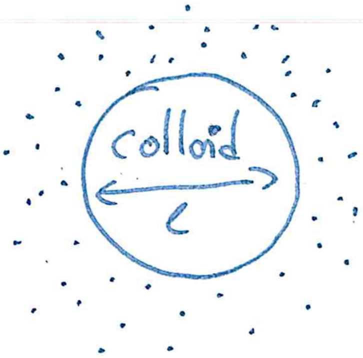
These three chapters correspond to a set of lectures I give in Master Course on Physics of complex systems in Paris.

Chapter 2 shows why the motion of a micrometric particle in an equilibrated solvent can be modelled by a Langevin equation.

Since this equation contains a random force, an initial condition x_0 generates an ensemble of different trajectories $\{x(t)\}$. The position at time t is thus also a random variable $x(t)$ whose statistics is described by a probability distribution $P(x(t)=x;t)$ whose time-evolution is given by a Fokker-Planck equation which is constructed and discussed in chapter 4. To do so, I use Itô Formula whose derivation will be sketched in my second lecture and is detailled in Chapter 3.

Chapter II : the Langevin Equation

Idea: show that a single, mesoscopic particle inserted in an equilibrated fluid relaxes to equilibrium, i.e. $P(q) \propto e^{-\beta E(q)}$ and characterize its dynamics.



liquid molecules $\sim 10^{-10}$ m (3.4 Å for water)
colloid $l \sim 10^{-6}$, area $\sim 10^{-12}$ m^2
area of water molecules $\sim 10^{-20}$ m^2 } 10^8 water molecules in contact with colloid
$\Rightarrow$ lots of random collisions

I/ Introduction

Colloid: M, x, p ; Fluid particles $m_i = 1$, q_i, p_i

Hamiltonian $$H = \frac{p^2}{2M} + V(x) + \underbrace{\sum_i V_{FC}(x-q_i)}_{\equiv H_{FC}\text{ ; interactions between fluid and colloid}} + \underbrace{\sum_i \frac{p_i^2}{2} + \sum_{i,j} V_{FF}(q_i - q_j)}_{H_{FF}\text{ interactions between fluid particles}}$$

Equations of motions: $\dot{x} = \frac{p}{M}$; $\dot{p} = -V'(x) - \sum_i V'_{FC}(x-q_i)$ (*)

fluid particles $\dot{q}_i = p_i$; $\dot{p}_i = V'_{FC}(x - q_i) - \sum_{j \neq i} V'_{FF}(q_i - q_j)$

Problem: ① impossible to solve ; ② too much information

Idea: eliminate q_i, p_i to get a self consistent equation for x & p.

Intuitively: Imagine that the colloid is at rest at time t, i.e. $p = 0$.
Then, by symmetry there is no net force on average.
$\Rightarrow \langle \sum_i V'_{FC}(x - q_i) \rangle = 0$ where $\langle \cdots \rangle$ is an average over | repeated samples realisations.

Imagin that, suddenly, there is sae motion $X(t+dt) \neq X(t)$
i.e. $X(t+dt) = X(t) + \Delta$; $\Delta \simeq \frac{P(t)dt}{M} \neq 0$ then

$$\sum_i V'_{FC}(X(t+dt)-q_i) \simeq \sum_i V'_{FC}(X(t)-q_i) + \Delta V''_{FC}(x(t)-q_i)$$

$$\langle \text{———} \rangle \simeq \underbrace{\langle \text{———} \rangle}_{\simeq 0} + \Delta \langle V''_{FC}(x(t)-q_i) \rangle$$

$\Rightarrow$ < force felt by colloid> $\propto \Delta = \frac{P(t)dt}{M} \propto p(t) \Rightarrow$ friction!
The motion of the colloid breaks the isotropy of space and generate a non-zero net force from the fluid.

Idea $\dot{p} = -V'(x) - \gamma p$ + fluctuations ; let's derive it!

