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# Diffusion in small time in incomplete sub-Riemannian manifolds

I. BAILLEUL and J. NORRIS<sup>1</sup>

**Abstract.** For incomplete sub-Riemannian manifolds, and for an associated second-order hypoelliptic operator, which need not be symmetric, we identify two alternative conditions for the validity of Gaussian-type upper bounds on heat kernels and transition probabilities, with optimal constant in the exponent. Under similar conditions, we obtain the small-time logarithmic asymptotics of the heat kernel, and show concentration of diffusion bridge measures near a path of minimal energy. The first condition requires that we consider points whose distance apart is no greater than the sum of their distances to infinity. The second condition requires only that the operator not be too asymmetric.

## 1 – Introduction

Let  $M$  be a possibly unbounded connected smooth manifold, which is equipped with a smooth sub-Riemannian structure  $X_1, \dots, X_m$  and a positive smooth measure  $\nu$ . Thus,  $X_1, \dots, X_m$  are smooth vector fields on  $M$  which, taken along with their commutator brackets of all orders, span the tangent space at every point, and  $\nu$  has a positive smooth density with respect to Lebesgue measure in each coordinate chart. Consider the symmetric bilinear form  $a$  on  $T^*M$  given by

$$a(x) := \sum_{\ell=1}^m X_\ell(x) \otimes X_\ell(x).$$

Let  $\mathcal{L}$  be a second order differential operator on  $M$  with smooth coefficients, such that  $\mathcal{L}1 = 0$  and  $\mathcal{L}$  has principal symbol  $a/2$ . In each coordinate chart,  $\mathcal{L}$  takes the form

$$\mathcal{L} = \frac{1}{2} \sum_{i,j=1}^d a^{ij}(x) \frac{\partial^2}{\partial x^i \partial x^j} + \sum_{i=1}^d b^i(x) \frac{\partial}{\partial x^i} \quad (1.1)$$

for some smooth functions  $b^i$  on the coordinate chart. Write  $p$  for the Dirichlet heat kernel of  $\mathcal{L}$  in  $M$  with respect to  $\nu$ , and write  $B = (B_t : t \in [0, \zeta))$  for the associated diffusion process. For  $x, y$  of  $M$  and  $t \in (0, \infty)$ , set

$$\Omega^{t,x,y} := \left\{ \omega \in C([0, t], M) : \omega_0 = x \text{ and } \omega_t = y \right\}.$$

Consider the case where  $B_0 = x$ . While the explosion time  $\zeta$  of  $B$  may be finite, we can still disintegrate the sub-probability law  $\mu^{t,x}$  of  $B$  restricted to the event  $\{\zeta > t\}$  by a unique family of probability measures  $(\mu^{t,x,y} : y \in M)$ , weakly continuous in  $y$ , such that

$$\mu^{t,x,y}(\Omega^{t,x,y}) = 1$$

and

$$\mu^{t,x}(d\omega) = \int_M \mu^{t,x,y}(d\omega) p(t, x, y) \nu(dy).$$

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The probability measures  $\mu^{t,x,y}$  are called *bridge measures*. It will be convenient to consider these measures all on the same space  $\Omega^{x,y} := \Omega^{1,x,y}$ . So define  $\sigma_t : \Omega^{t,x,y} \rightarrow \Omega^{x,y}$  by  $\sigma_t(\omega)_s := \omega_{st}$  and define  $\mu_t^{x,y}$  on  $\Omega^{x,y}$  by

$$\mu_t^{x,y} := \mu^{t,x,y} \circ \sigma_t^{-1}.$$

We focus mainly on two problems, each associated with a choice of the endpoints  $x$  and  $y$ , and with the limit  $t \rightarrow 0$ . The first is to *give conditions for the validity of Varadhan's asymptotics for the heat kernel*

$$t \log p(t, x, y) \rightarrow -\frac{d(x, y)^2}{2}, \quad (1.2)$$

where  $d$  is the sub-Riemannian distance. The second is to *give conditions for the weak limit*

$$\mu_t^{x,y} \rightarrow \delta_\gamma \quad (1.3)$$

where  $\gamma$  is a path of minimal energy in  $\Omega^{x,y}$ . We wish to understand, in particular, what can be said without symmetry or ellipticity of the operator  $\mathcal{L}$ , and *without compactness or even completeness of the underlying space  $M$* . The heat kernel and the bridge measures have a global dependence on  $\mathcal{L}$ , while the limit objects have a more local character, so the limits depend on some localization of diffusion in small time. We will give two sufficient conditions for this localization, the first generalizing from the Riemannian case a criterion of Hsu [8] and the second requiring a ‘sector condition’ which ensures that the asymmetry in  $\mathcal{L}$  is not too strong. We will thus give new conditions for the validity of (1.2) and (1.3), which do not require completeness, symmetry or ellipticity; no control on the diffusivity  $a$  or the symmetrizing measure  $\nu$  is needed either. In a companion paper [3], we have further investigated the small-time fluctuations of the diffusion bridge around the minimal path  $\gamma$ , which reveal a Gaussian limit process.

We define from the quadratic form  $a$  the energy  $I(\gamma)$  of an  $M$ -valued path  $\gamma$  and the distance functions on  $M$  in the classical way; see the Notations paragraph at the end of this section.

Let  $K$  be a closed set in  $M$ . Write  $p_{K^c}$  for the Dirichlet heat kernel of  $\mathcal{L}$  in  $K^c$ , extended by 0 outside  $K^c \times K^c$ . Define

$$p(t, x, K, y) := p(t, x, y) - p_{K^c}(t, x, y). \quad (1.4)$$

Then

$$p(t, x, K, y) = p(t, x, y) \mu_t^{x,y} \left( \left\{ \omega \in \Omega^{x,y} : \omega_s \in K \text{ for some } s \in [0, 1] \right\} \right).$$

We call  $p(t, x, K, y)$  the *heat kernel through  $K$* . In the case where  $K^c$  is relatively compact, we write  $p(t, x, K)$  for the hitting probability for  $K$ , given by

$$p(t, x, K) := \mathbb{P}_x(T \leq t) = 1 - \int_{K^c} p_{K^c}(t, x, y) \nu(dy) \quad (1.5)$$

where  $T := \inf\{t \in [0, \zeta) : B_t \in K\}$ .<sup>2</sup> Define also

$$\begin{aligned} d(x, K) &:= \inf \{d(x, z) : z \in K\} \\ d(x, K, y) &:= \inf \left\{ d(x, z) + d(z, y) : z \in K \right\} \end{aligned}$$

<sup>2</sup>Note that

$$p(t, x, K) \geq \int_M p(t, x, K, y) \nu(dy) \geq \int_K p(t, x, y) \nu(dy)$$

and the first inequality is strict if the process explodes, while the second inequality is always strict because the process returns to  $U$  with positive probability after hitting  $K$ .

and note that

$$d(x, K) + d(y, K) \leq d(x, K, y).$$

Define

$$d(x, \infty) := \sup \left\{ d(x, K) : K \text{ closed and } M \setminus K \text{ relatively compact} \right\}.$$

It is clear that  $d(\cdot, \infty)$  is either finite or identically infinite. By the sub-Riemannian version of the Hopf-Rinow theorem, the second case occurs if and only if  $M$  is complete for the sub-Riemannian metric. Note that the triangle inequality does not apply ‘at  $K$ ’ or ‘at  $\infty$ ’, and  $d(x, K)$  may exceed  $d(x, \infty)$  if  $M \setminus K$  is not relatively compact.

**1. Theorem** – Suppose that there is a smooth 1-form  $\beta$  on  $M$  such that

$$\mathcal{L}f = \frac{1}{2} \operatorname{div}(a \nabla f) + a(\beta, \nabla f) \quad (1.6)$$

where the divergence is understood with respect to  $\nu$ . Then, for all  $x, y \in M$  and any closed set  $K$  in  $M$  with  $M \setminus K$  relatively compact, we have

$$\limsup_{t \rightarrow 0} t \log p(t, x, K) \leq -d(x, K)^2/2 \quad (1.7)$$

and

$$\limsup_{t \rightarrow 0} t \log p(t, x, K, y) \leq -(d(x, K) + d(y, K))^2/2. \quad (1.8)$$

Moreover, if there is a finite positive constant  $\lambda$  such that

$$\sup_{x \in M} a(\beta, \beta)(x) \leq \lambda^2 \quad (1.9)$$

then, for any closed set  $K$  in  $M$ ,

$$\limsup_{t \rightarrow 0} t \log p(t, x, K, y) \leq -d(x, K, y)^2/2. \quad (1.10)$$

Moreover, all the above upper limits hold uniformly in  $x$  and  $y$  in compact subsets of  $M \setminus \partial K$ .

The sector condition (1.9) limits the strength of the asymmetry of  $\mathcal{L}$  with respect to  $\nu$  and plays the role of a uniform bound on the drift. We will deduce from Theorem 1 the small-time logarithmic asymptotics of the heat kernel.

**2. Theorem** – Suppose that  $\mathcal{L}$  has the form (1.6). Define

$$S := \left\{ (x, y) \in M \times M : d(x, y) \leq d(x, \infty) + d(y, \infty) \right\}.$$

Then, as  $t \rightarrow 0$ , uniformly on compacts in  $S$ ,

$$t \log p(t, x, y) \rightarrow -d(x, y)^2/2. \quad (1.11)$$

Moreover, if  $\mathcal{L}$  satisfies (1.9), then (1.11) holds uniformly on compacts in  $M \times M$ .

