

Geodesics and Approximate Heat Kernels

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Abstract

We use the gradient flow on the path space to obtain estimates on the heat kernel $k(t, x, y)$ on a complete Riemannian manifold. This approach gives a sharp formula for the small-time asymptotics of $k(t, x, y)$ and an upper bound for all time for pairs x and y are not conjugate. It also gives a theorem about convolutions of heat kernels that makes precise the intuition that heat flows in packets along geodesics.

On a complete Riemannian manifold M , the heat kernel $k(t, x, y)$ of the Laplacian exists and satisfies the semigroup property

$$k(t, x, y) = \int_M k(s, x, z)k(t-s, z, y)dv_z \quad (0.1)$$

for each $0 \leq s \leq t$. The problem of estimating the heat kernel for small time has a long history with at least four distinct approaches. The traditional Minakshisundaram-Pleijel expansions give parametrixes p_ℓ satisfying $k(t, x, y) = p_\ell(t, x, y) + O(t^\ell)$ as $t \rightarrow 0$; this statement is weaker than (0.4) for all ℓ whenever $x \neq y$ because the function e^ε/t approaches 0 faster than any power of t as $t \rightarrow 0$. In the geometric analysis literature bounds on $k(t, x, y)$ valid for all t were given by Cheng, Li and Yau [CLY] [LY], with further notable work by Cheeger, Gromov and Taylor [CGT], Davies [D] and Grigor'yan [G] (see [G] for additional references). These have the general form

$$k(t, x, y) \leq c(\varepsilon) t^{-n/2} e^{-\frac{d^2(x,y)}{(4+\varepsilon)}t}$$

for any $\varepsilon > 0$; this is also weaker than (0.4) for the same reason. There is a separate literature that estimates the heat kernel using stochastic processes. This approach produces bounds with the “sharp” exponent $-d^2(x, y)/4t$. In particular, in a brilliant but terse paper [M], S. Molchanov used stochastic processes to prove a version of Theorem A below (see also the exposition [A]).

This paper uses a new method, based on the gradient flow of the energy function on path space, that uses geometric analysis to produce bounds with sharp exponents.

Our first result is a global, small-time asymptotic formula for the heat kernel for points x and y away from the conjugate locus. For each $L > 0$, let $\mathcal{C}_L \subset M \times M$ be the

set of (x, y) such that y is conjugate to x along some geodesic with length at most L . For (x, y) in the complement of \mathcal{C}_L one is led, as we explain in Section 1, to the approximate heat kernel

$$k_L(t, x, y) = (4\pi t)^{-n/2} \sum_{\gamma} e^{-S(\gamma)} D_{\gamma}^{-1/2} \quad (0.2)$$

where the sum is on all locally minimal geodesics γ from x to y of length $\leq L$, D_{γ} is the Jacobian of the exponential map along γ , and $S(\gamma)$ is the energy of γ

$$S(\gamma) = \frac{1}{4} \int_0^t |\dot{\gamma}(s)|^2 ds. \quad (0.3)$$

We will prove that $k_L(t, x, y)$ gives the correct small-time asymptotics for the heat kernel. The statement is a slight extension of a result of Molchanov [M].

Theorem A ([M]). *Let M be a complete Riemannian manifold with Ricci curvature bounded below and positive injectivity radius. If $(x, y) \notin \mathcal{C}_L$ for some $L > d(x, y)$, then as $t \rightarrow 0$*

$$k(t, x, y) = k_L(t, x, y) (1 + O(t)) \quad (0.4)$$

More specifically, there is a bound $\left| \frac{k_L(t, x, y)}{k(t, x, y)} - 1 \right| \leq ct k(t, x, y)$ whenever $t < t_0$ where the constants c and t_0 are uniform for (x, y) in compact sets in $(M \times M) \setminus \mathcal{C}_L$.

Note that for each (x, y) only the minimal geodesics in the sum (0.2) contribute to the asymptotics. However, the difference between the lengths of the minimal geodesic and the next shortest geodesic from x to y is not uniform in (x, y) at points that are in the cutlocus but not the conjugate locus. Thus it is necessary to include non-minimal geodesics in order to get uniform bounds.

Theorem A has two useful consequences. The first is an upper bound on the heat kernel valid for all t for non-conjugate points x and y .

Theorem B. *Let (M, g) be a complete Riemannian manifold with Ricci curvature bounded below and positive injectivity radius. Then there is a constant c , uniform for (x, y) in compact sets in $(M \times M) \setminus \mathcal{C}_L$, such that*

$$k(t, x, y) \leq c k_L(t, x, y) \quad \forall t > 0. \quad (0.5)$$

More generally, let E be a vector bundle over (M, g) with a metric and a connection ∇ compatible with the connection, and let \mathcal{A} be an endomorphism of E satisfying $|\mathcal{A}\phi| \leq a|\phi|$ pointwise for all $\phi \in \Gamma(E)$. Then the kernel k^E of the operator $\nabla^ \nabla + \mathcal{A}$ satisfies*

$$|k^E(t, x, y)| \leq c e^{at} k_L(t, x, y) \quad \forall t > 0. \quad (0.6)$$

Theorem A also leads to a precise statement of the physical intuition that heat flows primarily along geodesics. This intuition also indicates that much of the integral (0.1) is superfluous: it should suffice to integrate over tubular neighborhoods of the geodesics from x to y . In fact, if heat is transported by particles which move at constant speed along geodesics from x to y in time t , then the integral (0.1) should be concentrated around the points $\gamma(s)$ where these particles are at time s . Our third theorem affirms this:

Theorem C. *Let M be a complete Riemannian manifold satisfying the conditions of Theorem B. Fix $(x, y) \in M \times M \setminus \mathcal{C}_L$ with $L > d(x, y)$. Let $\{\gamma_1, \dots, \gamma_n\}$ be the set of locally minimal geodesics from x to y of length $\leq L$ and let $B_s \subset M$ be the union of the geodesic balls $B(\gamma_i(s), \varepsilon)$, $i = 1, \dots, n$. Then the convolution (0.1) localizes in the sense that for each s , $0 < s < t$,*

$$k(t, x, y) \underset{t \rightarrow 0}{\approx} \int_{B_s} k(s, x, z) k(t - s, z, y) dv_z \quad (0.7)$$

where \approx means asymptotic to all orders of t as $t \rightarrow 0$. This statement is uniform on compact sets in $(M \times M) \setminus \mathcal{C}_L$.

Physics offers yet another viewpoint on these results. In ‘‘Euclidean’’ quantum mechanics the heat kernel $k(t, x, y)$ for the Hamilton operator $H = \Delta$ on a Riemannian manifold is expressed as an integral over the space \mathcal{P} of all paths γ from x to y in time t . This expression is based on the action (0.3) corresponding to H . It has the form

$$k(t, x, y) = \int_{\mathcal{P}} e^{-S(\gamma)} D\phi$$

where $D\phi$ is a measure on the Hilbert manifold \mathcal{P} . Because the integrand peaks sharply around the stable critical paths of S , the usual practice is to replace the integral over \mathcal{P} by the sum of the integrals over neighborhoods $U_\gamma \subset \mathcal{P}$ of the stable critical paths. These integrals are then approximated by the standard methods of evaluating (infinite-dimensional) Gaussian integrals. The resulting ‘‘semiclassical’’ approximation is

$$k(t, x, y) \sim (4\pi t)^{-n/2} \sum_{\gamma} e^{-S(\gamma)} D_\gamma^{-1/2}$$

- exactly as above! (The factors $(4\pi t)^{-n/2}$ and $D_\gamma^{-1/2}$ arise from the Fredholm determinant $(\det \text{Hess } S)^{-1/2}$). In terms of the geometry of M , the approximation of the integral over \mathcal{P} with the integral over the B_s amounts to considering only paths from x to y which lie in a tubular neighborhood of a stable critical path. Theorem C shows that this approximation is valid to all orders in t for small t .

All three theorems are proved by analyzing convolutions similar to the one obtained by substituting (0.2) into (0.1). Of course, if y is conjugate to x then the Jacobian factor

$D^{-\frac{1}{2}}$ in (0.4) is undefined. Thus the technical challenge is to estimate the contribution of points z that are nearly conjugate to x or y .

The key technique is to deform curves using the gradient flow of the energy function on the path space. We first associate the integral (0.1) with the piecewise-geodesic path γ_1 which goes from x to z in time s , then from z to y in time $t - s$. Regarding γ_1 as a point in the path space \mathcal{P} , we use the gradient flow of the energy function S to obtain a family of paths deforming γ_1 to a geodesic γ_0 joining x to y in time t , as illustrated in Figure 3. We then bound the convolution by analyzing how S changes under this deformation. As preliminaries, we describe the analytic properties of the path space in Section 3 and establish certain estimates on the gradient flow in Section 4. These led to the crucial ‘‘Energy Loss’’ Lemma 5.1. Sections 6 and 7 show how Theorems A, B and C follow from the Energy Loss Lemma and a well-known result of Cheng, Li and Yau.

1 The Approximate Heat Kernel

Let (M, g) be a smooth complete Riemannian manifold with Ricci curvature bounded below. The Laplacian $\Delta = d^*d$ on functions has a heat kernel $k(t, x, y)$; k is a distribution on $\mathbf{R}^+ \times M \times M$ satisfying

$$(\partial_t + \Delta_y)k(t, x, y) = 0 \tag{1.1}$$

$$\lim_{t \rightarrow 0} \int_M k(t, x, y), \phi(y) \rangle = \phi(x) \quad \forall x \in M \quad \text{and} \quad \phi \in C^\infty(M) \tag{1.2}$$

(the subscript on Δ_y signifies that the differentiation is applied to the y variable). The existence and uniqueness of the heat kernel is well-known (c.f. [Do]) and standard regularity results show that it is smooth for $t > 0$. It follows from uniqueness that k is a semigroup in t under convolution, that is, formula (0.1) holds. In this section we reinterpret the convolution in a way that leads naturally to the approximate heat kernel (0.2). Readers willing to take (0.2) as an ansatz can skip this section.

