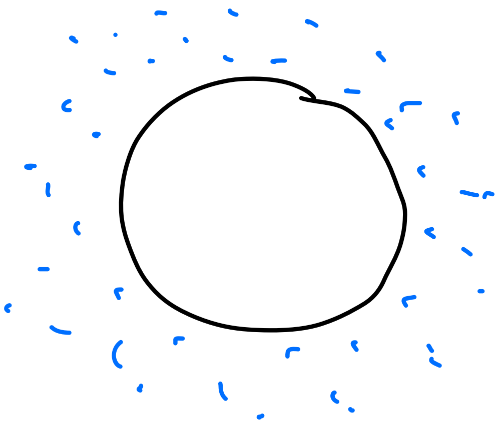
2/ The Langevin equation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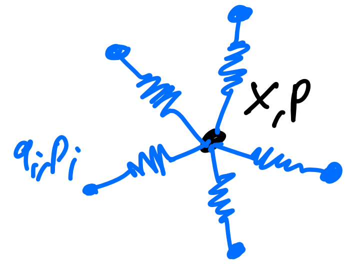


Eliminate $\{q_i, p_i\}$ to get

$$\boxed{M\dot{x} = p} \; ; \qquad \boxed{\dot{p} = -V'(x) - \int_0^t ds\, \dot{x}(s)\, K(t-s) + \xi(t)}$$

* Equilibrated fluid $\Rightarrow$ Fluctuations $\xi(t)$ given by GWN with

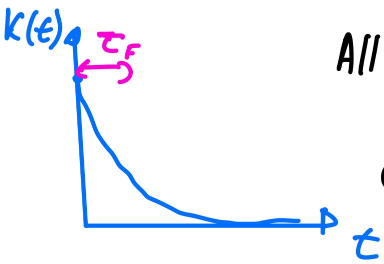
$$\langle \xi(t) \rangle = 0 \quad \& \quad \langle \xi(t)\, \xi(t') \rangle = k_B T\, K(t-t')$$

FDT

* $K(t-t') = \delta(t-t') \Rightarrow$ white noise $\left(\hat{K}(\omega) = 1\right)$

  $K(t-t') \neq \delta(t-t') \Rightarrow$ colored noise

Comment: $K(t)$ is a property of the fluid. Some fluid have memory, and are called "visco elastic", others do not and are typically called Newtonian fluid.



All fluids have finite memory time τ_F, if the time scale of the colloid dynamics τ_c is such that $\tau_c \gg \tau_F$, then the white noise is a good approximation. (water, $\tau_F \lesssim 1\,\mathrm{ps}$)

<u>Water</u>: Stokes-Einstein tells us that the diffusion constant of a particle of size R is $D = \frac{k_B T}{6\pi R \eta}$.

τ_c can be estimated as the time it takes to diffuse its size

$\Rightarrow \tau_c = \frac{R^2}{D}$. $\tau_c = \tau_F \Leftrightarrow R = 1\,\text{Å}$

For $R = 10^{-6}$, $\tau_c \gg \tau_F \Rightarrow$ water well described as Newtonian fluid.

<u>Comment:</u>

Note that $\xi(t)$ with $\langle \xi \rangle = 0$ & $\langle \xi(t)\xi(t') \rangle = 2\gamma kT \delta(t-t')$

and $\sqrt{2\gamma kT}\,\eta(t)$ with $\langle \eta \rangle = 0$ & $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$

are two GRV with the same average and covariance $\Rightarrow$ these processes are identical. One thus often write the Langevin equation as

$$\dot{q} = p \;;\; \dot{p} = -\gamma p - V'(x) + \sqrt{2\gamma kT}\,\eta .$$

We will <u>often</u> silently switch from one notation to the other.

2.1.4) The large damping limit

Naively, one would think that a large damping coefficient γ implies a large dissipation and thus no motion.

The life of a Brownian particle is <u>very</u> different.

Large friction γ $\Rightarrow$ slow system $\Rightarrow$ evolves on large time scale

consider $t = \gamma \tau$ with $\tau \sim O(1)$

$\Downarrow$ large; $\hookrightarrow O(1)$; $\hookrightarrow$ large

dynamics

$$m \frac{d^2x}{dt^2} = \frac{m}{\gamma^2}\frac{d^2x}{d\tau^2} = -\frac{\gamma}{\gamma}\frac{dx}{d\tau} - V'(x) + \sqrt{2\gamma kT}\,\underbrace{\eta(\gamma\tau)}_{=?} \qquad (\Delta)$$

Note that $\langle \eta(t)\eta(t')\rangle = \delta(t-t') = \delta(\gamma(\tau-\tau')) = \frac{1}{\gamma}\delta(\tau-\tau')$

$$= \frac{1}{\gamma}\langle \tilde{\eta}(\tau)\underbrace{\tilde{\eta}(\tau')}\rangle$$

