0.1 Continuous Diffusion

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We see now how to compute transition probabilities $W(x, t|x_0, 0)$ using the path integral formalism and some powerful variational techniques.
Consider a 1D harmonic oscillator, $\mathrm{d}x = -kx\,\mathrm{d}\tau$, in the *overdamped limit*, meaning with an extra term $\sqrt{2D}\,\mathrm{d}B$. Recall that $k = m\omega^2/\gamma$, and $F = -m\omega^2 x$. Then:

$$W(x, t|x_0, 0) = \int \prod_{\tau=0}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi D\,\mathrm{d}\tau}} \exp\left(-\frac{1}{4D}\int_0^t \mathrm{d}\tau\,(\dot{x}(\tau) + kx)^2\right)\delta(x(t) - x)$$

Previously, we computed this integral by evaluating:

$$\langle \exp\left(\frac{k^2}{4D}\int x^2(\tau)\,\mathrm{d}\tau\right)\delta(x(t) - x)\rangle_W$$

But now we use variational methods, so that:

$$W(x, t|x_0, 0) = \phi(t)\exp\left(-\frac{1}{4D}\operatorname{Stat}\int_0^t (\dot{x}(\tau) + kx(\tau))^2\,\mathrm{d}\tau\right)$$

where the Stat term evaluates to the integral computed at the stationary point x_c:

$$\int_0^t (\dot{x}_c(\tau) + kx_c(\tau))^2\,\mathrm{d}\tau$$

We can compute this in the *Lagrangian* formalism, by defining the action S:

$$S = \int_0^t L(\dot{x}, x)\,\mathrm{d}\tau \qquad L(\dot{x}, x) = (\dot{x} + kx)^2$$

Then the Lagrangian equations are:

$$x_c\colon 0 \overset{!}{=} \frac{\partial L}{\partial x}\Big|_{x_c} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}}\Big|_{x_c} = 2k(\dot{x}_c + kx_c) - 2(\ddot{x}_c + k\dot{x}_c) = 2(k^2 x_c - \ddot{x}_c)$$

as:

$$\frac{\partial L}{\partial x} = 2k(\dot{x} + kx)$$
$$\frac{\partial L}{\partial \dot{x}} = 2(\dot{x} + kx)$$

Then, by rearranging, we find the equation of motion:

$$\ddot{x}_c = k^2 x_c$$

with the boundary conditions $x_c(0) = x_0$ and $x_c(t) = x$ (the two extrema of the path).
Note that the classical equation of motion, in absence of friction and thermal noise, is just:

$$m\ddot{x} = -m\omega^2 x \Rightarrow \ddot{x} = -\omega^2 x$$

Here the solution is an *oscillating function*, i.e. $x(t) = A\sin(\omega t + \varphi)$, which is very different from that of $\ddot{x}_c = k^2 x_c$. This last one is solved by a linear combination of exponentials:

$$x_c(\tau) = Ae^{k\tau} + Be^{-k\tau}$$

Imposing the boundary conditions, we find:

$$\begin{aligned} x_0 &\overset{!}{=} A + B \\ x &\overset{!}{=} Ae^{kt} + Be^{-kt} \end{aligned}$$

which is a set of two equations in two unknowns, with solution:

$$A = \frac{x - x_0 e^{-kt}}{2\sinh(kt)}; \qquad B = -\frac{(x - x_0 e^{kt})}{2\sinh(kt)}$$

Then:

$$\dot{x}_c = k(Ae^{kt} - Be^{-kt}) \quad x_c(\tau) = Ae^{k\tau} + Be^{-k\tau}$$

and we can plug these into the integral:

$$\int_0^t (\dot{x}_c(\tau) + kx_c(\tau))^2 \, \mathrm{d}\tau$$

leading to the solution:

$$\begin{aligned} W(x,t|x_0,0) &= \int \prod_{\tau=0}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi D \, \mathrm{d}\tau}} \exp\left(-\frac{1}{4D}\int_0^t \mathrm{d}\tau \, (\dot{x}(\tau) + kx)^2\right) \delta(x(t) - x) = \\ &= \Phi(t) \exp\left(-\frac{k}{2D}\frac{(x - x_0 e^{-kt})^2}{(1 - e^{-2kt})}\right) \end{aligned}$$

We can also evaluate the more general $W(x,t|x_0,t_0)$ just by substituting $t \to t - t_0$. $\Phi(t)$ is just the normalization constant, which is computed by:

$$1 \overset{!}{=} \mathrm{d}x \, W(x,t|x_0,0) = \Phi(t)\sqrt{\frac{2\pi D}{k}(1 - e^{-2kt})}$$

