Multi-scale diffusions on biological interfaces

C. Chevalier and F. Debbasch
Université Pierre et Marie Curie-Paris6, UMR 8112, ERGA-LERMA,
3 rue Galilée, 94200 Ivry, France.
chevalier_claire@yahoo.fr, fabrice.debbasch@gmail.com

Many situations of physical and biological interest involve diffusions on manifolds. It is usually assumed that irregularities in the geometry of these manifolds do not influence diffusions. The validity of this assumption is put to test by studying Brownian motions on nearly flat 2D surfaces. It is found by perturbative calculations that irregularities in the geometry have a cumulative and drastic influence on diffusions, and that this influence typically grows exponentially with time. The corresponding characteristic times are computed and discussed.

1 Introduction

Stochastic process theory is one of the most popular tools used in modelling time-asymmetric phenomena, with applications as diverse as economics ([21, 22]), traffic management ([20, 15]), biology ([16, 2, 10, 8]), physics ([23]) and cosmology ([5]). Many diffusions of biological interest, for example the lateral diffusions ([4, 17]), can be modelled by stochastic processes defined on surfaces ([12, 13, 9, 18]). In practice, the geometry of the surface is never known with infinite precision, and it is common to ascribe to the surface an approximate, mean geometry and to assume irregularities in the geometry have, in the mean, a negligible influence on diffusion phenomena ([4, 1, 3, 6, 19]). The aim of this article is to investigate if this last assumption is indeed warranted.

To this end, we model the surface by a fixed base manifold $\mathcal{M}$ and focus on

Brownian motion. We introduce two metrics on $\mathcal{M}$. The first one, g, represents the real, irregular geometry of the manifold; what an observer would consider as the approximate, mean geometry is represented by another metric, which we call $\bar{g}$; to keep the discussion as general as possible, both metrics are allowed to depend on time.

We compare the Brownian motions in the approximate metric $\bar{g}$ to those in the real, irregular metric g by comparing their respective densities with respect to a reference volume measure, conveniently chosen as the volume measure associated to $\bar{g}$. Explicit computations are presented for diffusions on nearly flat surfaces whose geometry fluctuates on spatial scales much smaller than the scales on which these diffusions are observed. We investigate in particular if the densities generated by Brownian motions in the real, irregular metric g coincide on large scales with the densities generated by Brownian motions in the approximate metric $\bar{g}$. We perform a perturbative calculation and find that, generically, these densities differ, even on large scales, and that the relative differences of their spatial Fourier components grow exponentially in time; we also evaluate how the corresponding characteristic time scales with the amplitude of the geometry fluctuations and the wave vector of the scale at which Brownian motion is observed. Our general conclusion is that geometry fluctuations have a cumulative memory effect on Brownian motion and that their influence on diffusions cannot be neglected.

2 How to compare Brownian motions in different geometries

2.1 Definition of Brownian motion

Let $\mathcal{M}$ be a fixed real base manifold of dimension d, whose geometry is described by the possibly time dependent metric $g(t)$. This metric endows $\mathcal{M}$ with a natural volume measure which will be denoted hereafter by $\mathrm{dVol}_{g(t)}$. If C is a chart on $\mathcal{M}$ with coordinates $x = (x^i), i = 1, ..., d$, integrating against $\mathrm{dVol}_{g(t)}$ comes down to integrating against $\sqrt{\det g_{ij}} d^d x$, where the $g_{ij}(t)$'s are the components of g in the coordinate basis associated to C.

The standard definition of Brownian motions on manifolds does not apply apply to time dependent geometries because it does not conserve probability in this case. We therefore need to extend the standard definition. We introduce an auxilliary time *independent* metric γ on $\mathcal{M}$; the density of $\mathrm{dVol}_{g(t)}$ with respect to dVol_γ will be denoted by $\mu_{g(t)|\gamma}$. We define the Brownian motion in the time-dependent metric $g(t)$ as the stochastic process whose density n with respect to $\mathrm{dVol}_{g(t)}$ obeys the following generalized diffusion equation:

$$\frac{1}{\mu_{g(t)|\gamma}} \partial_t \left(\mu_{g(t)|\gamma} n \right) = \chi \Delta_{g(t)} n, \tag{1}$$

where $\Delta_{g(t)}$ is the Laplace-Beltrami operator associated to g ([7]). Given an arbitrary coordinate system (x), equation (1) transcribes into:

$$\partial_t \left(\sqrt{\det g_{kl}} n \right) = \chi \partial_i \left(\sqrt{\det g_{kl}}\, g^{ij} \partial_j n \right), \tag{2}$$

which shows that the Brownian motion in $g(t)$ does not actually depend on γ. A straightforward calculation also shows that () conserves the normalization of the density n.