We will deduce from Theorem 1 also the following concentration estimate for the bridge measures  $\mu_t^{x,y}$  on  $\Omega^{x,y}$ . A path  $\gamma \in \Omega^{x,y}$  is *minimal* if  $I(\gamma) < \infty$  and

$$I(\gamma) \leq I(\omega) \text{ for all } \omega \in \Omega^{x,y}.$$

We will say that  $\gamma$  is *strongly minimal* if, in addition, there exist  $\delta > 0$  and a relatively compact open set  $U$  in  $M$  such that

$$I(\gamma) + \delta \leq I(\omega) \text{ for all } \omega \in \Omega^{x,y} \text{ which leave } U.^3 \quad (1.12)$$

<sup>3</sup>When  $M$  is complete for the sub-Riemannian distance, all metric balls are relatively compact, so every minimal path is strongly minimal. Also, if there is a unique minimal path  $\gamma \in \Omega^{x,y}$ , which is strongly minimal, then, by a weak compactness argument, for all relatively compact domains  $U$  containing  $\gamma$ , there is a  $\delta > 0$  such that (1.12) holds.

**3. Theorem** – Suppose that  $\mathcal{L}$  has the form (1.6). Let  $x, y \in M$  and suppose that there is a unique minimal path  $\gamma \in \Omega^{x,y}$ . Suppose either that

$$d(x, y) < d(x, \infty) + d(y, \infty),$$

or that the drift in  $\mathcal{L}$  satisfies the boundedness assumption (1.9) and  $\gamma$  is strongly minimal. Write  $\delta_\gamma$  for the unit mass at  $\gamma$ . Then

$$\mu_t^{x,y} \rightarrow \delta_\gamma \quad \text{weakly on } \Omega^{x,y} \text{ as } t \rightarrow 0.$$

Theorems 1, 2 and 3 are our main results; they are proved in Section 5 as a consequence of Proposition 6 and Proposition 7 that give Gaussian-type upper bounds, for heat kernels and hitting probabilities respectively. The proof of the latter builds on the extension to the incomplete case of the dual characterization for complete sub-Riemannian metrics, proved by Jerison and Sanchez-Calle [11], given here in Section 3.

**Notations.** For an absolutely continuous path  $\gamma : [0, 1] \rightarrow M$ , the energy  $I(\gamma)$  is given by

$$I(\gamma) = \inf \int_0^1 \langle \xi_t, a(\gamma_t)\xi_t \rangle dt$$

where the infimum is taken over all measurable paths  $\xi : [0, 1] \rightarrow T^*M$  such that  $\xi_t \in T_{\gamma_t}^*M$  for all  $t$  and, for almost all  $t$ ,

$$\dot{\gamma}_t = a(\gamma_t)\xi_t.$$

If  $\gamma$  is not absolutely continuous or there is no such path  $\xi$ , then we set  $I(\gamma) = \infty$ . The sub-Riemannian distance is given by

$$d(x, y) = \inf \left\{ \sqrt{I(\gamma)} : \gamma \in \Omega^{x,y} \right\}.$$

It is known that  $d$  defines a metric on  $M$  which is compatible with the topology of  $M$ .

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## 2 – Discussion and review of related works

- The small-time logarithmic asymptotics for the heat kernel (1.2) or (1.11) were proved by Varadhan [21] in the case when  $M = \mathbb{R}^d$  and  $a$  is uniformly bounded and uniformly positive-definite. Azencott [1] considered the case where  $a$  is positive-definite but  $M$  is possibly incomplete for the associated metric  $d$ . He showed [1, Chapter 8, Proposition 4.4], that the condition

$$d(x, y) < \max \{d(x, \infty), d(y, \infty)\} \tag{2.1}$$

is sufficient for a Gaussian-type upper bound which implies the small time logarithmic asymptotics (1.2). In particular, completeness is sufficient. He showed also [1, Chapter 8, Proposition 4.10], that such an upper bound holds for  $p_U(t, x, y)$ , without further conditions, whenever  $U$  is a relatively compact open set in  $M$ . Azencott also gave an example [1, Chapter 8, Section 2], which shows that (1.2) can fail without a suitable global condition on the operator  $\mathcal{L}$ . Hsu [8] showed that Azencott's condition (2.1) for (1.2) could be relaxed to

$$d(x, y) \leq d(x, \infty) + d(y, \infty) \tag{2.2}$$

and gave an example to show that (1.2) can fail without this condition.

Azencott and Hsu's methods in [1] and [8] work 'outwards' from relatively compact subdomains  $U$  in  $M$  and make essential use of the following identity, which allows to control  $p$  in terms of  $p_U$ . See [1, Chapter 2, Theorem 4.2]. Let  $U, V$  be open sets in  $M$  with  $V$  compactly contained in  $U$ . Then, for  $x \in M$  and  $y \in V$ , we have the decomposition

$$p(t, x, y) = 1_U(x)p_U(t, x, y) + \int_{[0,t] \times \partial V} p_U(t-s, z, y) \mu_x(ds, dz) \quad (2.3)$$

where

$$\mu_x = \sum_{n=1}^{\infty} \mu_x^n, \quad \mu_x^n([0, t] \times A) = \mathbb{P}_x(B_{T_n} \in A, T_n \leq t)$$

where we set  $S_0 = 0$  and define recursively for  $n \geq 1$

$$T_n := \inf \left\{ t \geq S_{n-1} : B_t \in V \right\}, \quad S_n := \inf \left\{ t \geq T_n : B_t \notin U \right\}.$$

This can be combined with the estimate

$$\mu_x([0, t] \times \partial V) \leq C(U, V)t, \quad C(U, V) < \infty$$

to obtain estimates on  $p(t, x, y)$  from estimates on  $p_U(t, x, y)$ . The same identity (2.3) is also used elsewhere to deduce estimates under local hypotheses from estimates requiring global hypotheses. See for example [12] on hypoelliptic heat kernels, and [6] on Hunt processes.

- Varadhan's asymptotics (1.2) were extended to the sub-Riemannian case by Léandre [13, 14] under the hypothesis

$$M = \mathbb{R}^d \quad \text{and} \quad X_0, X_1, \dots, X_m \text{ are bounded with bounded derivatives of all orders.} \quad (2.4)$$

Here,  $X_0$  is the vector field on  $M$  which appears when we write  $\mathcal{L}$  in Hörmander's form

$$\mathcal{L} = \frac{1}{2} \sum_{\ell=1}^m X_\ell^2 + X_0.$$

Our Theorem 2 extends (1.2) to a general sub-Riemannian manifold for operators  $\mathcal{L}$  of the form (1.6), subject either to Hsu's condition (2.2), understood for the sub-Riemannian metric, or to the sector condition (1.9).

- A powerful approach to analysis of the heat equation emerged in the work of Grigor'yan [5] and Saloff-Coste [18, 19]. They showed that a local volume-doubling inequality, combined with a local Poincaré inequality, implies a local Sobolev inequality, which then allows to prove regularity properties for solutions of the heat equation by Moser's procedure, and then heat kernel upper bounds by the Davies–Gaffney argument. This was taken up in the general context of Dirichlet forms by Sturm who proved a Gaussian upper bound [20, Theorem 2.4] under such local conditions, without completeness and for non-symmetric operators. Moreover, in this bound, the intrinsic metric appears with the correct constant in the exponent, which allows to deduce the correct logarithmic asymptotic upper bound (1.2). This intrinsic metric corresponds in our context to the dual formulation of the sub-Riemannian metric. Our Gaussian upper bounds can be seen as applications of Sturm's result. For greater transparency, we will re-run part of the argument in our context, rather than embed in the general framework and check the necessary hypotheses. The approach thus adopted no longer relies on working outwards from well-behaved heat kernels using (2.3), but reduces the global aspect to a certain sort of  $L^2$ -estimate for solutions of the heat equation, which requires no completeness in the underlying space. One finds that the sector condition (1.9) on the drift is enough to prevent pathologies in the  $L^2$ -estimate, thus dispensing with the need for condition (2.2) on the end-points  $x, y$ .

This is a significant extension: for example, (1.9) is satisfied trivially by all symmetric operators  $\mathcal{L}f = \frac{1}{2} \operatorname{div}(a\nabla f)$ , without any control on the diffusivity  $a$  or the symmetrizing measure  $\nu$  near infinity.

- The small-time convergence of bridge measures is known in the case of Brownian motion in a complete Riemannian manifold by a result of Hsu [7] and in the case of Hörmander's type operators  $\mathcal{L} = \frac{1}{2} \sum_{\ell=1}^m X_\ell + X_0$ , on a closed manifold, with no horizontality assumption on the drift  $X_0$ , by a result of Bailleul [2]. It is also known under the assumption (2.4) and subject to the condition that  $a(x)$  is positive-definite by work of Inahama [9] on  $\mathbb{R}^d$ . While the limit is the expected one, given the well-known small-time large deviations behaviour of diffusions, a statement such as Theorem 3 appears new, both for incomplete manifolds and in the unbounded sub-Riemannian case.

