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Effective large-scale description of lateral diffusions on fluctuating interfaces

Claire Chevalier\(^1\) and Fabrice Debbasch\(^2\)

\(^1\) Université Pierre et Marie Curie-Paris6, UMR 7600, LPTMC, 4 place Jussieu, 75255 Paris, France. \(^2\) Université Pierre et Marie Curie-Paris6, UMR 8112, ERGA-LERMA, 3 rue Galilée, 94200 Ivry, France

E-mail: \(^1\) claire.chevalier26@gmail.com \(^2\) fabrice.debbasch@gmail.com

Abstract. The non-linear coupling between lateral diffusions on an interface and the geometry of this interface is studied numerically on a simple 1D model which presents the same kind of non-linearities as fully 2D ones. It is found that small-scale geometry fluctuations influence the diffusion at all scales, including scales much larger than those of the fluctuations. At large enough scales, the diffusion can be approximately described by introducing an effective or renormalized diffusion coefficient. Several theoretical estimates for this coefficient are introduced and compared to the value derived from numerical simulations.

1. Introduction

Lateral diffusions on interfaces are of great biological importance \([1, 2, 3, 4, 5, 6]\). They are usually modelled by 2D diffusions on ‘simple’ surfaces like a plane, a sphere or an ellipsoid. Yet, the geometry of real biological interfaces fluctuates in time and space \([7, 5]\); these fluctuations are coupled non-linearly to diffusions and, thus, influence transport in a non-trivial manner. The problem has been addressed recently in \([8, 9, 10, 11]\). This contribution focuses on a simple 1D model of diffusion which presents the same kind of non-linearities as a fully 2D Brownian motion on a fluctuating surface. The main conclusion is that small scale geometry fluctuations profoundly influence diffusions at all scales, including scales much larger than the typical scales of the fluctuations. In particular, the effective large-scale aspects of diffusions cannot be generically described through a renormalized diffusion coefficient and, even when they can, this coefficient generically depends on time and space in a non trivial manner.

2. General framework

2.1. Basics

A curved surface is a 2D differentiable manifold \([12]\) \(\mathcal{M}\) equipped with a Riemannian metric \(g\). The metric codes for all local geometric properties of \(\mathcal{M}\). Given a coordinate system \(x = (x^1, x^2)\) on \(\mathcal{M}\), the metric \(g\) is represented by its components \(g_{ij}\), which generally depend on the time \(t\) and on both coordinates. The metric \(g\) defines a line element \(dl^2\) and a surface element \(dS_g\) on \(\mathcal{M}\). In coordinates, \(dl^2 = g_{ij} dx^i dx^j\) and \(dS_g = \sqrt{\det g_{kl}(t, x)} dx^2\).

Suppose now that the geometry of \(\mathcal{M}\) can be naturally interpreted as the superposition of a mean (or reference) geometry, represented by a mean (or reference) metric \(\bar{g}\) and some fluctuations. The fluctuations are represented by the difference \(h = g - \bar{g}\). Consider a Brownian
motion \([13, 14, 15, 16]\) \(B_g\) in \(g\) which starts at time \(t = 0\) from some given point \(O\) (with coordinates \(x = 0\)). This stochastic process is fully characterized in law by its density \(n_g(t, x)\) with respect to \(dS_g\), which obeys the diffusion equation:

\[
\frac{\partial}{\partial t} \left( \sqrt{\det g_{kl}(t, x)} n_g(t, x) \right) = \frac{1}{2} \frac{\partial}{\partial x^i} \left( \sqrt{\det g_{kl}(t, x)} g^{ij}(t, x) \frac{\partial}{\partial x^j} n_g(t, x) \right)
\]

with initial condition \(n_g(0, x) = \delta(x)\). The same process can be alternately characterized by its density \(N_g\) with respect to \(dS_g = \sqrt{\det g_{kl}(t, x)} d^2x\); the identity \(n_g dS_g = N_g dS_g\) gives

\[
n_g(t, x) = \frac{\sqrt{\det g_{kl}(t, x)}}{\sqrt{\det g_{kl}(t, x)}} N_g(t, x).
\]