Problem: this is far too difficult $\Rightarrow$ make two approximations

① V_{FC} generic $\Rightarrow$ too complicated $\Rightarrow$ use harmonic oscillators

② $M \gg 1$; motion of colloid is slow and we assume that the fluid dynamics makes it equilibrate so that, at $t=0$,

$$P(q_1, \ldots, q_N; p_1, \ldots, p_N) \propto e^{-\beta[H_{FP}(X, \{q_i, p_i\}) + H_{FF}(\{q_i, p_i\})]}$$

II An exactly solvable case: the Ford, Kac and Mazur model

(Also known as Caldeira-Leggett for its quantum version)

Ref: J. Math. Phys. 6, 504 (1965)

$$H = \sum_j \left(\frac{p_j^2}{2} + \frac{\omega_j^2}{2}(q_j - X)^2 \right) + \frac{P^2}{2M} + V(X)$$

A) A self-consistent dynamics for X & P

Equations of motion: $\dot{q}_i = p_i$ ① ; $\dot{p}_i = -\omega_j^2 (q_j - X)$ ②

$$M\dot{X} = P \quad ③ \quad ; \quad \dot{P} = -V'(X) - \sum_j \omega_j^2 (X - q_j) \quad ④$$

Note $A_j \equiv X - q_j$

Todo: assume $x(t)$ given; solve formally ① + ② as functions of $x(t)$; inject back in ③ + ④ to get self-consistent equations.

~~Homogeneous solution:~~

① + ②: $\ddot{q}_j = -\omega_j^2 q_j + \omega_j^2 x$

Homogeneous solution: $q_j^H = A\cos\omega_j t + B\sin\omega_j t$

General solution: $q_j(t) = q_j^H(t) + q_j^P(t)$ with $q_j^P(t)$ a particular solution of ① + ②

$\Rightarrow$ look for $Y(t)$ s.t. $\mathcal{L}Y(t) = \omega_j^2 x(t)$ with $\mathcal{L} = \frac{d^2}{dt^2} + \omega_j^2$

let f be such that $\mathcal{L}f(t) = 0$ and look for $Y(t) = \int_0^t dt' f(t-t')x(t')$

then $Y'(t) = f(0)x(t) + \int_0^t dt' f'(t-t')\, x(t')dt'$

$Y''(t) = f(0)x'(t) + f'(0)x(t) + \int_0^t dt' f''(t-t')\, x(t')dt'$

$$\mathcal{L}Y = f(0)x'(t) + f'(0)x(t) + \int_0^t dt' \underbrace{\left[f''(t-t') + \omega_j^2 f(t-t')\right]}_{=\mathcal{L}f = 0} x(t')dt'$$

Need $f(0) = 0$ and $f'(0) = \omega_j^2 \Rightarrow f(t) = \omega_j \sin\omega_j t$

$Y(t) = \int_0^t \omega_j \sin\omega_j(t-t')\, x(t')dt'$

Initial conditions: $q_j(t=0) \equiv q_j(0)$; $p_j(t=0) \equiv p_j(0)$

ok because $m_j = 1$ so that $p_j(0) = \dot{q}_j(0)$

$$\Rightarrow \boxed{q_j(t) = q_j(0)\cos\omega_j t + \frac{p_j(0)}{\omega_j}\sin\omega_j t + \omega_j \int_0^t \sin\omega_j(t-t')\, x(t')dt'}$$

Solely depends on the constants $q_j(0), p_j(0), \omega_j$; the variable t and the trajectory $x(t)$.

Going back to ③ + ④ $\rightarrow$ simplify $A_j = x - q_j$

$$A_j = \underbrace{X(t) - \int_0^t x(t')\,\omega_j \sin\omega_j(t-t')dt'}\; - q_j(0)\cos\omega_j t - \frac{p_j(0)}{\omega_j}\sin\omega_j t$$

$$= X(t) - \left[X(t')\cos\omega_j(t-t')\right]_0^t + \int_0^t \frac{p(t')}{M}\cos\omega_j(t-t')dt' - [\ldots]$$

$$A_j = X(0)\cos\omega_j(t) + \int_0^t \frac{p(t')}{M}\cos\omega_j(t-t')dt' - q_j(0)\cos\omega_j t - \frac{p_j(0)}{\omega_j}\sin\omega_j t$$