In the limit $t \to \infty$ the transition probability becomes:

$$W(x,t|x_0,0) = \sqrt{\frac{k}{2\pi D}} \underbrace{\exp\left(-\frac{k}{2D}x^2\right)}_{e^{-\beta U(x)}}$$

as:

$$\frac{k}{2D} = \beta\frac{m\omega^2}{2} \quad U(x) = \frac{m\omega^2}{2}x^2$$

Consider now the general case (not the overdamped limit):

$$\begin{aligned} \mathrm{d}x\,(\tau) &= v(\tau)\,\mathrm{d}\tau \\ \mathrm{d}v\,(\tau) &= -\frac{\gamma}{m}v(\tau)\,\mathrm{d}\tau + \frac{\gamma\sqrt{2D}}{m}\,\mathrm{d}B \end{aligned}$$

Recall in fact that in the overdamped limit we consider $\gamma/m \to \infty$, leading to $\mathrm{d}x\,(\tau) = \sqrt{2D}\,\mathrm{d}B$, which is similar to the expression we obtained for Brownian motion.
In principle we could consider:

$$\begin{cases} \mathrm{d}x\,(\tau) = v(\tau)\,\mathrm{d}\tau + 2\hat{D}\sqrt{\mathrm{d}\hat{B}} \\ \mathrm{d}v\,(\tau) = -\frac{\gamma}{m}v(\tau)\,\mathrm{d}\tau + \frac{\gamma\sqrt{2D}}{m}\,\mathrm{d}B \end{cases}$$

with B and $\hat{B}$ being two *independent* random motions, so that:

$$\mathrm{d}P\,(\Delta B_1, \Delta\hat{B}_1, \dots, \Delta B_N, \Delta\hat{B}_N) = \prod_{i=1}^{N} \frac{\mathrm{d}B_i}{\sqrt{4\pi\Delta t_i}}\frac{\mathrm{d}\hat{B}_i}{\sqrt{4\pi\Delta t_i}} \exp\left(-\frac{1}{2}\sum_i \frac{\Delta B_i^2}{\Delta t_i} - \frac{1}{2}\sum_i \frac{\Delta\hat{B}_i^2}{\Delta t_i}\right)$$

In the continuum limit:

$$\mathrm{d}P\,(\{x,v\}) = \prod_{\tau=0}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi\hat{D}\,\mathrm{d}\tau}}\frac{\mathrm{d}v(\tau)}{4\pi D\gamma^2/m^2} \exp\left(-\frac{m^2}{4D\gamma^2}\int_0^t \mathrm{d}\tau\,\left(\dot{v}(\tau) + \frac{\gamma}{m}v(\tau)\right)^2 - \frac{1}{4\hat{D}}\int_0^t \mathrm{d}\tau\,(\dot{x}(\tau) - v(\tau))^2\right)$$

In the limit $\hat{D} \to 0$:

$$\prod_i \mathrm{d}\Delta x_i\,\delta\left(\frac{\Delta x_i}{\Delta t_i} - v_i\right) \to \prod_\tau \mathrm{d}x\,(\tau)\delta(\dot{x}(\tau) - v(\tau))$$

leading to:

$$\prod_i \frac{\mathrm{d}\Delta x_i}{\sqrt{4\pi\hat{D}\Delta t_i}} \exp\left(-\frac{1}{4\hat{D}}\left[\frac{\Delta x_i}{\Delta t_i} - v_i\right]\right)^2$$

and

$$\mathrm{d}x = v\,\mathrm{d}\tau + \sqrt{2\hat{D}}\,\mathrm{d}\hat{B} \Rightarrow \frac{(\mathrm{d}\hat{B})^2}{\mathrm{d}\tau} = \frac{(\mathrm{d}x - v\,\mathrm{d}\tau)^2}{\sqrt{2\hat{D}}\,\mathrm{d}\tau}$$

So we have:

warning! accuracy not 100%

$$\begin{aligned} \mathrm{d}P\,(\{x,v\}) = \left(\prod_{\tau=0^+}^{k} \mathrm{d}x\,(\tau)\right) \prod_{\tau=0^+}^{t} \frac{\mathrm{d}v\,(\tau)}{\sqrt{4\pi D\,\mathrm{d}\tau}} \exp\left(-\frac{m^2}{4D\gamma^2}\int_0^t \mathrm{d}\tau\,(\dot{v} + \frac{\gamma}{m}v)^2\right)\cdot \\ \cdot\left(\prod_\tau \delta(\dot{x}(\tau) - v(\tau))\delta(x(t) - x_0 - \int_0^t v(\tau)\,\mathrm{d}\tau)\right) \end{aligned}$$

$$\int \mathrm{d}P\left(\{x,v\}\right)\delta(x(t)-x)\delta(v(t)-v) = W(x,v,t|x_0,v_0,0) =$$

