Brief survey of stoch. equations

in the overdamped limit for the position

$$\dot{x} = \frac{1}{M\gamma}[\underbrace{F(x)}_{\substack{\text{ext}\\\text{force}}} + \underbrace{\xi}_{\text{noise}}]$$

$\boxed{\begin{array}{l}\text{Gardiner Handbook of Stoch process}\\ \text{Risken The Fokker-Planck eq}\end{array}}$

$$\langle \xi(t) \rangle = 0 \qquad \langle \xi(t)\,\xi(t')\rangle = \frac{2M\gamma}{\beta}\delta(t-t')$$

ϵ

we can define a scaled "noise" term $\eta(t)$ such that

$$\dot{x} = \frac{1}{M\gamma}F(x) + \sqrt{\epsilon}\,\eta(t) \qquad \text{here} \qquad \frac{1}{M\gamma}\xi = \sqrt{\epsilon}\,\eta$$

correlation

where

$$\langle \eta(t)\,\eta(t')\rangle = \delta(t-t') \qquad \frac{1}{M^2\gamma^2}\frac{2M\gamma}{\beta}\delta(t-t') = \epsilon\,\delta(t-t')$$

$$\boxed{\epsilon = \frac{2}{M\gamma\beta}} \sim \text{position}$$

in the Langevin eq for momenta the Ornstein-Uhlenbeck process is the solution of

$$\dot{p} = -\gamma p + \xi$$

again

$$\dot{p} = -\gamma p + \sqrt{\epsilon}\,\eta(t) \qquad \text{here} \qquad \underbrace{\langle \xi(t)\,\xi(t')\rangle}_{\frac{2M\gamma}{\beta}\delta(t-t')} = \epsilon\,\underbrace{\langle \eta(t)\,\eta(t')\rangle}_{\delta(t-t')}$$

$$\frac{2M\gamma}{\beta}\delta(t-t') = \epsilon\,\delta(t-t')$$

$$\boxed{\epsilon = \frac{2M\gamma}{\beta}} \sim \text{momenta}$$

position $\dot{x} = \frac{1}{M\gamma} F(x) + \sqrt{\epsilon}\,\eta(t)$

momentum $\dot{p} = -\gamma p + \sqrt{\epsilon}\,\eta(t)$

belong to the general form

$$\boxed{\dot{x} = f(x) + \sqrt{\epsilon}\,\eta(t)}$$ general Langevin

position $x = x$ $\frac{F(x)}{M\gamma} = f(x)$ $\epsilon = \frac{2}{M\gamma\beta}$

momentum $x = p$ $F(x) = -\gamma x$ $\epsilon = \frac{2M\gamma}{\beta}$

if $f(x) = -\gamma x$ (as for momentum)

$$\dot{x} = -\gamma x + \sqrt{\epsilon}\,\eta(t)$$

solution is

$$x(t) = e^{-\gamma t} x(0) + \sqrt{\epsilon}\int_0^t dt'\, e^{-\gamma(t-t')}\,\xi(t')$$

Ornstein-Uhlenbeck process

x is a functional of the history of ξ

if $f(x) = 0$

$\dot{x} = \sqrt{\epsilon}\,\eta$ $x(t) = x(0) + \underbrace{\sqrt{\epsilon}\int_0^t dt'\,\eta(t')}_{\text{Wiener process}}$

$X(t)$ is a stochastic process

a random time-dependent variable

time here's just the name of the variable

~~we can~~

let's write the general Langevin in a diff form

$$\boxed{dx = f(x)dt + \sqrt{\epsilon}\, dW(t)} \quad \text{— Itô differential form}$$

since $W(t) = \int_0^t dt' \xi(t')$ we define $dW(t)$ as that process which have

$$\begin{cases} \langle dW(t) \rangle = 0 \\ \langle dW(t)\, dW(t') \rangle = \delta(t-t')\, dt \end{cases}$$

discretisation (Euler)

$$\Delta x = \int_t^{t+\Delta t} dX(t) = X(t+\Delta t) - X(t)$$

$$X(t+\Delta t) - X(t) = f(X(t))\Delta t + \sqrt{\epsilon}\, \Delta W(t)$$

$$\Delta W(t) = \int_t^{t+\Delta t} dt' \eta(t')$$

now

$\langle \Delta W(t)\, \Delta W(t') \rangle =$
- $= 0$ if t & t' are not in the same time interval
- $\langle \Delta W^2(t) \rangle = \Delta t$ if t & t' lie in the same time-interval

How to simulate a stochastic process

$$X(t_{k+1}) = X(t_k) + f(X(t_k))\Delta t + \sqrt{\epsilon \Delta t}\, g(t_k)$$

$g(t_k)$ is a gaussian random number of variance $= 1$ for that

Itô sense

$$\langle g(t_k)\, g(t_j) \rangle = \delta_{kj}$$

therefore averages are average over a sequence of (gaussian) random uncorrelated number

average over ξ

Example: Wiener process $f = 0$

$$X_{k+1} = X_k + \sqrt{\epsilon \Delta t}\, g_k$$

X_0

$X_1 = X_0 + \sqrt{\epsilon \Delta t}\, g_0$

$X_2 = X_1 + \sqrt{\epsilon \Delta t}\, g_1 = X_0 + \sqrt{\epsilon \Delta t}\, g_0 + \sqrt{\epsilon \Delta t}\, g_1$