The metric determines a volume density whose square root $\sqrt{dv_x}$ trivializes the real line bundle H of half-densities. We can consider Δ acting on half-densities on M . The corresponding heat kernel, still denoted k , is an element of the space $\mathcal{D}(M \times M)$ of distributional half-densities on $M \times M$ and satisfies (1.1) and (1.2) above. Explicitly, k acts on half-densities ϕ by

$$(k * \phi)(x) = \int_M \left[k(t, x, y) \sqrt{dv_x} \otimes \sqrt{dv_y} \right] \cdot \left[\phi(y) \sqrt{dv_y} \right] = \left(\int_M k(t, x, y) \phi(y) dv_y \right) \sqrt{dv_x}$$

Similarly, the convolution formula (0.1) can be written as

$$\int_M \left[k(t, x, y) \sqrt{dv_x} \otimes \sqrt{dv_y} \right] \cdot \left[k(s, y, z) \sqrt{dv_y} \otimes \sqrt{dv_z} \right] = k(t + s, x, z) \sqrt{dv_x} \otimes \sqrt{dv_z}.$$

The cotangent space T^*M has a symplectic form ω and a canonical half-density δ defined by $\delta^2 = \omega^n$. Letting $\pi : T^*M \rightarrow M$ be the projection and $V = \ker \pi_*$ be the vertical subspace, we get an exact sequence

$$0 \rightarrow \pi^*T^*M \rightarrow T^*(T^*M) \rightarrow V \rightarrow 0$$

and hence an isomorphism

$$\Lambda^{2n}(T^*(T^*M)) = \pi^*\Lambda^n(T^*M) \otimes \Lambda^n(V)$$

of bundles over T^*M . A choice of Riemannian metric determines volume elements of unit length in $\Lambda^n(T^*M)$ and V and we can then write, with the obvious notation,

$$\delta = \pi^* \sqrt{dv_x} \otimes \sqrt{dv_\xi}.$$

The half-densities on $M \times M$ and T^*M are linked by the map $\exp : T^*M \rightarrow M \times M$, which can be thought of either as the usual exponential map composed with the metric isomorphism $T^*M \cong TM$ or as the composition of the unit-time geodesic flow in T^*M with the projection $\pi : T^*M \rightarrow M$. For each $(x, \xi) \in T^*M$ the image of the line segment $(x, t\xi), 0 \leq t \leq 1$ under \exp_x is a geodesic γ from x to $y = \exp_x(\xi)$. The pullback of the density dv_y by \exp_x is then a multiple of dv_ξ which we will write as $D(x, \xi) = D(x, y) = D_\gamma$, labeling it by either $(x, \xi) \in T^*M$, by $(x, y) \in M \times M$, or by the geodesic γ . In fact, D is the square root of the absolute value of $\det d\exp_x(\xi) : \Lambda^n(T_\xi^*(T^*M)) \rightarrow \Lambda^n(T_y^*(M))$. We also have $\exp_x^* \sqrt{dv_x} = \pi^* \sqrt{dv_x}$ and hence

$$\exp_x^* \left(\sqrt{dv_x} \otimes \sqrt{dv_y} \right) (x, \xi) = D^{\frac{1}{2}}(x, \xi) \delta.$$

If x and y are not conjugate along $\gamma(t)$ then \exp is a local diffeomorphism near (x, ξ) in $M \times M$, so we can write the above equation in the form

$$(\exp^{-1})^* \delta = D_\gamma^{-\frac{1}{2}} \sqrt{dv_x} \otimes \sqrt{dv_y}. \quad (1.3)$$

The local diffeomorphism also defines a smooth distance function $r_\gamma(x, y) = |\exp^{-1}(y)|$ which gives the distance from x to y measured along geodesics close to γ .

To first approximation one expects that heat diffuses from the point $x \in M$ along geodesics emanating from x . These pullback to lines in T_x^*M under the exponential map from x . It is therefore natural to consider the euclidean heat kernel on T_x^*M , regarding it as a multiple of δ :

$$k_0(t, x, \xi) = (4\pi t)^{-n/2} e^{-\frac{|\xi|^2}{4t}} \delta. \quad (1.4)$$

This defines a distributional half-density on T^*M . A smooth half-density on $M \times M$ pullsback via the exponential map to a smooth half-density on T^*M and hence the distributional half-density k_0 pushes forward to the half-density $\exp_* k_0$ defined by the L^2 pairing

$$\langle \exp_* k_0, \phi \rangle = \langle k_0, \exp^* \phi \rangle$$

for all smooth half-densities ϕ on $M \times M$.

Now suppose that x and y are not conjugate along any geodesic joining them. Then the set $\{\xi\}$ of inverse images of y under \exp_x is in one-to-one correspondence with the set of geodesics from x to y . For each such ξ formula (1.3) holds in some neighborhood of (x, ξ) in T^*M . Hence the *local* pushforward is

$$(\exp_* k_0)(t, x, y) = (4\pi t)^{-\frac{n}{2}} e^{-r_\gamma^2/4t} D_\gamma^{-\frac{1}{2}} \sqrt{dv_x} \otimes \sqrt{dv_y}.$$

Since the geodesic γ has constant velocity $\dot{\gamma}$ the factor in the exponent is the energy of the path, namely

$$S(\gamma) = \frac{1}{4} \int_0^t |\dot{\gamma}(s)|^2 ds = \frac{r_\gamma^2}{4t}. \quad (1.5)$$

Summing on all geodesics γ from x to y then yields the complete pushforward

$$(\exp_* k_0)(t, x, y) = (4\pi t)^{-\frac{n}{2}} \sum_\gamma e^{-S(\gamma)} D_\gamma^{-\frac{1}{2}} \sqrt{dv_x} \otimes \sqrt{dv_y}. \quad (1.6)$$

Lemma A.1 shows that the expression on the right is symmetric in x and y . This formula is a natural first guess for the heat kernel acting on half-densities on M . We will next see how it compares to the true heat kernel.

2 The Proof of Theorem A

This section presents key parts of the proof that the pushforward formula (1.6) is asymptotic to the heat kernel as $t \rightarrow 0$, and thus provides a small-time approximation to the heat kernel. Along the way we use two facts, Lemma 2.1 and Proposition 2.2, that are proved in later sections.

We start by introducing some notation that is designed to control the difficulties encountered at the conjugate locus. First, we limit the length of geodesics by fixing a number $L > 0$ and working with the sets

$$\Gamma(x, y; L) = \{\text{stable geodesics from } x \text{ to } y \text{ of length } < L \}. \quad (2.1)$$

These determine an “ L -conjugate locus” \mathcal{C}_L consisting of those points $(x, y) \in M \times M$ with $D_\gamma(x, y) = 0$ along some $\gamma \in \Gamma(x, y; L)$. We can use the values of D_γ to define neighborhoods

$$\mathcal{C}_L(\delta) = \{(x, y) \in M \times M \mid D_\gamma(x, y) < \delta^2 \text{ for some } \gamma \in \Gamma(x, y; L)\}$$

of $\mathcal{C}_L = \mathcal{C}_L(0)$ in $M \times M$. With this notation we have the following lemma, which is needed to ensure that our estimates are uniform away from \mathcal{C}_L .

Lemma 2.1. *Given L and a compact set $A \subset (M \times M) \setminus \mathcal{C}_L$, the set (2.1) is finite and its cardinality is bounded by a constant $\Gamma = \Gamma(L, A)$:*

$$|\Gamma(x, y; L)| \leq \Gamma \quad \forall (x, y) \in A. \quad (2.2)$$

Furthermore, there is a small constant $\delta_A > 0$ and a large constant B so that, for each $(x, y) \in A$ and each $\gamma \in \Gamma(x, y; L)$, the δ_A -tubular neighborhood of the γ does not intersect the set

$$\mathcal{C}_L(1/B) = \{(x, y) \mid D_\gamma^{-\frac{1}{2}}(x, y) > B \text{ for some } \gamma \in \Gamma(x, y; L)\}.$$

Lemma 2.1 is proved at the end of Section 3.

Henceforth, fix L and a compact set $A \subset (M \times M) \setminus \mathcal{C}_L$. For each $(x, y) \in A$ and each geodesic $\gamma \in \Gamma(x, y; \lambda)$ the function

$$k_\gamma(t, x, y) = (4\pi t)^{-\frac{n}{2}} e^{-\frac{r^2}{4t}}$$

is well-defined and smooth in a neighborhood of (x, y) as is the approximate heat kernel

$$k_L(t, x, y) = \sum_{\gamma \in \Gamma(x, y; L)} k_\gamma(t, x, y) D_\gamma^{-\frac{1}{2}}. \quad (2.3)$$

Theorem A asserts that $k_L(t, x, y)$ is asymptotic to the heat kernel $k(t, x, y)$ for small t .