$$= \int \prod_{\tau=0^+}^{t} \frac{\mathrm{d}v\left(\tau\right)}{\sqrt{4\pi D\,\mathrm{d}\tau\,\gamma/m^2}} \exp\left(-\frac{m^2}{4D\gamma}\int_0^t \left(\dot{v}+\frac{\gamma}{m}v\right)^2 \mathrm{d}\tau\right)\delta(v(t)-v)\,\delta\left(x-x_0-\int_0^t v(\tau)\,\mathrm{d}\tau\right) =$$

$$= \Phi(t)\exp\left(-\frac{m^2}{4D\gamma}\int_0^t (\dot{v}_c(\tau)+\frac{\gamma v_c(\tau)}{m})^2\,\mathrm{d}\tau\right)$$

To stationarize the exponential, we need to impose the constraint:

$$x-x_0 = \int_0^t v(\tau)\,\mathrm{d}\tau$$

Recall that if we want to find the stationary points of $F(z_1,\ldots,z_k)$ on the manifold (= subjected to the constraints) $\Phi(z_1,\ldots,z_k)$, we use the Lagrange multipliers:

$$\frac{\partial}{\partial z_i}(F(z_1,\ldots,z_k)+\lambda\Phi(z_1,\ldots,z_k)) = 0$$

We find all the coordinates as functions of λ ($z_i(\lambda)$) and then search the λ^* such that:

$$\Phi(z_1(\lambda^*),\ldots,z_k(\lambda^*)) = 0$$

In our case:

$$\int_0^t \left(\dot{v}+\frac{\gamma}{m}v\right)^2 \mathrm{d}\tau \qquad (\leftarrow F)$$

$$\int_0^t v(\tau)\,\mathrm{d}\tau - (x-x_0) = 0 \qquad (\leftarrow \Phi)$$

leading to:

$$\int_0^t \left(\dot{v}+\frac{\gamma}{m}v\right)^2 \mathrm{d}\tau + \lambda\left[\int_0^t v(\tau)\,\mathrm{d}\tau-(x-x_0)\right]$$

$$\int_0^t \underbrace{\left[\left(\dot{v}+\frac{\gamma}{m}v\right)^2+\lambda v(\tau)\right]}_{L(v,\dot{v})}\mathrm{d}\tau - \lambda(x-x_0)$$

Finding the Euler-Lagrange equation for the second one:

$$0 = \left(\frac{\partial L}{\partial v}-\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{v}}\right)\Big|_{v=v_0} = \lambda + 2\left(\frac{\gamma}{m}\right)^2 v_c - 2\ddot{v}_c = 0 \Rightarrow \ddot{v}_c = \left(\frac{\gamma}{m}\right)^2 v_c + \lambda$$

The homogeneous solution is again a combination of exponentials:

$$v_c(\tau) = A\exp\left(-\frac{\gamma}{m}\tau\right) + B\exp\left(\frac{\gamma}{m}\tau\right)$$

and then we add an inhomogeneous term $+\lambda(m/\gamma)^2$, so that we have 3 parameters, with 3 constraints :

$$v_c(0) = v_0 \qquad v_c(t) = v \qquad \int_0^t v(\tau)\,\mathrm{d}\tau = (x-x_0)$$

The highlighted part comes from:

$$\int \mathrm{d}x_1 \dots \mathrm{d}x_N \, \delta(x_1 - x_0 - v_0\Delta t_1)\delta(x_2 - x_1 - v_1\Delta t_2)\dots\delta(\overbrace{x_N}^{x} - x_{N-1} - v_{N-1}\Delta t_N)\delta(x_N - x) =$$
$$= \int \mathrm{d}x_2 \dots \mathrm{d}x_N \, \delta(x_2 - x_0 - (v_0\Delta t_1 + v_1\Delta t_2))\delta(x_3 - x_2 - \Delta t_3 v_2)\dots =$$
$$= \int \mathrm{d}x_N \, \delta(x_N - x_0 - \sum_i \Delta t_i v_{i-1})\delta(x_N - x)$$