Inserting the above relation into eq. (1) leads to the diffusion equation obeyed by \(N_g\):

\[
\frac{\partial}{\partial t} \left( \sqrt{\det g_{kl}(t, x)} N_g(t, x) \right) = \frac{1}{2} \frac{\partial}{\partial x^i} \left( \sqrt{\det g_{kl}(t, x)} g^{ij}(t, x) \frac{\partial}{\partial x^j} \left( \frac{\sqrt{\det g_{kl}(t, x)}}{\sqrt{\det g_{kl}(t, x)}} N_g(t, x) \right) \right).
\]

Consider now a Brownian motion \(B_g\) in \(\bar{g}\) which also starts at point \(O\). This process is fully characterized in law by its density \(N_{\bar{g}}\) with respect to \(dS_g\). The two Brownian motions \(B_g\) and \(B_{\bar{g}}\) are compared with each other by comparing their respective densities \(N_g\) and \(N_{\bar{g}}\) with respect to the reference surface element \(dS_g\).

### 2.2. The 1D problem

Consider in the 2D \((x, y)\)-Euclidean plane a curve defined by the equation \(y = H(x)\). The squared line element along the rope, \(dl^2 = dx^2 + dy^2 = (1 + H'^2(x)) dx^2\), defines a 1D metric \(g\) of single coordinate component \(g_{xx} = 1 + H'^2(x)\). In 1D, this component coincides with \(\det g_{kl}\). The inverse metric \(g^{-1}\) has \(g^{xx} = 1/g_{xx}\) as single coordinate component. Since the problem is 1D, the line element \(dl\) also plays the role of the surface element \(dS_g\). Thus, the Brownian motion along the rope starting at \(x = 0\) is characterized by its density \(n_g(t, x)\) with respect to \(dl\). The differential equation obeyed by \(n_g(t, x)\) is obtained by inserting the above expressions for \(g^{xx}\) and \(\sqrt{\det g_{kl}}\) into eq. (1); this equation reads:

\[
\frac{\partial}{\partial t} \left( \sqrt{1 + H'^2(x)} n_g(t, x) \right) = \frac{1}{2} \frac{\partial}{\partial x} \left( \frac{1}{\sqrt{1 + H'^2(x)}} \frac{\partial}{\partial x} n_g(t, x) \right),
\]

with initial condition \(n_g(0, x) = \delta(x)\).

We retain for \(H\) the following simple form:

\[
H(x) = a (\cos(2\pi(K + \Delta K)x) - \cos(2\pi K x)),
\]

and choose \(a = 0.6\), \(K = 10^{-1}\), \(\Delta K = 10^{-2}\). The rope then presents ‘small scale’ oscillations of wave numbers \(10^{-1}\) and \(1.1 \cdot 10^{-1}\) around the straight line (‘plane’) with metric \(\bar{g} = 1\); the difference \(\Delta K = 10^{-2}\) between the wave numbers of these oscillations defines the ‘large scale’ \(1/10^{-2} = 100\). The associated ‘geometry’ is thus ‘flat’ (straight line, equivalent to the plane) with oscillations of amplitude \(\alpha = 4\pi^2 a^2\). The metric component \(g_{xx}\) reads:

\[
g_{xx} = 1 + \alpha \left( K^2 + K \Delta K + \frac{1}{2} \Delta K^2 \right) - \alpha K(K + \Delta K) \cos(2\pi \Delta K x)
+ \alpha K(K + \Delta K) \cos(2\pi(2K + \Delta K)x) - \frac{K^2}{2} \cos(4\pi K x)
- \alpha \frac{(K + \Delta K)^2}{2} \cos(4\pi(K + \Delta K)x);\]

\[\text{(6)}\]
the fluctuations thus generate in the metric both an offset in the lower 0 mode and contributions at wave-numbers $2\pi\Delta K$, $2 \times 2\pi K$, $2\pi(2K + \Delta K)$ and $2 \times 2\pi(K + \Delta K)$. As far as the inverse metric $g^{xx}$ or the volume factor $\sqrt{\det g_{xx}}$ are concerned, the fluctuations thus also generate an offset in the 0 mode, together with an infinite number of contributions at wave-numbers, larger or equal to $\Delta K$. One thus expects the fluctuations to influence diffusions, not only on 'small' scales comparable to $K^{-1}$, but also on 'large' scales, including scales of order $\Delta K^{-1}$ and larger ones. The form (5) has no direct physical relevance but is the simplest one which makes all interesting dynamical effects manifest; the form (5) is thus best suited for a detailed analysis of all significant physical effects.