All in all:

$$\dot{p} = -V'(x) - \int_0^t \frac{p(t')}{M} \sum_j \omega_j^2 \cos\omega_j(t-t')\,dt' + \sum_j \left\{ \omega_j p_j(0) \sin\omega t + \omega_j^2 (q_j(0) - x(0)) \cos\omega_j t \right\}$$

or $$\dot{p} = -V'(x) - \int_0^t \frac{p(t')}{M} K(t-t')\,dt' + \xi(t) \qquad (**)$$

where $K(u) = \sum_j \omega_j^2 \cos(\omega_j u)$

$\xi(u) = \sum_j \left\{ \omega_j p_j(0) \sin(\omega_j t) + \omega_j^2 (q_j(0) - x_j) \cos\omega_j t \right\}$

B) Fluctuations ξ and dissipation K

In principle, $(**)$ is a deterministic equation. In practice, $q_j(0)$ and $p_j(0)$ are impossible to know precisely and they fluctuate widely $\Rightarrow$ use their statistics.

Fluid equilibrated at $t=0 \Rightarrow P(q(0), -, q(N), p(0), -, p(N)) \propto e^{-\beta\left[\sum_j \frac{p_j(0)^2}{2} + \frac{\omega_j^2}{2}(q_j(0)-x\right.}$ ok because $m_j = 1$.

i.e. $P(\{q_i(0), p_i(0)\}) = \prod_i e^{-\beta \frac{p_i(0)^2}{2} - \beta (q_i(0)-x)^2} \equiv \prod_i P_i(q_i(0), p_i(0))$

$\Rightarrow$ independent Gaussian variables.

α) The fluctuations ξ

$\xi(t)$ is a linear combination of the Gaussian variables $q_i(0), p_i(0)$; it is thus a Gaussian variable.

Proof: Let us show that if $\xi = \mu a + \nu b$ with $p(a) = \frac{1}{\sqrt{2\pi\sigma_a}} e^{-\frac{a^2}{2\sigma_a}}$ and $p(b) = \frac{1}{\sqrt{2\pi\sigma_b}} e^{-\frac{b^2}{2\sigma_b}}$ then ξ is Gaussianly distributed.

① $P(\xi_0) = \int P(\xi)\, \delta(\xi - \xi_0)\, d\xi$ (definition of dirac function)

$= \langle \delta(\xi - \xi_0) \rangle_\xi$ (definition of average)

② $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ixk}\, \hat{\delta}(k)\, dk$ (Fourier transform)

$\hat{\delta}(k) = \int_{-\infty}^{+\infty} e^{-ixk} \delta(x) dx = 1 \Rightarrow \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ixk}\, dk$

① + ② $\Rightarrow P(\xi_0) = \langle \delta(\xi - \xi_0) \rangle_\xi = \langle \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\lambda \, e^{i\lambda(\xi - \xi_0)} \rangle$

$$P(\xi_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} da \int_{-\infty}^{+\infty} db \int_{-\infty}^{+\infty} d\lambda \, e^{-i\lambda\xi_0} e^{i\lambda(\mu a + \partial b)} \frac{1}{\sqrt{2\pi\sigma_a}} e^{-\frac{1}{2}\frac{a^2}{\sigma_a}} e^{-\frac{1}{2}\frac{b^2}{\sigma_b}} \frac{1}{\sqrt{2\pi\sigma_b}} \qquad (***)$$

③ Gaussian integral: $\int_{-\infty}^{+\infty} dx \, e^{-\frac{1}{2}ax^2 + bx} = \sqrt{\frac{2\pi}{a}} \, e^{\frac{b^2}{2a}}$

$$(***) + ③ \Rightarrow P(\xi_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\lambda}{\sqrt{2\pi\sigma_a}} e^{-i\lambda\xi_0} \sqrt{2\pi\sigma_a} \, e^{-\frac{\lambda^2\mu^2\sigma_a}{2}} \frac{\sqrt{2\pi\sigma_b} \, e^{-\frac{\lambda^2\partial^2\sigma_b}{2}}}{\sqrt{2\pi\sigma_b}}$$

$$P(\xi_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\lambda \, e^{-i\lambda\xi_0} e^{-\frac{1}{2}\lambda^2(\mu^2\sigma_a + \partial^2\sigma_b)} = \frac{1}{\sqrt{2\pi(\mu^2\sigma_a + \partial^2\sigma_b)}} e^{-\frac{\xi_0^2}{2(\mu^2\sigma_a + \partial^2\sigma_b)}}$$

$\Rightarrow \xi$ is a random variable distributed following a Gaussian law of zero mean and variance $\mu^2\sigma_a + \partial^2\sigma_b$.