**Remark.** *We have not attempted to minimize regularity assumptions for coefficients but note that their use for upper bounds is limited to certain basic tools. The analysis [16] of metric balls, in particular the volume-doubling inequality (3.2), is done for the case where  $X_1, \dots, X_m$  are smooth. Also the Poincaré inequality (3.6) is proved in [10] in this framework. These points aside, for upper bounds, the smooth assumptions on  $a$ ,  $\nu$  and  $\beta$  are used only to imply local boundedness. While the dual characterization of the distance function is unaffected by modification of  $a$  on a Lebesgue null set, the definition as an infimum over paths is more fragile, and current proofs that these give the same quantity rely on the continuity of  $a$ . In contrast to the Riemannian case [17], for lower bounds in the sub-Riemannian case, in particular for Léandre's argument using Malliavin calculus, current methods demand more regularity.*

### 3 – Dual formulation of the sub-Riemannian distance

We review some basic analytic facts for sub-Riemannian manifolds before extending Jerison and Sanchez-Calle's dual formulation of the sub-Riemannian distance [11] to possibly incomplete settings.

#### 3.1 – Analytic ingredients

The set-up of Section 1 is assumed. Nagel, Stein & Wainger's analysis [16] of the sub-Riemannian distance and of the volume of sub-Riemannian metric balls implies the following statements. There is a covering of  $M$  by charts  $\phi : U \rightarrow \mathbb{R}^d$  such that, for some constants  $\alpha(U) \in (0, 1]$  and  $C(U) \in [1, \infty)$ , for all  $x, y \in U$ ,

$$C^{-1}|\phi(x) - \phi(y)| \leq d(x, y) \leq C|\phi(x) - \phi(y)|^\alpha. \quad (3.1)$$

Moreover, there is a covering of  $M$  by open sets  $U$  such that, for some constant  $C(U) \in (1, \infty)$ , for all  $x \in U$  and all  $r \in (0, \infty)$  such that  $B(x, 2r) \subseteq U$ , we have the volume-doubling inequality

$$\nu(B(x, 2r)) \leq C\nu(B(x, r)). \quad (3.2)$$

Moreover, in [16, Theorem 1], a uniform local equivalent for  $\nu(B(x, r))$  is obtained, which implies that, for all  $x \in M$ ,

$$\lim_{r \rightarrow 0} \frac{\log \nu(B(x, r))}{\log r} = N(x). \quad (3.3)$$

Here,  $N(x)$  is given by

$$N(x) = N_1(x) + 2N_2(x) + 3N_3(x) + \dots \quad (3.4)$$

where  $N_1(x) + \dots + N_k(x)$  is the dimension of the space spanned at  $x$  by brackets of the vector fields  $X_1, \dots, X_m$  of length at most  $k$ . While the limit (3.3) is in general not locally uniform, there is also the following uniform asymptotic lower bound on the volume of small balls, for any compact set  $F$  in  $M$ ,

$$\limsup_{r \rightarrow 0} \sup_{x \in F} \frac{\log \nu(B(x, r))}{\log r} \leq N(F) \quad (3.5)$$

where

$$N(F) := \sup_{x \in F} N(x) < \infty.$$

We recall also the local Poincaré inequality proved by Jerison [10]. There is a covering of  $M$  by open sets  $U$  such that, for some constant  $C(U) < \infty$ , for all  $x \in U$  and all  $r \in (0, \infty)$  such that  $B(x, 2r) \subseteq U$ , for all  $f \in C_c^\infty(M)$ , we have

$$\int_{B(x, r)} |f - \langle f \rangle_{B(x, r)}|^2 d\nu \leq Cr^2 \int_{B(x, 2r)} a(\nabla f, \nabla f) d\nu \quad (3.6)$$

where  $\langle f \rangle_B := \frac{1}{\nu(B)} \int_B f d\nu =: \int_B f d\nu$  is the average value of  $f$  on  $B$ . As Saloff-Coste claimed [19, Theorem 7.1], the validity of Moser's argument, given (3.2) and (3.6), extends with minor modifications to suitable non-symmetric operators. This leads to the following parabolic mean-value inequality.

**4. Proposition** – *Let  $\mathcal{L}$  be given as in equation (1.6) and let  $U$  be a relatively compact open set in  $M$ . Then there is a constant  $C(U) < \infty$  with the following property. For any non-negative weak solution  $u$  of the equation  $(\partial/\partial t)u_t = \mathcal{L}u_t$  on  $(0, \infty) \times U$ , for all  $x \in U$ , all  $t \in (0, \infty)$  and all  $r \in (0, \infty)$  such that  $B(x, 2r) \subseteq U$  and  $r^2 \leq t/2$ , we have*

$$u_t(x)^2 \leq C \int_{t-r^2}^t \int_{B(x, r)} u_s^2 d\nu ds. \quad (3.7)$$

Moreover, the same estimate holds if  $\mathcal{L}$  is replaced by its adjoint  $\hat{\mathcal{L}}$  under  $\nu$ .

For a detailed proof, the reader may check the applicability of the more general results [4, Theorem 1.2] or [15, Theorem 4.6].

### 3.2 – Dual formulation of the sub-Riemannian distance

In Riemannian geometry, the distance function has a well known dual formulation in terms of functions of unit gradient. Jerison & Sanchez-Calle [11] showed that this dual formulation extends to complete sub-Riemannian manifolds. We now show that such a dual formulation holds without completeness, and for the distances to and through a given closed set.

**5. Proposition** – *For all  $x, y \in M$  and any closed subset  $K$  of  $M$ , we have*

$$d(x, K, y) = \sup \left\{ w^+(y) - w^-(x) : w^-, w^+ \in \mathcal{F} \text{ with } w^+ = w^- \text{ on } K \right\} \quad (3.8)$$

and

$$d(x, K) = \sup \left\{ w(x) : w \in \mathcal{F} \text{ with } w = 0 \text{ on } K \right\}, \quad (3.9)$$

where  $\mathcal{F}$  is the set of all locally Lipschitz functions  $w$  on  $M$  such that  $a(\nabla w, \nabla w) \leq 1$  almost everywhere.



**Proof** – Denote the right hand sides of (3.8) and (3.9) by  $\delta(x, K, y)$  and  $\delta(x, K)$  for now.

First we will show that  $\delta(x, K, y) \leq d(x, K, y)$ . Let  $\omega \in \Omega^{x,y}$  and suppose that  $\omega$  is absolutely continuous with driving path  $\xi$  and that  $\omega_t \in K$ . Let  $w^-, w^+ \in \mathcal{F}$ , with  $w^+ = w^-$  on  $K$ . It will suffice to consider the case where  $\omega|_{[0,t]}$  and  $\omega|_{[t,1]}$  are simple, and then to choose relatively compact charts  $U_0$  and  $U_1$  for  $M$  containing  $\omega|_{[0,t]}$  and  $\omega|_{[t,1]}$  respectively. Then, given  $\varepsilon > 0$ , since  $a$  is continuous, for  $i = 1, 2$ , we can find smooth functions  $f_i^-, f_i^+$  on  $U_i$  such that  $|f_i^\pm(z) - w^\pm(z)| \leq \varepsilon$  and  $a(\nabla f_i^\pm, \nabla f_i^\pm)(z) \leq 1 + \varepsilon$  for all  $z \in U_i$ . Then

$$w^+(y) - w^-(x) = w^+(y) - w^+(\omega_t) + w^-(\omega_t) - w^-(x) \leq f_1^+(y) - f_1^+(\omega_t) + f_0^-(\omega_t) - f_0^-(x) + 4\varepsilon$$

and

$$\begin{aligned} & f_1^+(y) - f_1^+(\omega_t) + f_0^-(\omega_t) - f_0^-(x) \\ &= \int_0^t \langle \nabla f_0^-(\omega_s), \dot{\omega}_s \rangle ds + \int_t^1 \langle \nabla f_1^+(\omega_s), \dot{\omega}_s \rangle ds \\ &= \int_0^t \langle \nabla f_0^-(\omega_s), a(\omega_s) \xi_s \rangle ds + \int_t^1 \langle \nabla f_1^+(\omega_s), a(\omega_s) \xi_s \rangle ds \\ &\leq \left( \int_0^t a(\nabla f_0^-, \nabla f_0^-)(\omega_s) ds + \int_t^1 a(\nabla f_1^+, \nabla f_1^+)(\omega_s) ds \right)^{1/2} \left( \int_0^1 a(\xi_s, \xi_s) ds \right)^{1/2} \\ &\leq \sqrt{(1 + \varepsilon)I(\omega)}. \end{aligned}$$

Hence  $w^+(y) - w^-(x) \leq \sqrt{I(\omega)}$ . On taking the supremum over  $w^\pm$  and the infimum over  $\omega$ , we deduce that

$$\delta(x, K, y) \leq d(x, K, y). \quad (3.10)$$

For  $w \in \mathcal{F}$  with  $w = 0$  on  $K$  and for  $y \in K$ , we can take  $w^- = -w$  and  $w^+ = 0$  in (3.8) to see that  $\delta(x, K) \leq \delta(x, K, y)$ . Hence, on taking the infimum over  $y \in K$  in (3.10), we obtain

$$\delta(x, K) \leq d(x, K).$$

Now we prove the reverse inequalities. Consider a smooth symmetric bilinear form  $\bar{a}$  on  $T^*M$  such that  $\bar{a} \geq a$  and  $\bar{a}$  is everywhere positive-definite. Write  $\bar{I}$  for the associated energy function and write  $\bar{d}$  and  $\bar{\delta}$  for the distance functions obtained by replacing  $a$  by  $\bar{a}$  in the definitions of  $d$  and  $\delta$ . Set

$$w^+(z) = \bar{d}(x, K, z), \quad w^-(z) = \bar{d}(x, z), \quad w(x) = \bar{d}(x, K).$$

