0.1 Stochastic Differential Calculus

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We want now to generalize the ordinary calculus rules to the stochastic case.
We obtained a stochastic differential equation from the Master Equation. Then, to understand the underlying physics, we introduced the *Langenvin equation* (in the Overdamped limit):

$$\mathrm{d}x(t) = f(x(t),t)\,\mathrm{d}t + \sqrt{2D(x(t),t)}\,\mathrm{d}B(t)$$

with $f = F_{\text{ext}}/\gamma$.
The meaning of $\mathrm{d}B(t)$ is clear only passing to *finite differences*, where $\mathrm{d}B \to \Delta B$ is distributed according to:

$$\Delta B \frac{1}{\sqrt{2\pi\Delta t}} \sim \exp\left(-\frac{(\Delta B)^2}{2\Delta t}\right)$$

If we consider a *stochastic integral*:

$$\int g\,\mathrm{d}B$$

we need to discretize it and take the continuum limit (in the mean square convergence).
In the more general case, we want to integrate wrt $(\mathrm{d}B)^n$. We will now show that:

$$(\mathrm{d}B)^n = \begin{cases} \mathrm{d}B & n=1 \\ \mathrm{d}t & n=2 \\ 0 & n>2 \end{cases}$$

Example 1 (Integral in $\mathbf{d}\boldsymbol{B}^{\mathbf{2}}$)**:**

Consider a *non-anticipating* function $G(\tau)$, and the following integral:

$$I = \int G(\tau)(\mathrm{d}B\,(\tau))^2$$

With *non-anticipating* we mean that $G(\tau)$ does not depend on $B(s)-B(\tau)\forall s > \tau$, i.e. it does not depend on the *future*. Discretizing:

$$I = \mathrm{ms}-\lim \sum_{i=1}^{n} G(t_{i-1})\Delta B_i^2$$

For simplicity, we will denote $G_{i-1} \equiv G(t_{i-1})$, $\Delta B_i \equiv B_i - B_{i-1} \equiv B(t_i) - B(t_{i-1})$ and $t_i - t_{i-1} = \Delta t_i$.
We want to prove that:

$$\int_0^t G(\tau)(\mathrm{d}B(\tau))^2 \stackrel{?}{=} \int_0^t G(\tau)\,\mathrm{d}\tau = \lim_{n\to\infty}\sum_i G(t_{i-1})\Delta t_i$$

So we take their average difference squared and compute the limit:

$$\langle\left(\sum_{i=1}^{n} G_{i-1}\Delta B_i^2 - \sum_{i=1}^{n} G_{i-1}\Delta t_i\right)^2\rangle \xrightarrow[n\to\infty]{?} 0$$

Then, proceeding similarly to last lecture:

$$= \langle\left[\sum_{i=1}^{n} G_{i-1}((\Delta B_i)^2 - \Delta t_i)\right]^2\rangle = \langle\sum_{i=1}^{n} G_{i-1}((\Delta B_i)^2 - \Delta t_i)\sum_{j=1}^{n} G_{j-1}((\Delta B_j)^2 - \Delta t_j)\rangle =$$

$$= \sum_{i=1}^{n}\langle G_{i-1}^2((\Delta B_i)^2 - \Delta t_i)^2\rangle + 2\sum_{i<j}^{n}\langle G_{i-1}((\Delta B_i)^2 - \Delta t_i)G_{j-1}\,((\Delta B_j)^2 - \Delta t_j)\rangle$$

Note that the yellow term *does not depend* on $\Delta B_j = B_j - B_{j-1} = B(t_j) - B(t_{j-1})$ (recall that G is *non-anticipating*). Thus, the yellow and blue terms are *independent* of each other, and so we can factorize the average:

$$= \sum_{i=1}^{\infty}\langle G_{i-1}^2((\Delta B_i)^2 - \Delta t_i)^2\rangle + 2\sum_{i<j}^{n}\langle G_{i-1}((\Delta B_i)^2 - \Delta t_i)G_{j-1}\rangle\langle(\Delta B_j)^2 - \Delta t_j\rangle$$