__exercise:__ redo with non-zero mean random variables.

__Comment:__ if y is a Gaussian random variable of law $p(y) = \frac{1}{\sqrt{2\pi\sigma_y}} e^{-\frac{1}{2}\frac{(y-y_0)^2}{\sigma_y}}$ then $p(y)$ is entirely characterized by $\langle y \rangle = y_0$ and $\langle y^2 \rangle_c = \sigma_y$.

Going back to $\xi(t) \Rightarrow$ sum of Gaussian variables and hence Gaussian
$\Rightarrow$ entirely characterized by two first cumulants. True for all t
$\Rightarrow$ need to compute $\langle \xi(t) \rangle$ and $\langle \xi(t)\, \xi(t') \rangle$

$$* \langle \xi(t) \rangle = \sum_j \omega_j \sin(\omega_j t) \langle p_j(0) \rangle + \omega_j^2 \cos\omega_j t \, \langle q_j(0) - x_j(0) \rangle = 0$$

$$\langle \xi(t)\,\xi(t')\rangle = \Big\langle \Big[\sum_j \omega_j p_j(0)\sin(\omega_j t) + \omega_j^2\,(q_j(0)-x_j)\cos(\omega_j t)\Big]\Big[\sum_i \omega_i p_i(0)\sin(\omega_i t') + \omega_i^2\,(q_i(0)-x_i)\cos(\omega_i t')\Big]\Big\rangle$$

$\rightarrow$ terms involving $\langle p_i(0)^2\rangle$; $\langle (q_i-x)^2\rangle$ and cross terms $\langle p_i p_{j\neq i}\rangle$ or $\langle (q_i-x)(q_{j\neq i}-x)\rangle$

Since $p_i, (q_j-x)$ are independent variables of zero mean, the cross term vanish.

Using the distributions of p_i and q_i, one gets

$$\langle p_i p_j\rangle = \delta_{ij}\, kT \text{ and } \langle (q_i-x)(q_j-x)\rangle = \delta_{ij}\,\frac{kT}{\omega_j^2} \text{ and } \langle p_i\,(q_j-x)\rangle = 0$$

$$\Rightarrow \langle \xi(t)\,\xi(t')\rangle = \sum_j \omega_j^2\, kT \sin(\omega_j t)\sin(\omega_j t') + \omega_j^4\,\frac{kT}{\omega_j^2}\cos(\omega_j t)\cos(\omega_j t')$$

$$= \sum_j \omega_j^2\, kT \cos[\omega_j(t-t')] = kT\, K(t-t')$$

Comment: $K(t-t')$ characterizes the friction from the medium, i.e. the mean force stemming from a speed $p(t')$ at a later time t.
$\xi(t)$ characterizes the fluctuations around this mean behaviour.
$\boxed{\langle \xi(t)\,\xi(t')\rangle = kT\, K(t-t')}$ is a fluctuation-dissipation relation typical of equilibrium dynamics (cf. D. Machanna's lectures)

Comment: $\dot{p}(t)$ depends on $p(t')$ for $t'<t$. The system has a memory, stored in the surrounding fluid. Its dynamics at time t does not solely depends on its position in phase space $(x(t), p(t))$.
This is the definition of a non-Markovian dynamics. Here, this results from projecting away some degrees of freedom since the initial dynamics for $x, p, q_1, \dots q_N, p_1, \dots, p_N$ was Markovian.

(B) The damping term $K(t-t')$

All the oscillators may have different frequencies $\Rightarrow g(\omega)$ the density of operators having a frequency ω (or rather in $[\omega, \omega+d\omega]$)

$$K(t-t') = \sum_j \omega_j^2 \cos[\omega_j(t-t')] \simeq \int_0^\infty d\omega\, g(\omega) \cos[\omega(t-t')]$$

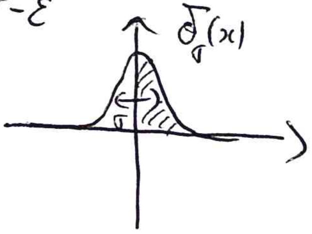
$g(\omega)$ determines $K(t)$.