Proof of Theorem A. Fix L and A as above, and let δ_A and B be the constants produced by Lemma 2.1. Choose a smooth cutoff function $\beta_B : [0, \infty) \rightarrow \mathbf{R}$ with $\beta_B(x) = x$ for $x \leq B$, $\beta_B(x) = 0$ for $x \geq 2B$ and $|\beta'| \leq 2$ and $|\beta''| \leq 4/B$ everywhere. We will consider the truncated approximate heat kernel

$$\bar{k}_L(t, x, y) = \sum_{\gamma \in \Gamma(x, y; \lambda)} k_\gamma(t, x, y) \beta(D_\gamma^{-\frac{1}{2}}). \quad (2.4)$$

This agrees with (2.3) for all (x, y) in A and it is smooth, symmetric under the interchange $x \leftrightarrow y$, and it vanishes for $(x, y) \in \mathcal{C}_L(1/2B)$. Since k and \bar{k}_L are symmetric and Δ is self-adjoint we have

$$(\partial_t + \Delta_x)(k - \bar{k}_L)(t, x, y) = - [(\partial_t + \Delta_y)\bar{k}_L](t, x, y).$$

Solving this inhomogeneous heat equation on $[0, \delta]$ gives

$$(k - \bar{k}_L)(t, x, y) = \int_M k(t - \delta, x, z) (k - \bar{k}_L)(\delta, z, y) dv_z - \int_\delta^t ds \int_M k(t - s, x, z) [(\partial_t + \Delta_z)\bar{k}_L(s, z, y)] dv_z. \quad (2.5)$$

For (x, y) near the diagonal of $M \times M$, the principle term of \bar{k}_L – the term corresponding to the unique minimal geodesic – agrees with the euclidean heat kernel to highest order

in t and r , and for each $x \neq y$ both $k(\delta, x, y)$ and $\bar{k}_L(\delta, x, y)$ vanish as $\delta \rightarrow 0$. It follows, using properties (1.1) and (1.2), that the first integral in (2.5) vanishes in the limit $\delta \rightarrow 0$, leaving

$$(k - \bar{k}_L)(t, x, y) = - \int_0^t ds \int_M k(t-s, x, z) [(\partial_t + \Delta_z) \bar{k}_L](s, z, y) dv_z. \quad (2.6)$$

We next fix x and y and explicitly calculate the integrand. The integrand vanishes on the neighborhood

$$N_{2B} = \{z \in M \mid (z, y) \in \mathcal{C}_L(1/2B)\}$$

of the conjugate locus to y . For each z not in N_{2B} and each geodesic γ from y to z , the functions r (the distance from y to z measured along geodesics close to γ), $k_\gamma(s, \cdot, y)$ and $D_\gamma(\cdot, y) = D_\gamma(y, \cdot)$ are well-defined in a neighborhood \mathcal{O}_γ of z . By direct calculation,

$$\begin{cases} \partial_t k_\gamma &= \left[\frac{r^2}{4t^2} - \frac{n}{2t} \right] k_\gamma \\ \nabla k_\gamma &= -\frac{\nabla r^2}{4t} k_\gamma = -\frac{r}{2t} k_\gamma \frac{\partial}{\partial r} \\ \Delta_z k_\gamma &= -\left[\frac{\Delta r^2}{4t} + \frac{r^2}{4t^2} \right] k_\gamma. \end{cases}$$

on \mathcal{O}_γ . By Lemma A.2 we also have $\Delta r^2 + 2n = 4r D_\gamma^{\frac{1}{2}} \nabla_r D_\gamma^{-\frac{1}{2}}$. Consequently,

$$\begin{aligned} (\partial_t + \Delta_z) k_\gamma D_\gamma^{-\frac{1}{2}} &= [(\partial_t + \Delta_z) k_\gamma] D_\gamma^{-\frac{1}{2}} - 2\langle \nabla k_\gamma, \nabla D_\gamma^{-\frac{1}{2}} \rangle + k_\gamma \Delta D_\gamma^{-\frac{1}{2}} \\ &= E_\gamma k_\gamma D_\gamma^{-\frac{1}{2}} \end{aligned} \quad (2.7)$$

where $E_\gamma = -D_\gamma^{\frac{1}{2}} \Delta_z D_\gamma^{-\frac{1}{2}}$. To include β , note that $\nabla(\beta \circ D_\gamma^{-\frac{1}{2}}) = \beta' \nabla D_\gamma^{-\frac{1}{2}}$ and $\Delta(\beta \circ D_\gamma^{-\frac{1}{2}}) = \beta' \Delta D_\gamma^{-\frac{1}{2}} - \beta'' \cdot |\nabla D_\gamma^{-\frac{1}{2}}|^2$ where β' and β'' are evaluated at $D_\gamma^{-\frac{1}{2}}$. Calculating as in (2.7), we obtain

$$(\partial_t + \Delta_z) k_\gamma \beta \circ D_\gamma^{-\frac{1}{2}} = (\beta E_\gamma + \frac{r}{t}(\beta' - \beta) D_\gamma^{\frac{1}{2}} \nabla_r D_\gamma^{-\frac{1}{2}} + F_\gamma) k_\gamma D_\gamma^{-\frac{1}{2}}$$

where $F_\gamma = (\beta - \beta') E_\gamma - \beta'' D_\gamma^{\frac{1}{2}} |\nabla D_\gamma^{-\frac{1}{2}}|^2$. Note that (i) β has support on $M \setminus N_{2B}$ and is the identity on $M \setminus N_B$, and (ii) $\beta - \beta'$ and β'' have support on the set $N(1/B) \setminus N(1/2B)$ where $|D_\gamma^{-\frac{1}{2}}| \leq 2B$.

Let c_1 be the supremum of E_γ on $(M \times M) \setminus \mathcal{C}_L(1/2B)$ and let c_2 and c_3 be, respectively, the supremums of $|(\beta' - \beta) \nabla_r D_\gamma^{-\frac{1}{2}}|$ and $|F_\gamma|$ on the compact set $\mathcal{C}_L(1/B) \setminus \mathcal{C}_L(1/2B)$. After summing on γ we have

$$|(\partial_t + \Delta_x) \bar{k}_L| \leq \begin{cases} c_1 \bar{k}_L & \text{on } M \setminus N_B \\ 2B \sum_{\gamma \in \Gamma(z, y; L)} (c_2 + \frac{r^2}{s} c_3) k_\gamma & \text{on } N_B \setminus N_{2B}. \end{cases}$$

Inserting this into (2.6) and again noting that the heat kernel $k(t, x, y)$ is non-negative gives the inequality

$$|(k - \bar{k}_L)(t, x, y)| \leq c_1 \int_0^t ds \int_{M \setminus N_{2B}} k(t-s, x, z) \bar{k}_L(s, z, y) dv_z + 2B \cdot I \quad (2.8)$$

where

$$I = \sum_{\gamma \in \Gamma(z, y; L)} \int_0^t \left(c_2 + \frac{r_\gamma}{s} c_3 \right) ds \int_{N_B \setminus N_{2B}} k(t-s, x, z) k_\gamma(s, z, y) dv_z \quad (2.9)$$

The technically difficult part of the proof is bounding the integral I . This will be done in Section 7, where we will establish the following bound.

Proposition 2.2. *There are constants C , δ and $t_0 > 0$, uniform for (x, y) in compact sets in $M \times M \setminus \mathcal{C}_L$, such that the integral (2.9) satisfies*

$$I \leq C e^{-\delta/t} \bar{k}_L(t, x, y)$$

for all $t < t_0$.

The function $e^{-\delta/t}$ approaches 0 faster than any power of t as $t \rightarrow 0$. For our purposes it is enough to note that we can choose a constant $t_1 < \min\{t_0, \frac{1}{2}\}$, depending only on C and δ , so that $C e^{-\delta/t} \leq t$ whenever $t < t_1$. Then (2.8) gives

$$|(k - \bar{k}_L)(t, x, y)| \leq c_1 \Phi(t, x, y) + t \bar{k}_L(t, x, y) \quad (2.10)$$

where

$$\Phi(t, x, y) = \int_0^t ds \int_M k(t-s, x, z) \bar{k}_L(s, z, y) dv_z.$$

To bound $\Phi(t, x, y)$, note that (2.10) implies that $\bar{k}_L \leq 2k + 2c_1 \Phi$ for $t < t_1$. Substituting into the definition of Φ and using the semigroup property, we have

$$\begin{aligned} |\Phi(t, x, y)| &\leq 2 \int_0^t ds \int_M k(t-s, x, w) k(s, w, y) dv_z \\ &\quad + 2c_1 \int_0^t ds \int_0^s du \int_M k(t-s, x, w) \int_M k(s-u, w, z) \bar{k}_L(u, z, y) dv_z dv_w \\ &\leq 2tk(t, x, y) + 2c_1 \int_0^t ds \int_0^t du \int_M k(t-u, x, z) \bar{k}_L(u, z, y) dv_z \\ &\leq 2tk(t, x, y) + 2c_1 t \Phi(t, x, y). \end{aligned}$$

(in the middle, we have extended the s -integration from $[0, u]$ to $[0, t]$, noting that $k \bar{k}_L \geq 0$). Thus $|\Phi| \leq ctk$ for small t . But then (2.10) implies that

$$|(k - k_\lambda)(t, x, y)| \leq c_1 tk(t, x, y)$$

for t sufficiently small. Thus the proof of Theorem A will be complete once we have established Lemma 2.1 and Proposition 2.2. \square

Remark 2.3. In light of the pushforward formula (1.6) it is natural to take $L = \infty$ in (2.1). The proof shows that this can be done provided that the conjugate locus $C \subset M \times M$ is closed and that $D^{\frac{1}{2}}\Delta D^{-\frac{1}{2}}$ is a bounded function on TM . This holds, for example, when M has non-positive curvature.