Note that both the metric $g$ and the initial condition $n_g(0, x)$ are symmetric with respect to $x = 0$ and that the density $n_g$ has therefore this same symmetry property at all times. Plots below are thus given only for $x \geq 0$.

Let us replace $x$ by another coordinate, say $X$, defined by:

$$dX = \sqrt{1 + H^2(x)}dx,$$

and $X(0) = 0$. By definition of $X$, the metric component $g_{XX}$ equals unity and the $X$-coordinate expression of the 'surface' element $dS_g$ is simply $dX$. The density of a process with respect to $dS_g$ is a scalar and is independent of the choice of coordinates. If one uses the $X$-coordinate, the process is thus represented by the function $\tilde{n}_g(t, X) = n_g(t, x(X))$, which obeys (1) with $g_{XX} = 1$ i.e. the standard diffusion equation $\partial_t \tilde{n}_g = (1/2) \times \partial_{XX} \tilde{n}_g$. Since the initial condition is $\tilde{n}_g(0, X) = \delta(X)$, one obtains immediately the standard expression $\tilde{n}_g(t, X) = (1/\sqrt{2\pi t}) \exp(-X^2/(2t))$ for the density of the Brownian motion with respect to $dS_g = dX$, expressed as a function of $t$ and $X$. This in turn furnishes the density $n_g(t, x)$ or, equivalently, $N_g(t, x)$, provided one knows $X$ as a function of $x$. Obtaining this function directly from (7) involves computing a so-called oscillatory integral. It is therefore advisable to proceed indirectly by first expanding the integrand in powers of $a$ around $a = 0$, thus obtaining a simple trigonometric series, and, then, to compute the integral of this series. This method works as long as the series converges. For the retained values of $K$ and $\Delta K$, the series converges for all (positive) $a < a^*$ where $a^*$ is slightly superior to 0.6. The presented results thus correspond to a fluctuation amplitude close to the amplitude for which the retained numerical method breaks down and computational accuracy suffers. In practice, the expansion in power series of $a$ has been pushed to order 30 and the relative amplitude of the corresponding neglected rest is typically $10^{-7}$.

3. Results

3.1. Description

The unperturbed Brownian motion starting at point $x = 0$ associates the time $\tau(k) = 2 \ln 2/(2\pi k)^2$ to any spatial scale $k^{-1}$; $\tau(k)$ is the time at which the half-width of the Gaussian density coincides with the scale $k^{-1}$ and represents physically the time before which the diffusion does not 'see' the scale $k^{-1}$. The effects of small-scale geometry fluctuations on the large-scale $\Delta K^{-1}$ are thus best studied after time $\tau(\Delta K) \sim 351$. One also expects effects to be cumulative. All results below are thus presented at time $t_0 = 10^4 \sim 30 \tau(\Delta K)$, which is large enough for large-scale effects to be fully developed. The complete time evolution of the diffusion will be presented in full detail in a future article.

The density $N_g(10^4, x)$ and the relative density contrast $\Delta N/N_g$ at time $t = 10^4$ are plotted against the $x$-coordinate $x$ in Fig. 1 and Fig. 2.

The length $1/\Delta K = 100$ is clearly much larger than the metric fluctuation amplitude $a = 0.6$; yet, the relative density contrast is not small compared to unity and neglecting the geometry fluctuations would lead a typical relative error of at least 20%. The density $N_g(10^4, x)$ also
Figure 1. Plot of the density $N_g$ with respect to $x$ at fixed $t$ ($t = 10^4$).

Figure 2. Plot of the relative density contrast $(N_g - \bar{N}_g)/N_g$ with respect to $x$ at fixed $t$ ($t = 10^4$).

displays small-scale oscillations around a function that resembles a Gaussian. This qualitative assessment is confirmed by inspecting the spatial Fourier transform of $N_g$ at time $t = 10^4$, which is plotted in Fig. 3.