2.2 What to compare

Let us introduce a new metric $\bar{g}(t)$ on $\mathcal{M}$, which describes what an observer would consider as the approximate, mean geometry of the manifold; the real, irregular metric of $\mathcal{M}$ is still denoted by $g(t)$.

Consider an arbitrary point O in $\mathcal{M}$ and let B_t be the Brownian motion in $g(t)$ that starts at O. The density n of B_t with respect to $\mathrm{dVol}_{g(t)}$ obeys the diffusion equation:

$$\frac{1}{\mu_{g(t)|\gamma}} \partial_t \left(\mu_{g(t)|\gamma} n \right) = \chi \Delta_{g(t)} n. \tag{3}$$

We denote by $\bar{B}_t$ the Brownian motion in $\bar{g}(t)$ that starts at point O and by $\bar{n}$ its density with respect to $\mathrm{dVol}_{\bar{g}(t)}$; this density obeys:

$$\frac{1}{\mu_{\bar{g}(t)|\gamma}} \partial_t \left(\mu_{\bar{g}(t)|\gamma} \bar{n} \right) = \chi \Delta_{\bar{g}(t)} \bar{n}. \tag{4}$$

We will compare the two Brownian motions by comparing on large scales their respective densities with respect to a reference volume measure on $\mathcal{M}$. From an observational point of view, the best choice is clearly $\mathrm{dVol}_{\bar{g}(t)}$, the volume measure associated to the approximate, mean geometry of the manifold. The density N of B_t with respect to $\mathrm{dVol}_{\bar{g}(t)}$ is given in terms of n by:

$$N = \mu_{g(t)|\bar{g}(t)} n, \tag{5}$$

where $\mu_{g(t)|\bar{g}(t)}$ is the density of $\mathrm{dVol}_{g(t)}$ with respect to $\mathrm{dVol}_{\bar{g}(t)}$. The transport equation obeyed by N can be deduced from (3) and reads:

$$\frac{1}{\mu_{g(t)|\gamma}} \partial_t \left(\mu_{\bar{g}(t)|\gamma} N \right) = \chi \Delta_{g(t)} \left(\frac{1}{\mu_{g(t)|\bar{g}(t)}} N \right). \tag{6}$$

The precise question investigated in this article is: how does the density N obeying (6) differ on large scales from the density $\bar{n}$ obeying (4)? Since this question is extremely difficult to solve in its full generality, we now concentrate on nearly flat 2D surfaces.

3 Brownian motions on nearly flat 2D surfaces

3.1 Method

We choose $\mathbb{R}^2$ as base manifold $\mathcal{M}$ and retain $\bar{g} = \eta$, the flat Euclidean metric on $\mathbb{R}^2$. The real, irregular metric on $\mathbb{R}^2$ is still denoted by $g(t)$ and we define $h(t)$ by $g^{-1}(t) = \eta^{-1} + \varepsilon h(t)$, where ε is a small parameter tracing the nearly flat character of the surface. From now on, we will use the metric η (*resp.* the inverse of η) to lower (*resp.* raise) all indices.

Let us choose a chart C where $\eta_{ij} = \mathrm{diag}(1, 1)$. The tensor field $h(t)$ is then represented by its components $h^{ij}(t, x)$. A particularly simple but very illustrative form for these components is:

$$h^{ij}(t, x) = \sum_{nn'} h^{ij}_{nn'} \cos\left(\omega_{n'} t - k_n.x + \phi_{nn'}\right), \tag{7}$$

where $k_n.x = k_{n1}x^1 + k_{n2}x^2$ and both integer indices run through arbitrary finite sets. Let us remark that perturbations $h(t)$ proportional to η amount to a simple modification of the conformal factor linking the 2D metric $g(t)$ to the flat metric η. We further impose that $| k_n | \geq k^*$ for all n, where k^* is a certain wave number separating the small scales ($| k | \geq k^*$) from the large ones ($| k | \ll k^*$).

The solution of (**??**) is searched for as a perturbation series in the amplitude ε of the fluctuations:

$$N(t, x) = \sum_{m \in N} \varepsilon^m N_m(t, x). \tag{8}$$

Setting to 0 both coordinates of the point O where the diffusion starts from, we further impose, for all x, that $N_0(0, x) = \delta(x)$ and $N_m(0, x) = 0$ for all $m > 0$. Equation (**??**) can then be rewritten as the system

$$\partial_t N_m = \chi \Delta_\eta N_m + \chi S_m[h, N_r], m \in \mathbb{N}, r \in \mathbb{N}_{m-1} \tag{9}$$

where the source term S_m is a functional of the fluctuation h and of the contributions to N of order strictly lower than m. In particular,

$$\begin{aligned}
S_0 &= 0 \\
S_1 &= \partial_i \left(h^{ij} \partial_j N_0 + \frac{1}{2} N_0 \eta^{ij} \eta_{kl} \partial_j h^{kl} \right) \\
S_2 &= \partial_i \left(h^{ij} \partial_j N_1 + \frac{1}{2} \left(N_0 h^{ij} + N_1 \eta^{ij} \right) \eta_{kl} \partial_j h^{kl} - \frac{1}{4} N_0 \eta^{ij} \eta_{mk} \eta_{nl} \partial_j \left(h^{mn} h^{kl} \right) \right).
\end{aligned} \tag{10}$$

