Functional integral methods

Fokker-Planck gives us $P(x,t)$.
But what if we want to know the probability of a whole trajectory $P[x(t)]$?

$\dot{x} = f(x) + \xi(t)$

We know $P[\xi]$, want to know $P[x]$!

Simple example: Suppose we have a stochastic variable X with probability density $P_X(X)$, and $Y = f(X)$.
What is $P_Y(Y)$? $\quad P_X(X)\,dX = P_Y(Y)\,dY$!

$$P_Y(Y) = \int dX\, P_X(X)\, \delta(Y - f(X)) = \{\text{change integration variable}\} =$$
$$= \int dY \frac{dX}{dY} P_X(X(Y))\, \delta(Y - f(X)) = P_X(f^{-1}(Y)) \frac{dX}{dY}.$$ Now generalize!

$P[\xi]$? ξ Gaussian white noise: But $\langle \xi^2(t) \rangle = 2B\,\delta(0)$ undefined!

Obtain $P[\xi]$ as the continuum limit of a discrete process:

$$P(\xi_i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\xi_i^2}{2\sigma^2}}$$

$$P(\xi_1, \xi_2, \ldots, \xi_N) = \prod_{i=1}^{N} P(\xi_i) \sim e^{-\frac{1}{2\sigma^2} \sum_{i=1}^{N} \xi_i^2 \frac{\Delta t}{\Delta t}}$$

Take limit $\Delta t \to 0$, $N \to \infty$, $N\Delta t = t$, $\sigma^2 \Delta t = \text{const} = 2D$

$$\Rightarrow P[\xi(t)] \sim e^{-\frac{1}{4D}\int_0^t \xi^2(t)\,dt}$$

To calculate an average of some $f[\zeta]$:

$$\langle f[\zeta] \rangle = \int f[\zeta]\, e^{-\frac{1}{4D}\int \zeta^2(t)\,dt}\, [d\zeta]$$

Functional integral or Path integral

where $[d\zeta] = \lim_{N\to\infty} \prod_{i=1}^{N} \left(\frac{d\zeta_i}{\sqrt{2\pi\sigma_N^2}} \right)$

Generalizing the recipe above we write

$$P[X(t)] = \int [d\zeta]\, e^{-\frac{1}{4D}\int \zeta^2(t)\,dt}\, \delta[X - X_{sol}]$$

solution of Langevin eq.

Functional δ-function $= \lim_{N\to\infty} \prod_{i=1}^{N} \delta(x_i - x_{i,sol})$

Now change variables in the $\delta[\,]$ functional from x to ζ:

$$\delta[X - X_{sol}] = \delta[\dot{x} - f(x) - \zeta(t)]\, J(x)$$

The δ-functional enforces x to solve the Langevin eq.

~~$J(x)$ = the Jacobian of the transformation~~

$$= \left| \frac{\delta(\dot{x} - f(x) - \zeta(t))}{\delta(x(t'))} \right| = \left| \det(\partial_t - f'(x)) \right|$$

More about this later

$$P[x(t)] = \int [d\zeta]\, e^{-\frac{1}{4D}\int \zeta^2(t)\,dt}\, \delta[\dot{x} - f(x) - \zeta(t)]\, J(x) =$$

$$= C\, e^{-\frac{1}{4D}\int (\dot{x} - f(x))^2\,dt}\, J(x) = C\, e^{-S[x]}\, J(x)$$

S = Onsager-Machlup functional

Can use this to calculate averages, e.g.,

$$\langle x(t_1)\, x(t_2) \cdots x(t_n)\rangle = \int [dx]\, e^{-S[x]}\, x(t_1)\cdots x(t_n)\, J[x]$$

Define a generating functional

$$Z[\eta] = \int [dx]\, e^{-S + \int \eta(t)\, x(t)\, dt}\, J[x]$$

We now have a formulation of the problem which resembles the Feynman path integral in quantum mechanics. Can use the full machinery of quantum field theory.

