Notes on Brownian motion

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1 SDE basics

We will begin by reviewing basics about stochastic differential equations and the various regularization procedures used to make them well-defined. As a physicist, one is tempted to ignore details like these, but understanding them turns out to be crucial for producing SDEs that converge correctly to thermal equilibrium. A nice reference which dispelled some of my confusion on regularization conventions is [2]. Throughout, $\phi = (\phi_1, \dots, \phi_d)$ will denote a d-component object evolving according to a general SDE, and ∂_a will be used as shorthand for $\partial/\partial\phi^a$. In this section, ϕ will be assumed to take values in $\mathbb{R}^d$; the extension to the case where ϕ describes a point on a d-dimensional Riemannian manifold will be considered in the next section.

A typical Langevin equation one might imagine writing down for ϕ is

$$\partial_t \phi^a \stackrel{?}{=} f^a(\phi) + \lambda^{ab}(\phi)\xi^b, \tag{1}$$

where ξ is a white noise field with zero mean and unit variance:[1]

$$\langle \xi(t) \rangle = 0, \qquad \langle \xi^a(t)\xi^b(t') \rangle = \delta^{ab}\delta(t-t'). \tag{2}$$

When considering discritized regularizations of (1), it will be helpful to define the Wiener process $W(t)$ as the time integral of the noise (now switching to vector notation):

$$W(t) \equiv \int_0^t dt'\, \xi(t'). \tag{3}$$

One easily verifies that $\langle W(t)^2 \rangle = t$, as befitting a continuous-time random walk. In the math literature, (1) is often written in discritized form as

$$d\phi \stackrel{?}{=} f\, dt + \lambda\, dW, \tag{4}$$

where dW is morally $\dot{W} dt \to \xi dt$.

The $\stackrel{?}{=}$ in (4) is present because this "equation" does not make sense without specifying a bit more information about the definition of $g\, dW$. To understand why,

[1] Any nonzero mean can be absorbed into the drift term f, and any non-unit variance can be absorbed by a rescaling of g.

consider integrating (4) by summing up values of $d\phi$ at different discrete time steps. Doing this produces

$$\phi(t) = \phi(0) + \sum_{i=0}^{N\to\infty} \big(f[\phi(t_i^{ev})](t_{i+1} - t_i) + \lambda[\phi(t_i^{ev})](W(t_{i+1}) - W(t_i)) \big), \tag{5}$$

where the time $t_i \leq t_i^{ev} \leq t_{i+1}$ at which we evaluate the functions f, g is a choice left up to us. For the non-stochastic term, this choice is irrelevant: modifications to t_i^{ev} only modify the f part of the summand by terms of order $(t_{i+1} - t_i)^2$, which die in the continuum ($N \to \infty$) limit. For the stochastic term, the choice matters: since the noise is discontinuous in time, we obtain different results if the noise amplitude $\lambda(\phi(t))$ for the ith time step is determined before or after ϕ absorbs the fluctuations imparted to it by $W(t_{i+1}) - W(t_i)$.

The Ito prescription

A natural choice is to let $t_i^{ev} = t_i$ be the beginning of the interval, so that the instantaneous noise strength at the ith step is determined before the noise acts. This is choice is called the *Ito prescription*, and its primary benefit is the fact that the amplitude $\lambda(\phi(t_i^{ev}))$ and noise $W(t_{i+1}) - W(t_i)$ are uncorrelated. When we write derivatives in the usual way, we implicity mean that we are working with this convention:

$$d\phi = f\, dt + \lambda\, dW \qquad \text{(Ito)}. \tag{6}$$

The fact that g and dW are uncorrelated at each step means that, for any function $h(\phi(t))$,

$$\langle \int_{t_1}^{t_2} dt\, h(\phi(t))\, \frac{dW}{dt} \rangle = 0, \tag{7}$$

where the $\langle \cdot \rangle$ indicate averaging over noise realizations. As a particular example, consider computing $\langle \phi(t+\varepsilon) - \phi(t) \rangle$ to leading order in ε. With this prescription we obtain the expected

$$\frac{1}{\varepsilon}\langle \phi(t+\varepsilon) - \phi(t) \rangle = f[\phi(t)] + \langle \lambda[\phi(t)] dW_\varepsilon(t) \rangle = f[\phi(t)], \tag{8}$$

where

$$dW_\varepsilon(t) \equiv W(t+\varepsilon) - W(t). \tag{9}$$

The variance is also the expected

$$\frac{1}{\varepsilon}\langle (\phi^a(t+\varepsilon) - \phi^a(t))(\phi^b(t+\varepsilon) - \phi^b(t)) \rangle = \lambda^{ac}[\phi(t)]\lambda^{bc}[\phi(t)], \tag{10}$$

where we used

$$\langle dW_\varepsilon^a dW_{\varepsilon'}^b \rangle = \delta^{ab} \min(\varepsilon, \varepsilon'). \tag{11}$$