$\hookrightarrow$ unitary GWN

$$\Rightarrow \eta(t=\gamma\tau) = \frac{1}{\sqrt{\gamma}}\tilde{\eta}(\tau)$$

$$(\Delta) \Leftrightarrow \underbrace{\frac{m}{\gamma^2}\frac{d^2x}{d\tau^2}}_{\xrightarrow[\gamma\to\infty]{} 0} = -\frac{dx}{d\tau} - V'(x) + \sqrt{2kT}\,\tilde{\eta}(\tau)$$

overdamped Langevin equation

$$\boxed{\frac{dx}{d\tau} = -V'(x) + \sqrt{2kT}\,\tilde{\eta}(\tau)} \qquad (\Delta\Delta)$$

Speed = Sum of forces

Aristotelian physics :-)

Thanks to the fluctuation dissipation relation, damping & noise scale the same way and both survive in the $\gamma \to \infty$ limit.

$\Rightarrow$ motion survives on time scale $t \sim \gamma$.

$\Rightarrow$ inertia is irrelevant (speed = Σ forces)

($\Delta\Delta$) is the love of theoretician (up to setting $k=1$) but it has weird units.

$$[\gamma] = \frac{M}{T} \Rightarrow \tau = \frac{t}{\gamma} \text{ measured in } s^2 . kg^{-1} \ldots$$

To compare with experiments, restore the real units:

$$\frac{dx}{dt} = -\frac{1}{\gamma} V'(x) + \sqrt{2\frac{kT}{\gamma}}\,\eta(t)$$

Mobility: Apply a constant force $-V'(x) = F_0$

Then the average speed is $\langle v \rangle = \langle \frac{dx}{dt} \rangle = \frac{1}{\gamma} F_0$

The mobility μ is defined as $\mu = \frac{\langle v \rangle}{F_0} = \frac{1}{\gamma}$

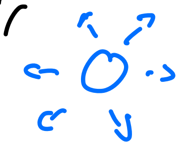
It measures the response of the particle to an external drive.

The overdamped Langevin equation then reads

$$\boxed{\dot{x} = -\mu V'(x) + \sqrt{2\mu kT}\,\eta(t)}$$

Comment: μ is a property of the fluid that can be computed independently.

For water, one can use Stokes equation to show that, for a sphere of radius R, $\gamma = 6\pi R \underbrace{\eta}_{\text{dynamic viscosity of water}}$



dynamic viscosity of water $\simeq 9.10^{-4}\ \mathrm{kg\ m^{-1} s^{-1}}$

Rotational diffusion  $\gamma_R = 8\pi R^3 \eta$

As $R \to 0$ $\gamma_R \ll \gamma$ & it's easier to rotate than to move.

Summary:

Large object connected to many equilibrated fluid molecules

$\Downarrow$ "coarse-graining" eliminate degrees of freedom

Dynamical equation for the object that is <u>stochastic</u>, depends on a small number of parameters $(kT, \gamma, \ldots)$ that can be measured independently.

The Langevin equation is the $PV = NkT$ of non-equilibrium statistical mechanics $\Rightarrow$ let's learn how to use it.

Chapter 2: Itō calculus

In the absence of external potential, the simplest dynamics of an overdamped colloid is given by

$$\dot{x}(t) = \sqrt{2D}\,\eta(t) \qquad (1)$$

where $\eta(t)$ is a Gaussian white noise satisfying $\langle \eta(t) \rangle = 0$
$\langle \eta(t)\eta(t') \rangle = \delta(t-t')$

1) The breakdown of standard calculus

$\eta(t)$ is a random variable $\Rightarrow$ new value at every time
$\Rightarrow$ far from continuous

Is (1) a reasonable ODE? (Answer: not really)

History: 1785 Jan Ingenhousz observes the random motion of coal particles at the surface of water

1827: Robert Brown describes the motion of pollen grain suspended in water

1905: Einstein makes a convincing connection to atomistic theory

1906: Smoluchowski
1908: Langevin
} birth of stochastic differential equations.

1918: Wiener
1944: Itō
} solid mathematical basis $\Rightarrow$ hard problem!

