

Considering a simpler Langevin dynamics under the following equations

$$\begin{cases} \dot{x} &= v \\ \dot{v} &= \frac{F(x)}{m} - \gamma v + \frac{\xi(t)}{m} \end{cases}$$

where (x, v) are position and velocity. $F(x) = -\partial_x U(x)$ which is the position-dependent force. The m, γ are mass and friction coefficient. The $\xi(t)$ represents randomness defines the Wiener noise in the Ito convention:

$$\langle \xi(t)\xi(t') \rangle = \frac{2m\gamma}{\beta} \langle dW_t dW_{t'} \rangle = \frac{2m\gamma}{\beta} \delta(t - t')$$

This equation describes a dynamics equivalent to an evolution of probability density $f(x, v; t)$ through Fokker-Planck equation:

$$\frac{\partial f(x, v; t)}{\partial t} = -\hat{L}f(x, v; t)$$

where

$$\hat{L} \equiv \frac{F(x)}{m} \frac{\partial}{\partial v} + v \frac{\partial}{\partial x} - \gamma \left(\frac{\partial}{\partial v} v + \frac{1}{m\beta} \frac{\partial^2}{\partial v^2} \right)$$

The probability density f evolves through

$$f(x, v, t + \Delta t) = e^{-\Delta t \hat{L}} f(x, v; t)$$

The operator \hat{L} is separated into three parts, and the iteration is approximated through Lie-Trotter formula,

$$\begin{aligned} e^{-\Delta t \hat{L}} &\approx e^{-\Delta t \hat{L}_x} e^{-\Delta t \hat{L}_v} e^{-\Delta t \hat{L}_\gamma} \\ &\approx e^{-(\Delta t/2) \hat{L}_\gamma} e^{-(\Delta t/2) \hat{L}_v} e^{-(\Delta t/2) \hat{L}_x} e^{-(\Delta t/2) \hat{L}_v} e^{-(\Delta t/2) \hat{L}_\gamma} \end{aligned}$$

where

$$\begin{aligned} \hat{L}_x &= v \frac{\partial}{\partial x} \\ \hat{L}_v &= \frac{F(x)}{m} \frac{\partial}{\partial v} \\ \hat{L}_\gamma &= -\gamma \left(\frac{\partial}{\partial v} v + \frac{1}{m\beta} \frac{\partial^2}{\partial v^2} \right) \end{aligned}$$

The integration can then be taken into two parts.

I. \hat{L}_γ - Diffusion in momentum space

This first part is a diffusion in momentum space

$$f(v^+ \equiv v(t^+), t^+) = e^{-(\Delta t/2) \hat{L}_\gamma} f(v, t)$$

which corresponds to the evolution of f

$$\frac{\partial f}{\partial t} = -\frac{\hat{L}_\gamma}{2} f = \frac{\gamma}{2} \left[\frac{\partial}{\partial v} (vf) + \frac{1}{m\beta} \frac{\partial^2 f}{\partial v^2} \right]$$

which has a solution [“The Fokker-Planck Equation Second Edition”, H. Risken] of

$$f(v^+, t^+ | v, t) \propto \exp \left[-\frac{m\beta}{2} \frac{(v^+ - ve^{-\frac{\gamma}{2}\Delta t})^2}{1 - e^{-\gamma\Delta t}} \right] = \exp \left[-\frac{1}{2} \left(\frac{v^+ - \mu_v}{\sigma_v} \right)^2 \right]$$

This step can then be performed by sampling from a Normal distribution $N(\mu_v, \sigma_v)$,

$$\begin{aligned} v(t^+) &\sim N(\mu_v, \sigma_v) \\ &= \mu_v + \sigma_v N(0, 1) \\ &= v(t) e^{-\frac{\gamma}{2}\Delta t} + \sqrt{\frac{1}{m\beta} (1 - e^{-\gamma\Delta t})} N(0, 1) \\ &= c_1 v(t) + c_2 N(0, 1) \end{aligned}$$

I. (\hat{L}_x, \hat{L}_v) - Deterministic canonical transformation in phase space

Both \hat{L}_v and \hat{L}_x are deterministic canonical transformation in phase space. Applying $f(v', t') = f(v(t + \Delta t), t + \Delta t) = e^{-(\Delta t/2)\hat{L}_v} f(v(t), t)$, and observing that by doing the transformation $p = t + \frac{F(x)}{2m}v$ and $q = \frac{F(x)}{2m}t - v$, we have

$$\frac{\partial f}{\partial t} + \frac{F(x)}{2m} \frac{\partial f}{\partial v} = \left[1 + \left(\frac{F(x)}{2m} \right)^2 \right] \frac{\partial f}{\partial p} \Big|_q = 0$$

The solution is then $f(v, t) = f(q) = f(\frac{F(x)}{2m}t - v)$. With the boundary condition $v(0) = v$, the solution must be a delta function

$$f(v, t) = f\left(\frac{F(x)}{2m}t - v\right) = \delta\left(\frac{F(x)}{2m}t - v\right)$$

$$\Delta v = \frac{F(x)}{2m} \Delta t$$

Similarly, the operation of \hat{L}_x during $\Delta t/2$ is equivalent to $\Delta x = v(\Delta t/2)$.