Taken together, $S_0(t, x) = 0$ and $N_0(0, x) = \delta(x)$ imply that N_0 coincides with the Green function of the standard diffusion equation on the flat plane; note that N_0 is thus normalized to unity at all times. Moreover, the fact that S_m is a divergence for all m implies that the normalizations of all N_m's are conserved in time. The initial condition $N_m(0, x) = 0$ for all x and $m > 0$ then implies that all N_m's with $m > 0$ remain normalized to zero and only contribute to the local density of particles, and not to the total density.

Equation is best solved in (spatial) Fourier space and leads, for all $m \neq 0$, to

$$\frac{\hat{N}_m(t,k)}{\hat{N}_0(t,k)} = \int_0^t \hat{S}_m(t',k)\exp(\chi k^2 t')dt'. \tag{11}$$

3.2 Results

First order terms

Let us fix a certain 'observation scale' $k = k^* O(\nu)$, where $\nu \ll 1$. One then has:

$$\frac{\hat{N}_1(t,k)}{\hat{N}_0(t,k)} = \sum_{n,n',\sigma} I^{\sigma}_{nn'}(k)\left[\exp\left(i\sigma\omega_{n'}t - (k_n^2 + 2\sigma k.k_n)\chi t\right) - 1\right] \tag{12}$$

with $\sigma = \pm 1$ and

$$I^{\sigma}_{nn'}(k) = \frac{A^{\sigma}_{nn'}(k)\exp(i\phi_{nn'})}{i\sigma\omega_{n'} + (k^2 - (k+\sigma k_n)^2)\chi}, \tag{13}$$

where the $A^{\sigma}_{nn'}(k)$'s are polyonomials in the components of k, with coefficients depending on the metric perturbation amplitudes $h^{ij}_{nn'}$. For a typical perturbation, $A^{\sigma}_{nn'}(k) \sim\mid k \mid\mid k_n \mid$, while $A^{\sigma}_{nn'}(k) \sim\mid k \mid^2$ for perturbations proportional to the Euclidean metric η.

The time dependence of $\hat{N}_1/\hat{N}_0$ is controled by the real exponentials in (12), which essentially decreases as $\exp(-k_n^2\chi t)$. The first order relative contribution $\varepsilon\hat{N}_1/\hat{N}_0$ thus tends towards a quantity $L_1(k)$ which is linear in the $I^{\pm}_{nn'}(k)$'s; the typical relaxation time is $\tau_1 \sim 1/(\chi k_n^2)$, which is much smaller than the diffusion time $1/(\chi k^2)$ associated to scale k. Moreover, the limit $L_1(k)$ scales as $O(\varepsilon\nu)$, except for perturbations h proportional to η, for which it scales as $O(\varepsilon\nu^2)$; $L_1(k)$ is therefore always much smaller than ε and, in particular, tends to zero with ν *i.e.* as the scale separation tends to infinity. The effect of the k_n Fourier mode on scales characterized by a wave vector k verifying $\mid k \mid\ll\mid k_n \mid$ is thus in practice negligible.

Second order terms

The exact expression of these $\hat{N}_2/\hat{N}_0$ is extremely complicated and does not deserve full reproduction here. Of interest is that $\hat{N}_2/\hat{N}_0$ contains contributions whose amplitudes potentially grows exponentially in time. One of these reads

$$\begin{aligned} D_1(t,k) \quad &= \sum_{n,n',\sigma_1,\sigma_2,\sigma_3} I^{\sigma_1}_{nn'}(k+\sigma_2 k_p) A^{\sigma_2}_{pp'}(k) J^{\sigma_1\sigma_3}_{nn'pp'}(k) \times \\ &\left[\exp\left(i(\sigma_1\omega_{n'} + \sigma_2\omega_{p'})t - \left((k_n + \sigma_1\sigma_2 k_p)^2 + 2k.(k_n + \sigma_1\sigma_2 k_p)\right)\chi t\right) - 1\right] \end{aligned} \tag{14}$$

with $\sigma_i = \pm 1$ $(i = 1, 2, 3)$ and

$$J_{nn'pp'}^{\sigma_1\sigma_3}(k) = \frac{\exp\left(i\sigma_1\sigma_3\phi_{pp'}\right)}{i\sigma_1(\omega_{n'} + \sigma_3\omega_{p'}) + (k^2 - (k + \sigma_1(k_n + \sigma_3 k_p))^2)\chi}. \tag{15}$$

