq d_\phi(x,y) + 2\sqrt{\lambda}\sigma(\phi)$$

so

$$\limsup_{\sigma(\psi)\to 0} d_\psi(x,y) \leq \liminf_{\sigma(\phi)\to 0} d_\phi(x,y).$$

This shows that $d_\phi(x,y)$ converges as $\sigma(\phi) \to 0$. We denote the limit by $d_0(x,y)$ and note the following inequalities, obtained on passing to the limit in certain inequalities above:

(i) $d_0(x,y) \leq d_0(x,z) + d_0(z,y)$,
(ii) $(\sqrt{\lambda})^{-1}|x-y| \leq d_0(x,y) \leq \sqrt{\lambda}|x-y|$,
(iii) $d_0(x,y) \geq d(x,y)$,
(iv) $d_\phi(x,y)^2 \geq \int_{\mathbb{R}^n} \phi(z) d_0(x-z, y-z)^2 dz$.

We postpone the argument which shows that $d_0 = d$ until we can give it for a general manifold M, since we would have to repeat it then anyway.

Next we prove two localization results. Given an open set $U \subseteq \mathbb{R}^n$, denote by $\rho = \rho_U$ the Euclidean distance to the boundary

$$\rho(x) = \inf\{|z-x| : z \notin U\}, \qquad x \in U.$$

Let a^{-1} be a metric on U with $\lambda = \lambda(U) < \infty$. Let a_1^{-1}, a_2^{-1} be extensions of a^{-1} to $\mathbb{R}^n$ and suppose that $\lambda^1(\mathbb{R}^n), \lambda^2(\mathbb{R}^n) < \infty$. Denote by d_0^1, d_0^2 the corresponding distance functions. We introduce a neighbourhood of the diagonal in $U \times U$: define

$$\Lambda(U) = \{(x,y) \in U \times U : \rho(x) + \rho(y) > \lambda|y-x|\}.$$

Recall that $U(\varepsilon) = \{x \in U : \rho(x) > \varepsilon\}$.

Proposition 3.3. *We have*

$$d_0^1 = d_0^2 \qquad \textit{on } \Lambda(U).$$

Proof. Suppose $(x,y) \in \Lambda(U)$. Choose $\varepsilon > 0$ so that

$$\rho(x) + \rho(y) > \lambda|y-x| + 2\varepsilon.$$

Let ϕ be a probability density function, supported in the ball of radius ε in $\mathbb{R}^n$. Let $\gamma : [0,1] \to \mathbb{R}^n$ be Lipschitz, with $\gamma(0) = x, \gamma(1) = y$. If $\gamma_s \notin U(\varepsilon)$ for some s, then for $i = 1,2$

$$d_\phi^i(x,y)^2 \leq \lambda|y-x|^2 < \lambda^{-1}\big(\rho(x)+\rho(y)-2\varepsilon\big)^2 \leq \int_0^1 |\dot\gamma_s|^2_{a_i^{-1}*\phi} ds.$$

On the other hand, if $\gamma_s \in U(\varepsilon)$ for all s, then

$$\int_0^1 |\dot\gamma_s|^2_{a_1^{-1}*\phi} ds = \int_0^1 |\dot\gamma_s|^2_{a_2^{-1}*\phi} ds.$$

On taking the infimum over γ we find

$$d^1_\phi(x,y) = d^2_\phi(x,y).$$

The claim follows on letting $\varepsilon \to 0$. $\square$

We denote by d_0^U the common restriction to $\Lambda(U)$ provided by Proposition 3.3.

We return to the case of a general Lipschitz Riemannian manifold M, with distance function d. The distance function corresponding to an open set $U \subseteq M$ is given by

$$d^U(x,y) = \sup\{w(y) - w(x)\}$$

where the supremum is taken over Lipschitz functions $w : U \to \mathbb{R}$ with $|\nabla w| \le 1$ almost everywhere in U. Of course $d^U \ge d$ on $U \times U$. For each $x \in M$ the set

$$\{z \in M : d(x,z) \le r\}$$

is compact for all sufficiently small $r > 0$. Denote by $d(x,\infty)$ the supremum of such r. Define a neighbourhood of the diagonal in $M \times M$ by

$$\Delta(M) = \{(x,y) \in M \times M : d(x,y) < d(x,\infty) + d(y,\infty)\}.$$

Note that, if U is a chart with $\lambda(U) < \infty$, then $\Lambda(U) \subseteq \Delta(U)$.