0.2 Another problem

Consider a particle in a potential $U(x)$ that goes to 0 at infinity, and has a local minimum separated by a *barrier*. If the energy is sufficiently low, the particle can become *trapped* inside this minimum. However, in the presence of thermal noise, there is a possibility of escape.
Before solving this problem, we focus on a simpler case: that of a particle confined in an interval $[a, b]$:

$$\mathrm{d}x = \frac{F}{\gamma} + \sqrt{2D}\,\mathrm{d}B \qquad F = -U'$$

so that the Fokker-Planck equation becomes:

$$\dot{p}(x, t|x_0, t_0) = \partial_x[U'P + D\partial_x P]$$

Suppose that the boundary conditions are *reflecting* in a and *absorbing* in b.
Expanding the notation:

$$\dot{p}(x, t|x_0, t_0) = \partial_x \underbrace{[-A(x)p(x, t|x_0, t_0) + \partial_x(D(x)p(x, t|x_0, t_0))]}_{-J(x,t)}$$

with:

$$D(x) \equiv D = \frac{k_B T}{\gamma} \qquad A(x) = -U'(x)$$

In a, the *reflecting* boundary condition means that:

$$J(a, t) = 0 \qquad \forall t$$

as the *inward* flux and *outward* one are the same, and so their sum is 0.
In b, however, the *absorbing* boundary condition means that the probability to find the particle here is exactly 0:

$$p(b, t|x_0, t_0) = 0$$

The *survival probability*, i.e. the probability of the particle still being inside the interval $[a, b]$ is:

$$p_{\text{surv}}(t, x_0) = \int p(x, t|x_0, t_0)\,\mathrm{d}x$$

which is generally not 1, as the boundary in b leads to a *violation* of the probability conservation (as here the particle "disappears"). Note, in fact, that $p(b,t|x_0,t_0) = 0$ does not mean that the flux here is null:

$$\begin{aligned} J(b,t) &= \cancel{A(b)p(b,t|x_0,t_0)} - \partial_x(D(x)p(x,t|x_0,t_0)) = \\ &= \cancel{-(\partial_x D)p(b,t|x_0,t_0)} - D(b)\partial_x p(x,t|x_0,t_0)|_{x=b} \neq 0 \end{aligned}$$

We define $T(x)$ as being the *lifetime* of the particle, i.e. the instant when the particle reaches b for the first time. Then:

$$p_{\text{surv}}(t,x_0) = \mathbb{P}(T(x_0) > t)$$

That is, the survival probability is the probability that the particle *has not yet reached* b during the time interval $[0,t]$.
Consider now the *forward* F-P equation:

$$\partial_t p(x,t|x_0,t_0) = \partial_x[-A(x)p(x,t|x_0,t_0) + \partial_x(D(x)p(x,t|x_0,t_0))]$$

while the *backward* F-P equation is:

$$\partial_{t_0} p(x,t|x_0,t_0) = -A(x_0)\partial_{x_0} p(x,t|x_0,t_0) - D(x_0)\partial^2_{x_0} p(x,t|x_0,t_0)$$

as here we are deriving wrt the *initial coordinates*.
We can derive it from the ESCK relation:

$$\int \mathrm{d}x'\, p(x,t|x',t')p(x',t'|x_0,t_0) = p(x,t|x_0,t_0) \quad \forall t' \in (t,t_0)$$

If we differentiate both sides wrt t' we get 0, as $p(x,t|x_0,t_0)$ does not depend on t'. So:

$$0 = \int_a^b \mathrm{d}x'\, [\partial_{t'} p(x,t|x',t') \cdot p(x',t'|x_0,t_0) + p(x,t|x',t')\, \partial_{t'} p(x',t'|x_0,t_0)\,]$$

We then apply the forward F-P equation to the highlighted term, and then integrate by parts, forgetting the boundary conditions, we arrive at:

$$= \int_a^b \mathrm{d}x'\, [\partial_{t'} p(x,t|x',t') + A(x')\partial_{x'} p(x,t|x',t') + D(x')\partial^2_{x'} p(x,t|x',t')]p(x',t'|x_0,t_0) + \text{Boundary terms}$$

Considering now the limit $t' \to 0$, $p(x',t'|x_0,t_0) = \delta(x'-x_0)$, and so the integral can be computed, leading to the *backward* F-P.
Returning to our case, if A and D are time independent, we have:

$$p(x,t|x_0,t_0) = p(x,t-t_0|x_0,0)$$

Differentiating:

$$\partial_{t_0} p(x,t|x_0,t_0) = -\partial_t p(x,t-t_0|x_0,0)$$

Substituting in the backwards F-P:

$$-\partial_t p(x,t|x_0,t_0) = -A(x_0)\partial_{x_0} p(x,t|x_0,t_0) - D(x_0)\partial^2_{x_0} p(x,t|x_0,t_0)$$

One boundary condition is just:

$$p(x,t|x_0,t_0)\Big|_{x_0=b} = 0 \quad \forall t, t_0$$

meaning that if the particle *starts* at the absorbing boundary, it immediately disappears. However, it is not obvious that the other boundary condition is:

$$\partial_{x_0} p(x,t|x_0,t_0)\Big|_{x_0=a} = 0$$

and we will prove it during the next lecture.