Why? two important problems

1. Formal solution of (1) $x(t) = \int_0^t ds\,\sqrt{2D}\,\eta(s) + \underbrace{x(0)}_{=0 \text{ for simplicity}}$

$$\frac{x(t+\tau) - x(t)}{\tau} \equiv \frac{\Delta X}{\tau} = \frac{1}{\tau}\int_t^{t+\tau} ds\,\sqrt{2D}\,\eta(s) \quad \text{random variable}$$

$$\left\langle \frac{\Delta X}{\tau} \right\rangle = \frac{1}{\tau}\int_t^{t+\tau} ds\,\sqrt{2D}\,\underbrace{\langle \eta(s) \rangle}_{=0} = 0$$

$$\left\langle \frac{\Delta X^2}{\tau^2} \right\rangle = \frac{2D}{\tau^2}\underbrace{\int_t^{t+\tau} ds \int_t^{t+\tau} du\, \underbrace{\langle \eta(s)\eta(u) \rangle}_{\delta(s-u)}}_{1} = \frac{2D\tau}{\tau^2} = \frac{2D}{\tau} \xrightarrow[\tau \to 0]{} \infty$$

$\frac{\Delta X}{\tau}$ scales as $\frac{1}{\sqrt{\tau}} \Rightarrow$ not differentiable! Q: how to give a proper meaning to (1)?

Mathematicians: You do not, only $x(t) = \int_0^t ds\,\sqrt{2D}\,\eta(s)$ is well defined $\Rightarrow$ Wiener process $\quad dx = \sqrt{2D}\,d\eta$ is acceptable

Physicists: Yes, fine, but let's still use it because it is a useful notation...

2. Eq (1) describes a random motion and we expect $\langle x^2(t) \rangle \sim 2Dt$

$$(x(t) - x(0))^2 = 2D\int_0^t ds \int_0^t du\, \eta(s)\eta(u) \Rightarrow \langle x^2(t) \rangle = 2Dt$$

correct diffusive scaling.

Alternative derivation: $\quad \frac{d}{dt} x^2(t) = 2x(t)\,\dot{x}(t) = \sqrt{8D}\,x(t)\eta(t) \qquad (2)$

$$\frac{d}{dt}\langle x^2(t) \rangle = \sqrt{8D}\,\langle x(t)\,\eta(t) \rangle$$

$$\left.\begin{aligned}&x(t): \text{position reached at time } t\\ &\eta(t): \text{random kick received } \underline{\text{at}} \text{ time } t\end{aligned}\right\} \text{causality} \Rightarrow \text{uncorrelated}$$

$$\langle x(t)\,\eta(t)\rangle = \langle x(t)\rangle \underbrace{\langle \eta(t)\rangle}_{=0} = 0 \qquad (3)$$

$$\Rightarrow \frac{d}{dt}\langle x^2(t)\rangle = 0 \Rightarrow \langle x^2(t)\rangle = C^{st} \Rightarrow \text{paradox!}$$

Conclusion: (2) & (3) are incompatible.

Itō convention:

We choose to stick to (3) and we will have to fix the chain rule (a). To do so, we will use what is called Itō stochastic calculus. Alternatively, physicists often like to keep (2), but then (3) does not hold. This is the path of Stratonovich calculus on which I will comment later on.

Comment: The proper mathematical treatment of stochastic equations relies on integrating them over a time step dt to write

$$dx = f(x)\,dt + d\xi$$

and on giving a proper mathematical sense to integrals of the form

$$\int f(x)\,d\xi$$

Here, we will stick to physics notation. The reading of chapters 1-5 of the book "Stochastic differential equations", by Bernt Øksendal, forms a solid mathematical reference for interested readers.

2) Itō formula: the modified chain rule

Q°: How does $f(x(t))$ evolve when $x(t)$ is solution of

$$\dot{x}(t) = F(x(t)) + \eta(t) \qquad (4)$$

and $\eta(t)$ is a Gaussian white noise (GWN) such that
$\langle \eta(t) \rangle = 0$ & $\langle \eta(t)\, \eta(t') \rangle = \Gamma\, \delta(t-t')$

[Or, equivalently, $\dot{x} = F + \sqrt{\Gamma}\, \xi(t)$ & $\langle \xi(t)\, \xi(t') \rangle = \delta(t-t')$]

Comment: Formal solution of (4):

$$dx = x(t+dt) - x(t) = \underbrace{\int_t^{t+dt} \underbrace{F(x(s))}_{\simeq F(x(t)) + O(s-t)} ds}_{\simeq F[x(t)]dt + o(dt)} + \underbrace{\int_t^{t+dt} \eta(s)\, ds}_{d\eta(t)} \qquad (5)$$

What do we know about $d\eta$?

$$\langle d\eta \rangle = 0 \quad ; \quad \langle d\eta^2 \rangle = \int_t^{t+dt} ds \int_t^{t+dt} du\, \langle \eta(s)\, \eta(u) \rangle = \Gamma\, dt$$

$d\eta \sim \sqrt{dt}$ unusual

Comment: To simulate (4), the simplest way is to use (5)

$$x(t+dt) = x(t) + dt\, F(x(t)) + \sqrt{2\Gamma dt}\; u, \quad \text{where } p(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{u^2}{2}}$$

Chain rule: To evaluate $\frac{df(x(t))}{dt}$, let us first compute

$$\frac{f(x(t+dt)) - f(x(t))}{dt} = \frac{f(x(t)+dx) - f(x(t))}{dt} = \frac{1}{dt} \sum_{k=1}^{\infty} \frac{(dx)^k}{k!} f^{(k)}(x(t)) \qquad (6)$$

Since $\frac{df(x(t))}{dt} = \lim_{dt \to 0} \frac{f(x(t+dt)) - f(x(t))}{dt}$, we need to retain in (6) (10)

all terms that do not vanish as $dt \to 0$. Since dx contain $d\eta$, which scale as $\sqrt{dt}$, $(dx)^2$ will contribute.