A "disadvantage" of the Ito prescription is that the normal rules of calculus do not apply. Specifically, the chain rule for the derivative of a function $h(\phi)$ is modified as

$$dh = \partial_a h\, d\phi^a + \frac{1}{2}(\partial_a \partial_b h)\lambda^{ad}\lambda^{bd} dt, \tag{12}$$

which is (a multivariate version of) *Ito's lemma*. Heuristically, this is arrived at by realizing that the term $\frac{1}{2}(\partial_a\partial_b h)d\phi^a d\phi^b$ in the Taylor expansion of h is *not* parametrically smaller than the linear term, as it contains a piece like $(\lambda\, dW)^2$, which is not subleading on account of $(dW)^2 = dt$ in expectation. More details can be found in the appropriate (rather abstrusely written) chapter of Zinn-Justin.

The Stratonovich prescription

Another acceptible choice—although only one of infinitely many other acceptible ones—is to fix $t_i^{ev} = (t_{i+1} + t_i)/2$ to be the midpoint of the ith time interval. This choice is called the *Stratonovich prescription*, and it is customary to put a $\circ$ to denote that one is working in this prescription:

$$d\phi = f\, dt + g \circ dW \qquad \text{(Stratonovich)}. \tag{13}$$

One benefit of this choice is that the chain rule is *not* modified in this prescription (see any stochastic analysis book). However, since the noise strength and noise are correlated during each step, the expectation value of quantities linear in the noise do *not* necessarily vanish:

$$\langle \int_{t_1}^{t_2} dt\, h(\phi(t)) \circ \frac{dW}{dt} \rangle \neq 0. \tag{14}$$

In particular, the expectation value of $\langle \phi(t+\varepsilon) - \phi(t)\rangle$ is now, again to leading order in ε, (writing $\phi(t) \to \phi$ to save space)

$$\begin{aligned} \frac{1}{\varepsilon}\langle \phi^a(t+\varepsilon) - \phi^a\rangle &= f^a(\phi) + \frac{1}{\varepsilon}\langle \big(\lambda^{ac}(\phi) + \partial_b\lambda^{ac}(\phi)(\phi^b(t+\varepsilon/2) - \phi^b)\big)\, dW^c_\varepsilon\rangle \\ &= f^a(\phi) + \frac{1}{\varepsilon}\partial_b\lambda^{ac}(\phi)\lambda^{bd}(\phi)\langle dW^d_{\varepsilon/2} dW^c_\varepsilon\rangle \\ &= f^a(\phi) + \frac{1}{2}\partial_b\lambda^{ac}(\phi)\lambda^{bc}(\phi). \end{aligned} \tag{15}$$

On the other hand, the variance is the same as in the Ito prescription:

$$\frac{1}{\varepsilon}\langle(\phi^a(t+\varepsilon) - \phi^a(t))(\phi^b(t+\varepsilon) - \phi^b(t))\rangle = \lambda^{ac}[\phi(t)]\lambda^{bc}[\phi(t)]. \tag{16}$$

Thus the Stratonovich prescription gives results which differ from the Ito one by the imposition of an additional contribution to the drift force. Note that the difference is only present when $\lambda(\phi)$ is a nontrivial function of ϕ—if g is simply constant, the two prescriptions are equivalent. Unfortunately (or fortunately, depending on one's taste), we will be required to think about nonlinear noise of this form when studying Brownian motion on curved manifolds.

The Fokker-Planck equation

We now derive the FP equation in these two prescriptions. The usual derivation is done using the Kramers-Moyal expansion, but the way in which the Taylor expansion works has always seemed a bit mysterious to me. We instead take the following variational approach. Let $h(\phi, t)$ be a function which vanishes as $|t| \to \infty$ but which is otherwise arbitrary. Consider the expectation value over ϕ of the integral $\int (dh/dt)dt = 0$. Letting $P(\phi,t)$ be the probability of observing ϕ at time t,

$$0 = \int D\phi \int dt\, P(\phi,t) \left(\partial_t h + \partial_a h \langle d\phi_\varepsilon^a \rangle + \frac{1}{2}\partial_a\partial_b h \langle d\phi_\varepsilon^a d\phi_\varepsilon^b \rangle \right), \tag{17}$$

where $d\phi_\varepsilon \equiv \phi(t+\varepsilon) - \phi(t)$. Integrating by parts,

$$0 = \int D\phi \int dt\, h \left(-\partial_t P - \partial_a (P\langle d\phi_\varepsilon^a \rangle/\varepsilon) + \frac{1}{2}\partial_a\partial_b (P\langle d\phi_\varepsilon^a d\phi_\varepsilon^b \rangle/\varepsilon) \right). \tag{18}$$