Let us choose $g(\omega) = \frac{2\gamma}{\pi \omega^2}$; then $K(t) = \frac{2\gamma}{\pi}\int_0^\infty \cos\omega t\, d\omega = \frac{2\gamma}{\pi}\int_{-\infty}^{+\infty} \frac{e^{i\omega t}}{2} d\omega = 2\gamma\,\delta(t)$

The damping term then reads $\int_0^t \frac{p(t')}{M} 2\gamma\, \delta(t-t')$

Comment: $\int_{-\varepsilon}^{\varepsilon} f(t)\delta(t)dt = f(0)$ but $\int_0^{\varepsilon} f(t)\delta(t)dt = ?$

Idea



$\delta(x) = \lim_{\sigma\to 0} \delta_\sigma(x)$ use only one side $\int_0^{\varepsilon} f(t)\delta(t)dt = \frac{f(0)}{2}$

Thus $\int_0^t \frac{p(t)}{m} 2\gamma\delta(t-t')\,dt' = \frac{\gamma}{m} p(t)$ and the dynamics reduces to

$$\begin{cases} \dot{q} = p \\ \dot{p} = -V'(x) - \frac{\gamma}{m} p + \xi(t) \end{cases}$$

with $\xi(t)$ a Gaussian white noise such that

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

This is the celebrated Langevin equation. (1908)

Comment: $K(t)$ is a property of the fluid. Some have memory (visco-elastic media); others don't (Newtonian fluids).

III The large damping limit (a.k.a. the over-damped limit)

Naively, large damping means large dissipation $\Rightarrow$ loss of energy
$\Rightarrow$ no motion

The life of a Brownian particle is very different.

$\dot{x} = v$; $m\dot{v} = -\gamma v - V'(x) + \xi(t)$ with $\langle \xi(t)\,\xi(t')\rangle = 2\gamma kT\,\delta(t-t')$

or equivalently $m\dot{v} = -\gamma v - V'(x) + \sqrt{2\gamma kT}\,\eta(t)$ with $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$

⚠ Normalisation with sloppily appear in or in front of the noise in the following.

Large friction: slow system $\Rightarrow$ evolution over a very long time-scale

tentative scaling $t = \gamma\,\tau$
$\uparrow$ large, $\uparrow$ large, $\tau \to \mathcal{O}(1)$?

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

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

Introduce GRW $\tilde{\eta}(\tau)$ such that $\langle\tilde{\eta}\rangle = 0$ $\langle \tilde{\eta}(\tau)\tilde{\eta}(\tau')\rangle = \delta(\tau-\tau')$

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

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

Thanks to fluctuation-dissipation theorem, $-\gamma v$ and $\sqrt{2\gamma kT}\,\eta$ follow the same scaling as $\gamma \to \infty \Rightarrow$ motion survives

Comment: (**) is nice and simple but $[\gamma] = \frac{M}{T}$

$\tau = \frac{\epsilon}{\gamma}$ is a time counted in $s^2\, kg^{-1}$:-)

Real physicists (i.e. experimentalists) often use proper units $\dot{x} = -\frac{1}{\gamma} V'(x) + \sqrt{\frac{2kT}{\gamma}}\,\eta(t)$

Mobility: If one applies a constant force F to the colloid

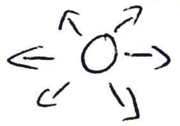
$$\dot{x} = v = \frac{F}{\gamma} + \sqrt{\frac{2kT}{\gamma}}\,\eta \Rightarrow \langle v \rangle = \frac{F}{\gamma} \equiv \mu F$$

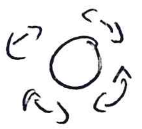
$\mu = \frac{1}{\gamma}$ is called the mobility of the particle; it measures the response of the colloid to an external force.

Comment $\mu = \frac{d\langle v \rangle}{dF}$ looks like a non-equilibrium property (constant drive, no steady-state, etc.) but it is related to $\langle \xi(t)\xi(t') \rangle$ which can be measured in the absence of F $\Rightarrow$ equilibrium property.

Comment: μ can be computed using hydrodynamics (Stokes equation)

Sphere $\gamma = 6\pi R \eta$ where η is the dynamic viscosity of the solvent.