$\vdots$

$$X_n = X_0 + \underbrace{\sqrt{\epsilon \Delta t}\, g_0 + \sqrt{\epsilon \Delta t}\, g_1 \cdots \sqrt{\epsilon \Delta t}\, g_{n-1}}_{\text{sum of } n \text{ gaussian random \#}}$$

$$\langle (x_n - x_0)^2 \rangle = \langle \left(\sqrt{\varepsilon \Delta t} \sum_{0k}^{n-1} g_k \right)^2 \rangle =$$

$$= \varepsilon \Delta t \sum_{0k}^{n-1} \sum_{0e}^{n-1} \langle \underbrace{g_k g_e}_{\delta_{ke}} \rangle = \varepsilon \Delta t \underbrace{\sum_{0k}^{n-1} 1}_{n} = \varepsilon \underbrace{n \Delta t}_{t}$$

The Fokker-Planck equation

Given a process $x(t)$ which satisfy the generalised Langevin

$$\dot{x} = f(x) + \sqrt{\varepsilon}\,\eta(t)$$

then the distribution of x $P(x)$ satisfy the F-P equation

$$\frac{\partial P(x,t)}{\partial t} = \underbrace{-\frac{\partial}{\partial x}(FP)}_{\text{Drift}} + \underbrace{\frac{\varepsilon}{2}\frac{\partial^2 P}{\partial x^2}}_{\text{Diffusion}}$$

$\Rightarrow$ proof as an Exercise

$P(x,t)$ is a time-dependent distribution function and F-P play the role of Boltzman eq for collisions it is ~~int~~ differential and not integro-differential

Multiplicative Noise

a more general F-P can be associated to

a more general Langevin

$$\dot{x} = f(x) + \underbrace{\cancel{\sqrt{\#}}\, g(x)\, \eta(t)}_{\text{Multiplicative noise}}$$

$$\frac{\partial P}{\partial t} = -\underbrace{\frac{\partial}{\partial x} D^{(1)} P}_{\text{Drift}} + \underbrace{\frac{\partial^2}{\partial x^2} D^{(2)} P}_{\text{Diffusion}}$$

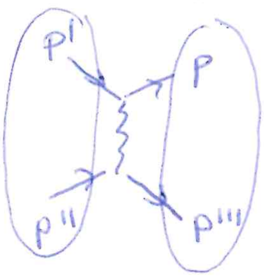
$$D^{(1)} = f(x) + \frac{1}{2} g'(x) g(x)$$

$$D^{(2)} = g^2(x)/2$$

if $g(x) = \sqrt{\epsilon}$ $\qquad D^{(1)} = f(x) \quad D^{(2)} = \frac{\epsilon}{2}$

Relation with Boltzmann eq

$$\frac{\partial f(p,t)}{\partial t} = \int d^3p'\, d^3p''\, d^3p''' \Big\{ \underbrace{W_{p'p'' \to pp'''}\, \overset{(2)}{f(p') f(p'')}}_{(in)} - \underbrace{W_{pp''' \to p'p''}\, f(p)\, f(p''')}_{(out)} \Big\}$$



this is a 2 particle process

$$(in) \quad \int d^3p' \Big[\overbrace{\int d^3p''\, d^3p'''\, W_{p'p'' \to pp'''}\, f(p'')}^{W(p|p')} \Big] f(p')$$

$$(out) \quad \int d^3p''' \Big[\underbrace{\int d^3p' \int d^3p''\, W_{pp''' \to p'p''}\, f(p''')}_{W(p'''|p)} \Big] f(p)$$

therefore generally speaking the B-E

is a sort of

$\boxed{\text{Master Equation}}$

$$\frac{\partial P(x,t)}{\partial t} = \underset{(\text{in})}{\int dx' \, W(x|x') P(x',t)} - \underset{(\text{out})}{\int dx' \, W(x'|x) P(x,t)}$$

$W(x|x')$ transition probability from $x' \to x$

$W(x'|x)$ " " " $x \to x'$

which is integro-differential

the Kramers-Moyal expansion express the integro-differential operator as a sum of ∞ differential operator (the sum is ∞)

$$\int dx' [W(x|x') P(x') - W(x'|x) P(x)] =$$

$$= \sum_{1}^{\infty} {}_n \frac{(-1)^n}{n!} \left[\frac{\partial^n}{\partial x^n} \alpha_n(x) P(x,t) \right]$$

$$\alpha_n(x) = \int dx' (x'-x)^n W(x'|x)$$

$\boxed{\text{Fokker-Planck is obtained retaining } n=1,2}$

Important differences

Master Eq: $W(x|x')$ & $W(x'|x)$

do not depend on time

do not depend on P itself

Isolated system
BBGKY

Boltzmann
(Molecular Chaos)