Proposition 3.4. *For any open set $U \subseteq M$ we have*

$$d^U = d \qquad \text{on } \Delta(U).$$

Proof. Suppose that $(x,y) \in \Delta(U)$ and that $w : U \to \mathbb{R}$ is Lipschitz, with $|\nabla w| \le 1$ almost everywhere. Then

$$w(y) - w(x) < d^U(x,\infty) + d^U(y,\infty).$$

By adding a constant to w, we can assume that

$$w(x) > -d^U(x,\infty), \quad w(y) < d^U(y,\infty).$$

Hence the cut-off functions

$$w^-(z) = -\big(w(x) + d^U(x,z)\big)^-, \quad w^+(z) = \big(w(y) - d^U(y,z)\big)^+$$

are Lipschitz, of compact support, and satisfy $|\nabla w^\pm| \le 1$ almost everywhere. See for example [S1]. Set $\tilde w = w^- \vee w \wedge w^+$. Then $\tilde w(x) \le w(x)$, $\tilde w(y) \ge w(y)$, $\tilde w$ is Lipschitz, of compact support, and $|\nabla \tilde w| \le 1$ almost everywhere. Hence, if $U \subseteq M$, we can extend $\tilde w$ to M by setting $\tilde w = 0$ on $M \setminus U$. The claim follows on optimizing over w. $\square$

Proposition 3.5. *Assume that U is a chart with $\lambda(U) < \infty$. Then*

$$d_0^U \geq d \qquad \text{on } \Lambda(U).$$

Proof. The restriction of the metric to U extends to a metric $\tilde{a}^{-1}$ on $\mathbb{R}^n$. Denote by $\tilde{d}$ the associated distance function. Then for $(x, y) \in \Lambda(U)$,

$$d_0^U(x, y) = \tilde{d}_0(x, y) \geq \tilde{d}(x, y) = d^U(x, y) = d(x, y)$$

by Propositions 3.3 and 3.4. □

We now extend the definition of d_0 to M. Define

$$d_0(x, y) = \inf \sum_{i=1}^{k} d_0^{U_i}(z_{i-1}, z_i)$$

where the infimum is taken over all integers $k \geq 1$, all sequences of charts $U_1, \ldots, U_k$ with $\lambda(U_i) < \infty$, and all sequences of points $z_0, \ldots, z_k$ with $z_0 = x$, $z_k = y$ and $(z_{i-1}, z_i) \in \Lambda(U_i)$ for all i. Consistency with the old definition, when M has a global chart U with $\lambda(U) < \infty$, is an easy consequence of Proposition 3.3. The following properties hold:

(i) $d_0(x, y) \leq d_0(x, z) + d_0(z, y)$,
(ii) $d_0(x, y) \leq \sqrt{\lambda(U)}|x - y|$ for $(x, y) \in \Lambda(U)$,
(iii) $d_0(x, y) \geq d(x, y)$.

Property (iii) follows from Proposition 3.5 and the triangle inequality for d.

Theorem 3.6. *We have $d_0 = d$.*

Proof. Fix $x \in M$ and set $w(y) = d_0(x, y)$. We shall show that w is Lipschitz, with $|\nabla w| \leq 1$ almost everywhere. This implies that

$$d(x, y) \geq w(y) - w(x) = d_0(x, y).$$

Combined with (iii) above, this proves the theorem.

We can cover M by charts U with $\lambda(U) < \infty$. Then we can cover each chart U by Euclidean balls N such that for some $\rho > 0$, for all $y, y' \in N$ and all $|z| \leq \rho$, we have $(y - z, y' - z) \in \Lambda(U)$. Then for $y, y' \in N$ and $|z| \leq \rho$

$$\begin{aligned} |w(y - z) - w(y' - z)| &\leq d_0^U(y - z, y' - z) \\ &= \tilde{d}_0(y - z, y' - z) \leq \sqrt{\lambda(U)}|y - y'|, \end{aligned}$$

where $\tilde{d}_0$ corresponds to some extension $\tilde{a}^{-1}$ of the metric from U to the whole of $\mathbb{R}^n$. This shows, by taking $z = 0$, that w is Lipschitz on N, so has a bounded weak derivative on N.