However, recall that:

$$\langle(\Delta B_j)^2 - \Delta t_j\rangle = \langle(\Delta B_j)^2\rangle - \Delta t_j = 0$$

and so only the first term remains. Again, we can separate two independent terms:

$$= \langle\sum_{i=1}^{n} G_{i-1}^2((\Delta B_i)^2 - \Delta t_i)^2\rangle = \sum_{i=1}^{n}\langle G_{i-1}^2\rangle\langle(((\Delta B_i)^2 - \Delta t_i^2)\rangle$$

Then, focus on a single term:

$$\begin{aligned}\langle((\Delta B_i)^2 - \Delta t_i)^2\rangle &= \langle\Delta B_i^4 - 2\Delta t_i(\Delta B_i)^2\rangle + \Delta t_i^2 = \\ &= \underbrace{\langle(\Delta B_i)^4\rangle}_{3(\Delta t_i)^2} - 2\Delta t_i\underbrace{\langle(\Delta B_i)^2\rangle}_{\Delta t_i} + \Delta t_i^2 = 2\Delta t_i^2\end{aligned}$$

Substituting back into the sum:

$$\begin{aligned}&= \langle\left[\sum_{i=1}^{n} G_{i-1}((\Delta B_i)^2 - \Delta t_i)\right]^2\rangle = 2\sum_{i=1}^{n} G_{i-1}^2\Delta t_i^2 \\ &\le 2\left(\max_{i\le j\le n}\Delta t_j\right)\sum_{i=1}^{n} G_{i-1}^2\Delta t_i \xrightarrow[n\to\infty]{} 2\cdot 0\cdot\int_0^t G^2\,\mathrm{d}\tau = 0\end{aligned}$$

This proves that $(\mathrm{d}B)^2 = \mathrm{d}t$.

$\boxed{\textbf{Example 2 (The case with } n > 2\textbf{):}}$

We want now to show that:

$$\int_0^t G(\tau)(\mathrm{d}B\,(\tau))^n = \mathrm{ms} - \lim \sum_{i=1}^n G(t_{i-1})\Delta B_i^n = 0$$

Again, we discretize and consider the average distance squared:

$$\langle \left(\sum_{i=1}^n G_{i-1}(\Delta B_i)^n \right)^2 \rangle = \sum_{i=1}^n G_{i-1}^2 (\Delta B_i)^{2n} + 2 \sum_{i<j} \langle G_{i-1} G_{j-1} (\Delta B_i)^n (\Delta B_j)^n \rangle$$

Suppose, for simplicity, that G is bounded, i.e. $|G| < K$. Then, as G is non-anticipating, we can factorize the averages (as we did before). If n is **odd** , the second term vanishes:

$$= \sum_i \langle G_{i-1}^2 \rangle (\Delta t_i)^n \frac{(2n)!}{2^n n!} \leq \frac{K^2 (2n)!}{2^n n!} \sum_{i=1}^n (\Delta t_i)^n \leq \frac{K^2 (2n)!}{2^n n!} \max_{i \leq j \leq n} (\Delta t)^{n-1} \underbrace{\sum_{i=1}^n \Delta t_i}_{t} \xrightarrow[n\to\infty]{} 0$$

Otherwise, if n is even, the following holds instead:

$$\leq 2K^2 \left(\frac{n!}{2^{n/2}(n/2)!} \right)^2 \sum_{i<j} \Delta t_i^{n/2} \Delta t_j^{n/2} \leq 2K^2 \left(\frac{n!}{2^{n/2}(n/2)!} \right)^2 \left(\max_{i \leq l \leq n} \Delta t_l \right)^{2(n/2-1)} \sum_{i<j} \underbrace{\Delta t_i \Delta t_j}_{\leq t^2}$$

and by taking the limit $n \to \infty$ it goes to 0, proving the thesis.

Example 3 (Other cases)**:**

Consider now:

$$\int G(\tau)\,\mathrm{d}B(\tau)\,\mathrm{d}\tau = 0$$

In fact, as $(\mathrm{d}B)^2 = \mathrm{d}\tau$, $\mathrm{d}B\,\mathrm{d}u = 0$ because $(\mathrm{d}B)^n = 0\ \forall n > 2$.