For $k \geq 3$ $\frac{(dx)^k}{dt} = \mathcal{O}(\sqrt{dt}) \to 0$ as $dt \to 0$.

Let us look at the terms order by order.

$k=1$ $\frac{dx}{dt} f'(x) \Rightarrow$ standard chain rule

$k=2$ $\frac{1}{2}\frac{dx^2}{dt} f''(x) \simeq \frac{1}{2dt}\left(F(x(t))\,dt + d\eta\right)^2 f''(x)$

$$= \Big(\underbrace{F(x(t))^2\,dt}_{\substack{\to 0 \\ dt \to 0}} + \underbrace{2F(x(t))\,d\eta}_{\substack{\sim\sqrt{dt} \to 0 \\ dt \to 0}} + \underbrace{\frac{d\eta^2}{dt}}_{?}\Big)\frac{f''(x)}{2}$$

$d\eta^2 = \int_t^{t+dt} ds \int_t^{t+dt} du\, \eta(s)\eta(u)$ is a random variable whose average value is $\sigma\,dt$: $d\eta^2 = \sigma\,dt +$ fluctuations

As $dt \to 0$, the fluctuations of $d\eta^2$ becomes negligible and it stops acting as a random variable so that we write $d\eta^2 \text{ "="}\ \sigma\,dt$.

This equality is for stochastic variables: mathematically, it is a convergence in L_2-Norm.

The $k=2$ term thus contributes $\frac{\sigma}{2} f''(x(t))$, leading to

$$\boxed{\frac{d}{dt}\left[f(x(t))\right] = f'(x(t))\,\dot{x}(t) + \frac{\sigma}{2} f''(x(t))} \quad (7)$$

For those who like more mathematical derivations.

2.1) Evolution of $f(x(t))$

$$x(t+dt) = x(t) + F(x(t))\,dt + d\eta(t) + o(dt) \quad : \quad d\eta(t) = \int_t^{t+dt} ds\, \eta(s)$$

Discretize time $t_j = j\,dt$; $t = N dt$

Trick: $f(x(t)) = f(x(0)) + \sum_{j=0}^{N-1} f(x(t_{j+1})) - f(x(t_j))$

Idea: N large, $dt \to 0$, with $t = N dt$ fixed to expand

$$f(x(t_{j+1})) - f(x(t_j)) \simeq \frac{\partial f}{\partial x}\Big|_{t_j} \cdot dx_j + \frac{1}{2}\frac{\partial^2 f}{\partial x^2} \cdot dx_j^2$$

where $dx_j = x(t_{j+1}) - x(t_j) \simeq F(x(t_j))\,dt + d\eta(t_j)$

Then identify $f(x(t)) - f(x_0) = \int_0^t ds\, \frac{df}{ds}(x(s))$ to get $\frac{df}{ds}(x(s))$

To lighten notations, we denote $O(t_j)$ by O_j

$$f(x(t)) - f(x(0)) = \sum_{j=0}^{N-1} \underbrace{f'(x_j)\,dx_j}_{1} + \frac{1}{2} f''(x_j)\left[\underbrace{F_j^2 dt^2}_{2} + \underbrace{2F_j\,dt\,d\eta_j}_{3} + \underbrace{d\eta_j^2}_{4}\right]$$

Analyse term by term in the limit $dt \to 0$

$$1 = \sum_j f'(x_j)\frac{dx_j}{dt}\,dt \underset{dt\to 0}{\sim} \int_0^t f'(x(s))\,\dot{x}(s)\,ds = \int_0^t f'(x(s))\left[F(x(s)) + \eta(s)\right]$$

$$2 = dt \sum_j \frac{1}{2} f''(x_j) F(x_j)\,dt \sim dt \int_0^t ds\, \frac{1}{2} f''(x(s))\, F(x(s)) = O(dt) \underset{dt\to 0}{\longrightarrow} 0$$

$$3 = \sum_j dt\, f''(x_j)\, F(x_j)\, d\eta_j \equiv A \quad \text{random variable} \to \text{scale?}$$

$$\langle A\rangle = \sum_j dt \underbrace{\left\langle f''(x_j)\, F(x_j) \int_{t_j}^{t_j+dt} \eta(s)\,ds \right\rangle}_{\langle f''(x_j)\, F(x_j)\rangle \left\langle \int_{t_j}^{t_j+dt} \eta(s)\,ds \right\rangle} \quad \text{Itô}$$