Note that  $w^+ = w^-$  and  $w = 0$  on  $K$ . Since  $\bar{a}$  is positive-definite, the functions  $w^-, w^+$  and  $w$  are locally Lipschitz, and their weak gradients  $\nabla w^\pm$  and  $\nabla w$  satisfy, almost everywhere,

$$\bar{a}(\nabla w^\pm, \nabla w^\pm) \leq 1, \quad \bar{a}(\nabla w, \nabla w) \leq 1.$$

Hence

$$\begin{aligned} \bar{d}(x, K, y) &= w^+(y) - w^-(x) \leq \bar{\delta}(x, K, y) \leq \delta(x, K, y), \\ \bar{d}(x, K) &= w(x) \leq \bar{\delta}(x, K) \leq \delta(x, K). \end{aligned}$$

We will show that, for all  $\varepsilon > 0$  and all  $c \in [1, \infty)$ , we can choose  $\bar{a}$  so that, for all  $x, y \in M$  with  $d(x, y) \leq c$ ,

$$d(x, y) \leq \bar{d}(x, y) + \varepsilon.$$

Then, for this choice of  $\bar{a}$ , we have also, for all closed sets  $K$  with  $d(x, K), d(y, K) \leq c - 1$ ,

$$d(x, K, y) \leq \bar{d}(x, K, y) + 2\varepsilon, \quad d(x, K) \leq \bar{d}(x, K) + \varepsilon.$$

Since  $\varepsilon > 0$  and  $c \geq 1$  are arbitrary, this completes the proof. The idea in choosing  $\bar{a}$  is as follows. While we have no control over the behaviour of  $a$  near  $\infty$ , neither do we have any constraint on how small we can choose  $\bar{a} - a$  near  $\infty$ . Given  $\varepsilon > 0$ , this will allow us to choose  $\bar{a}$  so that, for any path  $\bar{\gamma} \in \Omega^{x,y}$  with  $\bar{I}(\bar{\gamma}) < \infty$ , we can construct another path  $\gamma \in \Omega^{x,y}$  with  $I(\gamma) \leq \bar{I}(\bar{\gamma}) + \varepsilon$ .

It will be convenient to fix smooth vector fields  $Y_1, \dots, Y_p$  on  $M$  which span the tangent space at every point, so that

$$a_0(x) = \sum_{i=1}^p Y_i(x) \otimes Y_i(x)$$

is a positive-definite symmetric bilinear form on  $T^*M$ . There exists an exhaustion of  $M$  by open sets  $(U_n : n \in \mathbb{N})$ , such that  $U_n$  is compactly contained in  $U_{n+1}$  for all  $n$ . Set  $U_0 = \emptyset$ . Let  $(\delta_n : n \in \mathbb{N})$  be a sequence of constants, such that  $\delta_n \in (0, 1]$  for all  $n$ , to be determined. There exists a positive smooth function  $f$  on  $M$  such that  $f \leq \delta_n$  on  $M \setminus U_{n-2}$  for all  $n$ . We take  $\bar{a} = a + f^2 a_0$ . Write  $d_0$  and  $I_0$  for the distance and energy functions associated with  $a + a_0$ . Recall that we write  $\bar{d}$  and  $\bar{I}$  for the distance and energy functions associated with  $\bar{a}$ . Then  $d_0 \leq \bar{d} \leq d$ . Set  $\varepsilon_n = d_0(\partial U_n, \partial U_{n+1})$ . By the sub-Riemannian distance estimate (3.1), there are constants  $\alpha_n \in (0, 1]$  and  $C_n < \infty$ , depending only on  $n$  and on the open sets  $(U_n : n \in \mathbb{N})$  and the vector fields  $X_1, \dots, X_m$  and  $Y_1, \dots, Y_p$ , such that, for all  $x, y \in U_{n+2}$ ,

$$d(x, y) \leq C_n d_0(x, y)^{\alpha_n}.$$

Fix a constant  $c \in [1, \infty)$ . Fix  $x, y \in M$  with  $d(x, y) \leq c$  and suppose that  $\omega \in \Omega^{x,y}$  satisfies  $\bar{I}(\omega) \leq c^2$ . There exist absolutely continuous paths  $h : [0, 1] \rightarrow \mathbb{R}^m$  and  $k : [0, 1] \rightarrow \mathbb{R}^p$  such that, for almost all  $t$ ,

$$\dot{\omega}_t = \sum_{\ell=1}^m X_\ell(\omega_t) \dot{h}_t^\ell + \sum_{i=1}^p f(\omega_t) Y_i(\omega_t) \dot{k}_t^i$$

and

$$\int_0^1 |\dot{h}_t|^2 dt + \int_0^1 |\dot{k}_t|^2 dt = \bar{I}(\omega).$$

By reparametrizing  $\omega$  if necessary, we may assume that  $|\dot{h}_t|^2 + |\dot{k}_t|^2 = \bar{I}(\omega)$  for almost all  $t$ . Consider for now the case where  $\omega_t \in U_{n+1} \setminus U_{n-1}$  for all  $t$  for some  $n$  and define a new path  $\gamma$  by

$$\dot{\gamma}_t = \sum_{\ell=1}^m X_\ell(\gamma_t) \dot{h}_t^\ell, \quad \gamma_0 = x.$$

Then  $I(\gamma) \leq \bar{I}(\omega)$ . By Gronwall's lemma, there is a constant  $A_n \in [1, \infty)$ , depending only on  $n$  and on the open sets  $(U_n : n \in \mathbb{N})$  and the vector fields  $X_1, \dots, X_m$  and  $Y_1, \dots, Y_p$ , such that

$$d_0(\gamma_1, y) \leq D A_n \delta_n$$

provided that

$$c A_n \delta_n \leq \varepsilon_{n-2} \wedge \varepsilon_{n+1}. \quad (3.11)$$

We will ensure that (3.11) holds, and hence that  $\gamma_1 \in U_{n+2}$ . Then

$$d(x, y) \leq d(x, \gamma_1) + d(\gamma_1, y) \leq \sqrt{\bar{I}(\omega)} + C_n d_0(\gamma_1, y)^{\alpha_n} \leq \sqrt{\bar{I}(\omega)} + C_n c A_n \delta_n^{\alpha_n}.$$

We return to the general case. Then there is an integer  $k \geq 1$  and there is a sequence of times  $t_0 \leq t_1 \leq \dots \leq t_k$  and there is a sequence of positive integers  $n_1, \dots, n_k$  such

that  $t_0 = 0$ ,  $t_k = 1$ , and  $|n_{j+1} - n_j| = 1$  and  $\omega_{t_j} \in \partial U_{n_{j+1}}$  for  $j = 1, \dots, k-1$ , and

$$\omega_t \in \bar{U}_{n_{j+1}} \setminus U_{n_{j-1}}$$

for all  $t \in [t_{j-1}, t_j]$  and all  $j = 1, \dots, k$ , and, if  $k \geq 2$ ,  $\omega_t \in \partial U_{n_1}$  for some  $t \in [t_0, t_1]$ . Set

$$S_n = \{t_j : j \in \{1, \dots, k-1\} \text{ and } n_{j+1} = n\}, \quad \chi_n = |S_n|.$$

Since  $\omega$  must hit either  $\partial U_{n+1}$  or  $\partial U_{n-1}$  immediately prior to any time in  $S_n$ , we have

$$(\varepsilon_{n-1} \wedge \varepsilon_n) \chi_n \leq c.$$

We have shown that

$$d(\omega_{t_{j-1}}, \omega_{t_j}) \leq (t_j - t_{j-1}) \sqrt{\bar{I}(\omega)} + C_{n_j} c A_{n_j} \delta_{n_j}^{\alpha_{n_j}}$$

so

$$d(x, y) \leq \sum_{j=1}^k d(\omega_{t_{j-1}}, \omega_{t_j}) \leq \sqrt{\bar{I}(\omega)} + C_{n_1} c A_{n_1} \delta_{n_1}^{\alpha_{n_1}} + \sum_{n=1}^{\infty} C_n c A_n \chi_n \delta_n^{\alpha_n}.$$

Now we can choose the sequence  $(\delta_n : n \in \mathbb{N})$  so that (3.11) holds and

$$2 \sum_{n=1}^{\infty} \frac{C_n c^2 A_n \delta_n^{\alpha_n}}{\varepsilon_{n-1} \wedge \varepsilon_n} \leq \varepsilon.$$

Then, on optimizing over  $\omega$ , we see that  $d(x, y) \leq \bar{d}(x, y) + \varepsilon$  whenever  $d(x, y) \leq c$ , as required.  $\triangleright$

## 4 – Gaussian-type upper bounds

Recall the definition  $p(t, x, K, y)$  of the heat kernel via  $K$  given in (1.4) and the definition of the hitting probability  $p(t, x, K)$  given in (1.5).

