Heat-content and diffusive leakage from material sets in the low-diffusivity limit

Nathanael Schilling, Daniel Karrasch** and Oliver Junge

Department of Mathematics, Technical University of Munich, Germany

E-mail: schillna@ma.tum.de, karrasch@ma.tum.de and oj@tum.de

Received 3 August 2020, revised 28 June 2021
Accepted for publication 28 July 2021
Published 14 September 2021

Abstract

We generalize leading-order asymptotics of a form of the heat content of a submanifold (van den Berg & Gilkey 2015) to the setting of time-dependent diffusion processes in the limit of vanishing diffusivity. Such diffusion processes arise naturally when advection–diffusion processes are viewed in Lagrangian coordinates. We prove that as diffusivity $\varepsilon$ goes to zero, the diffusive transport out of a material set $S$ under the time-dependent, mass-preserving advection–diffusion equation with initial condition given by the characteristic function $\mathbb{1}_S$, is $\sqrt{\varepsilon/\pi} \int_{\partial S} d\mathcal{A} + o(\sqrt{\varepsilon})$. The surface measure $d\mathcal{A}$ is that of the so-called geometry of mixing, as introduced in (Karrasch & Keller 2020). We apply our result to the characterisation of coherent structures in time-dependent dynamical systems.

Keywords: finite time coherent sets, heat content, advection diffusion equation

Mathematics Subject Classification numbers: 35B25, 60G07, 58J32, 58J35.

(Some figures may appear in colour only in the online journal)

1. Motivation

Consider the advection–diffusion process of a passive scalar $u$ by a sufficiently regular, possibly time-dependent, volume-preserving vector field $V$ as described by the advection–diffusion
regardless of the initial condition equation (3) henceforth as we work in Lagrangian coordinates exclusively. Here, equation

\[ \partial_t u = -\text{div}(uV) + \varepsilon \Delta u, \]  

and some initial condition \( u(0, \cdot) = u_0 \). Let \( \Phi_0^\varepsilon \) denote the flow map (from time 0 to time \( t \)) induced by \( V \). For \( \varepsilon = 0 \), there is only advection and the time-\( t \) solution operator mapping \( u(0, \cdot) \) to \( u(t, \cdot) \) under equation (1) is given by a coordinate change by the flow map of \( V \), i.e., \( u(t, \Phi_0^\varepsilon(x)) = u_0(x) \). The coordinates induced by the flow map \( \Phi_0^\varepsilon \) are well known as Lagrangian coordinates. We refer to flow-invariant space-time sets as material sets.

For any non-negative \( \varepsilon \), we are interested in the leakage of \( u = u \) from a full-dimensional material set \( S \) with smooth boundary over the time interval \([0, t]\) under equation (1). Let us denote this material outflow by

\[ T_0^\varepsilon(S, u_0, \varepsilon) := \int_S u_0 \, dx - \int_{\Phi_0^\varepsilon(S)} u_\varepsilon(t, x) \, dx. \]

In the advection-only case, flow-invariance directly implies

\[ T_0^\varepsilon(S, u_0, 0) = 0, \]

regardless of the initial condition \( u_0 \) and set \( S \). In simple terms, no mass can leak out of a material set if there is no diffusion.

For \( \varepsilon > 0 \), however, the situation is different: in general, \( T_0^\varepsilon(S, u_0, \varepsilon) \) does not vanish, and the asymptotics of \( T_0^\varepsilon(S, u_0, \varepsilon) \) as \( \varepsilon \to 0 \) are nontrivial and of both scientific and practical interest. In [15], leading-order asymptotics of \( T_0^\varepsilon(S, u_0, \varepsilon) \) for smooth \( u_0 \) compactly supported in the interior of the domain were derived, and in [20] they were additionally studied from a geometric point of view. In this work, we further expand the theory towards the natural case \( u_0 = 1_S \).

Let \( \tilde{u}_\varepsilon \) denote \( u_\varepsilon \) in Lagrangian coordinates, i.e., \( \tilde{u}_\varepsilon(t, \cdot) = u_\varepsilon(t, \cdot) \circ \Phi_0^\varepsilon \). Then equation (1) reads as

\[ \partial_t \tilde{u}_\varepsilon = \varepsilon \Delta \tilde{u}_\varepsilon, \]

where \( \Delta_c \) is the differential geometrical pullback of the Laplace operator by \( \Phi_0^\varepsilon \); see, for instance, [19, 22, 27]. With a common, slight abuse of notation, we will omit the tilde in equation (3) henceforth as we work in Lagrangian coordinates exclusively. Here,

\[ T_0^\varepsilon(S, 1_S, \varepsilon) = \int_S \, dx - \int_S u_\varepsilon(t, x) \, dx = \int_{\partial S} u_\varepsilon(t, x) \, dx, \]

since \( \int_S u_\varepsilon(t, x) \, dx = \int_{\partial S} u_\varepsilon(x) \, dx = \int S \, dx \) for all \( t \in [0, 1] \) by mass preservation. If equation (3) were the classical autonomous heat equation, then the leading-order coefficient (of order \( \varepsilon \)) in \( T_0^\varepsilon(S, 1_S, \varepsilon) \) is proportional to the surface area of \( \partial S \); see [28]. For a generalization to the nonautonomous case as in equation (3), it is a priori unclear whether one should again expect some kind of surface measure of \( \partial S \) in the leading-order coefficient: in the Lagrangian pullback geometry, \( \partial S \) has—in general—a different surface area at each time instance \( t \). Recently, [19] proposed a (weighted) geometry—the geometry of mixing to be recalled below—which was developed to specifically analyze advection–diffusion processes on finite-time intervals. This geometry, which has the mathematical structure of a weighted (Riemannian) manifold [19, 20], admits an area form \( d\overline{A} \) about which we show in this work that it, indeed, determines the leading-order asymptotics of material leakage out of material sets, namely

\[ T_0^\varepsilon(S, 1_S, \varepsilon) = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} d\overline{A} + o(\sqrt{\varepsilon}). \]
In our proof, we will work with a generalized form of the time-dependent Lagrangian heat equation (3), and do not assume that it is necessarily given as some advection–diffusion equation in Lagrangian coordinates.

2. Mathematical setting

Let $M$ be a smooth compact manifold (possibly with smooth boundary), and $\omega$ a non-vanishing volume form on $M$. Recall that $\omega$ naturally defines a divergence operator, acting on vector fields $V \in \Gamma(TM)$, by $(\text{div}_\omega V) \omega = L_V \omega$. Here, $\Gamma(TM)$ denotes the set of smooth sections of the tangent bundle and $L$ is the Lie derivative. If $(g_t)_{t \in [0,1]}$ is a smoothly-varying one-parameter family of Riemannian metrics on $M$, a weighted Laplace operator (cf [13]), acting on smooth functions $f \in C^\infty(M)$, is defined for each $t$ with the formula

$$\Delta_t f := \text{div}_\omega g_t^{-1} df.$$ 

The notation $g_t^{-1}$ shall be interpreted using the well-known natural identification of $g_t$ with a vector bundle morphism mapping a tangent vector $v$ to the cotangent vector $g_t(v, \cdot)$. As $g_t$ is positive definite at each point, this is in fact a vector bundle isomorphism and $g_t^{-1}$ is well-defined. Indeed, $f \mapsto g_t^{-1} df$ is the gradient induced by the metric $g_t$.

As mentioned earlier, our object of study is the time-dependent heat equation with diffusivity $\varepsilon > 0$ and initial value $u_0 \in L^2(M, \omega)$,

$$\partial_t u_\varepsilon = \varepsilon \Delta u_\varepsilon, \quad u_\varepsilon(0, \cdot) = u_0, \quad (4)$$

which is a generalization of the classical heat equation on $M$ for which $g_t$ is independent from $t$ and $\omega$ is the Riemannian volume form. We will look at equation (4) with boundary conditions given by either (a) $\partial M = \emptyset$, (b) homogeneous Dirichlet boundary or (c) homogeneous Neumann boundary. Of course, (a) is a special case of both (b) and (c).