$$\langle f''(x_j)\, F(x_j)\rangle \underbrace{\left\langle \int_{t_j}^{t_j+dt} \eta(s)\,ds \right\rangle}_{=0} \Rightarrow \langle A\rangle = 0$$

$$\langle A^2\rangle = \sum_{j,h=0}^{N} dt \langle f''(x_j)\, f''(x_h)\, F(x_j)\, F(x_h)\, d\eta_j\, d\eta_h\rangle$$

if $h>j$, $d\xi_h$ independent from the rest $\langle \ldots\rangle = \langle \ldots\rangle\langle d\eta_h\rangle = 0$

if $j<h$, $\langle \ldots\rangle = 0$ by symmetry

$$\langle A^2\rangle = \sum_j dt \langle f''(x_j)^2\, F(x_j)^2\rangle \underbrace{\langle d\eta_j^2\rangle}_{\sigma\, dt} \sim dt \int_0^t dt\, \sigma \langle f''(x_j)\, F(x_j)^2\rangle \xrightarrow[dt\to 0]{} 0$$

The typical scale of A vanishes as $dt \to 0$ (also holds for higher moments)

④ $= \sum_j \frac{1}{2} f''(x_j)\, d\eta_j^2$

$d\eta_j^2$ is a random variable of average σdt. Let's show that

$d\eta_j^2 = \sigma dt$ + negligible fluctuations.

$B = \sum_j \frac{1}{2} f''(x_j)\,[d\eta_j^2 - \sigma dt]$ is a random variable

$$\langle B\rangle = \sum_j \frac{1}{2} \langle f''(x_j)\,[d\eta_j^2 - \sigma dt]\rangle \overset{\text{Itô}}{=} \frac{1}{2}\sum_j \langle f''(x_j)\rangle \underbrace{\langle d\eta_j^2 - \sigma dt\rangle}_{=0}$$

$= 0$

$$\langle B^2\rangle = \sum_{j,h} \langle f''(x_j)\, f''(x_h)\,[d\eta_j^2 - \sigma dt]\,[d\eta_h^2 - \sigma dt]\rangle$$

As before, $j\neq h$ vanishes $\Rightarrow \langle B^2\rangle = \sum_j \langle f''(x_j)^2\rangle \langle (d\eta_j^2 - \sigma dt)^2\rangle$

$$\langle (d\eta_j^2 - \sigma dt)^2 \rangle = \langle d\eta_j^4 \rangle - 2\sigma\, dt \,\langle d\eta_j^2 \rangle + \sigma^2 dt^2$$

Since $d\eta_j$ is a GRV of 0 mean, $\langle d\eta_j^4 \rangle = 3\langle d\eta_j^2 \rangle^2 = 3\sigma^2 dt^2$

$$\langle B^2 \rangle = \sum_j \langle f''(x_j)^2 \rangle\, 2\sigma^2 dt^2 \sim dt\, 2\sigma^2 \int_0^t ds\, f''(x(s)) = \mathcal{O}(dt) \xrightarrow[dt\to 0]{} 0$$

$\langle B^2 \rangle \to 0$ shows that the random variables $\sum_j \frac{1}{2} f''(x_j)\, d\eta_j^2$ converges in norm L^2 to the limit of $\sum_j \frac{1}{2} f''(x_j)\, \sigma dt$ and we thus replace ④ by $\sum_j \frac{1}{2} f''(x_j)\, \sigma dt \sim \frac{1}{2}\int_0^t ds\, f''(x(s))$.

All in all:

$$f(x(t)) - f(x(0)) \underset{dt\to 0}{\simeq} \int_0^t ds \left[f'(x(s))\, \dot{x}(s) + \frac{\sigma}{2} f''(x(s)) \right]$$

which leads to Itō lemma:

$$\boxed{\frac{d}{dt}\left[f(x(t)) \right] = f'(x(t))\, \dot{x}(t) + \frac{\sigma}{2} f''(x(t))} \qquad (7)$$

Comment: This is a very useful formula that we will use a lot but we have shown this for the integral of (7) in the L_2 sense: $\langle \int (RHS - LHS)^2 ds \rangle = 0$.

This is not an exact, point-wise formula ⇒ do not do crazy thing like $g(RHS) = g(LHS)$ with g a non-linear function.

End of the mathematical aparte.