**6. Proposition** – *Let  $\mathcal{L}$  be given as in equation (1.6) and suppose that the drift in  $\mathcal{L}$  satisfies the sector/boundedness condition (1.9). Then there is a continuous function  $C : M \times M \rightarrow (0, \infty)$  such that, for all  $x, y \in M$  and all  $t \in (0, \infty)$ , for*

$$r = \min \left\{ \frac{t}{d(x, y)}, \sqrt{\frac{t}{4}}, \frac{d(x, \infty)}{4}, \frac{d(y, \infty)}{4} \right\}$$

we have

$$p(t, x, y) \leq \frac{C(x, y)}{\sqrt{\nu(B(x, r))} \sqrt{\nu(B(y, r))}} \exp \left\{ -\frac{d(x, y)^2}{2t} + \frac{\lambda^2 t}{2} \right\}. \quad (4.1)$$

Moreover, for any closed set  $K = M \setminus U$  in  $M$ , there is a continuous function  $C(\cdot, \cdot, K) : U \times U \rightarrow (0, \infty)$  such that, for all  $x, y \in U$  and all  $t \in (0, \infty)$ , for

$$r = \min \left\{ \frac{t}{d(x, K, y)}, \sqrt{\frac{t}{4}}, \frac{r(x, K)}{4}, \frac{r(y, K)}{4} \right\}, \quad r(x, K) = \min\{d(x, \infty), d(x, K)\}$$

we have

$$p(t, x, K, y) \leq \frac{C(x, y, K)}{\sqrt{\nu(B(x, r))} \sqrt{\nu(B(y, r))}} \exp \left\{ -\frac{d(x, K, y)^2}{2t} + \frac{\lambda^2 t}{2} \right\}. \quad (4.2)$$

The statements above remain true with the constant 4 replaced by 2, by the local volume-doubling inequality. The value 4 will be convenient for the proof.

**Proof** – We omit the proof of (4.1), which is a simpler version of the proof of (4.2). For (4.2), we will show that the argument used in [17, Theorem 1.2], for the case where  $a$  is positive-definite and  $\beta = 0$ , generalizes to the present context<sup>4</sup>. Consider the set  $\widetilde{M} := M^- \cup M^+$ , where  $M^\pm = K \cup U^\pm$  and  $U^-, U^+$  are disjoint copies of  $U = M \setminus K$ . Write  $\pi$  for the obvious projection  $\widetilde{M} \rightarrow M$ . For functions  $f$  defined on  $M$ , we will write  $f$  also for the function  $f \circ \pi$  on  $\widetilde{M}$ . Thus we will sometimes consider  $a$  as a symmetric bilinear form on  $T^*U^\pm$  and  $\beta$  as a 1-form on  $U^\pm$ . Define a measure  $\widetilde{\nu}$  on  $\widetilde{M}$  by

$$\widetilde{\nu}(A) := \nu(A \cap K) + \frac{1}{2}\nu(\pi(A \cap U^-)) + \frac{1}{2}\nu(\pi(A \cap U^+)).$$

Note that  $\nu = \widetilde{\nu} \circ \pi^{-1}$ . Now define

$$\widetilde{p}(t, x, y) = \begin{cases} p(t, x, y) + p_U(t, x, y), & \text{if } x, y \in U^\pm, \\ p(t, x, y) - p_U(t, x, y), & \text{if } x \in U^\pm \text{ and } y \in U^\mp, \\ p(t, x, y), & \text{if } x \in K \text{ or } y \in K. \end{cases}$$

Given bounded measurable functions  $f^-, f^+$  on  $M$  with  $f^- = f^+$  on  $K$ , write  $f$  for the function on  $\widetilde{M}$  such that  $f = f^\pm \circ \pi$  on  $M^\pm$ , and set  $\bar{f} = (f^- + f^+)/2$  and  $f^U = (f^+ - f^-)/2$ . Let  $\phi^-$  and  $\phi^+$  be smooth functions on  $M$ , of compact support, with  $\phi^- = \phi^+$  on  $K$  and define  $\phi$  on  $\widetilde{M}$  and  $\bar{\phi}$  and  $\phi^U$  on  $M$  similarly. For  $t \in (0, \infty)$ , define functions  $u_t$  on  $\widetilde{M}$ ,  $\bar{u}_t$  on  $M$  and  $u_t^U$  on  $U$  by

$$u_t(x) = \int_{\widetilde{M}} \widetilde{p}(t, x, y) f(y) \widetilde{\nu}(dy)$$

and

$$\bar{u}_t(x) = \int_M p(t, x, y) \bar{f}(y) \nu(dy), \quad u_t^U(x) = \int_M p_U(t, x, y) f^U(y) \nu(dy).$$

Then  $\bar{u}_t$  and  $u_t^U$  solve the heat equation with Dirichlet boundary conditions in  $M$  and  $U$  respectively. It is straightforward to check that  $u_t = u_t^\pm \circ \pi$  on  $M^\pm$ , where  $u_t^\pm = \bar{u}_t \pm u_t^U$  and we extend  $u_t^U$  by 0 on  $K$ . Hence

$$\int_{\widetilde{M}} \phi u_t d\widetilde{\nu} = \int_M \bar{\phi} \bar{u}_t d\nu + \int_U \phi^U u_t^U d\nu$$

and so

$$\begin{aligned} \frac{d}{dt} \int_{\widetilde{M}} \phi u_t d\widetilde{\nu} &= \frac{d}{dt} \int_M \bar{\phi} \bar{u}_t d\nu + \frac{d}{dt} \int_U \phi^U u_t^U d\nu \\ &= -\frac{1}{2} \int_M a(\nabla \bar{\phi}, \nabla \bar{u}_t) d\nu + \int_M a(\bar{\phi} \beta, \nabla \bar{u}_t) d\nu \\ &\quad - \frac{1}{2} \int_U a(\nabla \phi^U, \nabla u_t^U) d\nu + \int_U a(\phi^U \beta, \nabla u_t^U) d\nu \\ &= -\frac{1}{2} \int_{\widetilde{M}} a(\nabla \phi, \nabla u_t) d\widetilde{\nu} + \int_{\widetilde{M}} a(\phi \beta, \nabla u_t) d\widetilde{\nu}. \end{aligned} \tag{4.3}$$

Let  $(w^-, w^+)$  be a pair of bounded locally Lipschitz functions on  $M$  such that  $w^- = w^+$  on  $K$  and  $a(\nabla w^\pm, \nabla w^\pm) \leq 1$  almost everywhere. Define a function  $w$  on  $\widetilde{M}$  by setting

<sup>4</sup>The idea is to combine a standard argument for heat kernel upper bounds with a reflection trick. In terms of Markov processes, we give a random sign to each excursion of the diffusion process into  $U$ , viewing it as taking values in  $U^-$  or  $U^+$ . Then a generalization of the classical reflection principle for Brownian motion allows to express the density for paths from  $x$  to  $y$  via  $K$  in terms of this enhanced process. In fact the heat kernel  $\widetilde{p}$  for this process may be written in terms of  $p$  and  $p_U$ , and we find it technically simpler to define  $\widetilde{p}$  in those terms, rather than set up the enhanced process.

$w = w^\pm \circ \pi$  on  $M^\pm$ . Fix  $\theta \in (0, \infty)$  and set  $\psi = \theta w$ . We deduce from (4.3) by a standard argument that

$$\begin{aligned} \frac{d}{dt} \int_{\tilde{M}} (e^{-\psi} u_t)^2 d\tilde{\nu} &= - \int_{\tilde{M}} a(\nabla(e^{-2\psi} u_t), \nabla u_t) d\tilde{\nu} + 2 \int_{\tilde{M}} a(\beta e^{-2\psi} u_t, \nabla u_t) d\tilde{\nu} \\ &= - \int_{\tilde{M}} a(\nabla u_t, \nabla u_t) e^{-2\psi} d\tilde{\nu} + 2 \int_{\tilde{M}} a((\beta + \nabla\psi)u_t, \nabla u_t) e^{-2\psi} d\tilde{\nu} \\ &\leq \int_{\tilde{M}} a(\beta + \nabla\psi, \beta + \nabla\psi) (e^{-\psi} u_t)^2 d\tilde{\nu} \leq \rho \int_{\tilde{M}} (e^{-\psi} u_t)^2 d\tilde{\nu} \end{aligned}$$

where

$$\rho := \left\| a(\beta + \nabla\psi, \beta + \nabla\psi) \right\|_\infty \leq (\lambda + \theta)^2.$$

Then, by Gronwall's inequality,

$$\int_{\tilde{M}} (e^{-\psi} u_t)^2 d\tilde{\nu} \leq e^{\rho t} \int_{\tilde{M}} (e^{-\psi} f)^2 d\tilde{\nu}. \quad (4.4)$$

There exists a locally finite cover  $\mathcal{U}$  of  $U$  by sets of the form  $B(x, r(x, K)/4)$ , where we recall that  $r(x, K) = \min\{d(x, \infty), d(x, K)\}$ . For  $V := B(x, r(x, K)/4) \in \mathcal{U}$ , set  $\tilde{V} := B(x, 7r(x, K)/8)$ . Then  $\tilde{V}$  is a relatively compact open subset of  $U$ . By the triangle inequality, for all  $V \in \mathcal{U}$  and all  $x \in V$ , we have  $B(x, r(x, K)/2) \subseteq \tilde{V}$ . Fix  $V_1, V_2 \in \mathcal{U}$  and write  $C(V_i)$  for the constants appearing in the parabolic mean-value inequality for  $\mathcal{L}$  on  $\tilde{V}_1$  and for  $\hat{\mathcal{L}}$  on  $\tilde{V}_2$ . Fix  $x \in V_1$ ,  $y \in V_2$  and  $t \in (0, \infty)$ , and recall that we set

$$r = \min \left\{ \frac{t}{d(x, K, y)}, \sqrt{\frac{t}{4}}, \frac{r(x, K)}{4}, \frac{r(y, K)}{4} \right\}.$$