Let ϕ be a smooth probability density function, supported on the ball of radius ρ in $\mathbb{R}^n$. Set $w_\phi = w * \phi$ on N. Then, for $y, y' \in N$,

$$w_\phi(y) - w_\phi(y') = \int_{|z| \leq \rho} \phi(z)\big(w(y - z) - w(y' - z)\big)dz$$

so

$$\big(w_\phi(y)-w_\phi(y')\big)^2 \le \int_{|z|\le\rho} \phi(z)\big(w(y-z)-w(y'-z)\big)^2 dz$$
$$\le \int_{\mathbb{R}} \phi(z)\tilde{d}_0(y-z,y'-z)^2 dz \le \tilde{d}_\phi(y,y')^2.$$

We used the inequality (iv), written after Proposition 3.2, at the final step. Now $\tilde{a}^{-1}*\phi$ is continuous, so given $\varepsilon>0$, there is a $\delta\in(0,\rho)$ such that, for $y,y'\in N$,

$$(\tilde{a}^{-1}*\phi)(y') \le (1+\varepsilon)(\tilde{a}^{-1}*\phi)(y) = (1+\varepsilon)(a^{-1}*\phi)(y).$$

Set $\gamma_s = y+s(y'-y)$. Then

$$\tilde{d}_\phi(y,y')^2 \le \int_0^1 |\dot\gamma_s|^2_{\tilde{a}^{-1}*\phi(\gamma_s)} ds$$
$$\le (1+\varepsilon)\int_0^1 |\dot\gamma_s|^2_{\tilde{a}^{-1}*\phi(y)} ds$$
$$= (1+\varepsilon)|y-y'|^2_{a^{-1}*\phi(y)}.$$

Hence

$$|\nabla w_\phi|_{(a^{-1}*\phi)^{-1}} \le 1 \qquad \text{on } N.$$

On letting $\sigma(\phi)\to 0$, we obtain $|\nabla w|_a \le 1$ almost everywhere on N, as required.□

We mention that the problem of characterizing the distance function d in terms of paths has already been solved by De Cecco and Palmieri [DP1],[DP2], who showed that $d=\delta$, where

$$\delta(x,y) = \sup_N \left(\inf_{\gamma\perp N}\int_0^1 |\dot\gamma_s|^2_{a^{-1}} ds\right)^{1/2}$$

where the supremum is taken over all sets $N\subseteq M$ with $m(N)=0$ and where the infimum is taken over all Lipschitz paths $\gamma:[0,1]\to M$ such that $\gamma(0)=x$, $\gamma(1)=y$ and $\gamma(s)\notin N$ for almost all s.

Let us show directly, in the case where $M=\mathbb{R}^n$ and $\lambda(\mathbb{R}^n)<\infty$, that $\delta\le d_0$. Given $\varepsilon>0$, we can find a continuous probability density function ϕ, supported in the ball of radius ε, and a Lipschitz path $\gamma:[0,1]\to M$ with $\gamma(0)=x,\gamma(1)=y$ such that

$$\int_0^1 |\dot\gamma_s|^2_{a^{-1}*\phi} ds \le d_0(x,y)^2+\varepsilon.$$

Fix $N\subseteq\mathbb{R}^n$ with $m(N)=0$. Define for $z\in\mathbb{R}^n$

$$\eta_s(z) = \left(\frac{s}{\varepsilon}\wedge 1\wedge\left(\frac{1-s}{\varepsilon}\right)\right) z$$

and set

$$N^\gamma = \Big\{z\in\mathbb{R}^n : \int_0^1 1_{\gamma_s+\eta_s(z)\in N} ds > 0\Big\}.$$

By Fubini's theorem, $m(N^\gamma) = 0$, so we can find $z \notin N^\gamma$ with $|z| \le \varepsilon$ such that

$$\int_0^1 |\dot\gamma_s|^2_{a^{-1}(\gamma_s+z)}\,ds \le d_0(x,y)^2 + 2\varepsilon.$$

But then $\gamma + \eta(z) \perp N$ and

$$\int_0^1 |\dot\gamma_s + \dot\eta_s(z)|^2_{a^{-1}}\,ds \le d_0(x,y)^2 + C(\lambda)\varepsilon.$$

Since $\varepsilon > 0$ and N were arbitrary, this shows that $\delta \le d_0$.

It is easy to extend this inequality to general M, and to show that $\delta \ge d$. So we can recover De Cecco and Palmieri's result $d = \delta$ from Proposition 3.6.