Consider now:

$$\begin{aligned} \mathrm{d}(B(t))^n &= (B(t) + \mathrm{d}B(t))^n - (B(t))^n = \\ &= \sum_{k=1}^n \binom{n}{k} (\mathrm{d}B\,(t))^k B(t)^{n-k} \end{aligned}$$

We consider the non-trivial case, i.e when $n \geq 2$:

$$= n\,\mathrm{d}B\,(t) B^{n-1}(t) + \frac{n(n-1)}{2} \underbrace{(\mathrm{d}B\,(t))^2}_{\mathrm{d}t} B^{n-2}(t) + 0$$

If we set $n-1 = m$ we arrive at:

$$(m+1) B^m(t)\,\mathrm{d}B\,(t) = \mathrm{d}B(t)^{m+1} - \frac{m(m+1)}{2} B^{m-1}(t)\,\mathrm{d}t$$

Then:

$$\int_0^\tau B^m(t)\,\mathrm{d}B\,(t) = \frac{1}{m+1}\int_0^\tau \mathrm{d}(B(t))^{m+1} - \frac{m}{2}\int_0^\tau B^{m-1}(t)\,\mathrm{d}t$$

Note that, if $m=1$:

$$\int_0^\tau B(\tau)\,\mathrm{d}B\,(t) = \frac{1}{2}\int_0^\tau \mathrm{d}(B(t))^2 - \frac{1}{2}\int_0^\tau \mathrm{d}t$$

and so we arrive again at a formula we already seen:

$$\int_0^\tau B(t)\,\mathrm{d}t = \frac{1}{2}(B^2(\tau) - B^2(0)) - \frac{\tau}{2}$$

In the general case, for $m>0$:

$$\begin{aligned}\int_0^\tau B^m(t)\,\mathrm{d}B\,(t) &= \frac{1}{m+1}\int_0^\tau \mathrm{d}(B(t))^{m+1} - \frac{m}{2}\int_0^\tau B^{m-1}(t)\,\mathrm{d}t = \\ &= \frac{B^{m+1}(\tau) - B^{m+1}(0)}{m+1} - \frac{m}{2}\int_0^\tau B^{m-1}(t)\,\mathrm{d}t\end{aligned}$$

Note that we can generalize this to a generic function f of $B(t)$:

$$\begin{aligned}\mathrm{d}f(B(t)) &= f(B(t) + \mathrm{d}B\,(t)) - f(B(t)) = \\ &= f'(B(t))\,\mathrm{d}B\,(t) + \frac{1}{2}f''(B(t))(\mathrm{d}B(t))^2 + 0\end{aligned}$$

and so:

$$\mathrm{d}f = f'\,\mathrm{d}B + \frac{1}{2}f''\,\mathrm{d}t + O(\mathrm{d}t^{3/2})$$

0.2 Derivation of the Fokker-Planck equation

Starting from the Master Equation and taking the continuum limit we arrived at the Fokker-Planck equation:

$$\dot{\mathbb{P}}(x,t) = -\frac{\partial}{\partial x}\left[f(x,t)\mathbb{P}(x,t) - \frac{\partial}{\partial x}\mathbb{P}(x,t)D(x,t)\right]$$

($\mathbb{P}(x,t) \equiv W(x,t)$).
We want to derive from that the Langenvin equation:

$$\mathrm{d}x(t) = f(x(t),t) + \sqrt{2D(x(t),t)}\,\mathrm{d}B(t)$$

Note that in the Langenvin eq. $x(t)$ appears because we are talking about a *single trajectory*, while in $\mathbb{P}(x,t)$ x and t are independent variables, and $\mathrm{d}x\,\mathbb{P}(x,t)$ is the *density* of trajectories passing in $[x, x+\mathrm{d}x]$ at time t. So, to compute $\mathbb{P}(x,t)$, we need to *generate many trajectories* with the Langenvin equation, and count the ones satisfying the appropriate conditions (crossing $[x, x+\mathrm{d}x]$ at time t). We can do this by writing:

$$\mathbb{P}(x,t) = \langle \delta(x(t)-x) \rangle$$

In fact, if we integrate in $[x, x+\Delta x]$:

$$\int_x^{x+\Delta x} \mathbb{P}(x',t)\,\mathrm{d}x' = \langle \int_x^{x+\Delta x} \delta(x(t)-x')\,\mathrm{d}x' \rangle$$