2.2) Generalization to $f(x(t), t)$

The derivation above generalizes directly to

$$\boxed{\frac{d}{dt} f(x(t),t) = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\dot{x}(t) + \frac{\Gamma}{2}\frac{\partial^2 f}{\partial x^2}}$$

2.3) N-dimensional Itō formula

$\dot{x}_i = F_i(x_1, \ldots, x_N) + \eta_i$ where the $\{\eta_i\}$ are correlated GWN s.t.

$$\langle \eta_i(t)\rangle = 0 \quad \langle \eta_i(t)\eta_k(t')\rangle = \Gamma_{ik}\,\delta(t-t')$$

Thus

$$\boxed{\frac{d}{dt} f(x_1(t), \ldots, x_N(t)) = \sum_i \frac{\partial f}{\partial x_i}\dot{x}_i + \frac{1}{2}\sum_{i,k}\frac{\partial^2 f}{\partial x_i \partial x_k}\Gamma_{ik}} \qquad (\&)$$

Comment: Very useful in the presence of deterministic & stochastic variable.

E.g. $\dot{x} = v \;;\; m\dot{v} = -\gamma v - V'(x) + \sqrt{2\gamma k T}\,\eta(t)$

$\Leftrightarrow \quad \dot{x} = v + \xi_x \;;\; \dot{v} = -\frac{\gamma}{m}v - \frac{1}{m}V'(x) + \xi_y$

where $\langle \xi_x(t)\rangle = 0 \;;\; \langle \xi_x(t)\,\xi_x(t')\rangle = 0$

$\langle \xi_y(t)\rangle = 0 ; \; \langle \xi_y(t)\,\xi_y(t')\rangle = 2\gamma k T\,\delta(t-t')$

$\langle \xi_x(t)\,\xi_y(t')\rangle = 0$

$$\frac{d}{dt} f(x(t), v(t)) = \frac{\partial f}{\partial x}\dot{x} + \frac{\partial f}{\partial v}\dot{v} + \gamma k T\frac{\partial^2 f}{\partial v^2}$$

$\Rightarrow$ only the stochastic variable leads to a second order derivative.

2.4) Back to the paradox

$f(x(t)) = x^2(t)$ & $\dot{x}(t) = \sqrt{2D}\,\eta(t)$

$f'(x) = 2x$; $f''(x) = 2$

$$\frac{d}{dt} f(x(t)) = \frac{\partial f}{\partial x} \cdot \dot{x} + \frac{1}{2} \cdot \frac{\partial^2 f}{\partial x^2} \cdot 2D = 2x\dot{x} + 2D = 2D + \sqrt{8D}\, x\, \eta(t)$$

$$x^2(t) = 2Dt + \sqrt{8D} \int_0^t ds\, \eta(s)$$

$\rightarrow$ ① we recover $\langle x^2(t) \rangle = 2Dt$

② we can characterize the fluctuations of $x^2(t)$ around its mean $2Dt$.

Also works for higher moments:

$$\frac{d}{dt} \langle x^4(t) \rangle = 4 \langle x^3 \dot{x} \rangle + \frac{1}{2} \cdot 2D \cdot 12 \langle x^2 \rangle$$

$$= 4 \langle x^3 \rangle \underbrace{\langle \sqrt{2D}\,\eta(t) \rangle}_{=0} + 12\, D \underbrace{\langle x^2 \rangle}_{2Dt}$$

$\Rightarrow \langle x^4(t) \rangle = 12\, D^2 t^2 = 3 \times (2Dt)^2 = 3 \langle x^2(t) \rangle^2$ as expected for a GRV.

3) Probability of noise realization

If we say that $\{\eta(t)\}$ forms a set of GRV, it would be nice to be able to write their probability weight.

Start with N random variables η_j such that $\vec{\eta} = (\eta_1, \dots, \eta_N)$

$$P(\vec{\eta}) = \frac{1}{Z} \exp\left[-\frac{1}{2} \vec{\eta} \cdot (\Gamma\, \vec{\eta})\right] \qquad (9)$$

with Γ a matrix symmetric positive definite.

From the pset you know that $\langle \eta_i \eta_j \rangle = K_{ij}$, with $K = \Gamma^{-1}$.

Now let's call $t_i = i\,dt$ and $\eta_i = \eta(t_i)$ and take the limit $dt \to 0$ (13)
keeping $N dt = t$ fixed. We then rewrite

$$\vec{\eta}\cdot(\Gamma\vec{\eta}) = \sum_{i,j} \eta_i \Gamma_{ij} \eta_j = \sum_{i,j} dt^2\, \eta(t_i) \frac{\Gamma_{ij}}{dt^2} \eta(t_j)$$

$$\vec{\eta}\cdot(\Gamma\vec{\eta}) \sim \int dt\,dt'\, \eta(t)\eta(t')\Gamma(t,t') \quad \text{where } \Gamma(t_i,t_j) = \frac{1}{dt^2}\Gamma_{ij} \qquad (10)$$