We have computed the noise averages $\langle d\phi_\varepsilon^a d\phi_\varepsilon^b \rangle$ and $\langle d\phi_\varepsilon^a \rangle$ above in both prescriptions, which we need only to leading order in ε. Defining the effective drift

$$\widetilde{f}^a \equiv \begin{cases} f^a & \text{(Ito)} \\ f^a + \frac{1}{2}\partial_b \lambda^{ac}\lambda^{bc} & \text{(Strat)} \end{cases} \tag{19}$$

we have

$$0 = \int D\phi \int dt\, h \left(-\partial_t P - \partial_a (\widetilde{f}^a P) + \frac{1}{2}\partial_a\partial_b (\lambda^{ac}\lambda^{bc} P) \right). \tag{20}$$

Since h was chosen arbitrarily, we thus have

$$\partial_t P = \partial_a \left(-\widetilde{f}^a P + \frac{1}{2}\partial_b (\lambda^{ac}\lambda^{bc} P) \right) \tag{21}$$

which we may rewrite casewise as

$$\begin{aligned} \partial_t P &= \partial_a \left(-f^a P + \frac{1}{2}\partial_b (\lambda^{ac}\lambda^{bc} P) \right) & \text{(Ito)} \\ \partial_t P &= \partial_a \left(-f^a P + \frac{1}{2}\lambda^{ac}\partial_b (\lambda^{bc} P) \right) & \text{(Strat).} \end{aligned} \tag{22}$$

If we require that $P_{\text{eq}} \propto e^{-F/T}$ be a steady state, we evidently must choose f^a such that

$$\widetilde{f}^a = \frac{1}{2}\partial_b(\lambda^{ac}\lambda^{bc}) - \frac{1}{2T}\lambda^{ac}\lambda^{bc}\partial_b F. \tag{23}$$

Naively one may have written down only the second term, but we see that in both prescriptions, an additional force dependent on the derivatives of g must be added to ensure the correct steady state. With this choice of $\widetilde{f}$, the FP equation becomes, in either prescription,

$$\partial_t P = \partial_a \left(D^{ab} \left(\frac{1}{T}\partial_b F P + \partial_b P \right) \right) = \partial_a \left(D^{ab} P \partial_b \ln(P/P_{\text{eq}}) \right), \tag{24}$$

where

$$D^{ab} \equiv \frac{1}{2}\lambda^{ac}\lambda^{bc}. \tag{25}$$

It is thus reassuring to note that *after* recieving addition input from physics (in the form of the correct steady state distribution), the two regularization procedures produce identical FP equations.

2 Brownian motion on a Riemannian manifold

We now discuss how the results of the previous section are modified when ϕ lives on a general d-dimensional Riemannian manifold M equipped with a metric g. A reference for background reading on stochastic geometry is [1], which appears very intimidating at first pass but which is actually quite good.

Let us first consider what sort of FP equation we would like to obtain. For motion in the absence of a force, simple diffusion on M would correspond to[2]

$$\partial_t P \propto \Delta_M P, \tag{26}$$

where Δ_M is the Laplace-Beltrami operator (aka the covariant Laplacian), which acts on functions $\psi \in C^\infty(M)$ as

$$\Delta_M \psi = \mathrm{div}(\mathrm{grad}\,\psi), \tag{27}$$

where div and grad are the covariant divergence and gradient on M. In components,

$$\Delta_M \psi = \frac{1}{\sqrt{g}}\partial_i(\sqrt{g}g^{ij}\partial_j\psi). \tag{28}$$

To obtain $P = e^{-F/T}$ as a steady state, we should instead have

$$\partial_t P \propto \frac{1}{\sqrt{g}}\partial_i\left(\frac{1}{T}\sqrt{g}Pg^{ij}\partial_j F + \sqrt{g}g^{ij}\partial_j P\right). \tag{29}$$

The task is then to construct a model of Langevin dynamics which correctly reproduces the above FP equations, perhaps modified to take into account more general types of diffusion constants as with the D^{ab} derived above.

There are two approaches to writing down Brownian motion on M: intrinsic and extrinsic. We will mostly discuss the extrinsic approach. This approach relies on Nash's embedding theorem, which states that M can always be isometrically embedded in $\mathbb{R}^D$ for some $D \geq d$. The strategy is then to obtain Brownian motion on M by a suitable projection of Brownian motion on $\mathbb{R}^D$. We do this via the following theorem, the proof of which I was unable to find in the literature:

Theorem 1. *Let Π denote the tensor field which projects vector fields in $\mathbb{R}^D$ to vector fields in TM. Free Brownian motion on M, for which the Fokker-Planck equation reads $\partial_t P = \frac{1}{2}\Delta_M P$, is generated by the following Stratonovich SDE:*[3]

$$d\phi^a = \Pi^{ab} \circ dW^b, \tag{30}$$

where the dW^a are independent Wiener processes with unit variance.

[2] Note that we are working in conventions where P is *not* a density, viz. normalization of probability is $\int \sqrt{g}P = 1$ (thus the probability density is instead $\sqrt{g}P$).