Now, all trajectories that pass through $[x, x+\Delta x]$ at time t (i.e. such that $x(t) \in (x, x+\Delta x)$) *contribute* to that integral, and the others do not. So, if we take the average over the set of *all trajectories*, we find the *density* of trajectories passing through that *gate*, which is exactly $\mathbb{P}(x,t)$.
Consider now a generic function h. Its average over the trajectory is defined as:

$$\langle h(x(t)) \rangle = \int \mathrm{d}x\, \mathbb{P}(x,t) h(x)$$

Differentiating:

$$\mathrm{d}\langle h(x(t)) \rangle = \langle h(x(t+\mathrm{d}t)) - h(x(t)) \rangle = \mathrm{d}t \int \mathrm{d}x\, \dot{\mathbb{P}}(x,t) h(x)$$

We have now all the results we need to derive the Fokker-Planck equation. Start with:

$$\begin{aligned}
\mathrm{d}h &= h(x(t) + \mathrm{d}x\,(t)) - h(x(t)) = \\
&= h'((t))\,\mathrm{d}x\,(t) + \frac{1}{2} h''(x(t))(\mathrm{d}x\,(t))^2 + O((\mathrm{d}x)^3)
\end{aligned}$$

Using Langenvin:

$$\begin{aligned}
&(\mathrm{d}x\,(t))^2 = \mathrm{d}t^2\, f^2 + 2D\, \overbrace{(\mathrm{d}B)^2}_{\mathrm{d}t} + \cancel{f\sqrt{2D}\,\mathrm{d}B\,\mathrm{d}t} \\
&(\mathrm{d}x\,(t))^3 = O((\mathrm{d}t)^2)
\end{aligned}$$

Substituting back:

$$\begin{aligned}
\mathrm{d}h &= h'(f\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}B) + \frac{1}{2} h'' 2D\,\mathrm{d}t + O(\mathrm{d}t^2) = \\
&= \mathrm{d}t\,[h'f + h''D] + h'\sqrt{2D}\,\mathrm{d}B
\end{aligned}$$

$$\langle \mathrm{d}t\,(h'f + h''D) \rangle + \langle h'\sqrt{2D}\,\mathrm{d}B \rangle$$

Focus on the last term. Factorizing the average (ad D is non-anticipating...)

$$2\langle h'(x(t)) D(x(t),t)\,\mathrm{d}B(t) \rangle = 2\langle h'D \rangle \underbrace{\langle \mathrm{d}B \rangle}_{=0}$$

Thus:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle h(x(t))\rangle &= \langle h'(x(t))f(x(t),t) + h''(x(t))D(x(t),t)\rangle = \\ &= \int \mathrm{d}x\,\mathbb{P}(x,t)\left[h'(x)f(x,t) + h''(x)D(x,t)\right]\end{aligned}$$

Now:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle h(x(t))\rangle = \int \mathrm{d}x\,\dot{\mathbb{P}}(x,t)h(x)$$

We want to compare the two different expressions to get an expression for $\dot{\mathbb{P}}(x,t)$. Integrating by parts:

$$\int \mathrm{d}x\,\dot{\mathbb{P}}(x,t)h(x,t) = \mathbb{P}hf\Big|_{-\infty}^{+\infty} - \int \mathrm{d}x\,h(x)\frac{\partial}{\partial x}\left(\mathbb{P}(x,t)f(x,t)\right) + D\mathbb{P}h'\Big|_{-\infty}^{+\infty} - \int h'\frac{\partial}{\partial x}(\mathbb{P}D)\,\mathrm{d}x$$

Integrating by parts again:

$$-\int h'\frac{\partial}{\partial x}(\mathbb{P}D)\,\mathrm{d}x = -h\frac{\partial}{\partial x}(\mathbb{P}D)\Big|_{-\infty}^{+\infty} + \int h\frac{\partial^2}{\partial x^2}(\mathbb{P}D)\,\mathrm{d}x$$