<u>What do we know about $\Gamma(t,t')$?</u>

$$K = \Gamma^{-1} \Rightarrow \sum_h K_{ih}\Gamma_{hj} = \delta_{i,j} \quad (11) \quad \& \quad \sum_{j,h} K_{ih}\Gamma_{hj} f_j = \sum_j \delta_{ij} f_j = f_i$$

$$\Leftrightarrow \sum_{j,h} dt^2 K_{ih} \frac{\Gamma_{hj}}{dt^2} f_j = f_i$$

$$\Leftrightarrow \int dt''dt'\, K(t,t')\Gamma(t',t'')f(t'') = f(t) \qquad \text{with } K(t_i,t_j) = K_{ij}$$

$$\Leftrightarrow \int dt'' f(t'') \left[\int dt' K(t,t')\Gamma(t',t'')\right] = f(t)$$

Since this holds for any function f, one has that

$$\Rightarrow \boxed{\int dt' K(t,t')\Gamma(t',t'') = \delta(t-t'')}$$

This is the generalisation of $K\cdot\Gamma = \mathrm{Id}$ for convolution kernel.

<u>Going back to the GWN</u>: $\langle \eta(t)\eta(t')\rangle = 2kT\,\delta(t-t') = K(t,t')$

$\Leftrightarrow \langle \eta(t_i)\eta(t_j)\rangle = 2kT \dfrac{\delta_{ij}}{dt} \Rightarrow K_{ij} = 2kT\dfrac{\delta_{ij}}{dt}$. Eq (11) then leads

to $\Gamma_{jh} = \dfrac{1}{2k_BT} dt\,\delta_{jh}$ & Eq (10) $\Rightarrow \Gamma(t_i,t_j) = \dfrac{1}{2k_BT}\dfrac{\delta_{jh}}{dt} \to \dfrac{\delta(t_i-t_j)}{2k_BT}$

We then check that

$$\int dt\, K(t,t')\Gamma(t',t'') = \frac{2k_BT}{2k_BT}\int dt'\, \delta(t-t')\,\delta(t'-t'') = \delta(t-t'')$$

$$\Rightarrow P[\{\eta(t)\}] = \frac{1}{Z} \exp\left[-\frac{1}{4\mu T}\int dt\,dt'\,\eta(t)\eta(t')\delta(t-t')\right]$$

$$\boxed{P[\{\eta(t)\}] = \frac{1}{Z} \exp\left[-\frac{1}{4\mu T}\int dt\,\eta(t)^2\right]}$$:-)

Colored noise If $\langle \eta(t)\eta(t')\rangle = K(t-t')$

then $P[\{\eta(t)\}] = \frac{1}{Z} \exp\left[-\int dt\,dt'\,\eta(t)\,\Gamma(t-t')\,\eta(t')\right]$

when Γ is such that $\int dt'\,K(t-t')\,\Gamma(t'-t'') = \delta(t-t'')$

4) Probability of trajectories $\{x(t)\}$

If we know $P[\{\eta(t)\}]$ and we know $x(t,\{\eta(s)\})$, can we get $P[\{x(t)\}]$? Yes, but this is painful...

Changing variable N rdm variables $x_1, -, x_N$ & a new set of coordinates $y_i(x_1, -, x_N)$

Conservation of probability means that $P(x_1,-,x_N)\,dx_1 - dx_N = P(y_1,-,y_N)\,dy_1 - dy_N$

$$\Rightarrow P(y_1,-,y_N) = P(x_1,-,x_N)\cdot \underbrace{\frac{dy_1 - dy_N}{dx_1 - dx_N}}_{\text{Jacobian}}$$ of the change of variable

$$\Rightarrow P[\{x(t)\}] = P[\{\eta(t)\}] \,.\, \det J \quad \text{where } J \text{ "="} \frac{\partial \eta(t)}{\partial x(t')}$$

Q: How do we give a meaning to J ?

Let's time-discretize the Langevin equation $\dot{x} = f(x) + \eta(t)$ 15

x_0 fixed, $x_i = x(t_i)$, $t_i = i\,dt$. $x_1, \dots, x_N$ are N RVs. Then, we define

$$\tilde{\eta}_i \equiv \int_{t_{i-1}}^{t_i} \eta(s)\,ds \quad \text{so that } \tilde{\eta}_i \text{ leads from } x_{i-1} \text{ to } x_i:$$

$$x_{i+1} = x_i + \int_{t_i}^{t_{i+1}} f(x(s))\,ds + \tilde{\eta}_{i+1} \Rightarrow \tilde{\eta}_1, \dots, \tilde{\eta}_N \text{ are } N \text{ GRVs.}$$

$$\Rightarrow \frac{\partial \tilde{\eta}_{i+1}}{\partial x_j} = \frac{\partial}{\partial x_j}\Big[\underbrace{x_{i+1} - x_i}_{\text{easy}} - \underbrace{\int_{t_i}^{t_{i+1}} f(x(s))\,ds}_{=?}\Big]$$

$$= f(x_i)\,dt \;?$$
$$= f(x_{i+1})\,dt \;?$$
$$= f(x_i^\alpha)\,dt \quad \text{with } x_i^\alpha = \alpha x_{i+1} + (1-\alpha) x_i \;?$$

All appear equivalent to order dt... Let's keep α arbitrary for now.