3. The geometry of mixing

We write $P^\varepsilon_t$ for the time-$t$ solution operator of equation (4), and denote by $\langle \cdot, \cdot \rangle_0$ the $L^2(M, \omega)$ inner product. Throughout, we will identify the volume form $\omega$ with its induced measure. A (time) averaged version of equation (4) describes the leading-order behaviour of $P^\varepsilon_t$ as $\varepsilon \to 0$. Indeed, defining

$$\overline{\varepsilon} := \left( \int_0^1 g_t^{-1} dt \right)^{-1}, \quad \overline{\Delta} := \text{div}_\omega \overline{\varepsilon}^{-1} df, \quad \text{and} \quad \overline{P}^\varepsilon_t := \exp(\varepsilon t \overline{\Delta}),$$

it is true [20], see also [15, 21], that for $u_0 \in C^\infty_c(M)$, i.e., $u_0 \in C^\infty(M)$ with compact support in $M$,

$$\| P^\varepsilon_t u_0 - \overline{P}^\varepsilon_t u_0 \|_{L^\infty(M)} = O(\varepsilon^2), \quad \varepsilon \to 0. \quad (5)$$

The operator $\overline{\Delta}$ was called the dynamic Laplacian in [9], and is the natural Laplace operator of the weighted manifold $(M, \overline{\varepsilon}, \overline{\omega})$. This weighted manifold was coined geometry of mixing.

1The imposed boundary condition type in the definition of the semigroup $\exp(\varepsilon t \overline{\Delta})$ corresponds to the one (homogeneous Dirichlet/Neumann) imposed in equation (4), see also [20].
in [19]. On the surface $\partial S$ oriented by the $g$-unit outer normal vector field $\nu$, the geometry of mixing has a natural area form given by $dA(x) = \omega(x, \cdot)$; see [19, 20].

For non-smooth $u_0$, such as $u_0 = 1_S$, it is not clear whether we can expect a result like equation (5): even in the special case of the time-independent heat equation on the weighted manifold $(M, g, \omega)$, there are now terms of order $\varepsilon^4$ and its powers (which is in stark contrast to the case of smooth initial values). It is known, for example, that

$$\langle P_\varepsilon 1_S, 1_{M \setminus S} \rangle = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} dA + o(\varepsilon), \quad \varepsilon \to 0; \quad (6)$$

see [23, 28]. In this paper, we show that equation (6) remains true if $P_\varepsilon$ is replaced by $P_\varepsilon \Phi_0$, i.e. the following theorem which we prove in section 5.

**Theorem 1.** Let $S$ be a compact, full-dimensional submanifold of $M$ with smooth boundary, contained in the interior of $M$, and let $S' := M \setminus S$. Then

$$\langle P_\varepsilon 1_S, 1_{S'} \rangle = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} dA + o(\varepsilon), \quad \varepsilon \to 0. \quad (7)$$

4. Eulerian coherent pairs and Lagrangian coherent sets

In [10], the following concept of coherence has been introduced. Consider two spatial sets $S$ (at time 0) and $S'$ (at time 1), $L_\varepsilon$ a small perturbation of the transfer operator, i.e., the solution operator for equation (1) with $\varepsilon = 0$, where the perturbation strength scales with $\varepsilon > 0$. Then [10] proposed a coherence ratio

$$\rho_\varepsilon(S, S') := \langle L_\varepsilon 1_S, 1_{S'} \rangle / \omega(S) + \langle L_\varepsilon 1_{M \setminus S}, 1_{M \setminus S'} \rangle / \omega(M \setminus S'), \quad (8)$$

as a measure of coherence of the pair $(S, S')$. Verbally, this measures how much of $S$ is carried to $S'$ and how much of $M \setminus S$ is carried to $M \setminus S'$ by the ‘perturbed flow’. In yet other words, coherent pairs (see also [2]) $S$ and $S'$ are pairs of spatial sets such that there is little leakage under the action of $L_\varepsilon$.

Of course, choosing $S' = \Phi_0(S)$ results in no leakage (or, equivalently, coherence ratio equal to 1) in the non-diffusive case, notably for any choice of $S$, see equation (2). While, in that limit case, the problem of seeking ‘maximally coherent pairs’ becomes meaningless, one would expect that $S' = \Phi_0(S)$ is the right condition to perturb from when bringing weak diffusion into consideration.

We thus define the Lagrangian coherence ratio as

$$\tilde{\rho}_\varepsilon(S) := \rho_\varepsilon(S, \Phi_0(S)).$$

Seemingly trivial, this has conceptually deep implications. First, it removes one degree of freedom, the choice of $S'$. As a consequence, it changes the focus from Eulerian coherent pairs (of sets) to individual Lagrangian coherent sets. Moreover, it is clear that, for given $S$, the Lagrangian coherence ratio depends only on the type and the strength of the perturbation of the transfer operator. One implementation of a perturbation, as done in [10], is to convolve densities both before and after the purely advective transport with an explicitly-defined kernel, whose support is bounded by $\varepsilon$ away from 0. Another popular approach is to omit any explicit perturbation, and rely on ‘numerical diffusion’ (e.g., via box discretizations) instead;
The choice $L_\varepsilon = P_\varepsilon^1$, i.e., the solution operator to the Lagrangian advection–diffusion equation (3) was suggested in [19]—see [5] for the analogous Eulerian approach—as a physically natural perturbation candidate, that can also be given a stochastic interpretation. With this definition of $L_\varepsilon$, we can work with indicator functions directly when maximizing coherence measures like equation (8), instead of applying a two-step relaxation procedure as is sometimes done; see [4, 10, 17].

By theorem 1, if $\partial S$ is smooth and $\partial M = \emptyset$ (or with homogeneous Neumann boundary), then as $\varepsilon \to 0$,

$$\rho_\varepsilon(S, \Phi_1^0(S)) = \frac{\omega(S)}{\omega(S)} \frac{\sqrt{\pi} \int_{\partial S} \omega^1 dA}{\omega(S)} + \frac{\omega(M \setminus S)}{\omega(M \setminus S)} + o(\sqrt{\varepsilon}).$$

In other words, if we fix $\omega(S)$, the coherence ratio depends in leading order as $\varepsilon \to 0$ only on (a constant times) the area of $\partial S$ in the geometry of mixing. Smooth local minimizers of the area functional in a (weighted) manifold with respect to volume-preserving variations are well-known to be surfaces of constant generalized mean curvature; see [14, section 9.4E]. The above considerations hence suggest that sets bounded by such a minimizing surface be viewed as Lagrangian coherent sets in the low-diffusivity limit. This connection between the concept of coherent sets and that of the (generalized) isoperimetric problem is closely related to the connection described in [9]. At the same time, it has close ties to the studies of diffusive transport across material surfaces performed in [15, 16, 19].

5. Proof of the main theorem

5.1. Overview

Our proof consists of a reduction of equation (7) to the time-independent setting so that we can apply equation (6). In a first step, we perform this reduction for the case $M = \mathbb{R}^n$ in section 5.2 using stochastic methods. This avoids technical complications arising from dealing with manifold-valued stochastic processes. We then treat the general case where $M$ is an arbitrary compact manifold in a second step (section 5.3).

The structure of the first step is sketched in figure 1. On the top right-hand side we depict the averaged, i.e., time-independent, advection–diffusion equation for which we know
(equation (6)) the asymptotic behaviour of \( \langle P_1^\epsilon \mathbb{1}_S, \mathbb{1}_S \rangle_0 \) as \( \epsilon \to 0 \). On the top left there is the time-dependent advection–diffusion equation which is the subject of theorem 1. Each arrow represents a reduction or approximation step in the proof:

(a) The upper two arrows (blue) connect a stochastic differential equation (SDE) to its Kolmogorov backward PDE above it; see section 5.2.1.

(b) Central arrows (olive): each SDE is approximated by another SDE, inheriting the leading-order asymptotics we are interested in, see section 5.2.4. The use of this kind of SDE approximation to obtain PDE approximations is well known in the literature, see, e.g., [7, section 2.3].

(c) The lower arrow (black) highlights the fact that \( Y_t^\epsilon \) and \( \mathbf{Y}_t^\epsilon \) have the same law, and, as a consequence, they share the same the leading-order asymptotics of interest.

The reduction as a whole may be conceptualised as going along the arrows from the top right of figure 1 to the top left.

5.1.1. Technical issues caused by non-compactness. As \( \mathbb{R}^n \) is not compact, it may be that \( \mathbb{1}_{\mathbb{R}^n} \notin L^2(\mathbb{R}^n, \omega) \). This means that the \( \langle \cdot, \cdot \rangle_0 \) notation appearing in equation (7) must be clarified: we abuse notation by writing \( \langle f, g \rangle_0 := \int_M f(x) g(x) \omega \) whenever \( fg \in L^1(\mathbb{R}^n, \omega) \). Similar issues also play a role in the non-compact case. Since in theorem 1 we assume the set \( S \) to be compact anyway, in order to avoid unnecessary technical complications, we state the following simplifying assumption:

**Assumption 1.** There exists a bounded set \( B \) (containing \( S \) in its interior) so that both \( g_t \) and \( \omega \) are equal to the Euclidean metric and its volume form respectively outside of \( B \) for all \( t \in [0, 1] \).