$h(x,t)$ can be chosen arbitrarily, as a *test function*. We can then choose h to have a narrow peak centered on a certain x, so that all highlighted terms vanish. Then:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle h(x(t))\rangle &= \int \mathrm{d}x\,\dot{\mathbb{P}}(x,t)h(x) = \\ &= \int \mathrm{d}x\,h(x)\left[-\frac{\partial}{\partial x}(\mathbb{P}f) + \frac{\partial^2}{\partial x^2}(\mathbb{P}D)\right]\end{aligned}$$

This proves that the Langenvin equation is *equivalent* to the Fokker-Planck equation:

$$\begin{aligned}&\text{F-P} \qquad \dot{\mathbb{P}}(x,t) = -\frac{\partial}{\partial x}\left[f(x,t)\mathbb{P}(x,t) - \frac{\partial}{\partial x}\left(\mathbb{P}(x,t)D(x,t)\right)\right] \\ &\text{L} \qquad \mathrm{d}x\,(t) = \mathrm{d}t\,f(x(t),t) + \sqrt{2D(x(t),t)}\,\mathrm{d}B(t)\end{aligned}$$

0.3 The role of temperature

Recall the definition of $f(x,t)$:

$$f(x,t) = \frac{F_{\text{ext}}}{\gamma}; \qquad \gamma = 6\pi a\eta; \qquad F_{\text{ext}}(x) = -\frac{\partial V}{\partial x}(x)$$

Assuming D independent of x:

$$\dot{\mathbb{P}}(x,t) = \frac{\partial}{\partial x}\left[\frac{1}{\gamma}\frac{\partial V}{\partial x}\cdot\mathbb{P} + D\frac{\partial\mathbb{P}}{\partial x}\right]$$

We expect that a particle will reach, after some time, an equilibrium described by the Maxwell-Boltzmann distribution:

$$\mathbb{P}(x,t) \xrightarrow[t\to\infty]{} P_{\text{eq}}(x) = \frac{e^{-\beta V(x)}}{z} \qquad z = \int \mathrm{d}x\, e^{-\beta V(x)}; \qquad \beta = \frac{1}{k_B T}$$

At equilibrium, $\dot{\mathbb{P}} = 0$ (stationary solution):

$$\frac{\partial}{\partial x}\left[\frac{1}{\gamma}\mathbb{P}^* + D\frac{\partial}{\partial x}\mathbb{P}^*\right] = 0$$

We would like that $\mathbb{P}^* = \mathbb{P}_{\text{eq}}$. We then ask: how many stationary solution are there? If there is only one, does it coincide always with $\mathbb{P}_{\text{eq}}$?

Note that the terms in the parenthesis must be constant:

$$\Rightarrow [\dots] = \text{constant}$$

We assume that $\mathbb{P}^*$ vanishes at infinity (as it is normalized), and also its first derivative:

$$\mathbb{P}^*, \frac{\partial}{\partial x}\mathbb{P}^* \xrightarrow[x\to\infty]{} 0$$

Then $[\dots]$ must be 0:

$$\frac{\partial}{\partial x}\mathbb{P}^* = -\frac{1}{\gamma D}\frac{\partial V}{\partial x}\mathbb{P}^*$$

Dividing both sides by $\mathbb{P}^*$ and integrating:

$$\frac{\partial}{\partial x}\ln \mathbb{P}^*(x) = -\frac{1}{\gamma D}\frac{\partial V}{\partial x} \Rightarrow \ln \mathbb{P}^*(x) = -\frac{1}{\gamma D}V(x) + \text{const}$$

Exponentiating:

$$\mathbb{P}^*(x) = \exp\left(-\frac{1}{\gamma D}V(x)\right)\cdot K$$

Comparing to the Maxwell-Boltzmann distribution:

$$\frac{1}{\gamma D} = \beta \Rightarrow \gamma D = k_B T \Rightarrow D = \frac{k_B T}{6\pi\eta a}$$

This is the Einstein relation (*fluctuation-dissipation relationship*), found in 1905. As $D(x,t) \propto T$, the amplitude of stochastic oscillations in the Langenvin eq. is proportional to $\sqrt{T}$.

However, are we sure that this is true *for every initial condition*?