[3] We are not bothering to distinguish between upper and lower indices as we will be working entirely with vector fields embedded in $\mathbb{R}^D$ with the natural Euclidean metric.

Proof. A necessary requirement of the proposed SDE is that a system initialized on M must stay on M for all time. It is easy to check that (30) satisfies this requirement. Consider for example the case when M is codimension 1, so that we may define M as a level surface of some function Ψ. Then the projector Π is simply

$$\Pi = \mathbf{1} - \frac{|\partial\Psi\rangle\langle\partial\Psi|}{||\partial\Psi||^2}. \tag{31}$$

Since the Stratonovich calculus operates according to the conventional chain rule,

$$d\Psi(\phi) = \partial_a\Psi\Pi^{ab} \circ dW^b = 0, \tag{32}$$

on account of $\partial\Psi \in \ker(\Pi)$. An similar argument goes through when M has arbitrary codimension.

The FP equation for (30) is

$$\partial_t P = \frac{1}{2}\partial_a(\Pi^{ac}\partial_b(\Pi^{bc}P)), \tag{33}$$

and we claim that the RHS is equal to $\frac{1}{2}\Delta_M P$. We will prove this by making use of the fact that the lift of Δ_M to $\mathbb{R}^D$ is

$$\Delta_M\psi = \Pi^{ab}\partial_b(\Pi^{ac}\partial_c\psi), \tag{34}$$

which is a nontrivial result whose proof is deferred to a separate subsection. With this, we thus need only show that

$$\Pi^{ab}\partial_b(\Pi^{ac}\partial_c P) = \partial_a(\Pi^{ac}\partial_b(\Pi^{bc}P)). \tag{35}$$

The difference of the LHS and RHS is

$$\partial_a(\Pi^{ac}\partial_b\Pi^{bc}P) + \partial_a\Pi^{ac}\Pi^{ac}\partial_b P. \tag{36}$$

This however vanishes on account of

$$\partial_a\Pi^{ac}\Pi^{bc} = 0 \tag{37}$$

for all b, since the vector field $\partial_a\Pi^{ab}$ is orthogonal to TM.[4] This completes the proof. □

When (30) is written in Ito form, it becomes

$$d\phi^a = \frac{1}{2}\Pi^{bc}\partial_b\Pi^{ac}\,dt + \Pi^{ab}\,dW^b, \tag{38}$$

with $f^a_\Pi \equiv \frac{1}{2}\partial_b\Pi^{ac}\Pi^{bc}$ acting as an effective geometric force. When M is codimension 1, this term affords a simple geometric interpretation. In this case we may write $\Pi = \mathbf{1} - nn^T$ for a unit normal vector $n(\phi)$. Then

$$f^a_\Pi = -\frac{1}{2}n^a\partial\cdot n + \frac{1}{2}n^a n^c(n\cdot\partial)n^c. \tag{39}$$

The second term vanishes, while the first term is proportional to the mean curvature:

$$f^a_\Pi = Kn^a, \qquad K \equiv -\frac{1}{2}\partial\cdot n. \tag{40}$$

[4]For example, when M is codimension 1, we may write $\Pi^{ab} = \delta^{ab} - n^a n^b$ for some unit vector $n^a(\phi)$, and $\partial_a\Pi^{ac}\Pi^{bc}$ vanishes on account of $(n\cdot\partial)n = 0$.

Example 1. Consider Brownian motion on S^n. Then

$$d\phi^a = (\delta^{ab} - \phi^a \phi^b) \circ dW^b \tag{41}$$

where $|\phi|^2 = 1$. Checking that this gives the spherical Laplacian in cartesian coordinates is a straigthforward but tedious exercise. More physical insight is gained by transforming to coordinates intrinsic to the sphere. Consider as an example S^2, and write $\phi = (x, y, z)$. Since we may use the chain rule for Stratonovich calculus, transforming to spherical coordinates (θ, φ) is easily (if again tediously) done. After doing this and moving to the Ito prescription, some algebra yields

$$\begin{aligned} d\theta &= \cot(\theta)\, dt + dW^\theta \\ d\varphi &= \frac{1}{\sin(\theta)} dW^\varphi, \end{aligned} \tag{42}$$

where $dW^{\theta/\varphi}$ are independent linear combinations of the $dW^{x,y,z}$. The $1/\sin\theta$ term in $d\varphi$ appropriately reduces the noise strength when the particle is close to the poles. Similarly, the drift term $\cot(\theta)dt$ appearing in $d\theta$ acts as an effective force pushing the particle away from the poles of the sphere (where the area is small), ensuring a uniform steady state. In fact it is rather remarkable that the Stratonovich SDE in (θ, φ) coordinates is purely stochastic, with no compensating geometric force; in this prescription the correlation between the (θ, φ)-dependent noise strengths and the noise itself are thus responsible from steering the particle away from the poles.[5]