Alternative form:

Use the generalizations of $\delta(x) = \int_{-\infty}^{\infty} d\tilde{x}\, e^{+i\tilde{x}x}$

and $\int_{-\infty}^{\infty} e^{-\frac{a}{2}x^2 + ibx}\, dx = \sqrt{\frac{2\pi}{a}}\, e^{-\frac{1}{2a}b^2}$

$$P[x] = \int [d\zeta][d\tilde{x}]\, e^{-\frac{1}{4D}\int \zeta^2(t)\, dt + i\int \tilde{x}(t)(\dot{x} - f(x) - \zeta(t))\, dt}\, J$$

$$= \int [d\tilde{x}]\, e^{-\int D\tilde{x}^2 - i\tilde{x}(\dot{x} - f(x))\, dt}\, J(x)$$

Carrying out the $[d\tilde{x}]$ integral gives back the first form

Compare these with the Feynman path integral

$$\int [dx]\, e^{iS} = \int [dx]\, e^{i\int \left(\frac{m\dot{x}^2}{2} - U(x)\right)dt}$$

$$= \int [dx][dp]\, e^{i\int \left(p\dot{x} - \frac{p^2}{2m} - U\right)dt}$$

What about the Jacobian?

$$J(x) = \left| \det\left(\partial_t - f'\right) \right|$$

The value depends on how the Langevin equation is discretized.

$$\dot{x} = f(x) + \xi$$

Ito: $$\frac{x(t+\tau) - x(t)}{\tau} = f(x(t)) + \xi_\tau(t)$$

Stratonovich: $$\frac{x(t+\tau) - x(t)}{\tau} = \frac{f(x(t+\tau)) + f(x(t))}{2} + \xi_\tau(t)$$

Both are ok if used consistently.

Ito:

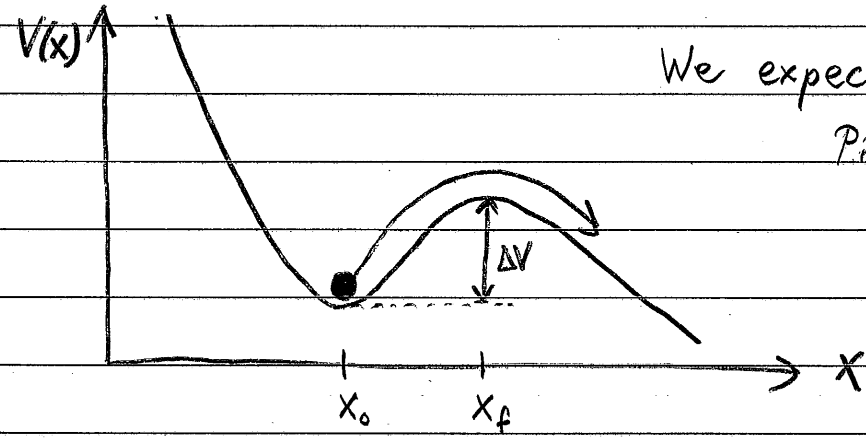
$$J(x) = \begin{vmatrix} \frac{1}{\tau} & -f' - \frac{1}{\tau} & 0 & \cdots \\ & \frac{1}{\tau} & -f' - \frac{1}{\tau} & \\ 0 & & \frac{1}{\tau} & \ddots \\ & & & \ddots \end{vmatrix} = \frac{1}{\tau^N} = \text{unimportant constant!}$$

Stratonovich: $$J(x) = \begin{vmatrix} \frac{1}{\tau} - \frac{1}{2}f' & -\frac{1}{\tau} - \frac{1}{2}f' & \\ & \ddots & \ddots \\ 0 & & \ddots \end{vmatrix} = \prod_{i=1}^{N} \left(\frac{1}{\tau} - \frac{1}{2}f'\right) =$$

$$= \frac{1}{\tau^N} e^{-\sum_i \frac{\tau}{2} f'} = \rightarrow \frac{1}{\tau^N} e^{-\int \frac{1}{2} f' dt}$$

Ex **Escape from a potential well**

Consider a Brownian particle trapped in a local minimum. What is the escape time?