5.2. Step 1: the case \( M = \mathbb{R}^n \)

On \( M = \mathbb{R}^n \), the initial value problem equation (4) takes the form

\[
\partial_t u = \epsilon \left( \sum_{i=1}^n b_i \partial_i u + \frac{1}{2} \sum_{i,j=1}^n a_{ij} \partial_{ij} u \right), \quad u(0, \cdot) = u_0.
\]  

Here, the space-time-dependent, real-valued functions \( a_{ij} \) and \( b_i \) depend on the metrics \( (g_t)_{t \in [0,1]} \) and the volume form \( \omega \). There are no coefficients of lower order because \( \Delta_t \mathbb{1}_{\mathbb{R}^n} = 0 \) for all \( t \in [0, 1] \). Assumption 1 yields that on the complement of \( B \), \( a_{ij} = \delta_{ij} \) and \( b_i = 0 \) in Cartesian coordinates. We have collected some results from the literature on parabolic PDEs in appendix C adapted to our setting which we will use in the sequel.

5.2.1. The Kolmogorov backwards equation. The time-1 solution operator of equation (9) is closely linked to the stochastic process governed by the SDE

\[
dX_t^\epsilon = \epsilon b(1 - t, X_t^\epsilon) \, dt + \sqrt{\epsilon} \sigma(1 - t, X_t^\epsilon) \, dW_t,
\]

with \( \sigma(t, x) = \sigma^T(t, x) \) and initial value \( X_0^\epsilon = X_0 \) independently of \( \epsilon \). It is well known that for a given \( n \)-dimensional Brownian motion \((W_t)_{t \in [0,1]} \), for \( t_0 \in [0,1] \) a unique strong solution to equation (10), starting at time \( t_0 \), exists provided that \( X_{t_0}^\epsilon \) is independent of \((W_t)_{t \in [0,1]} \) and that \( b \) and \( \sigma \) satisfy Lipschitz and growth conditions (cf also section 5.2.4). A direct consequence of smoothness and assumption 1 is that the Lipschitz and growth conditions...
are satisfied, as it is well known that $\sigma$ may be chosen to be smooth. To explicitly include the dependence of the process $(X'_t)_{t \in [0,1]}$ on the random variable $X_0$, we will write $E_{0,\omega}[\cdot]$ (given $x \in \mathbb{R}^d$) for the expected value under the assumption that $X_0 = x$ almost surely; in this case $X_0$ has law given by the Dirac delta measure centered at $x$. The Kolmogorov backwards-equation associated to equation (10) is a partial differential equation (PDE) for the function

$$\begin{align*}
w_c(t, x) &= E_{0,\omega}[u_0(X'_t)],
\end{align*}$$

provided that $u_0$ is sufficiently smooth, see [8, theorem 6.1]. This PDE reads

$$\partial_tw_c(t, x) = -\varepsilon \left( \sum_{i=1}^{n} b_i(1 - t, x)\partial_i w_c(t, x) + \frac{1}{2} \sum_{i,j=1}^{n} a_{ij}(1 - t, x)\partial_{ij} w_c(t, x) \right),$$

and moreover $w_c(t, x) \to w_c(x)$ as $t \to 1$. Thus, $u_c(t, x) = w_c(1 - t, x)$, as both sides satisfy equation (9) and solutions to parabolic PDEs are unique. As a consequence,

$$\begin{align*}
(P^t u_0)(x) &= u_c(1, x) = w_c(0, x) = E_{0,\omega}[u_0(X'_0)].
\end{align*}$$

(11)

This equation provides a probabilistic interpretation of the time-1 solution operator of equation (9) in terms of the SDE defined by equation (10).

5.2.2. Probabilistic interpretation of the heat content in a manifold. In equation (11) we assume the process $X'_t$ to start at the constant $x$ almost surely, i.e., we choose the initial value $X_0$ to have law equal to the point measure at $x$. We may, however, also treat the case in which the initial value $X_0$ of equation (10) is no longer a constant random variable.

Let $h : \mathcal{M} \to \mathbb{R}_{\geq 0}$ be a measurable function so that $h_\omega$ is a probability measure. We denote by $E_h[\cdot]$ the expected value in a probability space where $X_0$ has law $h_\omega$ independent of the Brownian motion $(W_t)_{t \in [0,1]}$. One may verify that

$$\langle x \mapsto E_{0,\omega}[u_0(X'_t)], h \rangle_0 = E_h[u_0(X'_0)]$$

holds in the case $u_0 = 1_A$, the extension to all $u_0 \in L^\infty(\mathbb{R}^d)$ follows from linearity and monotone convergence. Using equation (11) and remark 12, it follows that

$$\langle P^t u_0, h \rangle_0 = \langle x \mapsto E_{0,\omega}[u_0(X'_t)], h \rangle_0 = E_h[u_0(X'_0)].$$

(12)

We summarize that equation (12) proves a probabilistic interpretation of inner products of the form $\langle P^t u_0, h \rangle_0$ provided that (i) $u_0 \in L^\infty(\mathbb{R}^d)$, and (ii) $h \in L^1(\mathbb{R}^d, \omega)$ is nonnegative. The inner product appearing in equation (7) is not of the form just discussed as $1_{S'}$ is not in general in $L^1(\mathbb{R}^d, \omega)$. Observe, however, that for compact $S$,

$$\langle P^t 1_S, 1_{S'} \rangle_0 = \langle 1_{S'}, P^t 1_S \rangle_0,$$

which is proven in lemma 14 in appendix B. As a consequence of this and equation (12), the left-hand side of equation (7) may be re-written as

$$\langle P^t 1_S, 1_{S'} \rangle_0 = E_{1_S}[1_{S'}(X'_0)].$$

(13)

To see this, we first observe that the Markov property of SDEs [1, theorem 9.2.3] yields a time-1 transition function $p_\omega$ satisfying $p_\omega(x, A) = E_{0,\omega}[1_A(X'_1)]$ for $x \in \mathbb{R}^d$ and measurable $A \subset \mathbb{R}^d$. The definition of the inner product $\langle \cdot, \cdot \rangle_0$ yields

$$\langle x \mapsto E_{0,\omega}[1_A(X'_1)], h \rangle_0 = \int_{\mathbb{R}^d} p_\omega(x, \cdot) h(x) \omega = E_h[1_A(X'_0)].$$
provided that \( \omega(S) = 1 \), which can be assumed without loss of generality.

5.2.3. **Probabilistic interpretation of heat content in the averaged setting.** The steps above correspond to the left blue arrow in figure 1. The right blue arrow corresponds to repeating the same construction for the *averaged* equation \( \partial_t \overline{u} = \varepsilon \sum_{i=1}^n b_i \partial_i \overline{u} \). Here, the PDE of \( \overline{u} \) is given in coordinates by

\[
\partial_t \overline{u} = \varepsilon \left( \sum_{i=1}^n b_i \partial_i \overline{u} + \frac{1}{2} \sum_{i,j=1}^n \overline{a}_{ij} \partial_i \partial_j \overline{u} \right),
\]

with \( \overline{b}_i(x) = \int_0^1 b(t, x) dt \) and \( \overline{a}_{ij}(x) = \int_0^1 a_{ij}(t, x) dt \). The associated stochastic process is defined by the SDE

\[
d\overline{X}_t^i = \varepsilon \overline{b}_i(\overline{X}_t^i) dt + \sqrt{\varepsilon \overline{a}}(\overline{X}_t^i) dW_t,
\]

with \( \overline{a} \overline{\sigma}^T = \overline{\sigma} \). Given initial value \( \overline{X}_0^i = X_0 \), we see that analogously to equation (12),

\[
\langle \overline{P} u_0, h \rangle_0 = E_h[u_0(\overline{X}_1^i)]
\]

holds when \( u_0 \in L^\infty(M, \omega) \) and \( h \omega \) is a probability measure. Our aim is now to show that

\[
E_h[1_{S'}(\overline{X}_1^i)] = E_h[1_{S'}(\overline{X}_1^i)] + o(\sqrt{\varepsilon}), \quad \varepsilon \to 0,
\]

(15)
corresponding to \( h = 1_S \). In fact, we generalize to positive

\[ h \in C^\infty_S(M) \] ,

so that \( h \omega \) is a probability measure, and will look at the quantity \( E_h[1_{S'}(\overline{X}_1^i)] = \langle \overline{P} 1_{S'}, h \rangle_0 \) with the aim of showing

\[
E_h[1_{S'}(\overline{X}_1^i)] = E_h[1_{S'}(\overline{X}_1^i)] + o(\sqrt{\varepsilon}), \quad \varepsilon \to 0.
\]

Writing \( h = f 1_{S'} \), we know from [23, 28], that

\[
E_h[1_{S'}(\overline{X}_1^i)] = \langle \overline{P} 1_{S'}, f 1_{S'} \rangle_0 = \sqrt{\frac{\varepsilon}{\pi}} \int_{S'} f d\overline{\sigma} + o(\sqrt{\varepsilon}), \quad \varepsilon \to 0,
\]

(17)

which yields the asymptotic behaviour of the right-hand side of equation (16). Our aim in the next steps will be to prove equation (16).