The above discussion has focused only on free diffusion on M. If we want $P \propto e^{-F/T}$ as a steady state, we evidently must choose the drift term as

$$\widetilde{f}^a = \frac{1}{2}\partial_b \Pi^{ba} - \frac{1}{2T}\Pi^{ab}\partial_b F. \tag{43}$$

Thus the Langevin equations appropriate to the two situations are

$$\begin{aligned} d\phi^a &= \frac{1}{2}\left(\partial_b \Pi^{ba} - \frac{1}{T}\Pi^{ab}\partial_b F\right) dt + \Pi^{ab}\, dW^b \qquad \text{(Ito)} \\ d\phi^a &= -\frac{1}{2T}\Pi^{ab}\partial_b F + \Pi^{ab} \circ dW^b \qquad \text{(Strat)}. \end{aligned} \tag{44}$$

Note that since the gradient of F is projected by Π, the drift force it causes will not cause leakage of $\mathrm{supp}(P)$ out of M. The same is true for $\partial_b \Pi^{ba}$ in the Ito prescription, which cancels leakage of $\mathrm{supp}(P)$ caused by dW^b.

Finally, while all of the above has been formulated in an extrinsic approach (by embedding M into $\mathbb{R}^D$), the Langevin and FP equations we have derived may be easily transformed into intrinsic coordinates ϕ^i appropriate to M. This is done by recognizing that Π serves as the induced metric on M, which allows things to be written in more covariant forms a la (29). It is however still preferable to write things in terms of Wiener processes living in $\mathbb{R}^d$, $d = \dim M$. For this reason we introduce vielbeins e^i_a

[5] Of course the fact that these correlations produce a compensating drift force is no surprise, and was already displayed above in the definition of $\widetilde{f}^a$.

for the metric g on M, to which we couple an $\mathbb{R}^d$ Wiener process dW^a. The Langevin equation for free diffusion in this framework turns out to read

$$\begin{aligned} d\phi^i &= \frac{1}{2\sqrt{g}}\partial_j(g^{ij}\sqrt{g})\,dt + e^i_a\,dW^a \qquad \text{(Ito)} \\ d\phi^i &= e^i_a \circ dW^a \qquad \text{(Strat)}, \end{aligned} \tag{45}$$

whose FP equations can be checked to produce (29). We will omit the details due to laziness.

Appendix: Laplace-Beltrami operator in projected form

As above, let M be a d-dimensional Riemannian manifold embedded in $\mathbb{R}^D$. Our goal is to prove the following proposition, which provides a way of lifting the Laplace-Beltrami operator on M to $\mathbb{R}^D$:

Proposition 1. *The Laplace-Beltrami operator Δ_M of M is lifted to $\mathbb{R}^D$ takes the sum-of-squares form*

$$\Delta_M = \sum_{a=1}^{D} \Pi_a^2. \tag{46}$$

In components, $\Delta_M\psi = \sum_a \Pi^b_a\partial_b(\Pi^c_a\partial_c\psi)$ for any $\psi \in C^\infty(M)$.

The following proof is a translation of a result proved in [1] into human interpretable language.

Proof. In the proof (and as above), ∂ will be used to denote differentiation in $\mathbb{R}^D$, while ∇ will denote covariant differentiation in M. $a, b, c, \ldots$ will denote indices of objects in $\mathbb{R}^D$, and $i, j, k, \ldots$ will denote indices of objects in M.

Recall that in the present setting, the covariant derivative of a vector field $Y \in \Gamma(TM)$ along another vector field $X \in \Gamma(TM)$ ($\Gamma(TM)$ being the standard notation for vector fields on TM) is

$$\nabla_X Y = \Pi(\partial_X Y). \tag{47}$$

If we lift X, Y to vector fields on $\mathbb{R}^D$, in components this reads $X^a\nabla_a Y^b = \Pi^b_a X^c\partial_c Y^a$.[6]

Let $\nabla\psi = \Pi(\partial f) \in \Gamma(TM)$ be the gradient of $\psi \in C^\infty(M)$ lifted to a vector field on $\mathbb{R}^D$. Since ∇ is stabilized by Π, we may insert a resolution of the identity as

$$\nabla\psi = \sum_a e_a(e_a\cdot\nabla\psi) = \sum_a \Pi_a(\Pi_a\cdot\partial\psi), \tag{49}$$