The "Bath"
is the "System" itself

Open System
Langevin

Fokker-Planck

"Bath" do not
have feed back
from System

Stationary (Asymptotic) solution of one dimensional FP

$$\frac{\partial P}{\partial t} = 0 \Rightarrow P \propto e^{-\frac{2}{\epsilon}V}$$

if $F = -\frac{\partial V}{\partial x}$ proof as an exercise $\Rightarrow$

for a generalised Langevin (1d)

$$\dot{x} = F + \sqrt{\epsilon}\,\eta$$

- Velocity distribution

$$F(p) = -\gamma p \qquad V(p) = \frac{\gamma p^2}{2} \qquad \epsilon = \frac{2m\gamma}{\beta}$$

$$e^{-\frac{2}{\varepsilon}V(p)} = e^{-\frac{2\beta}{2m\gamma}\frac{\cancel{\gamma} p^2}{2}} = e^{-\beta\frac{p^2}{2m}} \quad \text{Maxwell}$$

- position distribution (overdamped)

$$\dot{x} = \frac{1}{m\gamma}\left[\overset{-\partial V/\partial x}{F} + \xi\right] = \frac{F}{m\gamma} + \sqrt{\epsilon}\,\eta$$

$$\varepsilon = \frac{2}{m\gamma\beta}$$

$$e^{-\frac{2}{\epsilon}V(x)} = e^{-\frac{2m\cancel{\gamma}\beta}{2}\frac{1}{m\cancel{\gamma}}V} = e^{-\beta V(x)}$$

Multidimensional F-P

Let's consider a multi-dimensional Itô stoch eq

$$\dot{x}_i = f_i(\underline{x}) + \sqrt{\epsilon_i}\,\eta_i$$ the associated F-P reads

$$\frac{\partial P}{\partial t} = -\sum_i \frac{\partial}{\partial x_i}(f_i P) + \sum_i \frac{\epsilon_i}{2}\frac{\partial^2}{\partial x_i^2}P$$

that can be further generalised to multiplicative non-diagonal noise term

F-P for Langevin

The Langevin equation in one variable reads for momenta & coordinate

$$\dot{x} = p/m$$

$$\dot{p} = -\gamma p + F + \sqrt{\epsilon}\,\eta \qquad \text{with } \boxed{\epsilon = \frac{2m\gamma}{\beta}}$$

then

$$\frac{\partial P(p,x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{p}{m}P\right) - \frac{\partial}{\partial p}\left[(-\gamma p + F)P\right] + \frac{\epsilon}{2}\frac{\partial^2}{\partial p^2}P$$

$$\frac{\partial P(pxt)}{\partial t} = -\frac{p}{m}\frac{\partial P}{\partial x} + \gamma P - (F - \gamma p)\frac{\partial P}{\partial p} + \frac{\epsilon}{2}\frac{\partial^2}{\partial p^2}P$$

$$= -\frac{p}{m}\frac{\partial P}{\partial x} - F\frac{\partial P}{\partial p} + \gamma P + \gamma p\frac{\partial P}{\partial p} + \frac{\epsilon}{2}\frac{\partial^2}{\partial p^2}P$$

Liouvillian

$$H = \frac{p^2}{2m} + V$$

$$\boxed{\frac{\partial P}{\partial t} + \{P, H\} = \underbrace{\gamma P + \gamma p\frac{\partial P}{\partial p} + \frac{\epsilon}{2}\frac{\partial^2}{\partial p^2}P}_{\text{"collision" term}}}$$

let' assume that

$$\lim_{t\to\infty} P(x,p,t) = \frac{1}{Z} e^{-\beta H(p,x)} = \frac{1}{Z} e^{-\beta\frac{p^2}{2m}} e^{-\beta V(x)} \quad \text{then } \{P,H\}=0$$

let's check whether this is also stationary

the ~~first member~~ r.h.s. is zero $\Leftarrow P \propto e^{-\beta V}$

$$\gamma P + \gamma p\left(-\beta\frac{p}{m}\right)P + \frac{\varepsilon}{2}\left\{-\beta/m\right\}P + \frac{\varepsilon}{2}\left(-\beta\frac{p}{m}\right)^2 P$$

$$\left(\cancel{\gamma P} - \cancel{\gamma p \frac{p^2}{m}} - \frac{\varepsilon\beta}{2m} - \frac{\varepsilon\beta^2 p^2}{2m^2}\right)P = 0$$

as $\epsilon = \frac{2m\gamma}{\beta}$

$$\frac{2m\gamma}{\beta}\,\cancel{\frac{\beta}{2m}} \qquad \cancel{\frac{2m\gamma}{\beta}\,\frac{\beta^2 p^2}{2m^2}}$$

and the Maxwell-Boltzmann distribution $e^{-\beta H(px)}$ is stationary

$$\frac{\partial P}{\partial t} = 0$$