5.2.4. **Approximation of stochastic processes.** We continue with the middle (green) arrows in figure 1, starting with the left one. Here, we will construct a family of stochastic processes \( (Y_t^i)_{t \in [0,1]} \) so that

\[
E \left[ |X_t^i - Y_t^i|^2 \right] \leq K \varepsilon^2
\]

(18)

for some \( K > 0 \) and all \( t \in [0,1] \) for sufficiently small \( \varepsilon \). In light of the arguments around equation (16), we will use this approximation to show that:

**Proposition 2.** If \( (Y_t^i)_{t \in [0,1]} \) satisfies equation (18), then for \( h \in C^\infty_S(M) \),

\[
E_h[1_{S'}(Y_t^i)] = E_h[1_{S'}(Y^i_t)] + o(\sqrt{\varepsilon}).
\]

(19)
Analogously, corresponding to the right-hand side of figure 1, if the family of processes \((\overline{Y}_t)_{t\in[0,1]}\) satisfies an inequality like equation (18) but with \(\overline{X}_t\) in place of \(X_t\), then

\[
E_h[1_S(\overline{X}_t)] = E_h[1_S(\overline{Y}_t)] + o(\sqrt{\varepsilon}).
\]

(20)

The processes \(Y_t\) and \(\overline{Y}_t\) will have the same law (this is the bottom arrow in figure 1), after we have proven this we may conclude that

\[
E_h[1_S(\overline{Y}_t)] = E_h[1_S(\overline{Y}_t)],
\]

which yields equation (16), which together with equations (19) and (20) shows (here \(h = 1_{\delta/2}\)), that

\[
E_h[1_S(X_t)] = E_h[1_S(\overline{X}_t)] + o(\sqrt{\varepsilon}) = \sqrt{\frac{\varepsilon}{\pi}} \int_A f dA + o(\sqrt{\varepsilon}).
\]

Before proving proposition 2, we will state a lemma needed in the proof. Let \(A\) be a (Borel) measurable subset of \(\mathbb{R}^n\). We denote by \(d(x, A) = \inf_{y\in A} |x - a|\) the Euclidean distance between a point \(x \in \mathbb{R}^n\) and the set \(A\). Let further \(A_\delta := \{x \in \mathbb{R}^n; d(x, \partial A) \leq \delta\}\) be the \(\delta\)-neighborhood of the boundary of \(A\).

**Lemma 3.** Let \((\Omega, \mathcal{A}, \mathbb{P})\) be some probability space and let \(E[X]\) denote the expectation of some random variable \(X\) on \(\Omega\) with respect to \(\mathbb{P}\). For \(\varepsilon \in [0, 1]\), let \(A'\) and \(B'\) be \((\mathbb{R}^n, \mathcal{B})\)-valued random variables with \(E[A' - B']^2 \leq C_0 = \varepsilon^2\) for some \(C_0 > 0\). Let \(R \in \mathcal{B}\) and assume that \(\mathbb{P}(A' \in R) \leq C_1\delta\) for sufficiently small \(\delta > 0\) and some \(C_1 > 0\). Then,

\[
|E[1_R(A')] - E[1_R(B')]| = o(\sqrt{\varepsilon}) \quad \varepsilon \to 0.
\]

**Proof.** The proof is given in appendix B, and is essentially an application of the Markov inequality. \(\square\)

**Proof of Proposition 2.** We will apply lemma 3 twice with \(R = S^\varepsilon\). For the first application, with \(A' = \overline{X}_t\) (corresponding to equation (19)), we will need to check that \(\mathbb{P}[X_t \in (S^\varepsilon)_\varepsilon] \leq C_1\delta\) for some constant \(C_1 > 0\). To see this is indeed the case, observe that \((S^\varepsilon)_\varepsilon = S_\delta\), and furthermore \(\mathbb{P}(X_t \in S_\delta) = E[1_{S_\delta}(X_t)]\). In the case that \(X_0\) has law \(f\), this is equal to \(E[f1_{S_\delta}(X_t)]\). Thus, if \(X_0\) has law \(f\) we have

\[
\mathbb{P}(X_t \in (S^\varepsilon)_\varepsilon) = \langle P^\varepsilon 1_{S^\varepsilon}, f \rangle > 0
\]

\[
\leq \|P^\varepsilon 1_{S^\varepsilon}\|_{L^1(M,\mathcal{M},\mu)} \|f\|_{\infty} \quad \text{(by Hölder’s inequality)}
\]

\[
\leq \omega(S) \|f\|_{\infty} \quad \text{(by mass preservation of } P^\varepsilon\}
\]

\[
\leq C_1\delta,
\]

for some \(C_1 > 0\), proving the claim. The proof required for the second application (with \(A = X_1\), i.e., equation (20)) that \(\mathbb{P}(\overline{X}_t \in S_\delta) = O(\delta)\) proceeds along the same lines. \(\square\)

**5.2.5. Approximation by a Gaussian process.** We now construct the processes required by proposition 2 satisfying equation (18). To this end, let \((Y_t)_{t\in[0,1]}\) be defined by

\[
d Y_t^i = \sqrt{\sigma} (1 - t, X_0) dW_t, \quad Y_0^i = X_0.
\]
where $X_0$ is independent of the Wiener process and bounded. Likewise, let $(\mathcal{T}_i^0)_{i \in [0,1]}$ be defined by
\[
d\mathcal{T}_i^0 = \sqrt{\varepsilon\sigma(X_0)}dW_i, \quad \mathcal{T}_0^0 = X_0.
\]

**Proposition 4 ([3]).** Let $(X_i^0)_{i \in [0,1]}$ be the stochastic process satisfying equation (10). The process $(Y_i^0)_{i \in [0,1]}$ approximates $(X_i^0)_{i \in [0,1]}$ in the sense that
\[
E \left[ |Y_i^0 - X_i^0|^2 \right] \leq K \varepsilon^2, \quad \text{for all } t \in [0,1].
\]

Similarly, let $(\mathcal{X}_i^0)_{i \in [0,1]}$ by the solution of equation (14), then $(\mathcal{T}_i^0)_{i \in [0,1]}$ approximates $(\mathcal{X}_i^0)_{i \in [0,1]}$ in the sense that
\[
E \left[ |\mathcal{T}_i^0 - \mathcal{X}_i^0|^2 \right] \leq K \varepsilon^2, \quad \text{for all } t \in [0,1].
\]

In both cases, $K > 0$ is a constant independent of $\varepsilon$ and $t$.

**Proof.** This is a special case of the result in [3]. We have adapted the proof of this special case in appendix A. \qed

The processes $(Y_i^0)_{i \in [0,1]}$ and $(\mathcal{T}_i^0)_{i \in [0,1]}$ may be thought of as being second-order approximations to the processes $(X_i^0)_{i \in [0,1]}$ and $(\mathcal{X}_i^0)_{i \in [0,1]}$ respectively. With proposition 2, we conclude the following.

**Proposition 5.** With $(X_i^0, Y_i^0, \mathcal{X}_i^0, \mathcal{T}_i^0)$ as defined above and $h \in \mathcal{C}_S^\infty(M)$,
\[
|E_h[1_{\mathcal{S}}(X_i^0)] - E_h[1_{\mathcal{S}}(Y_i^0)]| = o(\sqrt{\varepsilon}),
\]
\[
|E_h[1_{\mathcal{S}}(\mathcal{X}_i^0)] - E_h[1_{\mathcal{S}}(\mathcal{T}_i^0)]| = o(\sqrt{\varepsilon}).
\]

While these second-order approximations may differ pointwise, their laws are the same, this is the black arrow in figure 1 and the subject of the following lemma.