For $k \leq K_m = 7 \cdot 10^{-3}$ ($\log K_m \simeq -2.3$), the Fourier transform resembles a parabole. But the spectrum has also several small-scale pics, including ones around the base wave-number $K = 10^{-1}$ and one at the wave-number $\Delta K = 10^{-2}$. Note also that there is no pic of wave number smaller than $\Delta K$. In other words, $1/\Delta K$ is the largest ‘excited’ scale in the system. On the other hand, there is apparently no smallest excited scale. In particular, the small scale ($\log k \rightarrow 0$) pics are not numerical artefacts and correspond to scales which are naturally excited by the non-linearity of the problem. Observing the diffusion on large scales comes down to filtering the density $N_g$ and put to zero the contributions of all wave-numbers larger than a certain cut-off, say $K^*$. Let $N_g < (K^*)$ be the corresponding filtered density. If $K^*$ is larger than $K_m$, the pic at $\Delta K$ is not entirely filtered and the filtered density $N_g < (K^*)$ does not resemble a Gaussian; an example of this situation is plotted in Fig. 4 for $K^*$ larger, but of the same order than $K_m$. The larger $K^*$, more the filtered density $N_g <$ displays oscillations and resembles the unfiltered density $N_g$.

On the other hand, the filtered density $N_g < (K^*)$ does resemble a Gaussian if the cut-off $K^*$ is smaller than $K_m$, as shown in the example plotted on Fig. 5.

An effective, large-scale diffusion coefficient $D^< (K^*)$ can be associated to $N_g < (K^*)$ if the usual diffusion equation $\partial_t N_g < (K^*) = \partial_x (D^< (K^*) \partial_x N_g <)$ can be solved for $D^< (K^*)$. A straightforward analysis shows that no coefficient $D^< (K^*)$ can be associated to $N_g < (K^*)$ if $K^*$ is larger than $K_m$. Technically, this is due to the fact that $N_g < (K^*)$ has then more than one extremum. On the other hand, an effective diffusion coefficient can be associated to any $N_g < (K^*)$ with $K^*$ smaller
Figure 3. Plot of the decimal logarithm of the Fourier transform $\tilde{N}_g$ of the density $N_g$ with respect to the decimal logarithm of the wave number $k$, at fixed time $t = 10^4$.

Figure 4. Plot of $N_g^< (K^*)$ with respect to $x$ at fixed $t$ ($t = 10^4$) for $K^* = 1.6 \times 10^{-2} > \Delta K = 10^{-2}$.

Figure 5. Plot of $N_g^< (K^*)$ with respect to $x$ at fixed $t$ ($t = 10^4$) for $K^* = 4.0 \times 10^{-3} < \Delta K = 10^{-2}$.

than $K_m$. Figure 6 shows the relative discrepancy for $K^* = 4.0 \times 10^{-3}$ between $D^<(K^*)$ and
the real diffusion coefficient $D_0 = 1/2$ given by equation (4).

\[ \frac{D - D_0}{D_0} \]

\[ \text{Figure 6. Plot of the ratio } \frac{D^< - D_0}{D_0} \text{ with respect to } x \text{ at fixed } t (t = 10^4). \]

This coefficient depends on $x$ and is approximately 13% lower than the original, true coefficient $D_0 = 1/2$.

Though the precise shape of the function $D^<$ naturally depends on the choice of cutoff $K^*$, the order of magnitude of $D^<$ is found, perhaps surprisingly, to be actually cutoff-independent and the relative difference between real and effective diffusion coefficients remains around 13% for all reasonable cutoffs i.e. cutoffs which generate a smoothed density $N^<_g$ which looks like a Gaussian. It is therefore natural to wonder where this rather stable percentage comes from. The next Section is devoted to this problem.