[6] The fact that the projection gives the correct connection is proved by recalling that the Levi-Civita connection is the *unique* connection which is metric compatible, meaning that $X(g_M(Y,Z)) = g_M(\nabla_X Y, Z) + g_M(Y, \nabla_X Z)$, where $X, Y, Z \in TM$ and g_M is the induced metric on M. That the projected derivative does the job can be shown by lifting things to $\mathbb{R}^D$: letting $\cdot$ denote the standard inner product in $\mathbb{R}^D$, and using the fact that the embedded metric satisfies $g_M(X,Y) = X\cdot Y$ for all $X, Y \in \Gamma(TM)$,

$$\begin{aligned} X(g_M(Y,Z)) &= X(Y\cdot Z) = (\partial_X Y)\cdot Z + Y\cdot(\partial_X Z) \\ &= (\Pi(\partial_X Y))\cdot Z + Y\cdot(\Pi(\partial_X Z)) \\ &= g_M(\nabla_X Y, Z) + g_M(Y, \nabla_X Z), \end{aligned} \tag{48}$$

where we used the fact that $((\mathbf{1}-\Pi)\partial_X Y)\cdot Z = 0$ on account of $Z \in \Gamma(TM)$ (and likewise for $Z \leftrightarrow Y$).

where we used $\Pi_a \cdot \nabla\psi = \Pi_a \cdot \Pi\partial\psi = \Pi_a \cdot \partial\psi$. To get the Laplace-Beltrami operator, we need to take the covariant divergence of $\nabla\psi$, which is

$$\Delta_M \psi = \nabla \cdot (\nabla\psi) = \sum_a (\nabla \cdot \Pi_a)(\Pi_a \cdot \partial\psi) + \sum_a (\Pi_a \cdot \partial)(\Pi_a \cdot \partial\psi). \tag{50}$$

The theorem will then follow if we can show that the first term on the RHS vanishes. To do this, recall that the covariant divergence of a vector field $X \in \Gamma(TM)$ is

$$\nabla \cdot X = \sum_{i=1}^{d} g_M(V_i, \nabla_{V_i} X) = \sum_{i=1}^{d} V_i^a V_i^b \nabla_b X^a, \tag{51}$$

where the $\{V_i\}$ are a collection of vector fields on $\mathbb{R}^D$ that form an orthonormal basis for TM (and g_M is the induced metric on M). We then use a standard trick by going into Riemann normal coordinates, where the Christoffel symbols of the connection (locally) vanish. Then

$$\nabla \cdot \Pi_a = \sum_i g_M(V_i, \nabla_{V_i} \Pi_a) = \sum_i V_i g_M(V_i, \Pi_a) - g_M(\nabla_{V_i} V_i, \Pi_a), \tag{52}$$

since ∇ is compatible with g_M. But the vector fields $\nabla_{V_i} V_j = (\partial_i \delta_i^k + \Gamma_{il}^k \delta_j^l)\partial_k = 0$ vanish for all i, j, since the Christoffel symbols (locally) do. Therefore

$$\nabla \cdot \Pi_a = \sum_i V_i g_M(V_i, \Pi_a) = \sum_i V_i (V_i \cdot \Pi_a) = \sum_i V_i (V_i \cdot e_a) = \sum_i (\partial_{V_i} V_i \cdot e_a) \tag{53}$$

since $\partial e_a = 0$. Then we may finally show that

$$\begin{aligned} \sum_a (\nabla \cdot \Pi_a)(\Pi_a \cdot \partial\psi) &= \sum_{a,i} (\partial_{V_i} V_i, e_a) \Pi_a \cdot \partial\psi \\ &= \left(\sum_i \Pi \left[\sum_a (\partial_{V_i} V_i \cdot e_a) e_a \right] \right) \cdot \partial\psi \\ &= \sum_i (\Pi[\partial_{V_i} V_i]) \cdot \partial\psi \\ &= 0, \end{aligned} \tag{54}$$

since $\partial_{V_i} V_j$ is orthogonal to TM for all i, j on account of $\nabla_{V_i} V_j = 0$ and $\nabla_{V_i} V_j = \Pi(\partial_{V_i} V_j)$. This shows that

$$\Delta_M \psi = \sum_a (\Pi_a \cdot \partial)(\Pi_a \cdot \partial\psi), \tag{55}$$

completing the proof. □

3 Application: relaxation by weak thermal baths

Consider a situation in which a system described by a vector of thermodynamic variables ϕ is coupled to a bath at temperature T. In the limit where the strength of the coupling to the bath vanishes, we assume that the system undergoes dynamics that lead it to maximize an entropy function $S(\phi)$, and that it does so while conserving an energy function $E(\phi)$. From the above discussion we expect to be able to describe this case with an Ito-prescription Langevin equation of the form (letting dW^a be unit-variance Wiener processes as above)

$$d\phi^a = f_S^a\,dt + A_S\Pi^{ab}\,dW^b, \tag{56}$$

where $\Pi = \mathbf{1} - n_E n_E^T$ is the projector onto the isoenergy surface defined by the unit normal $n_E^a = (\partial^a E)/||\partial E||$, and A_S is a (in general ϕ-dependent) parameter determining the noise strength. Using the results developed above, the associated FP equation is

$$\partial_t P = \partial_a\left(-(f_S^a - A_S\Pi^{ab}\partial_b A_S - A_S^2 K_E n_E^a)P + \frac{1}{2}A_S^2\Pi^{ab}\partial_b P\right), \tag{57}$$

where $K_E = -\frac{1}{2}\partial_a n_E^a$ is the curvature of the isoenergy surface at ϕ. To ensure that $e^{S(\phi)}$ is a steady state, we evidently must choose

$$f_S^a = A_S\Pi^{ab}\partial_b A_S + A_S^2 K_E n_E^a + \frac{1}{2}A_S^2\Pi^{ab}\partial_b S. \tag{58}$$

Note that on physical grounds it seems reasonable to let $A_S = A_S[E(\phi)]$ be a function of the energy only; the first term on the RHS vanishes if this is true.