$\Rightarrow$ the matrix $\frac{\partial \tilde{\eta}_{i+1}}{\partial x_j}$ is an upper triangular matrix

$$\Rightarrow \det = \prod_i \frac{\partial \tilde{\eta}_i}{\partial x_i} = \prod_i \left(1 - \alpha\,dt\,f'(x_i^\alpha)\right) \simeq \prod_i e^{-\alpha dt f'(x_i^\alpha)}$$

$$\simeq e^{-\alpha \sum_i dt\, f'(x_{i+1}^\alpha)} \simeq e^{-\alpha \int_0^t ds\, f'(x(s))}$$

$$P[\{x(t)\}] = \frac{1}{Z} e^{-\int dt \left[\frac{\eta^2(t)}{4kT} + \alpha f'(x(s))\right]}$$

But we know that $\dot{x} = f(x) + \eta(t) \Rightarrow \eta(t) = \dot{x} - f(x)$

$$\Rightarrow \boxed{P[\{x(t)\}] = \frac{1}{Z} e^{-\int dt \frac{(\dot{x} - f(x))^2}{4kT} + \alpha f'(x(s))}}$$

Comment: Causality makes us again choose $\alpha = 0$. Then

$$P[\{x(t)\}] = \frac{1}{Z} e^{-\int dt \frac{(\dot{x} - f(x))^2}{4kT}}$$

Then, we need to use Itō calculus to compute time-derivatives in the integral.

If we use $\alpha = \frac{1}{2}$, we use what is called Stratonovich time discretization. We can use standard calculus in the exponent, but the computation of averages is harder since $\eta(t)$ and $x(t)$ are now correlated $\Rightarrow \langle x(t)\eta(t)\rangle \neq 0$.

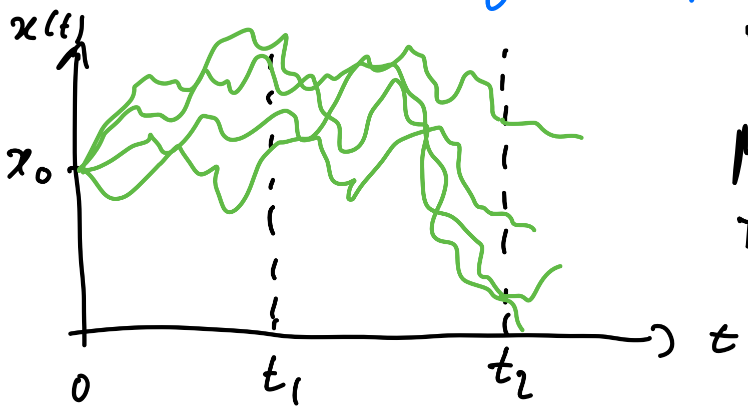
[Arnoulx de Pirey, Cugliandolo, Lecomte, van Wijland, Adv. Phys. 2023]
arXiv: 2211.09470

Chapter 3: The Fokker-Planck equation

Reference: Risken, "The Fokker-Planck equation", Springer

Take $x(t)$ such that $x(0)=x_0$ & $\dot{x}(t) = F(x(t)) + \xi(t)$ (1), where ξ is a GWN s.t. $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\, \xi(t') \rangle = 2D\,\delta(t-t')$

Consider several realizations of $x(t)$



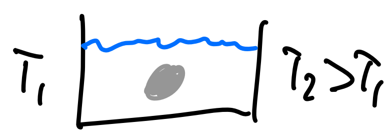
We denote by $P(x(t)=\bar{x}, t \mid x_0, 0)$ the probability that the process $x(t)$ reaches the position $\bar{x}$ at time t, given that it was at x_0 at time 0.

More concisely, we write $P(\bar{x}, t \mid x_0, 0)$ and stress that $\bar{x}$ & x_0 are numbers while $x(t)$ is a stochastic process.

Clearly $P(\bar{x}, t_1 \mid x_0, 0) \neq P(\bar{x}, t_2 \mid x_0, 0) \Rightarrow$ Q: how does $P(\bar{x}, t \mid x_0, 0)$ evolves in time?

1) The Fokker Planck Equation

In Eq (1), the statistics of $\xi(t)$ do not depend on $x(t)$. This is called an additive noise. Instead we can consider a case where, say, the temperature is inhomogeneous



Then $T(x)$ & the Langevin equation is of the type

$$\dot{x} = F(x) + \sqrt{2D(x)}\,\xi(t) \quad (2)$$