3 The Path Space

We begin by reviewing the global analysis of the energy function on the path space of a complete finite-dimensional Riemannian manifold (M, g) . Complete details can be found in [P].

Fix points $x, y \in M$ and let \mathcal{P}^∞ be the space of all smooth maps $\gamma : [0, 1] \rightarrow M$ with $\gamma(0) = x$ and $\gamma(1) = y$. The choice of an embedding $M \subset \mathbf{R}^N$ induces an inclusion $\mathcal{P}^\infty \hookrightarrow W^{1,2}([0, 1], \mathbf{R}^N)$ into the Sobolev space of $W^{1,2}$ maps $[0, t] \rightarrow \mathbf{R}^N$. The closure of \mathcal{P}^∞ in this topology is a smooth Hilbert manifold \mathcal{P} — the path space. A tangent vector $X \in T_\gamma\mathcal{P}$ is an $W^{1,2}$ vector field along the path γ in M that vanishes at the endpoints. By Hölder's inequality

$$|X(s') - X(s)| \leq \int_s^{s'} |X'| \leq \sqrt{|s' - s|} \|X\|_{H_1} \quad (3.1)$$

so X is Hölder continuous and by integration each $\gamma \in \mathcal{P}$ is Hölder continuous. Taking $s = 0$ and $X = \gamma_i - \gamma_j$ in (3.1) shows that $\sup |\gamma_i - \gamma_j| \leq \|\gamma_i - \gamma_j\|_{H_1}$. Consequently, each $\gamma \in \mathcal{P}$ is a Hölder continuous path in M .

There is a natural Riemannian metric on \mathcal{P} which induces the $W^{1,2}$ topology and is independent of the embedding of M in \mathbf{R}^N . It is defined by

$$\|X\|^2 = \int_0^1 |\nabla_T X|^2 + |X|^2 ds = \langle X, (1 - \nabla_T \nabla_T)X \rangle_{L^2} \quad (3.2)$$

where $X \in T_\gamma\mathcal{P}$ and $T = \dot{\gamma}$ is the tangent vector. With this metric \mathcal{P} is a complete, closed Riemannian Hilbert manifold.

Because X satisfies $2|X||X'| = (|X|^2)' = 2\langle X, \nabla_T X \rangle \leq 2|X||\nabla_T X|$ and vanishes at the endpoints we have, as in (3.1),

$$\begin{aligned} |X(s)| &\leq \min \left\{ \int_0^s |X'|, \int_s^1 |X'| \right\} \leq \min \{ \sqrt{s}, \sqrt{1-s} \} \left(\int_0^1 (|X'|)^2 \right)^{\frac{1}{2}} \\ &\leq \sqrt{2s(1-s)} \cdot \|\nabla_T X\|_{L^2}. \end{aligned} \quad (3.3)$$

Squaring and integrating with respect to s gives the Poincaré inequality $3\|X\|_{L^2}^2 \leq \|\nabla_T X\|_{L^2}^2$. Consequently, (3.2) and (3.3) give the bounds

$$\sup |X|^2 \leq \frac{1}{2} \|\nabla_T X\|_{L^2}^2 \quad \text{and} \quad \|X\| \leq \frac{4}{3} \|\nabla_T X\|_{L^2} \leq \frac{4}{3} \|X\|. \quad (3.4)$$

Below, the notation $\|X\|$ will always refer to the metric (3.2); when the L^2 norm is used it will be explicitly indicated.

Our aim is to study the gradient flow of the energy function $S(\gamma)$ of (0.1). This is naturally a function on the Riemannian manifold \mathcal{P}_t of H_1 paths from x to y in time $t > 0$ (constructed as above). However, because we are seeking estimates that are uniform in t it is convenient to embed $\mathcal{P}_t \hookrightarrow \mathcal{P} = \mathcal{P}_1$ by the rescaling $\gamma(s) \rightarrow \gamma(s/t)$, $0 \leq s \leq t$. The energy (0.3) then becomes the function

$$S(\gamma) = \frac{1}{4t} \int_0^1 |T(s)|^2 ds \quad (3.5)$$

on \mathcal{P} . This is a smooth function with differential

$$(dS)_\gamma(X) = \frac{1}{2t} \int_0^1 \langle \nabla_X T, T \rangle = \frac{1}{2t} \int_0^1 \langle X, \nabla_T T \rangle$$

for $X \in T_\phi \mathcal{P}$. The gradient is therefore defined by (from (3.2) and (3.4))

$$(1 - \nabla_T \nabla_T) \text{grad } S = \frac{1}{2} \nabla_T T.$$

Now consider the flow of the descending gradient vector field $V = -\text{grad } S$ on \mathcal{P} . Each integral curve $\phi(r)$ of V is defined for $0 \leq r < \infty$ (see [P] for details). Along $\phi(r)$

$$\frac{d}{dr} S(\phi(r)) = \langle dS, V \rangle = -\|V\|^2 \quad (3.6)$$

Hence S is decreasing and, since S is bounded below,

$$\int_0^\infty \|V\|^2 dr = S(\phi(0)) - S(\phi(\infty)) \quad (3.7)$$

is finite. Hence $\|V(r)\| \rightarrow 0$ as $r \rightarrow \infty$.

Palais-Smale Lemma. *Any sequence $\{\gamma_k\}$ in \mathcal{P} with $|S(\gamma_k)| < C$ and $\|(\text{grad } S)_{\gamma_k}\| \rightarrow 0$ has a convergent subsequence. \square*

This well-known lemma is proved by Palais in [P]. It implies that the integral curves $\phi(r)$ converges as $r \rightarrow \infty$ to a critical point of S . In the next section we will obtain estimates on these integral curves. Here we make some general preliminary remarks.

Let (M, g) be a Riemannian manifold with Levi-Civita connection ∇ . Each smooth function $f : M \rightarrow \mathbf{R}$ has a covariant Hessian defined as follows. For vector fields X, Y write $g(X, Y)$ as (X, Y) . Then

$$X \cdot Y \cdot f = X \cdot (\nabla f, Y) = (\nabla_X (\nabla f), Y) + (\nabla f, \nabla_X Y).$$

The Hessian is the second covariant derivative $\nabla^2 f$ of f :

$$Hf(X, Y) = (\nabla^2 f)(X, Y) = \nabla_X \nabla_Y \cdot f - \nabla_{\nabla_X Y} f = X \cdot Y \cdot f - df(\nabla_X Y).$$

This is a tensor on M that is symmetric because ∇ is torsion free. Its value at a critical point is independent of the metric and the connection.

If $v(t)$ is a flow line of the downward gradient vector field $V = -\nabla f$ then $f(v(t))$ satisfies $f'(t) = \nabla f(V) = -|V|^2$ as in (3.6), and

$$f''(t) = -V \cdot |V|^2 = -2(\nabla_V V, V) = 2(\nabla_V (\nabla f), V) = 2Hf(V, V). \quad (3.8)$$

We can apply this discussion to the path space \mathcal{P} , taking g to be the L^2 metric, h to be the $W^{1,2}$ metric (3.2), so L is the operator $1 - \nabla_T \nabla_T$. At each critical point the hessian is given by the usual second variation formula

$$HS_\gamma(X, X) = \frac{1}{2} \int_0^1 \langle X, -\nabla_T \nabla_T X + R(T, X)T \rangle \quad (3.9)$$

where R is the curvature tensor of (M, g) .

We conclude this section by using facts about the path space to prove Lemma 2.1.

Proof of Lemma 2.1: For each $x, y \in M$ the Palais-Smale Lemma implies that the set of all geodesics with energy less than L is compact. When $(x, y) \notin \mathcal{C}_L$, the geodesics from x to y of length $\leq L$ are also isolated, and hence $\Gamma(x, y; L)$ is finite. Its cardinality is locally bounded, so there is a uniform bound (2.2) for (x, y) in compact sets. For stable geodesics the Morse Index Theorem implies that $D_\gamma(x, \gamma(s)) > 0$ for all $s \in [0, 1]$. Consequently, there is a $\delta_\gamma > 0$ such that $\text{dist}(\gamma, \mathcal{C}_L) > 2\delta_\gamma$.

Next note that the energy function S on $\mathcal{P}(x, y)$ has a local minimum at each stable geodesic γ , and S is also smooth in the endpoints. Hence for each stable geodesic $\gamma \in \Gamma(x, y; L)$ there is a $\delta'_\gamma > 0$ and neighborhoods \mathcal{O}_γ^x and \mathcal{O}_γ^y such that for all $(z, w) \in \mathcal{O}_\gamma^x \times \mathcal{O}_\gamma^y$ there is a unique stable geodesic $\gamma' : [0, 1] \rightarrow M$ from z to w with $\text{dist}(\gamma, \gamma') < \delta'_\gamma$ in the $W^{1,2}$ Riemannian metric. By (2.5) the same bound holds for the C^0 distance: $d_{C^0}(\gamma, \gamma') < \delta'_\gamma$. Set $\delta_{(x,y)} = \min_\gamma \min\{\delta_\gamma, \delta'_\gamma\}$, where the first minimum is over all $\gamma \in \Gamma(x, y; L)$. We then have, for a new choice of \mathcal{O}_γ^x and \mathcal{O}_γ^y , that $d(\gamma', \mathcal{C}_L) > \delta_{(x,y)}$ for all stable geodesics from z to w of length at most L whenever

$$(z, w) \in \mathcal{O}_{(x,y)} = \bigcap_{\gamma \in \Gamma(x,y;L)} \mathcal{O}_\gamma^x \times \mathcal{O}_\gamma^y.$$

But the collection $\{\mathcal{O}_{(x,y)} \mid (x, y) \in A\}$ covers A . Choose a finite subcollection labeled by (x_k, y_k) , let δ_A be half the minimum of the corresponding numbers $\delta_{(x_k, y_k)}$, and choose B large enough that $\mathcal{C}_L(1/B)$ lies in the δ_A -neighborhood of \mathcal{C}_L . Lemma 2.1 holds for this δ_A and this B . \square

4 The Modified Gradient Flow

In this section we construct a flow on the path space that has all the essential properties of the gradient flow of the energy S and for which there is an estimate for the length of the flow lines. This flow is constructed in two steps. In Proposition 4.1 we modify the gradient flow obtain a flow with the desired properties and with a length estimate of the desired form. Unfortunately, the constant in this length estimate depends on the energy $S(\varphi(0))$ at the initial path of the flow; we require bounds which depend only on the length of this path $\varphi(0)$. This difficulty is surmounted by allowing each path to first flow along its image to reach the parameterization of least energy (Proposition 3.2). In this parameterization the length and energy are easily compared and the require bounds are obtained.