In the opposite limit where the coupling is strong, we assume that the dynamics leads the system to minimize $F(\phi) = E(\phi) - TS(\phi)$ for a fixed bath temperature T. In this case we may ignore the system's ability to self-equilibrate and write

$$d\phi = f_B^a\,dt + A_B\,dW^a, \tag{59}$$

where for simplicity the bath noise amplitude A_B is assumed to be independent of ϕ. We then obtain

$$\partial_t P = \partial_a\left(-f_B^a P + \frac{A_B^2}{2}\partial^a P\right), \tag{60}$$

and having $e^{-F/T}$ as a fixed point thus requires that we set

$$f_B^a = -\frac{A_B^2}{2T}\partial_a F. \tag{61}$$

We now consider the general case where both relaxation processes are active. We may write the full Langevin equation as

$$d\phi^a = g^a\,dt + (A_B\delta^{ab} + A_S\Pi^{ab})\,dW^b, \tag{62}$$

where g^a is to be determined by fixing the correct steady state distribution. Letting A_B be independent of ϕ and assuming that A_S depends only on $E(\phi)$, the associated FP equation is, after some simplifications,

$$\partial_t P = \partial_a\left(-\left(g^a - (A_S^2 + 2A_BA_S)K_E n^a\right)P + \frac{1}{2}\left(A_B^2\delta^{ab} + (A_S^2 + 2A_BA_S)\Pi^{ab}\right)\partial_b P\right). \tag{63}$$

From the above, we know that

$$g^a|_{A_S=0} = f^a_B, \qquad g^a|_{A_B=0} = f^a_S, \tag{64}$$

where $f^a_{B,S}$ are as in (61), (58). It thus may seem reasonable to simply add the bath and system drift forces together, by taking

$$g^a \to g^a_{\text{naive}} = f^a_B + f^a_S. \tag{65}$$

Doing this however does *not* produce $e^{-F/T}$ as a steady state, which we expect it to be as long as the system-bath coupling is nonzero. Indeed, inserting g^a_{naive} yields

$$\partial_t e^{-F/T} = \partial_a \left(2A_B A_S \left(K_E n^a_E - \frac{1}{2T}\Pi^{ab}\partial_b F \right) e^{-F/T} \right), \tag{66}$$

where we used $\Pi^{ab}\partial_b S = -\frac{1}{T}\Pi^{ab}\partial_b F$. Since $n_E \in \ker(\Pi)$, the terms inside the parenthesis cannot cancel, and $e^{-F/T}$ will not be a steady state. In order to fix this, we must add an additional term to the drift force proportional to $A_S A_B$ to cancel the above term. This means that $e^{-F/T}$ is a steady state only if we choose

$$\begin{aligned} g^a &= f^a_S + f^a_B + 2A_B A_S \left(K_E n^a_E - \frac{1}{2T}\Pi^{ab}\partial_b F \right) \\ &= \overline{A}^2_S K_E n^a_E + \frac{\overline{A}^2_S}{2}\Pi^{ab}\partial_b S - \frac{A^2_B}{2T}\partial_a F, \end{aligned} \tag{67}$$

where

$$\overline{A}^2_S \equiv A^2_S + 2A_B A_S. \tag{68}$$

Therefore we may describe the situation by saying that upon introducing the coupling to the bath, the Langevin equations of the system and bath in isolation may added together, *provided* one first renormalizes the system noise strength by sending $A_S \to \overline{A}_S$.

Appendix: anisotropic noise

The above analysis was performed assuming that the strengths of the noises dW^a were uniform in $\mathbb{R}^D$. In a more general setting, it is entirely possible for certain directions of the noise to be stronger than others; by FDT, this means simply that the transport coefficients determing the relaxation of ϕ^a may have anisotropy in $\mathbb{R}^D$ beyond the anisotropy present in $\partial_a F$ (or $\partial_a S$, as the case may be).