### 3.2. Interpretation

Equation (4) can be rewritten as

\[ \frac{\partial n_g}{\partial t} = \frac{1}{2g} \left[ \frac{\partial^2 n_g}{\partial x^2} - \frac{1}{2g} \frac{\partial g}{\partial x} \frac{\partial n_g}{\partial x} \right] \]

(8)

where $g(x) = g_{xx}(x) = 1 + H'^2(x)$. Since $g$ is oscillating at scales much smaller than the typical extension $L \sim 150$ of the density (at the chose observation time $t = 10^4$), the second term on the right-hand side of (8) essentially ‘averages’ to zero and the above form of the transport equation suggests that the effective diffusion coefficient is essentially the ‘average’ of $1/g$, or alternately, that the inverse effective diffusion coefficient is the average of $g$. Of course, the above statements make sense and, thus, can be validated or invalidated only after a precise definition of averages has been given. Two simple alternative definitions come to mind.

The first possible definition of averages is simply:

\[ < f >_1 = \lim_{x \to \pm \infty} \frac{1}{2X} \int_{-X}^{+X} f(x) dx \]

(9)

and the second one is:

\[ < f >_2 (t, K^*) = \int_{-\infty}^{+\infty} N^<_g(t, x) f(x) dx \]

(10)

Note that averages of the second type depend on both the transport (and thus on time) and the cutoff $K^*$.

Both types of averages have been evaluated for $f = 1/g$ and $f = g$, $t = 10^4$ and $K^* = 4 \times 10^{-3}$. One finds $< 1/g >_1 \sim 0.882$ and $< 1/g >_2 (10^4, 4 \times 10^{-3}) \sim 0.873$, corresponding respectively to $(D^< - D_0)/D_0 \sim -0.118$ and $(D^< - D_0)/D_0 \sim -0.127$, and $< g >_1 \sim 1.157$ and
<g>(10^4, 4 \times 10^{-3}) \sim 0.170, corresponding respectively to \((D^< - D_0)/D_0 \sim -0.136\) and \((D^< - D_0)/D_0 \sim -0.145\). The average relative importance of the \(\partial_x n\) term in (8) is measured by the product 
\[L < 1/2g \partial g/\partial x >_i\] where \(i = 1\) or \(2\) and \(L \sim 150\) is the typical spatial variation scale of \(N^<_g\). Both averages lead to a product of order \(10^{-15}\); this is actually smaller than the evaluated precision \((10^{-11})\) of the discrete Fourier transforms used in this contribution.

These results indicate that the second contribution to the right-hand side of (8) is indeed probably negligible on the average and, thus, that the effective large-scale dynamics should be describable by introducing an effective diffusion coefficient. They also indicate that the relative difference between the effective diffusion coefficient and the true diffusion coefficient should lie between \(-11\%\) and \(-15\%\), which is the correct order of magnitude. But none of these results really coincides with numerically observed relative differences \((D^< - D_0)/D_0\), which typically vary (with cutoff and position) between \(-0.131\) and \(-0.133\). Nevertheless, both \(1/g \sim 2\) and \(g \sim 1\) deliver rather good approximations for the effective diffusion coefficients.

4. Conclusion

We have presented numerical computations of a 1D diffusion which capture some essential properties of lateral diffusions on nearly flat interfaces. Our results show that small scale geometry fluctuations can influence diffusions at all scales, including scales much larger that the characteristic scales of these fluctuations. The large scale aspects of diffusion cannot always be described by simply introducing a renormalized diffusion coefficient and, even when they do, this coefficient depends on both space and time and is substantially different from the true diffusion coefficient. The order of magnitude of the correction seems to be predictable by averaging some functionals of the metric.

Let us now conclude by mentioning some interesting, yet still open problems. The geometry fluctuations studied in this Letter are time-independent and have a discrete spatial Fourier spectrum; one wonders if time-dependent fluctuations, and/or fluctuations with a richer spectrum (for example, a continuous spectrum) have a comparable impact on diffusions. Studying fluctuations around a compact shape like an ellipsoid (or a circle) is also mandatory if one wants to take into account finite size effects in lateral diffusions on cell membranes; in this vein the influence of fluctuations on first-passage times in certainly worth studying. Finally, determining when and how the large-scale average diffusion can be described by introducing an effective diffusion coefficient is a very interesting and still open homogenization problem. Further numerical computations should help in indicating which theorems could be proved about effective transport in fluctuating geometries.

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