We shall henceforth assume that x and y are not conjugate along any geodesic. (Sard's Theorem, applied to the exponential map, shows that all pairs (x, y) have this property except a set of measure zero in $M \times M$). The critical points of S on \mathcal{P} are then isolated and non-degenerate.

Fix L and let

$$\mathcal{P}(L) = \{\gamma \in \mathcal{P} \mid S(\gamma) < L^2\}. \quad (4.1)$$

By Hölders inequality each path $\gamma \in \mathcal{P}(L)$ has length

$$\ell(\gamma) \leq \sqrt{4S(\gamma)} < 2L, \quad (4.2)$$

so lies in the ball $B(x, 2L) \subset M$. It follows from the Palais-Smale Lemma that

- (i) there are a finite number $N(x, y, L)$ of such critical points in $\mathcal{P}(L)$, and
- (ii) there is a $\lambda = \lambda(x, y, L) > 0$ such that at each critical point γ_i the Hessian $\text{Hess } S_{\gamma_i}$ has no eigenvalue in $[-2\lambda, 2\lambda]$.

Since S is a smooth function on \mathcal{P} (ii) implies that there are neighborhoods $B(\gamma_i, \varepsilon)$ of the critical points on which the Hessian operator has no eigenvalues in $[-\lambda, \lambda]$. These $B(\gamma_i, \varepsilon)$ are disjoint for small ε . Finally, by making ε smaller if necessary and applying the Morse Lemma (cf. [P]), we can also arrange that

- (iii) there is a Morse coordinate system for S on each $B(\gamma_i, \varepsilon)$.

Proposition 4.1. *There is a vector field W on $\mathcal{P}(L)$ whose integral curves $\varphi(r)$ are piecewise smooth. Each ends at a stable critical point $\varphi(\infty)$ of S and satisfies*

$$\int_0^\infty \|W(\varphi(r))\| dr \leq C [S(\varphi(0)) - S(\varphi(\infty))]^{1/2} \quad (4.3)$$

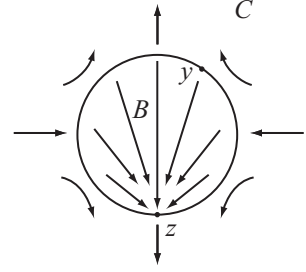
for some constant $C = C(L)$ independent of φ .

Proof. Let $\gamma_1, \dots, \gamma_k$ be the *stable* critical points of S in $\mathcal{P}(L)$. For sufficiently small $\varepsilon_1 > 0$ the ε_1 -ball around γ_i in Morse coordinates is a closed connected set A_i such that

$$S(\varphi) = S(\gamma_i) + \varepsilon_1^2, \quad \forall \varphi \in \partial A_i, \quad (4.4)$$

and such that every flow line of V which enters A_i remains in A_i . Similarly, around each unstable critical point γ_i , we choose an open ball B_i in the Morse coordinate system on $B(\gamma_i, \varepsilon)$. Write $\mathcal{P}(L)$ as the disjoint union $A \cup B \cup C$ where A is the union of the neighborhoods A_i of the stable critical points and B is the union of the neighborhoods B_i of the unstable critical points.

The vector field W is obtained by modifying the gradient vector field $V = -\text{grad } S$ in B as follows. At each unstable critical point γ choose a vector $X \in T_\gamma \mathcal{P}$ which is a negative direction of the Hessian of S . This X determines a flow line of the normalized gradient $V/\|V\|$ starting at γ . Let z be the point where this flow line first intersects ∂B_i . For each $y \in \partial B_i$ draw the line $\ell(r) = ry + (1-r)z$ in the Morse coordinate chart on B_i . Take W to be the unit tangent to $\ell(r)$ inside each B_i , and take $W = V = -\text{grad } S$ in $A \cup C$.



Every integral curve $\varphi(r)$ of W decomposes into connected components of $\varphi \cap A$, $\varphi \cap B$ and $\varphi \cap C$. Each such component is a smooth curve.

(a) First consider the flow of $W = V$ on one component A_i of A . As noted above $\varphi \cap A_i = \{\varphi(r) \mid r_0 \leq r \leq \infty\}$ and $\gamma = \varphi(\infty)$ is a critical point of S . Since the lowest eigenvalue of the Hessian is λ ,

$$S''(\varphi(r)) = 2\langle HS \rangle_{\varphi(r)}(V, V) \geq 2\lambda\|V\|^2 = -2\lambda S'(r).$$

Integration then gives $-S'(r) \leq -S'(r_0) \exp[2\lambda(r_0 - r)]$. But $S'(\infty)$ vanishes, so

$$-S'(r_0) = \int_{r_0}^{\infty} S''(s) ds \geq -2\lambda \int_{r_0}^{\infty} S'(s) ds = 2\lambda [S(r_0) - S(\infty)].$$

Since $W = V$ on A and $\|V\| = \sqrt{-S'}$ by (3.6), we have

$$\int_{\varphi \cap A} \|W\| \leq \sqrt{-S'(r_0)} \int_{r_0}^{\infty} e^{\lambda(r_0 - r)} dr \leq \sqrt{\frac{2}{\lambda}} \sqrt{S(\varphi(r_0)) - S(\gamma_i)} \quad (4.5)$$

(b) $\varphi \cap B$ has at most N components where N is the number of critical points in $\mathcal{P}_1(L)$. Each consists of the line segment $\ell(r)$ traversed at unit speed, so

$$\int_{\varphi \cap B} \|W\| \leq N \cdot \text{length } \ell(r) \leq 2\varepsilon N. \quad (4.6)$$

(c) On C , $W = V = -\text{grad } S$ and $\varphi \cap C$ is a union of segments $\varphi([s_i, t_i])$ of integral curves of V . The gaps $\varphi([t_i, s_{i+1}])$ occur when φ passes through B , so $S(\varphi(t_i)) > S(\varphi(s_{i+1}))$ by construction. Since there are no critical points adherent to C the P-S condition implies that $\|V\| > \alpha$ on C for some α . Hence by (3.7) and (4.1)

$$\begin{aligned} \int_{\varphi \cap C} \|W\| &\leq \alpha^{-1} \int_{\varphi \cap C} \|V\|^2 \leq \alpha^{-1} \sum_{i=0}^k [S(\varphi(s_i)) - S(\varphi(t_i))] \\ &\leq \alpha^{-1} [S(\varphi(0)) - S(\varphi(t_k))] \\ &\leq 2\alpha^{-1} L^2. \end{aligned}$$

Now fix an integral curve $\varphi(r)$ of W in $\mathcal{P}(L)$. As $t \rightarrow \infty$ it converges to a stable critical point γ of S . Let $\varphi(r_0)$ be the first point of $\varphi \cap A$.

(d) By (4.4) the change in S along $\varphi \cap A$ is $S(\varphi(r_0)) - S(\gamma) = \varepsilon_1^2$.

(e) Since $\varphi \cap B$ consists of at most N components each of length $\leq 2\varepsilon$, the total change in S along $\varphi \cap B$ is at most $2\varepsilon N$.

(f) S is decreasing along $\varphi \cap C$ by (3.6).