Write  $x^-$  and  $y^+$  for the unique points in  $U^-$  and  $U^+$  respectively such that  $\pi(x^-) = x$  and  $\pi(y^+) = y$ . Set

$$B^- := \left\{ z \in U^- : \pi(z) \in B(x, r) \right\}, \quad B^+ := \left\{ z \in U^+ : \pi(z) \in B(y, r) \right\}.$$

Take  $f^- = 0$  and choose  $f^+ \geq 0$  supported on  $B(y, r)$  and such that  $\int_M (f^+)^2 d\nu = 2$ . Then  $\int_{\tilde{M}} f^2 d\tilde{\nu} = 1$ . Note that  $w \leq w^-(x) + r$  on  $B^-$  and  $w \geq w^+(y) - r$  on  $B^+$ . Hence we obtain from (4.4), for all  $s \geq 0$ ,

$$e^{-2\theta(w^-(x)+r)} \int_{B^-} u_s^2 d\tilde{\nu} \leq e^{\rho s} e^{-2\theta(w^+(y)-r)}. \quad (4.5)$$

Since  $u_t^- \geq 0$  and  $(\partial/\partial t)u_t^- = \mathcal{L}u_t^-$  on  $(0, \infty) \times U$ , by the parabolic mean-value inequality, for all  $\tau \in (0, \infty)$  such that  $r^2 \leq \tau/2$ ,

$$u_\tau(x^-)^2 \leq C(V_1) \int_{\tau-r^2}^\tau \int_{B^-} u_s^2 d\tilde{\nu} ds \leq C(V_1) \nu(B(x, r))^{-1} e^{-2\theta(w^+(y)-w^-(x)-2r)+\rho\tau}. \quad (4.6)$$

Set  $v_s(z) = p(s, x, K, z)$ , then  $v_s \geq 0$  and  $(\partial/\partial s)v_s = \hat{\mathcal{L}}v_s$  on  $(0, \infty) \times D$ . By the parabolic mean-value inequality again,

$$\begin{aligned} p(t, x, K, y)^2 &\leq C(V_2) \int_{t-r^2}^t \int_{B(y, r)} p(s, x, K, z)^2 \nu(dz) ds \\ &\leq C(V_2) \int_{t-r^2}^t \int_{B^+} \tilde{p}(s, x^-, z)^2 \tilde{\nu}(dz) ds. \end{aligned}$$

Recall that  $r^2 \leq t/4$ . For each  $s \in [t - r^2, t]$ , we can take  $f^+ = c_\star p(s, x, K, \cdot) 1_{B(y, r)}$ , where  $c_\star$  is chosen so that  $\int_{\widetilde{M}} f^2 d\widetilde{\nu} = 1$ . For this choice of  $f^+$ , we have

$$u_s(x^-)^2 = \int_{B^+} \widetilde{p}(s, x^-, z)^2 \widetilde{\nu}(dz).$$

Hence

$$\begin{aligned} p(t, x, K, y)^2 &\leq \frac{C(V_2)}{\nu(B(y, r))} \int_{t-r^2}^t u_s(x^-)^2 ds \\ &\leq \frac{C(V_1)C(V_2)}{\nu(B(x, r))\nu(B(y, r))} e^{-2\theta(w^+(y) - w^-(x) - 2r) + \rho t}. \end{aligned}$$

Here, we applied (4.6) with  $\tau = s$ , noting that  $s \geq 3t/4$ , so  $r^2 \leq t/4 \leq s/2$ . We optimize over  $(w^-, w^+)$  and take  $\theta = d(x, K, y)/t$  to obtain

$$p(t, x, K, y) \leq \frac{C(V_1, V_2, x, y)}{\sqrt{\nu(B(x, r))}\sqrt{\nu(B(y, r))}} \exp\left\{-\frac{d(x, K, y)^2}{2t} + \frac{\lambda^2 t}{2}\right\}$$

where

$$C(V_1, V_2, x, y) := e^{2+\lambda d(x, K, y)/2} \sqrt{C(V_1)C(V_2)}.$$

Finally, since  $\mathcal{U}$  is locally finite, there is a continuous function  $C(\cdot, \cdot, K) : U \times U \rightarrow (0, \infty)$  such that  $C(V_1, V_2, x, y) \leq C(x, y, K)$  for all  $V_1, V_2 \in \mathcal{U}$  and all  $x \in V_1$  and  $y \in V_2$ .  $\triangleright$

**7. Proposition** – *Let  $\mathcal{L}$  be given as in equation (1.6). Let  $U$  be a relatively compact open set in  $M$  and set  $K := M \setminus U$ . There is a constant  $C(U) < \infty$  with the following property. For all  $x \in U$  and all  $t \in (0, \infty)$ , and for  $r = t/d(x, K)$ ,*

$$p(t, x, K) \leq \frac{C}{\sqrt{\nu(B(x, r))}} \exp\left\{-\frac{d(x, K)^2}{2t}\right\}. \quad (4.7)$$

**Proof** – We adapt the argument of the proof of Proposition 6. Since  $\nu(U) < \infty$  and  $p(t, x, K) \leq 1$ , it will suffice to consider the case where  $d(x, K)^2 \geq 2t$ . We modify the measure  $\nu$  and the 1-form  $\beta$  on  $K$ , if necessary, by multiplication by suitable smooth functions, so that  $\nu(K) \leq 1$  and  $a(\beta, \beta)(x) \leq \lambda^2$  for all  $x \in M$ , for some  $\lambda < \infty$ . This does not affect the value of  $p(t, x, K)$  for  $x \in U$ . Set  $f = 1 + 1_{U^+} - 1_{U^-}$  and define, for  $x \in \widetilde{M}$ ,

$$u_t(x) = \int_{\widetilde{M}} \widetilde{p}(t, x, y) f(y) \widetilde{\nu}(dy).$$

Then  $p(t, x, K) = u_t(x^-)$  for  $x \in U$ . Fix a locally Lipschitz function  $w$  on  $\widetilde{M}$  such that  $w = 0$  on  $K \cup U^+$  and  $a(\nabla w, \nabla w) \leq 1$  almost everywhere. Then, as we showed at (4.5), for all  $\theta \in [0, \infty)$ ,

$$\int_{\widetilde{M}} (e^{\theta w} u_t)^2 d\widetilde{\nu} \leq e^{\rho t} \int_{\widetilde{M}} f^2 d\widetilde{\nu} = e^{\rho t} (2\nu(U) + \nu(K))$$

where

$$\rho := \sup_{x \in M} a(\beta - \theta \nabla w, \beta - \theta \nabla w)(x) \leq (\lambda + \theta)^2.$$

By the same argument as that leading to (4.6), there is a constant  $C(U) < \infty$  with the following property. For all  $x \in U$  and all  $t \in (0, \infty)$ , for all  $r \in (0, \infty)$  such that  $B(x, 2r) \subseteq U$  and  $r^2 \leq t/2$ , we have

$$u_t(x^-)^2 \leq C \int_{t-r^2}^t \int_{B^-} u_s^2 d\widetilde{\nu} ds$$

where  $B^- := \pi^{-1}(B(x, r)) \cap U^-$ . Since  $d(x, K)^2 \geq 2t$ , we can take  $r = t/d(x, K)$ . Note that  $w \geq w(x^-) - r$  on  $B$ . Then

$$p(t, x, K)^2 = u_t(x^-)^2 \leq C \int_{t-r^2}^t \int_B u_s^2 d\tilde{\nu} ds \leq C \nu(B(x, r))^{-1} \exp \left\{ -2\theta(w(x^-) - r) + \rho t \right\}$$

and, by optimizing over  $\varepsilon$ ,  $\theta$  and  $w$ , using Proposition 5, we obtain

$$p(t, x, K) \leq \frac{C}{\sqrt{\nu(B(x, r))}} \exp \left\{ -\frac{d(x, K)^2}{2t} \right\}.$$

▷

## 5 – Proofs of Theorems 1, 2, 3

**Proof of Theorem 1** – The asymptotic upper bound (1.10) for the heat kernel through  $K$ , under condition (1.9), follows directly from the Gaussian upper bound (4.2) and the asymptotic lower bound (3.5) for the volume of small balls, on letting  $t \rightarrow 0$ . Similarly, the asymptotic upper bound (1.7) for the hitting probability for  $K$ , when  $M \setminus K$  is relatively compact, follows from (4.7) and (3.5). It remains to show (1.8). For this, we adapt an argument of Hsu [8] for the Riemannian case. Consider the  $\mathcal{L}$ -diffusion process  $(B_t : t \in [0, \zeta])$ . Set

$$T = \inf\{t \in [0, \zeta] : B_t \in K\}.$$

We use the identity

$$p(t, x, K, y) = \mathbb{E}_x \left[ p(t - T, B_T, y) 1_{\{T < t\}} \right]. \quad (5.1)$$