4. Lower bounds

In this section we establish the lower bound needed to complete the proof of Theorem 1.1. We also complete the proofs of Theorems 1.2 and 1.3. Recall that M is a Lipschitz Riemannian manifold, m is a Borel measure on M, and the basic assumption $(*)$ is in force. We have to show, for the Dirichlet heat kernel $p_0(t,x,y)$, for every compact set $K \subseteq M$ and every $\varepsilon > 0$, there is a $\delta > 0$ such that for all $t \in (0,\delta)$ and $x, y \in K$

$$t \log p_0(t,x,y) \ge -d_0(x,y)^2/4 - \varepsilon.$$

Whilst it would be nice to deduce such an asymptotic statement from a simple global lower bound, as we did for upper bounds in §2, this has not been achieved. Indeed our analysis allows that the rate of convergence in the lower estimate as $t \to 0$ may depend on the roughness of m and on the complexity of a minimizing sequence of paths for the distance function. In [N1],[N3] we proved estimates for heat kernels with rapidly oscillating coefficients, which show that this is inevitable.

We begin with the case where $M = \mathbb{R}^n$ with $\lambda(\mathbb{R}^n) < \infty$, where most of the analysis is done. In the subcase where μ is Lipschitz, the operator takes the form

$$Lf = \sum_{i,j=1}^n \frac{\partial}{\partial x^i}\left(a^{ij}(x)\frac{\partial f}{\partial x^j}\right) + \left(\frac{\partial \log \mu}{\partial x^i}\right) a^{ij}(x)\frac{\partial f}{\partial x^j}$$

and the global lower bound in [NS], together with §3, gives the desired asymptotics. Another subcase, where a is constant each side of a hyperplane and where μ is the associated Riemannian volume, was dealt with recently by Zheng [Z]. Our method for the general case is an elaboration of the method used in [NS], in which μ is approximated in $L^2(M)$ by a Lipschitz function.

Next we prove a lower bound for the Dirichlet heat kernel $p_0^U(t,x,y)$ of an open set $U \subseteq \mathbb{R}^n$ with $\lambda(U) < \infty$. The method uses the upper bound of Theorem 2.1 to control $p(t,x,\mathbb{R}^n \setminus U, y)$ together with the identity

$$p_0^U(t,x,y) = p(t,x,y) - p(t,x,\mathbb{R}^n \setminus U, y).$$

The general lower bound then follows by a chaining argument.

Theorem 4.1. *Assume that $M = \mathbb{R}^n$ and that $\lambda(\mathbb{R}^n) < \infty$. For every $R < \infty$ and $\varepsilon > 0$ there is a $\delta > 0$ such that for all $t \in (0, \delta)$ and $x, y \in \mathbb{R}^n$ with $|x|, |y| \le R$*

$$t \log p(t, x, y) \ge -d_0(x, y)^2/4 - \varepsilon.$$

Proof. Denote by ρ_τ the classical heat kernel in $\mathbb{R}^n$

$$\rho_\tau(x) = (4\pi\tau)^{-n/2} e^{-|x|^2/4\tau}.$$

Let d_τ denote the Riemannian distance function corresponding to the smoothed metric $a^{-1} * \rho_\tau$, which was written as d_{ρ_τ} in §3. We know by §3 that for all x, y

$$d_\tau(x, y) \to d_0(x, y) \qquad \text{as } \tau \to 0.$$

By equicontinuity, this convergence is uniform on compact sets.

Fix $R \in (0, \infty)$ and $\beta, \delta, \eta, \tau \in (0, 1/2)$. Fix also $t \in (0, 1]$ and $x, y \in \mathbb{R}^n$ with $|x|, |y| \le R$. We can find a Lipschitz path $\gamma : [0, t] \to \mathbb{R}^n$ such that

$$\gamma_s = \begin{cases} x & \text{for } s \le \beta t/2 \\ y & \text{for } s \ge (1 - \beta/2)t \end{cases}$$

and

$$\int_0^t |\dot\gamma_s|^2_{a^{-1} * \rho_\tau} ds = d_\tau(x, y)^2/(1 - \beta)t$$

and then moreover, for all s,

$$|\gamma_s| \le \lambda R, \quad |\dot\gamma_s| \le C|y - x|/t.$$

Choose $r \in (0, \infty)$ so that

$$\int_{|z|>r} \rho_\tau dz \le \lambda^{-4}\delta^2/2$$

and then $\sigma \in (0, \infty)$ so that

$$\int_{|z| \le R + r + \lambda R} (\rho_\sigma * \mu - \mu)^2 dz \le \lambda^{-2}\tau^{n/2}\delta^2/2.$$