**Lemma 6.** The random variables $Y_i^0 - X_0$ and $\mathcal{T}_i^0 - X_0$ have the same law, namely that of $\sqrt{\varepsilon\sigma(X_0)} W_1$.

**Proof.** Recall that $\overline{\eta}(x) := \int_0^1 a(t,x)dt$, $\overline{b}(x) := \int_0^1 b(t,x)dt$, and $\overline{\sigma}^T = \overline{\eta}$. As $Y_0 = X_0$, we see that $Y_i^0 - X_0 = \sqrt{\varepsilon} \int_0^1 \sigma(1 - t, X_0) dW_i$. If $X_0 = x$ then by [1, corollary 4.5.6], the random variable $Y_i^0 - X_0$ is a normal random variable with zero mean and covariance matrix $\int_0^1 \sigma(t,x)\sigma(t,x)^T dt = \varepsilon\overline{\eta}(x)$, which is (by the same argument) also the law of $\mathcal{T}_i^0 - X_0$. The random variable $\sqrt{\varepsilon\sigma(X_0)} W_1$ is a normal random variable with the same mean and covariance matrix, proving the claim for constant $X_0$. The processes $(Y_i^0)_{i \in [0,1]}$ and $(\mathcal{T}_i^0)_{i \in [0,1]}$ are not memoryless as the right-hand side depends on the initial value of the process. This can be worked around by suitably augmenting the state space, the claim of the lemma for nonconstant $X_0$ follows by making use of the Markov property for SDEs in this augmented state space. \qed

**Corollary 7.** For $h \in \mathcal{C}_S^\infty(M)$, one has that
\[
E_h \left[ 1_{\mathcal{S}}(Y_i^0) \right] = E_h \left[ 1_{\mathcal{S}}(\mathcal{T}_i^0) \right].
\]
**Proof.** This is a direct result of lemma 6. □

To summarize the reasoning so far: combining corollary 7 with proposition 5 yields for $h \in C^\infty_0(M)$, that

$$E_0[1_S(X^1)] = E_0[\varphi(X^1)] + o(\sqrt{\varepsilon}), \quad \varepsilon \to 0.$$ 

We know that $\langle P^\varepsilon 1_S, h \rangle_0 = E_0[1_S(X^1)]$. Writing $h = 1_Sf$, together with equation (17), we may see that

$$\langle P^\varepsilon 1_S, h \rangle_0 = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} f \, d\mathcal{A} + o(\varepsilon), \quad \varepsilon \to 0.$$ 

With $f \equiv 1$, applying lemma 14 completes the proof of theorem 1 on $\mathbb{R}^n$ in the setting of assumption 1.

### 5.3. Step 2: restriction to local data and geometry

In this section, we write $P^\varepsilon = P^\varepsilon_1$ and $P^\varepsilon = P^\varepsilon_1$.

#### 5.3.1. Only local data is asymptotically important.

Let $U$ be a compact, full-dimensional submanifold of $M$ with smooth boundary and with $S \subset U$. The inner product appearing on the left-hand side of equation (7) may be written as

$$\langle P^\varepsilon \varphi, I_{S(U)} \rangle_0 = \langle P^\varepsilon \varphi, I_{S(U)} \rangle_0 + \langle P^\varepsilon \varphi, I_{U^c} \rangle_0.$$ 

We start by showing that discarding the second term yields an error of $o(\varepsilon)$.

**Lemma 8.** Let either $M$ be compact, or $M = \mathbb{R}^n$ (together with assumption 1) and $S, U$ as above. Let $f \in L^\infty(M, \omega)$ with $\text{supp}(f) \subset U$. Then

$$\langle P^\varepsilon f, I_{U^c} \rangle_0 = o(\varepsilon), \quad \varepsilon \to 0.$$ 

**Proof.** Without loss of generality, assume $f \geq 0$. Pick some $h \in C^\infty_0(M)$ with $f \leq h$ and $\text{supp}(h) \subset U$. We compute:

$$0 \leq \langle P^\varepsilon f, I_{U^c} \rangle_0 \leq \langle P^\varepsilon h, I_{U^c} \rangle_0$$

$$= \langle P^\varepsilon h, I_{U} \rangle_0 - \langle P^\varepsilon h, I_{U^c} \rangle_0.$$ 

If $M$ is compact we are already done at equation (22), as by proposition 13, $P^\varepsilon h = h + \varepsilon \Delta h + O(\varepsilon^2)$ and $\varphi_{U^c} \in L^2(M, \omega)$. If $M = \mathbb{R}^n$, we observe that $\langle P^\varepsilon h, I_{U} \rangle_0 = \langle h, I_{U} \rangle_0 = \langle h, I_{U} \rangle_0$. Using proposition 13, $\langle P^\varepsilon h, I_{U} \rangle_0 = \langle h + \varepsilon \Delta h + o(\varepsilon), I_{U} \rangle_0$. Given that $h$ is compactly supported in the interior of $U$, the term $\langle \varepsilon \Delta h, I_{U} \rangle_0$ vanishes by the divergence theorem. We conclude that $\langle P^\varepsilon h, I_{U} \rangle_0 = \langle h, I_{U} \rangle_0 + o(\varepsilon)$ which yields the claim. □

#### 5.3.2. Only local geometry is asymptotically important.

Similarly, only local geometry affects the asymptotic behaviour of $\langle P^\varepsilon 1_S, 1_{S(U)} \rangle_0$.

**Lemma 9.** Let $M$ be either compact (with homogeneous Neumann or Dirichlet boundary conditions) or equal to $\mathbb{R}^n$ (together with assumption 1). Let $S \subset M$ be a compact, full-dimensional submanifold. Let $f \in C^\infty_0(M, \omega)$ with $\text{supp}(f) \subset U$. Let $P^\varepsilon$ be defined the same.
way as $P^\varepsilon$ via equation (4) but on $U$ with homogeneous Dirichlet boundary, i.e., $\bar{P}_t$ is the time-t solution operator to the time-dependent diffusion problem equation (4) on $U$ with Dirichlet boundary, and $\bar{P} := \bar{P}_t$. Then,
\[
\| (P^\varepsilon - \bar{P}^t) f \|_{L^\infty(U)} = o(\varepsilon), \quad \varepsilon \to 0.
\]

**Proof.** Let $e_\varepsilon(t) = (P^\varepsilon_t - \bar{P}^t) h$ for a generic positive $h \in C^\infty_c(\bar{U})$. The function $e_\varepsilon(t)$ satisfies the time-dependent heat equation $\partial_t e_\varepsilon = \varepsilon \Delta e_\varepsilon$ on $U$, with nonhomogeneous Dirichlet boundary $e_\varepsilon|_{\partial U} = P^\varepsilon_t h|_{\partial U} \geq 0$. By construction (and reasoning like the following is well known in the literature, cf [12]), $e_\varepsilon(0, \cdot) = 0$, and the weak maximum principle [18, theorem A.3.1] applied to $-e_\varepsilon(t)$ yields that on $U$ and $t \in [0, 1]$,
\[
(P^\varepsilon_t - \bar{P}^t) h \geq 0. \tag{23}
\]
By a continuity argument, equation (23) extends to positive $h \in L^\infty(M, \omega)$ with $\supp(h) \subset U$, including $f$. Going back to the case of a smooth $h$, we may pick $h \geq f$, and for this particular choice we get
\[
0 \leq (P^\varepsilon_t - \bar{P}^t) f \leq (P^\varepsilon_t - \bar{P}^t) h = e_\varepsilon(t),
\]
where both inequalities are a consequence of equation (23). We conclude for $e_\varepsilon$, once more with the maximum principle, that
\[
0 \leq \| e_\varepsilon \|_{L^\infty([0,1] \times U)} \leq \| P^\varepsilon_t h \|_{L^\infty([0,1] \times \partial U)}. \tag{24}
\]
With proposition 13, we see that $\| P^\varepsilon_t h - \tilde{h}^\varepsilon \|_{L^\infty([0,1] \times M)} = o(\varepsilon)$, where $\tilde{h}^\varepsilon(t, \cdot) := h + \varepsilon \int_0^t \Delta h \, ds$. In particular, this $L^\infty$ bound holds also on $[0, 1] \times \partial U$ as required in equation (24) (by construction, $\tilde{u}^\varepsilon$ vanishes on $\partial U$). This shows that $\| e_\varepsilon \|_{L^\infty([0,1] \times U)} = o(\varepsilon)$, proving the lemma. \qed