The right-hand sides of (14) contains four exponentials of given (n, n', p, p'); these involve the wave vectors $K_{np}^{\pm} = k_n \pm k_p$. Let us for the moment ignore the factors in front of these exponentials. Let k be an arbitrary wave vector and let $\theta^{\pm}$ be the angle between k and $K_{np}^{\pm}$. Each of the conditions $2k \mid \cos\theta^{\pm} \mid > \mid K_{np}^{-} \mid$ makes one of the four exponentials an increasing function of t. At second order, the spatial scales at which diffusions are influenced by the perturbation h are thus determined, not by the k_n's, but by the combinations $K_{np}^{\pm} = k_n \pm k_p$. Indeed, quite generally, the temporal behaviour of terms of order q, $q \geq 1$, will be determined by combinations of q wave vectors k_n. For perturbations h with a rich enough spectrum, these combinations correspond to all sorts of spatial scales and, in particular, to scales much larger than those over which h itself varies. Thus, h will generally influence diffusions on all spatial scales.

Let us elaborate quantitatively on this conclusion by further exploring the behaviour of $D_1(t, k)$. Suppose for example that the moduli of all k_n's are of the same order of magnitude, say k^*, but that there are some n and p for which $\mid K_{np}^{-} \mid \sim K^* O(\nu)$, where $\nu << 1$. The condition introduced above, which ensures that one of the exponentials involving K_{np}^{-} grows with t, then translates into $\mid k \mid > (2/\cos\theta^{-}) K^* O(\nu)$, and is realized for $\mid k \mid = K^* O(\nu)$ provided $\cos\theta^{-} \lesssim 1$. Let us check now that the factors in front of the exponentials do not tend towards zero with ν. Ignoring as before the influence of the frequencies ω_q, the quantity $I_{nn'}^{-}(k + k_p)$ (see (**??**)) scales as $A_{nn'}^{-}(k + k_p)/k_p^2$ *i.e.* as $k_p^2/k_p^2 = 1$. The quantity $\tilde{J}_{nn'pp'}^{-}(k)$ scales as $(Q_{np}(k))^{-1} = \left[2k.K_{np}^{-} - (K_{np}^{-})^2\right]^{-1}$. The factor in front of the exponential thus scales as $\mid k \mid\mid k_p \mid (Q_{np}(k))^{-1}$ for perturbations h not proportional to η, and as $k^2(Q_{np}(k))^{-1}$ otherwise. Taking into account that $\mid k \mid \sim \mid K_{np} \mid$ and putting $\cos\theta^{-} = 1$ to simplify the discussion, one finds that the factor in front of the exponentials scales as $\mid k_p \mid / \mid k \mid = O(1/\nu)$ if h is not proportional to η and as $O(1)$ otherwise. This factor therefore does not tend to zero with the separation scale parameter ν. Actually, for perturbations which are not proportional to η, this factor tends to infinity as ν tends to zero, a fact which only increases the influence of h on diffusions.

These estimates can be used to evaluate some characteristic times. For perturbations proportional to η, the second order term $\varepsilon^2 D_1$ reaches unity after a characteristic time $\tau_2^{\eta} \sim -(2/\nu^2 K^{*2}\chi) \ln\varepsilon$; for perturbations not proportional to η, the corresponding characteristic time is $\tau_2 \sim -(2/\nu^2 K^{*2}\chi) \ln(\varepsilon/\nu^{1/2}) << \tau_2^{\eta}$. These characteristic times are probably upper bound for the time at which the perturbation expansion ceases to be valid for scale k.

4 Conclusion

We have investigated how metric irregularities influence Brownian motion on a surface. We have performed explicit perturbative calculations for nearly flat surfaces and shown that the metric irregularities have a cumulative effect on Brownian motion; more precisely, we have found that the relative difference of the spatial Fourier components of the densities generated by a Brownian motion on the flat surface and a Brownian motion on the irregular surface grows exponentially with time on all spatial scales, including scales much larger than those characteristic of the metric perturbation; characteristic times have also been derived.

Let us conclude this article by mentioning some problems left open for further study. As stated in the introduction, many biological phenomena involve lateral diffusions on 2D interfaces. The results of this article show that the fluctuations of the interfaces profoundly affect these lateral diffusions; the discrepancies between real diffusions on irregular interfaces and idealized diffusions on highly regular surfaces are therefore probably observable and the biological consequences of these discrpancies should be carefully studied. The perturbative computations presented in this article should naturally be extended into full non perturbative treatments. Finally, the case of relativistic diffusions in fluctuating space-times is certainly worth investigating, notably in a cosmological context.

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