Set $\psi_s(z) = \rho_\tau(z - \gamma_s)$ and $\nu = \rho_s * \mu$. Then $\lambda^{-1} \le \nu(z) \le \lambda$ for all z. Moreover for all $s \in [0, t]$

$$\int_{\mathbb{R}^n} \left((\mu/\nu) - 1\right)^2 \psi_s dz \le \tau^{-n/2}\lambda^2 \int_{|z| \le R + r + \lambda R} (\mu - \nu)^2 dz + \lambda^4 \int_{|z|>r} \rho_\tau dz \le \delta^2.$$

Consider the probability measure π on $\mathbb{R}^n$ given by

$$d\pi/dm \propto \psi_{t/2}/\nu.$$

The normalizing constant is then

$$\alpha = \int_{\mathbb{R}^n} (\psi_{t/2}/\nu) dm$$

and by Jensen's inequality

$$1 - \alpha \leq \int_{\mathbb{R}^n} \big(1 - (\mu/\nu)\big)\psi_{t/2} dz \leq \delta.$$

In particular $\alpha \geq 1/2$, so $|d\pi/dm| \leq 2\lambda\tau^{-n/2}$.

We have

$$\begin{aligned} p(t,x,y) &= \int_{\mathbb{R}^n} p(t/2,x,z)p(t/2,z,y)m(dz) \\ &\geq C^{-1}\tau^{n/2}\int_{\mathbb{R}^n} p(t/2,x,z)p(t/2,z,y)\pi(dz) \end{aligned}$$

so by Jensen's inequality again

$$\log p(t,x,y) \geq -C + (n/2)\log\tau + \alpha^{-1}\{G(t/2) + \hat{G}(t/2)\} \tag{$\dagger$}$$

where

$$\begin{aligned} G(s) &= \int_{\mathbb{R}^n} (\psi_s/\nu)(z)\log p(s,x,z)m(dz), \\ \hat{G}(s) &= \int_{\mathbb{R}^n} (\psi_s/\nu)(z)\log p(s,z,y)m(dz). \end{aligned}$$

The following crude Gaussian bounds are due in the case $\mu \equiv 1$ to Aronson [A]. See for example [D2]. The extension to general μ is straightforward. Details may be found, for example, in [N3]. There is a constant $C(\lambda, n) < \infty$ such that, for all $t > 0$ and $x, y \in \mathbb{R}^n$,

$$C^{-1}t^{-n/2}e^{-C|y-x|^2/t} \leq p(t,x,y) \leq Ct^{-n/2}e^{-|y-x|^2/Ct}.$$

We deduce that

$$G(\beta t/2) \geq -C - (n/2)\log(\beta t/2) - C\tau/(\beta t).$$

Fix $\kappa > 0$ and set $p_s(z) = p(s,x,z) + \kappa$. Define

$$G_\kappa(s) = \int_{\mathbb{R}^n} (\psi_s/\nu)\log p_s dm.$$

Then by an obvious extension of Proposition 1.5, G_κ is differentiable almost everywhere with

$$\begin{aligned} G'_\kappa(s) = &\int_{\mathbb{R}^n} \langle\nabla\log p_s, a\nabla\log p_s\rangle(\psi_s/\nu)dm \\ &- \int_{\mathbb{R}^n} \langle\nabla\log\psi_s, a\nabla\log p_s\rangle(\psi_s/\nu)dm \\ &+ \int_{\mathbb{R}^n} \langle\nabla\log\nu, a\nabla\log p_s\rangle(\psi_s/\nu)dm \\ &+ \int_{\mathbb{R}^n} \langle\dot{\gamma}_s, \nabla\log p_s\rangle(\psi_s/\nu)dm \\ &+ \int_{\mathbb{R}^n} \langle\dot{\gamma}_s, \nabla\log p_s\rangle\big((\mu/\nu) - 1\big)\psi_s dz \\ &- \int_{\mathbb{R}^n} \langle\dot{\gamma}_s, \nabla\log\psi_s\rangle\big((\mu/\nu) - 1\big)(\log p_s)\psi_s dz \\ = &\; I_1 + I_2 + I_3 + I_4 + I_5 + I_6. \end{aligned}$$