**5.3.3. Remaining steps.** The statement of theorem 1 is thus reduced to one about
\[
\langle \mathbb{1}_S, P^\varepsilon \mathbb{1}_S \rangle_0,
\]
regardless of what manifold $P^\varepsilon$ is defined on, as long as this manifold is isometric to the original one on a neighborhood of $S$. By taking a smooth partition of unity $(f_i^L)_{i=1}^N$ so that $\sum_{i=1}^N f_i = 1$ on $S$ and each $f_i$ is supported in a single coordinate chart it is (by linearity) enough to prove that
\[
\langle f_i \mathbb{1}_S, P^\varepsilon \mathbb{1}_S \rangle_0 = \sqrt{\frac{\varepsilon}{\pi}} \int_{\partial S} f_i \, d\mathcal{A} + o(\sqrt{\varepsilon}),
\]
for each $i = 1, \ldots, N$. As each $f_i$ is supported in a single coordinate chart, we may pick a local isometry into $\mathbb{R}^n$ and prove the expression there. This is precisely the end result of what was proven in step 1, i.e., equation (21), so we are done.
Appendix A. Approximation of stochastic processes

Let \((\Omega, \mathcal{F}, \mathbb{P})\) be a probability space supporting a classical Wiener process \(W_t : \Omega \to \mathbb{R}^n\) for \(t \in [0, 1]\). Let \(b : [0, 1] \times \mathbb{R}^n \to \mathbb{R}^n\) and \(\sigma : [0, 1] \times \mathbb{R}^n \to \mathbb{R}^{n \times n}\) be measurable functions. Consider the stochastic initial value problem

\[
dX^\varepsilon_t = \varepsilon b(t, X^\varepsilon_t) \, dt + \sqrt{\varepsilon} \sigma(t, X^\varepsilon_t) \, dW_t, \quad X^\varepsilon_0 = X_0, \tag{25}
\]

with initial value \(X_0 \in L^2(\mathbb{P})\). If there is \(K > 0\) such that

\[
|b(t, X) - b(t, Y)| + |\sigma(t, X) - \sigma(t, Y)| \leq K |X - Y|,
\]

and

\[
|b(t, X)| + |\sigma(t, X)| \leq K \sqrt{1 + |X|^2},
\]

for all \(t \in [0, 1]\), then the initial value problem equation (25) has a \(\mathbb{P}\)-almost surely unique continuous solution [1, theorem (6.2.2)].

The following result is a special case of [3], we follow the proof there and track the dependence of constants involved on other values more explicitly. The precise value of \(C\), however, may change from line to line.

**Theorem 10.** Let \(X^\varepsilon_t\) be the unique solution of equation (25) and \(Y^\varepsilon_t\) the unique solution of the stochastic initial value problem

\[
dY^\varepsilon_t = \sqrt{\varepsilon} \sigma(t, X_0) \, dW_t, \quad Y^\varepsilon_0 = X_0.
\]

Then there exists \(C > 0\) such that for \(\varepsilon \leq 1\):

\[
E \left[ \sup_{0 \leq t \leq 1} |X^\varepsilon_t - Y^\varepsilon_t|^2 \right] \leq C \varepsilon^2. \tag{26}
\]

**Proof.** For \(t \in [0, 1]\), let

\[
\gamma(t, \varepsilon) := \frac{X^\varepsilon_t - Y^\varepsilon_t}{\varepsilon^2}, \quad \psi(t, \varepsilon) := E \left( \sup_{0 \leq s \leq t} |\gamma(s, \varepsilon)|^2 \right).
\]

In order to prove equation (26), it must be shown that that \(\psi(1, \varepsilon) \leq C\). By the definition of \(\gamma\),

\[
\varepsilon \gamma(t, \varepsilon) = \varepsilon \int_0^t b(s, X^\varepsilon_s) \, ds + \sqrt{\varepsilon} \int_0^t \sigma(s, X^\varepsilon_s) - \sigma(s, X_0) \, dW_s, \quad \varepsilon = a_1(t, \varepsilon), \quad \varepsilon \gamma(t, \varepsilon) = a_2(t, \varepsilon).
\]
and furthermore

\[ a_1(t, \varepsilon) = \varepsilon \left( \int_0^t b(s, X^\varepsilon_s) - b(s, Y^\varepsilon_s) \, ds + \int_0^t b(s, Y^\varepsilon_s) \, ds \right), \]

\[ |a_1(t, \varepsilon)| \leq \varepsilon K \left( \int_0^t \varepsilon |\gamma(s, \varepsilon)| \, ds + \int_0^t \sqrt{1 + |Y^\varepsilon_s|^2} \, ds \right). \]

Now, as \( t \leq 1 \), Jensen’s inequality (and \((a + b)^2 \leq 2(a^2 + b^2)\) twice) yields

\[ |a_1(t, \varepsilon)|^2 \leq 2\varepsilon^2 K^2 \left( \varepsilon^2 \left( \int_0^t |\gamma(s, \varepsilon)| \, ds \right)^2 + \left( \int_0^t \sqrt{1 + |Y^\varepsilon_s|^2} \, ds \right)^2 \right) \]

\[ \leq 2\varepsilon^2 K^2 \left( \varepsilon^2 \int_0^t |\gamma(s, \varepsilon)|^2 \, ds + 1 + 2|X_0|^2 + 2\varepsilon \int_0^t \frac{|Y^\varepsilon_s - X_0|^2}{\varepsilon} \, ds \right). \]

By monotonicity of the Lebesgue integral,

\[ \sup_{0 \leq s \leq t} |a_1(s, \varepsilon)|^2 \leq 4\varepsilon^2 K^2 \left( \varepsilon^2 \int_0^t |\gamma(u, \varepsilon)|^2 \, ds \right) + 1 \]

\[ + |X_0|^2 + \varepsilon \int_0^t \sup_{0 \leq u \leq s} \left| \frac{Y^\varepsilon_s - X_0}{\varepsilon} \right|^2 \, ds \].

Consequently,

\[ E \left( \sup_{0 \leq s \leq t} |a_1(s, \varepsilon)|^2 \right) \leq 4 K^2 \varepsilon^2 \left( \varepsilon^2 \int_0^t \psi(s, \varepsilon) \, ds \right) + 1 \]

\[ + E(|X_0|^2) + \varepsilon E \left( \int_0^t \sup_{0 \leq u \leq s} \left| \frac{Y^\varepsilon_s - X_0}{\varepsilon} \right|^2 \, ds \right). \] (27)

To deal with the \( a_2 \) term, we use the Itô isometry:

\[ E(|a_2(t, \varepsilon)|^2) = \varepsilon \int_0^t E \left( |\sigma(s, X^\varepsilon_s) - \sigma(s, X_0)|^2 \right) \, ds \]

\[ \leq \varepsilon \int_0^t K^2 E \left( |X^\varepsilon_s - X_0|^2 \right) \, ds \]

\[ \leq K^2 \varepsilon \int_0^t E \left( \left| Y^\varepsilon_s - X_0 + \varepsilon\gamma(s, \varepsilon) \right|^2 \right) \, ds \]

\[ \leq K^2 \varepsilon^2 \int_0^t E \left( \left( \frac{Y^\varepsilon_s - X_0}{\varepsilon} + \sqrt{\varepsilon} \gamma(s, \varepsilon) \right)^2 \right) \, ds \]

\[ \leq 2 K^2 \varepsilon^2 \left( \int_0^t E \left( \left| \frac{Y^\varepsilon_s - X_0}{\varepsilon} \right|^2 \right) \, ds + \varepsilon \int_0^t E(|\gamma(s, \varepsilon)|^2) \, ds \right) \]

\[ \leq 2 K^2 \varepsilon^2 \left( \int_0^t E \left( \left| \frac{Y^\varepsilon_s - X_0}{\varepsilon} \right|^2 \right) \, ds + \varepsilon \int_0^t \psi(s, \varepsilon) \, ds \right). \]
As \(a_2(t, \varepsilon)\) is a martingale, Doob’s maximal inequality for \(p = 2\) shows that

\[
E \left( \sup_{0 \leq s \leq t} |a_2(s, \varepsilon)|^2 \right) \leq 4E(|a_2(t, \varepsilon)|^2)
\]

\[
\leq 8 K^2 \varepsilon^2 \int_0^t E \left( \left| \frac{Y_s - X_0}{\sqrt{\varepsilon}} \right|^2 \right) ds + \varepsilon \int_0^t \psi(s, \varepsilon) ds.
\]