Consider first the bath only case, where no conservation laws are present. We may then write

$$d\phi^a = f^a_B\, dt + \sqrt{2T} M^{ab}_B\, dW^b \tag{69}$$

for some (in general ϕ-dependent) matrix M_B. Define the matrix

$$\Gamma_B \equiv M_B M^T_B. \tag{70}$$

Then using the above results, the requirement that $e^{-F/T}$ be a steady state fixes f^a_B so that the Langevin equation reads

$$d\phi^a = (T\partial_b\Gamma^{ab}_B - \Gamma^{ab}_B\partial_b F)dt + \sqrt{2T}M^{ab}\, dW^b. \tag{71}$$

It is worth reiterating that when the noise matrix M^{ab} has nontrivial dependence on ϕ, the drift force must contain a term which is independent of F. Using Ito's lemma, we can check how F changes in expectation:

$$\begin{aligned}\langle dF\rangle &= \partial_a F\,\langle d\phi^a\rangle + T\partial_a\partial_b F[MM^T]^{ab}\,dt\\ &= \big(\partial_a F(T\partial_b\Gamma_B^{ab} - \Gamma_B^{ab}\partial_b F) + T\Gamma_B^{ab}\partial_a\partial_b F\big)\,dt\\ &= \big(-(\partial F)^T\,\Gamma_B\,(\partial F) + T\partial_a(F\partial_b\Gamma_B^{ab})\big)\,dt,\end{aligned} \tag{72}$$

since in Ito's prescription the expectation of the dW piece vanishes. Γ_B is positive semidefinite, so $d\langle F\rangle/dt \le 0$ when Γ_B is ϕ-independent. While the total derivative term can change this when Γ_B has ϕ dependence, $H(P|P_{\rm eq})$ is always monontically decreasing, regardless of Γ_B. Indeed, the FP equation one obtains from this Langevin equation is

$$\partial_t P = \partial_a(\Gamma_B^{ab}(\partial_b F P + T\partial_b P)) = \partial_a(T\Gamma_B^{ab}P\partial_b\ln(P/P_{\rm eq})). \tag{73}$$

Thus as promised,

$$\begin{aligned}\partial_t H(P|P_{\rm eq}) &= \partial_t\int D\phi\,P\ln(P/P_{\rm eq})\\ &= \int D\phi\,\partial_t P\ln(P/P_{\rm eq})\\ &= T\int D\phi\,\partial_a(\Gamma_B^{ab}P\partial_b\ln(P/P_{\rm eq}))\ln(P/P_{\rm eq})\\ &= -T\int D\phi\,P[\partial\ln(P/P_{\rm eq})]^T\Gamma_B[\partial\ln(P/P_{\rm eq})]\\ &\le 0,\end{aligned} \tag{74}$$

where the second line follows from $\partial_t P$ being a total derivative and the last from the fact that Γ_B is PSD and P is everywhere non-negative.

A similar story goes through in the case of energy-preserving noise. Here we consider

$$d\phi = f_S\,dt + \sqrt{2}\Pi M_S\,dW. \tag{75}$$

Define the matrix

$$\Gamma_S \equiv \Pi M_S M_S^T\Pi. \tag{76}$$

Then fixing f_S to guarantee e^S as a steady state, the Langevin and FP equations are

$$d\phi^a = (\partial_b\Gamma_S^{ab} + \Gamma_S^{ab}\partial_b S)dt + \sqrt{2}\Pi^{ac}M_S^{cd}\,dW^d \tag{77}$$

and

$$\partial_t P = \partial_a(\Gamma_S^{ab}(-\partial_b SP + \partial_b P)) = \partial_a(\Gamma_S^{ab}P\partial_b\ln(P/P_{\rm eq})). \tag{78}$$

A similar statement about the monotonicity of $H(P|P_{\rm eq})$ of course holds here as well.

Finally, in the case where both types of relaxation processes are operative, we have

$$d\phi = f\,dt + \sqrt{2T}(M_B + \Pi M_S)\,dW. \tag{79}$$

Since we want $e^{-F/T}$ as the steady state, this is really no different than the unconstrained case considered above. It is sometimes conceptually helpful to break up Γ into energy-conserving and energy-nonconserving parts, although in general this separation can be rather arbitrary. In one convention, we may write the Langevin and FP equations as

$$d\phi^a = \left(T\partial_b\Gamma_B^{ab} - \Gamma_B^{ab}\partial_b F + \partial_b\Gamma_S^{ab} + \Gamma_S^{ab}\partial_b S\right) dt + \sqrt{2T}(M_B^{ab} + \Pi^{ac}M_S^{cb})dW^b \tag{80}$$

where

$$\Gamma_B = M_B M_B^T + \Pi M_S M_B^T + M_B M_S^T \Pi, \qquad \Gamma_S = \frac{1}{T}\Pi M_S M_S^T \Pi, \tag{81}$$

and

$$\partial_t P = \partial_a \left(\Gamma_B^{ab}(\partial_b F P + T\partial_b P) + \Gamma_S^{ab}(-\partial_b S P + \partial_b P)\right). \tag{82}$$

Note that $\partial_b\Gamma_S^{ab} = 0$ if $M_S = M_S[E(\phi)]$ is a function only of energy.

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