Note that  $\mathbb{P}_x(T \leq t) = p(t, x, K)$  and the estimate (4.7) applies. We estimate  $p(t, z, y)$  for  $z \in K$  using (2.3). Choose  $V$  relatively compact containing the closure of  $U$ . Then, for  $z \in \partial U$ ,

$$p(t, z, y) = 1_U(x) p_V(t, z, y) + \int_{[0, t) \times \partial U} p_V(t - s, z', y) \mu_x(ds, dz')$$

where

$$\mu_x([0, t] \times \partial U) \leq C(U, V) t, \quad C(U, V) < \infty.$$

For all  $z \in \partial U$ ,

$$p_V(t, z, y) \leq \frac{C_V(z, y)}{\sqrt{\nu(B(z, r(t, z)))} \sqrt{\nu(B(y, r(t, z)))}} \exp \left\{ -\frac{d(z, y)^2}{2t} + \frac{\lambda_V^2 t}{2} \right\}$$

where

$$r(t, z) = \min \left\{ \frac{t}{d(z, y)}, \sqrt{\frac{t}{4}}, \frac{d(z, \partial V)}{4}, \frac{d(y, \partial V)}{4} \right\}, \quad \lambda_V^2 = \sup_{z \in V} a(\beta, \beta)(z) < \infty.$$

Now

$$\inf_{z \in \partial U} d(z, y) = d(y, K), \quad \sup_{z \in \partial U} d(z, y) = C(U, y) < \infty$$

and, for  $r > 0$  sufficiently small

$$\inf_{z \in \bar{U}} \nu(B(z, r)) \geq r^{N(\bar{U})+1}.$$

For  $t > 0$  sufficiently small, we have  $r(t, z) = t/d(z, y)$  for all  $z \in \partial U$ , and then

$$\sqrt{\nu(B(z, r(t, z)))} \sqrt{\nu(B(y, r(t, z)))} \geq \left( \frac{t}{C(U, y)} \right)^{N(\bar{U})+1}.$$

Hence, for  $t > 0$  sufficiently small, and all  $z \in \partial U$ ,

$$p_V(t, z, y) \leq \frac{C_{U,V}(y)}{t^{N(\bar{U})+1}} \exp \left\{ -\frac{d(y, K)^2}{2t} + \frac{\lambda_V^2 t}{2} \right\}$$

where

$$C_{U,V}(y) = \sup_{z \in \partial U} C_V(z, y) \times C(U, y)^{N(\bar{U})+1}.$$

This estimate, along with (4.7), allows us to short-cut some steps in Hsu's argument. On substituting the estimates into (5.1) and using the elementary [8, Lemma 2.1], we conclude as claimed that

$$\limsup_{t \rightarrow 0} t \log p(t, x, K, y) \leq -(d(x, K) + d(y, K))^2/2.$$

▷

**Proof of Theorem 2** – First we will show the lower bound

$$\liminf_{t \rightarrow 0} t \log p(t, x, y) \geq -d(x, y)^2/2 \quad (5.2)$$

locally uniformly in  $x$  and  $y$ . Given  $\varepsilon > 0$ , there exists a simple path  $\gamma \in \Omega^{x,y}$ , with driving path  $\xi$  say, such that  $\sqrt{I(\gamma)} \leq d(x, y) + \varepsilon$ . We can and do parametrize  $\gamma$  so that  $a(\xi_t, \xi_t) = I(\gamma)$  for almost all  $t \in [0, 1]$ . Fix  $\delta > 0$  and consider the open set

$$U := \left\{ z \in M : d(z, \gamma_t) < \delta \text{ for some } t \in [0, 1] \right\}.$$

We can and do choose  $\delta$  so that  $U$  is compactly contained in the domain of a chart. Choose  $n \geq 1$  such that

$$\frac{d(x, y) + \varepsilon}{n} \leq \delta$$

and fix  $\eta \in (0, \delta/4)$ . For  $k = 0, 1, \dots, n$ , set  $t_k = k/n$  and  $x_k = \gamma_{t_k}$  and suppose that  $y_k \in B(x_k, \eta)$ . Then, for  $k = 1, \dots, n$ ,

$$\begin{aligned} d(y_{k-1}, y_k) &< d(x_{k-1}, x_k) + 2\eta = \sqrt{I(\gamma)}/n + 2\eta \leq (d(x, y) + \varepsilon)/n + 2\eta, \\ d(y_{k-1}, M \setminus U) + d(y_k, M \setminus U) &\geq 2(\delta - \eta) > (d(x, y) + \varepsilon)/n + 2\eta. \end{aligned}$$

We can identify the chart with a subset of  $\mathbb{R}^d$  and choose extensions  $\tilde{X}_0, \tilde{X}_1, \dots, \tilde{X}_m$  to  $\mathbb{R}^d$  of the restrictions of  $X_0, X_1, \dots, X_m$  to  $U$  such that the extended vector fields are all bounded with bounded derivatives of all orders, such that  $\tilde{X}_1, \dots, \tilde{X}_m$  is a sub-Riemannian structure on  $\mathbb{R}^d$ , and such that  $\tilde{X}_0 = \chi X_0$  for some smooth function  $\chi$  vanishing outside the chart. Then, by Léandre's lower bound [14, Theorem II.3] in  $\mathbb{R}^d$ , for  $k = 1, \dots, n$ , uniformly in  $y_{k-1}$  and  $y_k$ ,

$$\liminf_{t \rightarrow 0} t \log \tilde{p}(t, y_{k-1}, y_k) \geq -d(y_{k-1}, y_k)^2/2.$$

On the other hand, by Theorem 1, for  $k = 1, \dots, n$ , uniformly in  $y_{k-1}$  and  $y_k$ ,

$$\begin{aligned} \limsup_{t \rightarrow 0} t \log \tilde{p}(t, y_{k-1}, \mathbb{R}^d \setminus U, y_k) &\leq -d(y_{k-1}, \mathbb{R}^d \setminus U, y_k)^2/2 \\ &\leq -(d(y_{k-1}, M \setminus U) + d(y_k, M \setminus U))^2/2 \end{aligned}$$

Hence, by our choice of  $n$  and  $\eta$ , uniformly in  $y_{k-1}$  and  $y_k$ ,

$$\liminf_{t \rightarrow 0} t \log p_U(t, y_{k-1}, y_k) = \liminf_{t \rightarrow 0} t \log \tilde{p}_U(t, y_{k-1}, y_k) \geq -(d(x_{k-1}, x_k) + 2\eta)^2/2.$$



Now, by a standard chaining procedure, we obtain, uniformly in  $y_0$  and  $y_n$ ,

$$\liminf_{t \rightarrow 0} t \log p_U(t, y_0, y_n) \geq -\frac{n}{2} \sum_{k=1}^n (d(x_{k-1}, x_k) + 2\eta)^2 \geq -(d(x, y) + \varepsilon + 2\eta n)^2/2.$$

This implies (5.2), since  $p_U(t, x, y) \leq p(t, x, y)$  and  $\varepsilon$  and  $\eta$  may be chosen arbitrarily small.

It remains to show the upper bound

$$\limsup_{t \rightarrow 0} t \log p(t, x, y) \leq -d(x, y)^2/2 \quad (5.3)$$

locally uniformly in  $x$  and  $y$ . In the case where  $\mathcal{L}$  satisfies (1.9), this follows from Theorem 1 by taking  $K = M$ . On the other hand, given  $\varepsilon > 0$  and a compact set  $F$  in  $S$ , there is a relatively compact open set  $U$  in  $M$  such that, for  $K = M \setminus U$  and all  $(x, y) \in F$ ,

$$d(x, y) - \varepsilon \leq d(x, K) + d(y, K).$$

Now the restriction of  $\mathcal{L}$  to  $U$  satisfies (1.9), so

$$\limsup_{t \rightarrow 0} t \log p_U(t, x, y) \leq -d_U(x, y)^2/2 \leq -d(x, y)^2/2 \quad (5.4)$$

uniformly in  $(x, y) \in F$ , while, by Theorem 1,

$$\limsup_{t \rightarrow 0} t \log p(t, x, K, y) \leq -(d(x, K) + d(y, K))^2/2 \quad (5.5)$$

also uniformly in  $(x, y) \in F$ . Since  $p(t, x, y) = p_U(t, x, y) + p(t, x, K, y)$  and  $\varepsilon$  is arbitrary, (5.3) follows from (5.4) and (5.5).  $\triangleright$

In the following proof, we introduce an auxiliary real Brownian bridge, from 0 to 1 of speed  $\varepsilon$ . This is known to converge weakly to a uniform drift as  $\varepsilon \rightarrow 0$ . So this auxiliary process provides a new coordinate which acts as a surrogate for time, thereby allowing us to lift the small-time estimate for the heat kernel to a weak convergence result for the associated bridge.