Note that $I_1 > 0$. We exploit this fact using quadratic inequalities of the form $A^2 + AB \geq -B^2/4$ to obtain a lower bound for $G'_\kappa(s)$. We have

$$\begin{aligned}
(\eta/3)I_1 + I_2 &\geq -(C/\eta)\int_{\mathbb{R}^n} |\nabla \log \psi_s|^2 \psi_s dz \geq -C/\eta\tau, \\
(\eta/3)I_1 + I_3 &\geq -C\|\nabla \log \nu\|_\infty^2/\eta, \\
(1-\eta)I_1 + I_4 &\geq -\frac{1}{4(1-\eta)}\int_{\mathbb{R}^n} |\dot\gamma_s|^2_{a^{-1}(z)}(\mu/\nu)(z)\psi_s(z)dz \\
&\geq -\frac{1}{4(1-\eta)}\int_{\mathbb{R}^n} |\dot\gamma_s|^2_{a^{-1}(z)}\psi_s(z)dz - C|\dot\gamma_s|^2\int_{\mathbb{R}^n}\big((\mu/\nu)-1\big)^2\psi_s dz \\
&\geq -|\dot\gamma_s|^2_{a^{-1}*\rho_\tau}/4(1-\eta) - C\delta^2|y-x|^2/t^2, \\
(\eta/3)I_1 + I_5 &\geq -(C/\eta)|\dot\gamma_s|^2\int_{\mathbb{R}^n}\big((\mu/\nu)-1\big)^2\psi_s ds \\
&\geq -C\delta^2|y-x|^2/\eta t^2, \\
I_6 &\geq -(C/\eta)|\dot\gamma_s|^2\int_{\mathbb{R}^n}\big((\mu/\nu)-1\big)^2\psi_s dz - \eta\int_{\mathbb{R}^n}|\nabla \log \psi_s|^2(\log p_s)^2\psi_s dz.
\end{aligned}$$

To estimate this final integral we use the crude Gaussian bounnds above, which imply for $\beta t/2 \leq s \leq t/2$

$$\begin{aligned}
(\log p_s)^2 &\leq (1+|z-x|^2)^2/s^2 \\
&\leq C(1+|y-x|^4+|z-\gamma_s|^4)/\beta^2 t^2
\end{aligned}$$

where we have used

$$|z-x| \leq |z-\gamma_s| + |\gamma_s - x| \leq |z-\gamma_s| + Cs|y-x|/t.$$

Then

$$\int_{\mathbb{R}^n}|\nabla \log \psi_s|^2(\log p_s)^2\psi_s dz \leq C(1+|y-x|^4)/\beta^2\tau t^2.$$

Thus we obtain for $\beta t/2 \leq s \leq t/2$ the lower bound

$$\begin{aligned}
G'_\kappa(s) \geq &- |\dot\gamma_s|^2_{a^{-1}*\rho_\tau}/4(1-\eta) \\
&- (C/t^2)(\delta^2|y-x|^2/\eta + \eta(1+|y-x|^4)/\beta^2\tau) \\
&- C(1/\eta\tau + \|\nabla \log \nu\|_\infty^2/\eta).
\end{aligned}$$

Hence

$$\begin{aligned}
G_\kappa(t/2) &= G_\kappa(\varepsilon t/2) + \int_{\beta t/2}^{t/2} G'_\kappa(s) \\
&\geq -\frac{1}{4(1-\eta)}\int_0^{t/2}|\dot\gamma_s|^2_{a^{-1}*\rho_\tau}ds \\
&\quad - (C/t)(\delta^2|y-x|^2/\eta + \tau/\beta + \eta(1+|y-x|^4)/\beta^2\tau) \\
&\quad - Ct(1/\eta\tau + \|\nabla \log \nu\|_\infty^2/\eta).
\end{aligned}$$

The right-hand side is independent of $\kappa > 0$, so is also a lower bound for $G(t/2)$.

By symmetry there is an analogous lower bound for $\hat{G}(t/2)$. Hence, on substituting in (†), we obtain

$$
\begin{aligned}
t \log p(t,x,y) \geq & -d_\tau(x,y)^2/4(1-\eta)(1-\beta)(1-\delta) \\
& - C\big(\delta^2|y-x|^2/\eta + \tau/\beta + \eta(1+|y-x|^4)/\beta^2\tau\big) \\
& - Ct^2(1/\eta\tau + \|\nabla \log \nu\|_\infty^2/\eta).
\end{aligned}
$$

Given $\varepsilon > 0$, we can choose β, then τ, then η, then δ, so that for all $|x|, |y| \leq R$

$$
t \log p(t,x,y) \geq -d_0(x,y)^2/4 - \varepsilon - Ct^2(1/\eta\tau + \|\nabla \log \nu\|_\infty^2/\eta).
$$

The result follows. □

The following lemma is the first step in extending Theorem 4.1 to a general manifold M.