(28)

Let \(Z_t = \frac{Y_t - X_0}{\sqrt{\varepsilon}}\). One may readily verify that \(Z_t\) satisfies

\[
Z_t = \int_0^t \sigma(t, X_0) dW_t,
\]

and hence in particular \(Z_t\) does not depend on \(\varepsilon\), so we may write \(Z_t\) without the superscript \(\varepsilon\). Moreover, \(Z_t\) is an \(L^2\)-martingale. Thus, Doob’s inequality ensures that \(K_1 := 4E[Z_1^2]\) satisfies \(E \left( \sup_{0 \leq s \leq 1} |Z_s|^2 \right) \leq K_1\). Combining equation (27) with (28) and \((a + b)^2 \leq 2(a^2 + b^2)\), we obtain

\[
\varepsilon^2 \psi(t, \varepsilon) \leq 8 K^2 \varepsilon^2 \left( \varepsilon^2 \int_0^t \psi(s, \varepsilon) ds + 1 + E(|X_0|^2) + \varepsilon E \left( \sup_{0 \leq u \leq t} |Z_u|^2 \right) \right)
\]

\[
+ 16 K^2 \varepsilon^2 \left( \int_0^t E(|Z_t|^2) ds + \varepsilon \int_0^t \psi(s, \varepsilon) ds \right)
\]

\[
\leq 16 K^2 \varepsilon^2 \left( \varepsilon + \varepsilon^3 + \int_0^t \psi(s, \varepsilon) ds + 1 + E(|X_0|^2) + 1 + \varepsilon \int_0^t E \left( \sup_{0 \leq u \leq t} |Z_u|^2 \right) \right)
\]

Writing \(E(|X_0|^2) = K_2 < \infty\) we see that for suitable \(D > 0\),

\[
\psi(t, \varepsilon) \leq D \int_0^t \psi(s, \varepsilon) ds + 1 + 2K_1 + K_2,
\]

assuming \(\varepsilon \leq 1\). Grönwall’s lemma\(^3\), yields that \(\psi(1, \varepsilon)\) is uniformly bounded, proving the claim.

\(\Box\)

### Appendix B. Miscellaneous proofs

**Lemma 11.** Let \((\Omega, \mathcal{A}, \mathbb{P})\) be some probability space and let \(E[X]\) denote the expectation of some random variable \(X\) on \(\Omega\). For \(\varepsilon \in [0, 1]\), let \(A^\varepsilon\) and \(B^\varepsilon\) be \((\mathbb{R}^d, \mathcal{B})\)-valued random variables with \(E \left[ |A^\varepsilon - B^\varepsilon|^2 \right] \leq C_0 \varepsilon^2\) for some \(C_0 > 0\). Let \(R \in \mathcal{B}\) and assume that \(\mathbb{P}(A^\varepsilon \in R) \leq C_1 \delta\) for sufficiently small \(\delta > 0\) and some \(C_1 > 0\). Then:

\[
|E[1_R(A^\varepsilon)] - E[1_R(B^\varepsilon)]| = o(\sqrt{\varepsilon}), \quad \varepsilon \to 0.
\]

\(^3\)Observe that \(t \mapsto \psi(t, \varepsilon)\) is monotone (and hence measurable) and finite (cf [8, chapter 5, corollary 1.2]). By the monotone convergence theorem, if \(t_n \to t\) from below, then \(\psi(t_n, \varepsilon) \to \psi(t, \varepsilon)\). In particular, the almost-everywhere (in \(t\)) bound from the integral form of Grönwall’s lemma (see [6, appendix B.2]) holds everywhere.
Proof. Note that for $\omega \in \Omega$, the condition
\[
(A^\varepsilon(\omega) \in R \text{ and } B^\varepsilon(\omega) \in R) \text{ or } (A^\varepsilon(\omega) \notin R \text{ and } B^\varepsilon(\omega) \notin R)
\]
implies $1_R(A^\varepsilon(\omega)) = 1_R(B^\varepsilon(\omega))$. We thus may see that for any $\delta > 0$
\[
|E[1_R(A^\varepsilon)] - E[1_R(B^\varepsilon)]| \leq \mathcal{P}(A^\varepsilon \in R \text{ and } B^\varepsilon \notin R) + \mathcal{P}(A^\varepsilon \notin R \text{ and } B^\varepsilon \in R)
\]
\[
\leq 2\mathcal{P}(A^\varepsilon \in R^\delta \text{ or } |A^\varepsilon - B^\varepsilon| \geq \delta)
\]
\[
\leq 2\left(\mathcal{P}(A^\varepsilon \in R^\delta) + \mathcal{P}(|A^\varepsilon - B^\varepsilon| \geq \delta)\right).
\]
Now note that by the Markov inequality
\[
\mathcal{P}(|A^\varepsilon - B^\varepsilon| \geq \delta) \leq \frac{E[|A^\varepsilon - B^\varepsilon|^2]}{\delta^2} \leq \frac{C_2\varepsilon^2}{\delta^2}.
\]
By assumption, we therefore get for sufficiently small $\delta$ that
\[
|E(1_R(A^\varepsilon) - E(1_R(B^\varepsilon)))| \leq 2\left(C_1\delta + \frac{C_2\varepsilon^2}{\delta^2}\right).
\]
Choosing $\delta = \varepsilon^{0.6}$ makes the first term $o(\sqrt{\varepsilon})$. The second term is then proportional to $\varepsilon^2/\delta^2 = \varepsilon^{0.8} = o(\sqrt{\varepsilon})$, which proves the claim.

Appendix C. Parabolic PDEs

We collect here some useful technical facts about parabolic PDE of the form
\[
\partial_t u = \varepsilon \Delta u, \quad u(0, \cdot) = u_0(\cdot), \quad (29)
\]
where $\Delta u := \text{div}_{\omega} g_t^{-1} \text{div}u$ is a Laplace-like operator on a manifold $M$ for every $t \in [0, 1]$, and $(g_t)_{t \in [0,1]}$ is a smoothly varying nonvanishing family of Riemannian metrics. We write $P_t^\varepsilon$ for the time-$t$ solution operator, i.e., $u(\cdot, t) = P_t^\varepsilon u_0$. In the case that $M$ is a compact Riemannian manifold (possibly with Dirichlet boundary), we have summarized some well-known existence and uniqueness results for $u_0 \in L^2(M, \omega)$ in appendix D of [20]. If $M = \mathbb{R}^n$, we use in this document the assumption (assumption 1) that there exists a bounded set $B$ (containing $S$ in its interior) so that both $g_t$ and $\omega$ are equal to the Euclidean metric and its volume form respectively outside of $B$ for all $t \in [0, 1]$. Under this restriction, it is well-known that the time-$t$ solution operator $P_t^\varepsilon$ is well-defined for $u_0 \in C_0(\mathbb{R}^n)$, and a maximum principle for initial values in $C_0(\mathbb{R}^n)$ (continuous functions vanishing on infinity) holds. The solution $u_t(t, x) := P_t^\varepsilon u_0$ satisfies equation (29) everywhere on $(0, 1] \times \mathbb{R}^n$ if $u_0$ has compact support. Moreover, $P_t^\varepsilon$ is of the form $(P_t^\varepsilon u_0)(x) = \int_{\mathbb{R}^n} p_t(x, y) u_0(y) \omega$. We have here taken the somewhat unconventional step of using $\omega$ instead of the Lebesgue measure for the definition of the fundamental solution as this is the natural measure for problems like equation (29), recall that $\omega$ is equivalent to the $n$-dimensional Lebesgue measure $\ell^n$ under assumption 1. As a reference for these statements, see for instance [8, chapters 3–4], [25, chapter 3] and [24].
Remark 12. The measure \( p_\varepsilon(0, \cdot, \cdot, \cdot) \omega \) is a probability measure, so we may extend \( P_\varepsilon^{\ast} \) to act on \( u_0 \in L^\infty(\mathbb{R}^n) \). Moreover, if \( u_0 \uparrow u \) pointwise everywhere for a sequence of functions \( u_\varepsilon \in L^\infty(\mathbb{R}^n) \), then the monotone convergence theorem yields \( P_\varepsilon^{\ast} u_\varepsilon \uparrow P_\varepsilon^{\ast} u \).