We expect Arrhenius law

$$\text{Prob (escape)} \sim e^{-\frac{\Delta V}{kT}}$$

Strong friction limit $\Rightarrow$ overdamped dynamics

$$\gamma \dot{x} = F(x) + R(t), \qquad F = -\nabla V = -V'(x)$$

$$\dot{x} = \Gamma F(x) + J(t), \qquad \langle J(t) J(t') \rangle = 2D\, \delta(t-t')$$

$$D = \Gamma k T, \qquad \Gamma = 1/\gamma$$

"Action"

$$S = \int dt \, \frac{1}{4D} \left(\dot{x} - \Gamma F(x) \right)^2$$

$$P[x(t)]\,[dx] = e^{-S[x]}\,[dx] = \text{Prob of path } x(t)$$

Prob of escape $= P(x_f, t \,|\, x_0\, t_0) =$

$$= \int_{x(t_0)=x_0}^{x(t_f)=x_f} [dx]\, e^{-S[x]}$$

In general a very difficult integral!

We will use a saddle point approximation:

$$S[x] \approx S[x_{cl}] + \frac{1}{2}\iint dt\,dt'\,\delta x(t) A(t,t')\,\delta x(t') + \dots$$

x_{cl} minimizes S and $\delta x = x - x_{cl}$

$$P(x_f,t_f\,|\,x_0,t_0) \propto \underbrace{e^{-S[x_{cl}]}}_{\text{main contribution}} \underbrace{\int [d\delta x]\, e^{-\frac{1}{2}\int \delta x A \delta x}}_{\text{ignore for now}}$$

We expect this approximation to be fine when fluctuations are relatively small, i.e., at low T.

Minimize S:

$$S = \int \frac{1}{4D}\left(\dot{x}^2 + \Gamma^2F^2 - 2\Gamma F\dot{x}\right) dt$$

Start with last term: $-\int \frac{\Gamma}{2D} F(x)\,\dot{x}\,dt = \frac{\Gamma}{2D}\int_{t_0}^{t_f} \frac{dV}{dx}\frac{dx}{dt}\,dt =$

$$= \{D = \Gamma kT\} = \frac{1}{2kT}\left(V(x_f) - V(x_0)\right) = \underline{\frac{\Delta V}{2kT}}$$

$$\delta S_0 = \delta \int \frac{1}{4D}\left(\dot{x}^2 + \Gamma^2F^2\right) = 0 =$$

$$= \int \frac{1}{2D}\left(\dot{x}\,\delta\dot{x} + \Gamma^2 F F'\delta x\right) \underset{\text{partial int.}}{=} \int \frac{1}{2D}\underbrace{\left(-\ddot{x} + \Gamma^2 F F'\right)}_{=0}\delta x$$

$\ddot{x} = \Gamma^2 F F'$ Euler-Lagrange eq.

Multiply by $\dot{x}$ $\Rightarrow$

$$\Rightarrow \quad \ddot{x}\,\dot{x} = \Gamma^2 F(x) \frac{dF}{dx} \dot{x}$$

$$\frac{d}{dt}\left(\frac{\dot{x}^2}{2}\right) = \Gamma^2 \frac{d}{dt}\left(F^2\right)$$

$$\dot{x}^2 = \Gamma^2 F^2 + C$$

Fix using boundary conditions

Assume we start at the minimum of the potential $V(x)$

$\Rightarrow \quad F(x_0) = 0$ with zero velocity $\dot{x}(t_0) = 0 \Rightarrow C = 0$

$$\Rightarrow \quad \dot{x} = \pm \Gamma F$$

Which sign should we choose?

We want to go from the minimum to the maximum, i.e., against the force $\Rightarrow$ Choose $-$!

$$S_0 = \int dt \frac{1}{4D}\left(\underbrace{\dot{x}^2 + \Gamma^2 F^2}_{=}\right) = \int \frac{1}{2D}\left(\dot{x}^2\right) dt =$$

$$= \int_{t_0}^{t_f} \frac{1}{2D}\left(\underset{(+)}{-}\Gamma F\right)\dot{x} = \int \frac{\Gamma}{2D}\left(\underset{(-)}{+}\frac{dV}{dx}\right)\dot{x}\,dt = \underset{(-)}{+}\frac{\Delta V}{2kT}$$

$$S_{tot} = \frac{\Delta V}{2kT} \underset{(-)}{+} \frac{\Delta V}{2kT} = \frac{\Delta V}{kT}$$

$\Rightarrow$ Arrhenius law: Escape rate $\sim e^{-\frac{\Delta V}{kT}}$

Note: There may be simpler ways to get this!?