Lemma 4.2. *Let $U \subseteq M$ be a chart with $\lambda(U) < \infty$. For every $\varepsilon > 0$ and every compact set $K \subseteq \Delta(U)$, there is a $\delta > 0$ such that for all $t \in (0,\delta)$ and $(x,y) \in K$*

$$
t \log p_0^U(t,x,y) \geq -d_0^U(x,y)^2/4 - \varepsilon.
$$

Proof. The assertion is independent of $M \setminus U$ so, since U is a chart, we can assume that $M = \mathbb{R}^n$ and $\lambda(\mathbb{R}^n) = \lambda(U)$. In this case we have

$$
p_0^U(t,x,y) = p(t,x,y) - p(t,x,\mathbb{R}^n \setminus U, y).
$$

Given $K \subseteq \Delta(U)$ compact, there is an $\eta > 0$ such that, for all $(x,y) \in K$

$$
d(x,\mathbb{R}^n \setminus U, y)^2 \geq \big(d(x,\infty) + d(\infty,y)\big)^2 > d(x,y)^2 + 12\eta.
$$

By Theorems 2.1 and 4.1, given $\varepsilon > 0$, there is a $\delta > 0$ such that for all $t \in (0,\delta)$ and $(x,y) \in K$

$$
\begin{aligned}
t \log p(t,x,y) &\geq -d(x,y)^2/4 - \varepsilon \\
t \log p(t,x,\mathbb{R}^n \setminus U, y) &\leq -d(x,\mathbb{R}^n \setminus U, y)^2/4 + \varepsilon.
\end{aligned}
$$

Hence, provided that $\delta \leq \varepsilon \leq \eta$, we have

$$
\frac{p(t,x,\mathbb{R}^n \setminus U, y)}{p(t,x,y)} \leq e^{-\eta/t} \leq e^{-1}
$$

and

$$
\begin{aligned}
t \log p_0^U(t,x,y) &\geq t \log p(t,x,y) + t \log(1 - e^{-1}) \\
&\geq -d(x,y)^2/4 - 2\varepsilon.
\end{aligned}
$$

□

We can now complete the proof of Theorem 1.1. We have to show that, for every $\varepsilon > 0$ and every compact set $K \subseteq M$, there is a $\delta > 0$ such that for all $t \in (0, \delta)$ and $x, y \in K$

$$t \log p_0(t, x, y) \geq -d_0(x, y)^2/4 - \varepsilon.$$

Recall that the distance function d_0 is defined by

$$d_0(x, y) = \inf \sum_{i=1}^{k} d_0^{U_i}(z_{i-1}, z_i)$$

where the infimum is taken over all integers $k \geq 1$, all sequences of charts $U_1, \dots, U_k$ with $\lambda(U_i) < \infty$, and all sequences of points $z_0, \dots, z_k$ with $z_0 = x, , z_k = y$ and $(z_{i-1}, z_i) \in \Lambda(U_i)$ for all i. Hence, given $\varepsilon > 0$, we can cover $M \times M$ by open sets of the form $N_0 \times N_k$ where $k \geq 1$ is an integer and where there is a sequence of charts $U_1, \dots, U_k$ with $\lambda(U_i) < \infty$ and a sequence of open sets $N_1, \dots, N_{k-1}$ such that N_i is relatively compact for all i, $N_{i-1} \times N_i \subseteq \Lambda(U_i)$ for all $i \geq 1$, and

$$d_0(x_0, x_k) \geq \sum_{i=1}^{k} d_0^{U_i}(x_{i-1}, x_i) - \varepsilon$$

whenever $x_i \in N_i$ for all i.