For positive initial data, the time-dependent heat equation preserves the integral with respect to \( \omega \). This may be seen by adapting the proof of [8, section 6, theorem 4.7], but using the \( L^2(\mathbb{R}^n, \omega) \) adjoint (as opposed to the \( L^2(\mathbb{R}^n, d\ell) \) adjoint considered there) of \( M := \varepsilon \Delta + \partial_t \) which is given by \( M^{\ast} = \varepsilon \Delta + \partial_t \). The fundamental solution for \( M^{\ast} \) (adapted to \( \omega \) instead of the Lebesgue measure as before), denoted by \( p_\varepsilon^*(x, t, y, \tau) \) satisfies \( M^{\ast} p_\varepsilon^*(\cdot, \cdot, y, \tau) = 0 \) and (by mirroring the aforementioned proof) also \( p_\varepsilon^*(x, t, y, \tau) = p(y, \tau, x, t) \). As a consequence,

\[
\int (P_\varepsilon^{\ast} u_0)(x, t) \omega(x) = \int \int p(x, t, y, 0) u_0(y) \omega(y) \omega(x) = \int \int p_\varepsilon^*(y, 0, x, t) u_0(y) \omega(y) \omega(x) = \int \int p_\varepsilon^*(y, 0, x, t) \omega(x) u_0(y) \omega(y) = \int u_0 \omega,
\]

as \( p_\varepsilon^*(y, 0, \cdot, t) \omega \) is a probability measure. Of course, all of the arguments above may also be applied to \( \overline{\Delta} \). In addition, here it is known that \( \overline{\Delta} \) generates an analytic semigroup on \( L^p(\mathbb{R}^n) \) for \( p \in [1, \infty) \) [26, section 5.4, theorem 5.6], and on \( C^\infty(\mathbb{R}^n) \) [24].

We will make use of the following approximation result.

**Proposition 13 ([20, 21]).** If \( M \) is compact (possibly with smooth homogeneous Dirichlet/Neumann boundary) and \( u_0 \in C^\infty_c(\overline{M}) \) then

\[
(P_\varepsilon^{\ast} u_0)(x) = u_0 + \varepsilon \int_0^t (\varepsilon \Delta u_0)(x) \, dt + O(\varepsilon^2)
\]

uniformly in \((t, x) \in [0, 1] \times M \) as \( \varepsilon \to 0 \).

By adapting the proof in [20], this result can be extended to the case that \( M = \mathbb{R}^n \) assuming that the boundedness condition mentioned earlier holds. In fact, the case \( M = \mathbb{R}^n \) is close to the original setting of [21] on which the proof in [20] is based.

We conclude with the following useful property of \( P_\varepsilon^{\ast} \).

**Lemma 14.** Let \( S \subset \mathbb{R}^n \) be compact and measurable. Then

\[
\langle P_\varepsilon^{\ast} 1_S, 1_{S'} \rangle_0 = \langle 1_S, P_\varepsilon^{\ast} 1_{S'} \rangle_0.
\]

Note that \( P_\varepsilon^{\ast} \) is generally not self-adjoint.

**Proof.** Using the properties of \( P_\varepsilon^{\ast} \) mentioned above, we compute

\[
\langle P_\varepsilon^{\ast} 1_S, 1_{S'} \rangle_0 = \langle (P_\varepsilon(1_{\mathbb{R}^n} - 1_S))(1_{\mathbb{R}^n} - 1_S), 1_{S'} \rangle_0
\]
\[
\langle (P^e \mathbb{1}_S) \mathbb{1}_S + (\mathbb{1}_{R^n} - P^e \mathbb{1}_S - \mathbb{1}_S), \mathbb{1}_{R^n} \rangle_0 = 0.
\]

ORCID iDs

Daniel Karrasch https://orcid.org/0000-0001-9403-6511
Oliver Junge https://orcid.org/0000-0002-3435-307X

References

[1] Arnold L 1974 *Stochastic Differential Equations: Theory and Applications* (New York: Wiley)
[2] Banisch R and Kollet P 2017 Understanding the geometry of transport: diffusion maps for Lagrangian trajectory data unravel coherent sets *Chaos* 27 035804
[3] Blagoveshchenskii Y N 1962 Diffusion processes depending on a small parameter *Theory Probab. Appl.* 7 130–46
[4] Denner A 2017 Coherent structures and transfer operators *PhD Thesis* Technische Universität München
[5] Denner A, Junge O and Matthes D 2016 Computing coherent sets using the Fokker–Planck equation *J. Comput. Dyn.* 3 163–77
[6] Evans L C 2010 *Partial Differential Equations* (Graduate studies in Mathematics Volume 19) 2nd edn (Providence, RI: American Mathematical Society)
[7] Freidlin M I and Wentzell A D 2012 *Random Perturbations of Dynamical Systems* (Grundlehren der mathematischen Wissenschaften Volume 260) 3rd edn (Berlin: Springer)
[8] Friedman A 1975 *Stochastic Differential Equations and Applications* vol 1 (New York: Academic)
[9] Froyland G 2015 Dynamic isoperimetry and the geometry of Lagrangian coherent structures *Nonlinearity* 28 3587–622
[10] Froyland G and Padberg-Gehle K 2014 Almost-invariant and finite-time coherent sets: directional-ity, duration, and diffusion *Ergodic Theory, Open Dynamics, and Coherent Structures* (Springer Proceedings in Mathematics & Statistics Volume 70) ed W Bahsoun, C Bose and G Froyland (Berlin: Springer) pp 171–216
[11] Froyland G, Santitissadeekorn N and Monahan A 2010 Transport in time-dependent dynamical systems: finite-time coherent sets *Chaos* 20 043116
[12] Grigor’yan A 2006 Heat kernels on weighted manifolds and applications *The Ubiquitous Heat Kernel* (Contemporary Mathematics Volume 398) ed J Jorgenson and L Walling (Providence, RI: American Mathematical Society)
[13] Grigor’yan A 2009 *Heat Kernel and Analysis on Manifolds* (Number 47 in Studies in Advanced Mathematics) (Providence, RI: American Mathematical Society)
[14] Gromov M 2003 Isoperimetry of waists and concentration of maps *Geom. Funct. Anal.* 13 178–215
[15] Haller G, Karrasch D and Kogelbauer F 2018 Material barriers to diffusive and stochastic transport *Proc. Natl Acad. Sci. USA* 115 9074–9
[16] Haller G, Karrasch D and Kogelbauer F 2020 Barriers to the transport of diffusive scalars in compressible flows *SIAM J. Appl. Dyn. Syst.* 19 85–123
[17] Huisings W and Schmidt B 2006 *Metastability and Dominant Eigenvalues of Transfer Operators* (Berlin: Springer) pp 167–82
[18] Jost J 2011 *Riemannian Geometry and Geometric Analysis* (Universitext) 6th edn (Berlin: Springer)
[19] Karrasch D and Keller J 2020 A geometric heat-flow theory of Lagrangian coherent structures *J. Nonlinear Sci.* 30 1849–88
[20] Karrasch D and Schilling N 2020 A Lagrangian perspective on nonautonomous advection–diffusion processes in the low-diffusivity limit
[21] Kral M S 1991 On the averaging method in nearly time-periodic advection–diffusion problems *SIAM J. Appl. Math.* 51 1622–37
[22] Press W H and Rybicki G B 1981 Enhancement of passive diffusion and suppression of heat flux in a fluid with time varying shear *Astrophys. J.* 248 751–66
[23] Schilling N 2021 Short-time heat content asymptotics via the wave and Eikonal equations J. Geom. Anal. 31 172–81
[24] Stewart H B 1974 Generation of analytic semigroups by strongly elliptic operators Trans. Am. Math. Soc. 199 141
[25] Stroock D W and Varadhan S R S 2006 Multidimensional Diffusion Processes (Classics in Mathematics) (Berlin: Springer)
[26] Tanabe H 1997 Functional Analytic Methods for Partial Differential Equations (Monographs and Textbooks in Pure and Applied Mathematics Volume 204) (New York: Dekker)
[27] Thiffeault J-L 2003 Advection–diffusion in Lagrangian coordinates Phys. Lett. A 309 415–22
[28] van den Berg M and Gilkey P 2015 Heat flow out of a compact manifold J. Geom. Anal. 25 1576–601