**Proof of Theorem 3** – Consider first the case where  $\mathcal{L}$  satisfies (1.9) and  $\gamma$  is strongly minimal. We will show, for all  $\delta > 0$ , for

$$\Gamma_t(\delta) := \left\{ \omega_t : \omega \in \Omega^{x,y}, I(\omega) < d(x, y)^2 + \delta \right\}$$

and for

$$r = \delta^{1/4} (d(x, y)^2 + \delta)^{1/2}$$

that we have

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon \log \mu_\varepsilon^{x,y} \left( \left\{ \omega \in \Omega^{x,y} : d(\omega_t, \Gamma_t(\delta)) \geq r \text{ for some } t \in [0, 1] \right\} \right) \leq -\delta/2. \quad (5.6)$$

Then, since  $\gamma$  is the unique minimal path in  $\Omega^{x,y}$  and  $\gamma$  is strongly minimal, for all  $\rho > 0$ , there exists  $\delta > 0$  such that, for all  $\omega \in \Omega^{x,y}$ , we have  $I(\omega) \geq d(x, y)^2 + \delta$  whenever  $d(\omega_t, \gamma_t) \geq \rho$  for some  $t \in [0, 1]$ . Hence  $d(z, \gamma_t) < \rho$  for all  $z \in \Gamma_t(\delta)$  and all  $t \in [0, 1]$ . Then it follows from (5.6) that, as  $\varepsilon \rightarrow 0$ ,

$$\mu_\varepsilon^{x,y} \left( \left\{ \omega \in \Omega^{x,y} : d(\omega_t, \gamma_t) < r + \rho \text{ for all } t \in [0, 1] \right\} \right) \rightarrow 1$$

showing that  $\mu_\varepsilon^{x,y} \rightarrow \delta_\gamma$  weakly on  $\Omega^{x,y}$ .

Consider the operator  $\tilde{\mathcal{L}}$  and measure  $\tilde{\nu}$  on  $\tilde{M} = M \times \mathbb{R}$  given by

$$\tilde{\mathcal{L}} = \mathcal{L} + \frac{1}{2} \left( \frac{\partial}{\partial \tau} \right)^2, \quad \tilde{\nu}(dx, d\tau) = \nu(dx) d\tau$$

where  $\tau$  denotes the coordinate in  $\mathbb{R}$ . Then

$$\tilde{\mathcal{L}}f = \frac{1}{2}\tilde{\text{div}}(\tilde{a}\nabla f) + \tilde{a}(\tilde{\beta}, \nabla f)$$

where  $\tilde{\text{div}}$  is the divergence associated to  $\tilde{\nu}$  and where

$$\tilde{a}(x, \tau) = a(x) + \frac{\partial}{\partial \tau} \otimes \frac{\partial}{\partial \tau}, \quad \left\langle \tilde{\beta}(x, \tau), v \pm \frac{\partial}{\partial \tau} \right\rangle = \langle \beta(x), v \rangle, \quad v \in T_x M.$$

Moreover,  $\tilde{a}$  has a sub-Riemannian structure and

$$\tilde{a}(\tilde{\beta}, \tilde{\beta})(x, \tau) = a(\beta, \beta)(x) \leq \lambda^2$$

Write  $\Omega^{0,1}(\mathbb{R})$  for the set of continuous paths  $\sigma : [0, 1] \rightarrow \mathbb{R}$  such that  $\sigma_0 = 0$  and  $\sigma_1 = 1$ . For  $\sigma \in \Omega^{0,1}(\mathbb{R})$ , define

$$I(\sigma) = \begin{cases} \int_0^1 |\dot{\sigma}_t|^2 dt, & \text{if } \sigma \text{ is absolutely continuous,} \\ \infty, & \text{otherwise.} \end{cases}$$

Set  $\tilde{x} = (x, 0)$  and  $\tilde{y} = (y, 1)$ , and define

$$\tilde{K} := \tilde{M} \setminus \tilde{U}, \quad \tilde{U} := \left\{ (\gamma_t, \sigma_t) : (\gamma, \sigma) \in \tilde{\Gamma}(\delta), t \in [0, 1] \right\}$$

where

$$\tilde{\Gamma}(\delta) := \left\{ (\gamma, \sigma) \in \Omega^{x,y} \times \Omega^{0,1}(\mathbb{R}) : I(\gamma) + I(\sigma) < d(x, y)^2 + 1 + \delta \right\}.$$

Then  $\tilde{K}$  is closed in  $\tilde{M}$ . Write  $\beta_\varepsilon^{0,1}$  for the law on  $\Omega^{0,1}(\mathbb{R})$  of a Brownian bridge from 0 to 1 of speed  $\varepsilon$ . Then, with obvious notation,

$$\tilde{p}(t, \tilde{x}, \tilde{y}) = p(t, x, y) \frac{1}{\sqrt{2\pi}} e^{-1/(2t)}, \quad \tilde{\mu}_\varepsilon^{\tilde{x}, \tilde{y}}(d\omega, d\tau) = \mu_\varepsilon^{x,y}(d\omega) \beta_\varepsilon^{0,1}(d\tau).$$

By Theorem 1, we have

$$\limsup_{t \rightarrow 0} t \log \tilde{p}(t, \tilde{x}, \tilde{K}, \tilde{y}) \leq -\tilde{d}(\tilde{x}, \tilde{K}, \tilde{y})^2/2 = -(d(x, y)^2 + 1 + \delta)/2$$

so

$$\begin{aligned} \limsup_{\varepsilon \rightarrow 0} \varepsilon \log \tilde{\mu}_\varepsilon^{\tilde{x}, \tilde{y}}(\{(\omega, \tau) : (\omega_t, \tau_t) \in \tilde{K} \text{ for some } t \in [0, 1]\}) \\ \leq \limsup_{\varepsilon \rightarrow 0} \varepsilon \log \tilde{p}(\varepsilon, \tilde{x}, \tilde{K}, \tilde{y}) - \liminf_{\varepsilon \rightarrow 0} \varepsilon \log \tilde{p}(\varepsilon, \tilde{x}, \tilde{y}) \leq -\delta/2 \end{aligned} \quad (5.7)$$

where we have used the lower bound from Theorem 2. By standard estimates, we also have

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \log \beta_\varepsilon^{0,1}(\{\tau : |\tau_t - t| \geq \sqrt{\delta}/2 \text{ for some } t \in [0, 1]\}) = -\delta/2. \quad (5.8)$$

Suppose then that  $\omega \in \Omega^{x,y}$  and  $\tau \in \Omega^{0,1}(\mathbb{R})$  satisfy  $(\omega_t, \tau_t) \in \tilde{U}$  and  $|\tau_t - t| < \sqrt{\delta}/2$  for all  $t \in [0, 1]$ . Then, for each  $t \in [0, 1]$ , there exist  $s \in [0, 1]$  and  $\gamma \in \Omega^{x,y}$  and  $\sigma \in \Omega^{0,1}(\mathbb{R})$  such that

$$\omega_t = \gamma_s, \quad \tau_t = \sigma_s, \quad I(\gamma) < d(x, y)^2 + \delta, \quad I(\sigma) < 1 + \delta.$$

Then  $|\sigma_s - s| \leq \sqrt{\delta}/2$  so  $|t - s| \leq \sqrt{\delta}$  and so

$$d(\omega_t, \Gamma_t(\delta))^2 \leq d(\omega_t, \gamma_t)^2 = d(\gamma_s, \gamma_t)^2 \leq |t - s| I(\gamma) \leq \delta^{1/2} (d(x, y)^2 + \delta).$$

The estimates (5.7) and (5.8) thus imply (5.6).

We turn to the case where  $d(x, y) < d(x, \infty) + d(y, \infty)$ . Then there exists a relatively compact open set  $U$  in  $M$  such that, for  $K = M \setminus U$ ,

$$d(x, y) < d(x, K) + d(y, K).$$

Then, by Theorem 1,

$$\limsup_{\varepsilon \rightarrow 0} \varepsilon \log p(\varepsilon, x, K, y) \leq -(d(x, K) + d(y, K))^2/2 < -d(x, y)^2/2 \quad (5.9)$$

while, by Theorem 2,

$$\liminf_{\varepsilon \rightarrow 0} \varepsilon \log p(\varepsilon, x, y) \geq -d(x, y)^2/2. \quad (5.10)$$

Set

$$\Omega_U^{x,y} := \left\{ \omega \in \Omega^{x,y} : \omega_t \in U \text{ for all } t \in [0, 1] \right\}.$$

Then  $\gamma$  is the unique minimal path in  $\Omega_U^{x,y}$ ,  $\gamma$  is strongly minimal in  $\Omega_U^{x,y}$ , and

$$p(\varepsilon, x, y) \mathbf{1}_{\Omega_U^{x,y}}(\omega) \mu_\varepsilon^{x,y}(d\omega) = p_U(\varepsilon, x, y) \mu_\varepsilon^{x,y,U}(d\omega). \quad (5.11)$$

Consider the limit  $\varepsilon \rightarrow 0$ . Since the restriction of  $\mathcal{L}$  to  $U$  satisfies (1.9), by the first part of the proof, we have  $\mu_\varepsilon^{x,y,U} \rightarrow \delta_\gamma$  weakly on  $\Omega_U^{x,y}$ . Since

$$p(\varepsilon, x, y) = p_U(\varepsilon, x, y) + p(\varepsilon, x, K, y)$$

it follows from (5.9) and (5.10) that  $p_U(\varepsilon, x, y)/p(\varepsilon, x, y) \rightarrow 1$ . Hence, on letting  $\varepsilon \rightarrow 0$  in (5.11), we see that also  $\mu_\varepsilon^{x,y} \rightarrow \delta_\gamma$  weakly on  $\Omega^{x,y}$ .  $\triangleright$

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