By Lemma 4.2, there is a $\delta > 0$ such that for all $t \in (0, \delta)$ and $x_i \in \bar{N}_i$

$$t \log p_0(t, x_{i-1}, x_i) \geq -d_0^{U_i}(x_{i-1}, x_i)^2/4 - \varepsilon/k.$$

For any $\pi_1, \dots, \pi_k \geq 0$ with $\pi_1 + \dots + \pi_k = 1$, we have

$$p_0(t, x_0, x_k) \geq \int_{N_1} m(dx_1) \dots \int_{N_{k-1}} m(dx_{k-1}) \prod_{i=1}^{k-1} p(\pi_i t, x_{i-1}, x_i)$$

so for all $x_0 \in N, x_k \in N_k$

$$t \log p_0(t, x_0, x_k) \geq \sum_{i=1}^{k-1} t \log m(N_i) + \inf \sum_{i=1}^{k-1} t \log p(\pi_i t, x_{i-1}, x_i)$$

where the infimum is taken over all $x_1 \in N_1, \dots, x_{k-1} \in N_{k-1}$. We can find $x_1^* \in \bar{N}_1, \dots, x_{k-1}^* \in \bar{N}_{k-1}$ where this infimum is achieved. Take

$$\pi_i = d_0^{U_i}(x_{i-1}^*, x_i^*) / \sum_{j=1}^{k-1} d_0^{U_j}(x_{j-1}^*, x_j^*)$$

where $x_0^* = x_0, x_k^* = x_k$. Choose $\delta > 0$ sufficiently small that for all $t \in (0, \delta)$

$$\sum_{i=1}^{k-1} t \log m(N_i) \leq \varepsilon.$$

Then for $t \in (0, \delta)$ and $x_0 \in N_0, x_k \in N_k$ we have

$$\begin{aligned} t \log p_0(t, x_0, x_k) &\geq \sum_{i=1}^{k-1} t \log m(N_i) - \sum_{i=1}^{k-1} d_0^{U_i}(x_{i-1}^*, x_i^*)^2/4\pi_i - \varepsilon \\ &\geq -d_0(x_0, x_k)^2/4 - 3\varepsilon. \end{aligned}$$

This completes the proof of Theorem 1.1.

A small variation on the argument just used also gives the lower bound needed to complete the proof of Theorem 1.2. For we have for a non-empty closed set $K \subseteq M$ and $s \in (0, t)$

$$p_0(t, x, K, y) \geq \int_K p_0(s, x, z) p_0(t - s, z, y) m(dz)$$

and

$$d(x, K, y) = \inf_{z \in K} \big(d_0(x, z) + d_0(z, y)\big).$$

So, provided K is the closure of its interior we can re-run the preceding argument with $p_0(t, x, y)$ replaced by $p_0(t, x, K, y)$ and $d(x, y)$ replaced by $d(x, K, y)$, where we make the additional requirement that $N_i \subseteq K$ for some i.

Finally we prove the principle of not feeling the boundary, Theorem 1.3. Recall that for $U \subseteq M$ open we set

$$\Delta_M(U) = \{(x, y) \in U \times U : d(x, y) < d(x, M \setminus U, y)\}.$$

We have to show that, uniformly on compacts in $\Delta_M(U)$

$$\begin{aligned} p_{M \setminus U}(t, x, y)/p(t, x, y) &\to 1, \\ p_0^U(t, x, y)/p_0(t, x, y) &\to 1. \end{aligned}$$

We have

$$\begin{aligned} p_{M \setminus U}(t, x, y) &= p(t, x, y) - p(t, x, M \setminus U, y), \\ p_0^U(t, x, y) &= p_0(t, x, y) - p_0(t, x, M \setminus U, y). \end{aligned}$$

Given $K \subseteq \Delta_M(U)$ compact, there is an $\varepsilon > 0$ such that, for all $(x, y) \in K$

$$d(x, M \setminus U, y)^2 \geq d(x, y)^2 + 12\varepsilon.$$

By Theorems 2.1 and 4.3, there is a $\delta > 0$ such that, for all $t \in (0, \delta)$ and $(x, y) \in K$

$$\begin{aligned} t \log p_0(t, x, y) &\geq -d(x, y)^2/4 - \varepsilon, \\ t \log p(t, x, M \setminus U, y) &\leq -d(x, M \setminus U, y)^2/4 + \varepsilon \end{aligned}$$

so

$$\begin{aligned} p(t, x, M \setminus U, y)/p(t, x, y) &\leq e^{-\varepsilon/t}, \\ p_0(t, x, M \setminus U, y)/p_0(t, x, y) &\leq e^{-\varepsilon/t} \end{aligned}$$

and this is enough.

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