Combining (d), (e) and (f) we obtain

$$S(\varphi(0)) - S(\gamma) \geq \varepsilon_1^2 - 2\varepsilon N. \quad (4.7)$$

The ε in this equation is the radius of the neighborhoods B_i of the unstable critical points. These may be replaced by smaller neighborhoods B'_i inside $B(\gamma_i, \varepsilon')$ for any $\varepsilon' < \varepsilon$ without affecting (4.7). We may thus arrange that $S(0) - S(\gamma) \geq \frac{1}{2}\varepsilon_1^2$. Subsequently, (a), (b), and (c) give

$$\begin{aligned} \int_{\varphi} \|W\| &= \int_{r_0}^{\infty} \|V\| + \int_{\varphi \cap (B \cup C)} \|W\| \\ &\leq \sqrt{\frac{2}{\lambda}} [S(r_0) - S(\gamma)]^{1/2} + (2\varepsilon' N + 2\alpha^{-1} L^2) \\ &\leq \left[\sqrt{\frac{2}{\lambda}} + \frac{\sqrt{8}}{\varepsilon_1} (\varepsilon' N + \alpha^{-1} L^2) \right] [S(\varphi(0)) - S(\gamma)]^{1/2}. \quad \square \end{aligned}$$

Proposition 4.2. *Each path $\varphi \in \mathcal{P}_1$ can be deformed along its image to a path φ_0 with $S(\varphi_0) = \frac{1}{4}\ell^2(\varphi) \leq S(\varphi)$, and for each $\sigma \in [0, 1]$*

$$d^2(\varphi(\sigma), \varphi_0(\sigma)) \leq 8\sigma(1 - \sigma)[S(\varphi) - S(\varphi_0)]. \quad (4.8)$$

Proof. The image of φ is a path in M isometric to the interval $[0, \ell]$ in \mathbf{R} , where $\ell = \ell(\varphi)$. Thus we can regard φ as an element of the space \mathcal{Q} of $W^{1,2}$ maps from $[0, 1]$ to $[0, \ell]$. Note that \mathcal{Q} contains a unique geodesic, namely the path $\varphi_0(s) = s\ell$. Write $\varphi(s) = s\ell + \psi(s)$; the boundary conditions $\varphi(0) = 0$ and $\varphi(1) = \ell$ imply that $\psi(0) = \psi(1) = 0$, and hence

$$\begin{aligned} 4S(\varphi) &= \int_0^1 (\dot{\varphi})^2 ds = \int_0^1 (\ell + \dot{\psi})^2 ds = \ell^2 + 2\ell \int_0^1 \dot{\psi} ds + \int_0^1 \dot{\psi}^2 ds \\ &= 4S(\varphi_0) + \int_0^1 \dot{\psi}^2 ds. \end{aligned}$$

Now for fixed $\sigma \in [0, 1]$ the points $\varphi(\sigma)$ and $\varphi_0(\sigma)$ are joined by the path $p(r) = \sigma\ell + (1-r)\psi(\sigma)$, as r goes from 0 to 1. Hence

$$d^2(\varphi(\sigma), \varphi_0(\sigma)) \leq \left(\int_0^1 |p'(r)| dr \right)^2 = |\psi(\sigma)|^2 \leq 2\sigma(1-\sigma) \int_0^1 \dot{\psi}^2 ds$$

using (3.3). The proposition follows. \square

5 The Energy Loss Lemma

We now turn to the key geometric result: an estimate describing how much energy is lost as one deforms a path to a minimal geodesic. This estimate is used in the next section to bound the convolution of approximate heat kernels.

Energy Loss Lemma 5.1. *Fix $x, y \in M$. Suppose γ_1 is a geodesic from x to $z \in M$ in time s and γ_2 is a from z to y in time $t - s$. Then there is a stable geodesic γ_0 from x to y in time t such that $\gamma = \gamma_1 \cup \gamma_2$ satisfies*

$$S(\gamma) \geq S(\gamma_0) + \frac{\alpha r^2 t}{4s(t-s)} \tag{5.1}$$

where $r = d(z, p)$ is the distance from z to the point $p = \gamma_0(s/t)$. The constant α is uniform for (x, y) in compact sets $A \subset (M \times M) \setminus \mathcal{C}_L$.

Proof. When z is far from x , inequality (5.1) follows easily. Specifically, if $d(x, z) \geq 2d(x, y)$ and γ_0 is a minimal geodesic from x to y in time t , then $r \leq 2d(y, z)$ and $2r \leq 3d(x, z)$ by the triangle inequality. Hence for $0 \leq s \leq t$

$$\frac{d^2(x, z)}{4s} + \frac{d^2(z, y)}{4(t-s)} \geq \frac{7}{16} \frac{d^2(x, z)}{4s} + \frac{r^2}{16} \left(\frac{1}{s} + \frac{1}{t-s} \right) \geq \frac{d^2(x, y)}{4t} + \frac{r^2 t}{16s(t-s)},$$

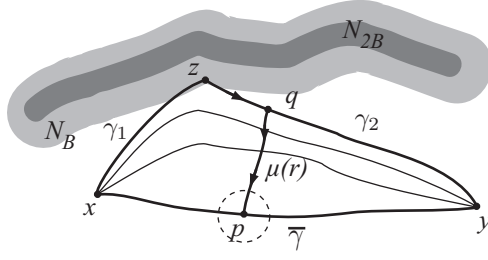


Figure 3: Deforming a path $\gamma = \gamma_1 \cup \gamma_2$ to a minimal geodesic $\bar{\gamma}$

so

$$S(\gamma) = S(\gamma_1) + S(\gamma_2) \geq S(\gamma_0) + \frac{r^2 t}{16s(t-s)}. \quad (5.2)$$

Symmetrically, (5.2) also holds if $d(y, z) \geq 2d(x, y)$. Thus it remains to consider the case when both $d(x, z) \leq 2d(x, y)$ and $d(y, z) \leq 2d(x, y)$. In this case the length of γ is bounded by

$$\ell(\gamma) \leq \ell(\gamma_1) + \ell(\gamma_2) \leq d(x, z) + d(z, y) + 2 \leq 4d(x, y).$$

Thus γ lies in $\mathcal{P}(L)$ for $L = 4d(x, y)$.

Now reparameterize γ by

$$\bar{\gamma}(\sigma) = \begin{cases} \gamma_1(\sigma t) & \text{for } 0 \leq \sigma \leq s/t \\ \gamma_2(\sigma t - s) & \text{for } s/t \leq \sigma \leq 1. \end{cases} \quad (5.3)$$

Then $\bar{\gamma}$ is an element of the space \mathcal{P}_1 of paths from x to y in time 1. We will deform $\bar{\gamma}$ in two steps.

First, using Proposition 4.2 we can deform $\bar{\gamma}$ along its image to a path $\hat{\gamma}$ with $4S(\hat{\gamma}) = \ell^2(\bar{\gamma}) \leq L^2$. Under this deformation the point $z = \bar{\gamma}(s/t)$ is carried along $\bar{\gamma}$ to the point $q = \hat{\gamma}(s/t)$. By Proposition 4.2 we have

$$d(z, q) \leq \sqrt{\frac{8s(t-s)}{t^2}} \left[S(\bar{\gamma}) - S(\hat{\gamma}) \right]^{\frac{1}{2}}. \quad (5.4)$$

Second, since $\hat{\gamma} \in \mathcal{P}_1(\frac{1}{4}L^2)$, we can use Proposition 3.1 to deform $\hat{\gamma}$ to a stable geodesic $\bar{\gamma}_0$. Under this deformation the point $q = \hat{\gamma}(s/t)$ is carried along a path $\mu(r)$ (see Figure 3) to the point $p = \bar{\gamma}_0(s/t)$. The tangent vector to $\mu(r)$ is $W_{\mu(r)}(s/t)$, where W is the vector field of Proposition 4.1. Hence using (3.3) and (4.3)

$$\begin{aligned} d(q, p) &\leq \int_0^\infty |\mu'| dr \leq \int_0^\infty \left| W_{\mu(r)} \left(\frac{s}{t} \right) \right| dr \\ &\leq \sqrt{\frac{2s(t-s)}{t^2}} \int_0^\infty \|W\| dr \\ &\leq c \sqrt{\frac{2s(t-s)}{t^2}} \left[S(\hat{\gamma}) - S(\bar{\gamma}_0) \right]^{\frac{1}{2}}. \end{aligned} \quad (5.5)$$

Combining (5.4), (5.5), and the triangle inequality, we have

$$r^2 \leq [d(z, q) + d(q, p)]^2 \leq c' \frac{s(t-s)}{t^2} [S(\bar{\gamma}) - S(\bar{\gamma}_0)] \quad (5.6)$$

where $c' = 16 + 4c^2$. Finally, write $\bar{\gamma} = \bar{\gamma}_1 \cup \bar{\gamma}_2$ and return to the original parameterization, going backwards through (5.3). From (3.5), the energies rescale according to $S(\bar{\gamma}_0) = tS(\gamma_0)$ and $S(\bar{\gamma}) = S(\bar{\gamma}_1) + S(\bar{\gamma}_2) = t[S(\gamma_1) + S(\gamma_2)]$. Substituting into (5.6), rearranging, and renaming c' then gives (5.1). \square

6 The Convolution Theorem

The theorems stated in the introduction are consequences of the energy loss Lemma 5. The basic idea of the proof can already be seen in the first proposition below, which show that the approximate heat kernel satisfies the localization property claimed for the true heat kernel in Theorem C.

At the start, we will use a result of Li and Yau. For this we will assume that M is a complete Riemannian manifold with Ricci curvature bounded below by $-\rho^2$ and with a bound

$$\text{Vol}(B(x, r)) \geq c_1 r^{n-p} \quad \forall r \leq r_0 \quad (6.1)$$

for some $p \geq 0$ and uniform constants c_1 and r_0 . This holds with $p = 0$ when the injectivity radius is bounded below. It also holds, for example, on the cylinder $\mathbf{R} \times S_\varepsilon^1$ where S_ε^1 is the circle of radius ε with $n - p = 1$ and a constant c_1 independent of ε and $r_0 = \infty$.

In this context, the upper bound of Li and Yau (Corollary 3.1 in [LY]) says that for each $0 < \beta < 1$ there are constants $c_2(\beta)$ and c_3 such that

$$k(t, x, y) \leq \frac{c_2(\beta)}{c_1} t^{\frac{p}{2}} e^{c_3 \beta \rho^2 t} k_\beta(t, x, y) \quad (6.2)$$

where

$$k_\beta(t, x, y) = (4\pi t)^{-\frac{n}{2}} \exp \left[-(1 - \beta) \frac{d^2(x, y)}{4t} \right] \quad (6.3)$$

for all $t < r_0^2$. This bound holds for all $x, y \in M$, even if x and y are conjugate. However, for small t and $\beta > 0$ the righthand side of (6.2) is exponentially larger than the bound obtained from Theorem A, and as $\beta \rightarrow 0$ we have $c_2(\beta) \rightarrow \infty$.

Recall our notation for approximate heat kernels: for fixed $L > 0$ and $(x, y) \in (M \times M) \setminus \mathcal{C}_L$ we have, for each geodesic γ from x to y with length $\leq L$, a function

$$k_\gamma(t, x, y) = (4\pi t)^{-\frac{n}{2}} e^{-S(\gamma)}. \quad (6.4)$$

Summing on all such geodesics gives our approximate heat kernel $k_L = \sum k_\gamma D_\gamma^{-\frac{1}{2}}$ as in (2.3).

Convolution Theorem 6.1. *Let M be a complete Riemannian manifold satisfying the conditions in (6.1). Fix $L > 0$ and $\delta > 0$ and $(x, y) \notin \mathcal{C}_L$. Let $\{\gamma_1, \dots, \gamma_n\}$ be the set of stable geodesics from x to y of length $\leq L$ and let $B_s(\delta) \subset M$ be the union of the geodesic balls $B(\gamma_i(s), \delta)$, $i = 1, \dots, n$. Then there are positive constants c_4, β_0, α and t_1 such that for each $\beta < \beta_0$, $t < t_1$ and each s , $0 < s < t$,*

$$\int_{M \setminus B_s(\delta)} k(t-s, x, z) k_\beta(s, z, y) dv_z \leq c_4(c_1, \rho, \delta) s t^{\frac{p}{2}} e^{-\alpha \delta^2/t} k_L(t, x, y). \quad (6.5)$$

The constants c_4, α, β_0 and t_1 uniform for (x, y) in compact sets $A \subset (M \times M) \setminus \mathcal{C}_L$.

Proof. Choose minimal geodesics γ_1 from x to z in time $t-s$ and γ_2 from z to y in time s . Then $S(\gamma_1) = d^2(x, z)/4(t-s)$ and $S(\gamma_2) = d^2(z, y)/4s$. Applying the Li-Yau bound (6.2) to the factor of k in the above integral, we have

$$I \leq c_1^{-1} c_2(\beta) e^{c_3 \beta \rho^2 t} (t-s)^{\frac{p}{2}} (16\pi^2 s(t-s))^{-\frac{n}{2}} \int_{M \setminus B_s(\delta)} e^{-(1-\beta)S(\gamma)} dv_z$$

where $\gamma = \gamma_1 \cup \gamma_2$ is the composite path as in Figure 3. After noting that $\beta < 1$ and $t < r_0^2$, we can bound the first three terms on the right by a single constant $c_4(\beta)$. Now set $\tau = \frac{4s(t-s)}{t}$ and apply Lemma 5.1: there is a locally minimal geodesic $\bar{\gamma}$ from x to y in time t so that

$$I \leq c_5(\beta, \rho) t^{-\frac{p-n}{2}} e^{-(1-\beta)S(\bar{\gamma})} \tau^{-\frac{n}{2}} \int_{M \setminus B_s(\delta)} e^{-(1-\beta)\frac{\alpha r^2}{\tau}} dv_z$$

where $r = r(z)$ is the distance from z to the point $p = \bar{\gamma}(s)$. The inequality is preserved if we replace $S(\bar{\gamma})$ by $S(\gamma_0)$ where γ_0 is a length-minimizing geodesic from x to y in time t . Note that $\beta S(\gamma_0) = \beta d^2(x, y)/4t \leq \beta d_A^2/4t$ where d_A is the diameter of A , and that $\tau \leq t$. Assuming that $\beta \leq \frac{1}{2}$ and $t \leq 1$, we then have:

$$I \leq c_5(\beta, \rho) t^{\frac{p}{2}} \left[t^{-\frac{n}{2}} e^{-S(\gamma_0)} D_{\gamma_0}^{-\frac{1}{2}} \right] e^{\frac{\beta}{4\tau} d_A^2} D_{\gamma_0}^{\frac{1}{2}} \tau^{-\frac{n}{2}} \int_{M \setminus B_s(\delta)} e^{-\frac{\alpha r^2}{2\tau}} dv_z.$$

The terms in brackets are bounded, up to a constant, by the approximate kernel $k_L(t, x, y)$. To evaluate the integral, we will pullback by the exponential map from the point $p = \bar{\gamma}(s)$, obtaining

$$I \leq c_6(\beta, \rho) t^{\frac{p}{2}} k_L(t, x, y) e^{\frac{\beta}{4\tau} d_A^2} D_{\gamma_0}^{\frac{1}{2}} \tau^{-\frac{n}{2}} \int_{T_p M \setminus B(0, \delta)} D(\xi) e^{-\frac{\alpha|\xi|^2}{2\tau}} dv_\xi. \quad (6.6)$$

where $D(\xi)$ is the Jacobian of the exponential map from p evaluated at $\xi \in T_p M$. There are well-known bounds for the Jacobian of the exponential map in terms of the Ricci curvature: by Lemma A.2 in the appendix we have:

$$|D_{\gamma_0}| \leq e^{(2n-2)\rho d_A} \quad \text{and} \quad |D(\xi)| \leq e^{(2n-2)\rho|\xi|}.$$

We can bound the exponent in the first inequality by writing $cd_A = c\sqrt{\frac{\tau}{\beta}} \cdot d_A\sqrt{\frac{\beta}{\tau}} \leq c^2\tau/\beta + \beta d_A^2/4\tau$. The second exponent can be similarly bounded using $c|\xi| \leq c^2\tau/\alpha + \alpha|\xi|^2/4\tau$. Inserting these inequalities into (6.6) yields

$$I \leq c_7(\beta, \rho) t^{\frac{n}{2}} k_L(t, x, y) e^{\beta d_A^2/2\tau} \tau^{-\frac{n}{2}} \int_{T_p M \setminus B(0, \delta)} e^{-\frac{\alpha|\xi|^2}{4\tau}} dv_\xi. \quad (6.7)$$

Finally, we apply Lemma 6.2 below with $m = 0$ and $x = \frac{\sqrt{\alpha}}{2}\xi$. Set $\beta_0 = \alpha\delta^2/8d_A^2$ and note that (6.3) shows that $k_\beta \leq k_{\beta_0}$ for $\beta \leq \beta_0$. Also, choose t_1 small enough that $t_1 < \min\{1, r_0^2\}$ and $(n-2)t_1 < \delta^2/8$. Then, noting that $\tau \leq t$, (6.7) implies

$$\begin{aligned} I &\leq c_7(\delta, \rho, \alpha, A) t^{\frac{n}{2}} k_L(t, x, y) e^{\frac{\beta}{2\tau}d_A^2} \tau e^{-\alpha\delta^2/8\tau} \\ &\leq c_8(\delta, \rho, \alpha, A) t^{\frac{n}{2}} k_L(t, x, y) \tau e^{-\alpha\delta^2/16\tau} \end{aligned}$$

whenever $t < t_1$. The inequality (6.5) of the lemma follows after renaming α and noting that $\tau \leq 4s$. \square

The final lines of the above proof used the following calculus fact.

Lemma 6.2. *For each $m \geq 0$ there is a constant $c(m, n)$ such that if $(n+m-2)\tau < \delta^2$ then*

$$\tau^{-\frac{n}{2}} \int_{\mathbf{R}^n \setminus B(0, \delta)} |x|^m e^{-\frac{|x|^2}{\tau}} \leq c(m, n) \delta^{m+\frac{n}{2}-2} \tau e^{-\frac{\delta^2}{2\tau}}. \quad (6.8)$$

Proof. Let ω_n be the volume of the unit sphere in \mathbf{R}^n . Note that the functions

$$f(\rho) = \int_{\mathbf{R}^n \setminus B(0, \rho)} |x|^m e^{-\frac{|x|^2}{\tau}} dv_x = \omega_n \int_\rho^\infty r^{m+n-1} e^{-\frac{r^2}{\tau}} dr$$

and $g(\rho) = \tau\omega_n \rho^{m+n-2} e^{-\rho/\tau}$ both vanish as $\rho \rightarrow \infty$ and satisfy $g'(\rho) \leq f'(\rho)$ for all $\rho \geq \delta$ when $(n+m-2)\tau < \delta^2$. Therefore $f(\delta) \leq g(\delta)$ whenever $(n+m-2)\tau < \delta^2$. Using the fact that $\tau^{-k} e^{-\delta/\tau} \leq c(k) \delta^{-k}$ for all $k, \tau, \delta > 0$, we have

$$\tau^{-\frac{n}{2}} \int_{\mathbf{R}^n \setminus B(0, \delta)} |x|^m e^{-|x|^2/\tau} \leq \omega_n \delta^{m+n-2} \tau e^{-\frac{\delta^2}{2\tau}} \left(\tau^{-\frac{n}{2}} e^{-\frac{\delta^2}{2\tau}} \right) \leq c(m, n) \delta^{m+\frac{n}{2}-2} \tau e^{-\frac{\delta^2}{2\tau}}.$$

\square

7 Proofs of the Main Theorems

This final section presents proofs of the three theorems stated in the introduction. The proof of Theorem A will be complete once we have established Proposition 2.2; Theorems B and C then follow easily. All are consequences of Convolution Theorem 6.1 or its proof. The proofs will involve the constants δ_A and $d_A = \text{diam}(A)$ introduced in the proof of Theorem 6.1.

Proof of Proposition 2.2. We must bound the integral I given by (2.9). By Lemma 2.1, there is a $\delta_A > 0$ so that the inner integral in I is over a region $N_B \setminus N_{2B}$ that does not intersect the balls $B(\gamma(s), \delta_A)$ for all $0 \leq s \leq t$ and all $\gamma \in \Gamma(x, y, L)$. Lemma 2.1 also shows that there is a bound $|\Gamma|$ on the cardinality of $\Gamma(x, y, L)$ for (x, y) in the compact set $(M \times M) \setminus N_{2B}$. Hence, using the notation of Theorem 6.1,

$$I \leq |\Gamma| \int_0^t ds \int_{M \setminus B_s(\delta_A)} k(t-s, x, z) \left(c_2 + \frac{r_\gamma}{s} c_3 \right) k_\gamma(s, z, y) dv_z \quad (7.1)$$

Now repeat the steps in the proof of Theorem 6.1: choose a minimal geodesic γ_1 from x to z in time $t-s$, replace $k(t-s, x, z)$ by (6.2), set $\tau = \frac{4s(t-s)}{t}$ and apply the Energy Loss Lemma 5.1. Each path $\gamma_1 \cup \gamma$ flows to a stable geodesic $\bar{\gamma}$, and we can again replace γ by a length-minimizing geodesic γ_0 in $\Gamma(x, y, L)$ that satisfies $S(\gamma_0) \leq S(\bar{\gamma})$. After pulling back by the exponential map and noting that $1/s \leq 4/\tau$, the inner integral in (7.1) is bounded, for $t \leq \min\{1, r_0^2\}$, by the expression (6.7) with its integral replaced by

$$\int_{T_p M \setminus B(0, \delta_A)} \left(c_2 + \frac{|\xi|}{\tau} c_3 \right) e^{-\frac{\alpha|\xi|^2}{4\tau}} dv_\xi. \quad (7.2)$$

By Lemma 6.2 with $x = \frac{\sqrt{\alpha}}{2} \xi$, this integral is bounded by $c(n, \delta_A) \tau^{\frac{n}{2}} \exp(-\alpha\delta_A^2/4\tau)$ provided that $(n-1)t_2 < \delta_A^2/8$. We then have

$$I \leq c(\beta, c_1, \rho, A) |\Gamma| t^{\frac{p}{2}} \bar{k}_L(t, x, y) \int_0^t e^{[2\beta d_A^2 - \alpha\delta_A^2]/4\tau} ds.$$

where c_1 is the constant in (6.1). Next set $\beta = \alpha\delta_A^2/4d_A^2$ and choose $t_2 \leq \min\{1, r_0^2\}$ small enough that $(n-1)t_2 < \delta_A^2/8$ and note that $\tau \leq t$. Then

$$I \leq c(c_1, \rho, A) t^{1+\frac{p}{2}} e^{-\alpha\delta_A^2/8t} k_L(t, x, y)$$

whenever $t \leq t_2$. If $p < -2$ we can also use the inequality $t^{-p/2} e^{-\varepsilon/t} \leq c(p, \varepsilon)$. This gives the inequality of Proposition 2.2 because $k_L(t, x, y) = \bar{k}_L(t, x, y)$ for all $(x, y) \in A$. \square

Proof of Theorem B. By Theorem A there is a $t_0 > 0$ such that $k(t, x, y) \leq c k_L(t, x, y)$ for all $t < t_0$. On the other hand, E.B. Davies proved in [D] that under the hypotheses

of Theorem B, the Li-Yau bound (6.2) holds for all $t > 0$ when, say, $\beta = 1/2$. Hence

$$k(t, x, y) \leq c(4\pi t)^{\frac{p-n}{2}} e^{-\frac{d^2(x,y)}{4t}} e^{\frac{d_A^2}{8t}}$$

for $t \geq t_0$. Again using the calculus inequality $t^{p/2} \exp(d_A^2/8t) \leq c(p, d_A) \exp(d_A^2/16t)$ we obtain, for $t \geq t_0$,

$$k(t, x, y) \leq c' e^{\frac{d_A^2}{8t_0}} k_L(t, x, y) \leq c'' k_L(t, x, y)$$

where c'' and t_0 again depend on c_1, δ, L and ρ and are uniform for (x, y) in compact sets in $(M \times M) \setminus \mathcal{C}_L$.

The corresponding bound (0.6) on the heat kernel for the bundle Laplacian $\nabla^* \nabla + \mathcal{A}$ follows using the comparison principle, exactly as in Taubes's paper [T], Proposition 5.2. \square

Finally, we will prove Theorem C in the following more explicit form.

Theorem C'. *Fix $\varepsilon > 0$, $(x, y) \in (M \times M) \setminus \mathcal{C}_L$, s with $0 < s < t$, and $B_s(\delta)$ as in the statement of Theorem B. Then there are constants C, ε and t_2 , uniform for (x, y) in compact sets $(M \times M) \setminus \mathcal{C}_L$, such that*

$$\left| k(t, x, y) - \int_{B_s(\delta)} k(s, x, z) k(t-s, z, y) \right| \leq C e^{-\varepsilon/t} k(t, x, y) \quad \forall t \leq t_2. \quad (7.3)$$

Proof. By (1.1) and the fact that $k(t, x, y) > 0$ the lefthand side of (7.3) is

$$I = \int_{M \setminus B_s(\delta)} k(s, x, z) k(t-s, z, y) dv_z.$$

Applying the bound (6.2) to the second factor of k shows that for each $\beta > 0$ there is a constant $c(\beta)$ such that

$$I \leq c(\beta) \int_{M \setminus B_s(\delta)} k(s, x, z) k_\beta(t-s, z, y) dv_z.$$

Theorem C' then follows immediately from the Convolution Theorem 6. \square

Appendix: The Exponential Jacobian

Let D_γ denote the Jacobian of the exponential map along a geodesic γ . This appendix reviews some basic properties of D_γ ; these are proved using Jacobi fields.

Jacobi fields along a geodesic $\gamma(r)$ are infinitesimal variations of γ through geodesics. Specifically, let ξ be the initial tangent vector $\dot{\gamma}(0)$ and choose a vector $\eta \in T_{\gamma(0)}M$. The map $\Phi(s, u) = \exp[s(\xi + u\eta)]$ defines a variation of $\gamma(s) = \Phi(s, 0)$ by geodesics $\gamma_u(s) = \Phi(s, u)$. The tangent vectors $T = \Phi_*\partial/\partial s$ satisfy the geodesic equation $\nabla_T T = 0$ and the variational vectors $X = \Phi_*\partial/\partial u$ satisfy the Jacobi equation

$$\nabla_T \nabla_T X = R(T, X)T. \quad (\text{A.1})$$

Solutions of (A.1) are called Jacobi fields along γ ; they form a $2n$ -dimensional space. For any two Jacobi fields X, Y the skew form

$$\omega(X, Y) = \langle \nabla_T X, Y \rangle - \langle X, \nabla_T Y \rangle$$

is constant along γ since $[\omega(X, Y)]' = 0$ by (A.1) and the symmetries of the curvature.

Lemma A.1. *Let γ be a geodesic from $p = \gamma(0)$ to $q = \gamma(r)$. The differentials of the exponential maps from p to q along γ and from q to p along $-\gamma$ are adjoint. Consequently $D = |\det(\text{dexp})|$ satisfies*

$$D_\gamma = D_{-\gamma}. \quad (\text{A.2})$$

Proof. Let $\xi = \dot{\gamma}(0)$ and $\eta = \dot{\gamma}(r)$ be the initial and final tangent vectors to γ . Then $q = \exp_p(r\xi)$ and $p = \exp_q(-r\eta)$. Choose vectors $x \in T_pM$ and $y \in T_qM$ and let $X(s), Y(s)$ be the Jacobi fields along γ with $X(0) = 0$, $(\nabla_T X)(0) = x$ and $Y(r) = 0$, $(\nabla_{-T} Y)(r) = y$. At q

$$\omega(X, Y) = -\langle X(r), y \rangle = -\langle (\text{dexp}_{(r\xi)})x, y \rangle$$

and at p

$$\omega(X, Y) = \langle x, Y(0) \rangle = \langle x, (\text{dexp}_{(-r\xi)})y \rangle.$$

These are equal since $\omega(X, Y)$ is constant along γ . □

Let γ be a locally minimal geodesic from $p = \gamma(0)$ to $q = \gamma(t)$, so no point of γ is conjugate to p . There are several functions defined in a neighborhood of q : the distance function $r = d(p, \cdot)$ (measured along geodesics close to γ), the energy function $S = r^2/4t$, and the Jacobian $D_\gamma(\cdot)$ of the exponential map from p , also measured along geodesics close to γ . These functions are related by the following version of the Laplacian Comparison Theorem.

Lemma A.2. *Let $-(n-1)\rho^2$ be an lower bound for the Ricci curvature of M . Then along each locally minimal geodesic γ of length r*

$$\Delta S_\gamma + \frac{n}{2t} = -\frac{r}{2t} D_\gamma^{-1} \nabla_r D_\gamma \tag{A.3}$$

with the bounds

$$\frac{1}{n-1} D^{-1} \nabla_r D \leq \frac{1}{r} [\rho r \coth(\rho r) - 1] \leq \rho, \quad D_\gamma(r) \leq \left(\frac{\sinh(\rho r)}{\rho r} \right)^{n-1} \leq e^{(2n-2)\rho r} \tag{A.4}$$

where the first and third inequalities hold when M has constant curvature $-\rho^2$ along γ .

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