Rotational diffusion  $\dot{\theta} = \sqrt{\gamma_R kT}\,\xi$; $\gamma_R = 8\pi R^3 \eta$

Summary: Large object connected to many equilibrated ones

statistical treatment

Dynamical equation which
- is stochastic
- depends on a small number of parameters ($kT, \gamma, \ldots$)

The Langevin equation is the $PV = NRT$ of non-equilibrium stat Mech

Chapter 3: Itō calculus

In the absence of external potential, the dynamics of our colloid in the overdamped limit is described by

$\dot{x}(t) = \sqrt{2D}\,\eta(t)$ (1) with $\eta(t)$ a Gaussian white noise

$\langle \eta(t) \rangle = 0 \quad \langle \eta(t)\eta(t') \rangle = \delta(t-t')$

I/ Is this really serious?

$\eta(t)$ is a random variable → new value at every time, uncorrelated with previous values ⇒ quite far from continuous, differentiable functions usually used in ordinary differential equations in physics.

History: → R. Brown, 1827, observation of the motion of pollen grains suspended in water. (Actually Jan Ingenhousz did the same with coal particle on the surface of alcohol in 1785)

→ Einstein, 1905, connection with atomistic theory

→ Smoluchowsky, 1906, Langevin, 1908 ⇒ birth of stochastic equations

Mathematical basis are hard to build: Wiener (1918), Itō (1944)

Why? Two important problems

① Formal solution of (1) $x(t) = \int_0^t \eta(t')\,dt' + x(0)$

$$\rightarrow \frac{x(t+\tau)-x(t)}{\tau} = \frac{1}{\tau}\int_t^{t+\tau} \eta(t')\,dt'$$

$$\left\langle \frac{x(t+\tau)-x(t)}{\tau} \right\rangle = \frac{1}{\tau}\int_t^{t+\tau} \langle \eta(t') \rangle\,dt' = 0 \qquad \text{OK ✓}$$

$$\left\langle \left(\frac{x(t+\tau) - x(t)}{\tau} \right)^2 \right\rangle = \frac{1}{\tau^2} \left\langle \int_t^{t+\tau} \eta(s)\,ds \int_t^{t+\tau} \eta(u)\,du \right\rangle = \frac{1}{\tau^2} \int_t^{t+\tau} ds \int_t^{t+\tau} du \underbrace{\langle \eta(s)\eta(u) \rangle}^{\delta(s-u)}$$

$$\forall s \in [t, t+\tau] \quad \int_t^{t+\tau} \delta(s-u)\,du = 1$$

$$\left\langle \left(\frac{x(t+\tau) - x(t)}{\tau} \right)^2 \right\rangle = \frac{1}{\tau^2} \int_t^{t+\tau} ds = \frac{1}{\tau} \xrightarrow[\tau \to 0]{} \infty$$

$x(t)$ is not differentiable $\Rightarrow$ what does $\dot{x}(t)$ mean?

Mathematicians: nothing, only $x(t) = \int_0^t \eta(s)\,ds$ means something $\rightarrow$ Wiener process

Physicists: Yeah, right, but let's still use it, because (1) is a useful notation!

② Diffusion $\quad x^2(t) = \int_0^t ds \int_0^t du\, \eta(s)\eta(u) \Rightarrow \langle x^2(t) \rangle = t$

$\rightarrow$ correct diffusive scaling

$\dot{x}(t) = \eta(t)$; $\frac{d}{dt} x^2(t) = 2x\dot{x} = 2x\eta$ (standard chain rule)

$\frac{d}{dt} \langle x^2(t) \rangle = \langle 2x\eta \rangle = 0$ since $\langle \eta = 0 \rangle$ and $x(t)$ is expected to be correlated only with $\eta(t' < t)$ (causality) so that we expect $\langle x(t)\eta(t) \rangle = \langle x(t) \rangle \langle \eta(t) \rangle$

But $\frac{d}{dt} \langle x^2(t) \rangle = 0$ incompatible with $\langle x^2(t) \rangle = t \Rightarrow$ paradox!

Comment: Not so obvious that $\langle x(t)\eta(t) \rangle = \langle x(t) \rangle \langle \eta(t) \rangle$

Indeed (1) $\Rightarrow x_1(t+dt) = x_1(t) + dt\, \eta(t)$ indeed means $\langle x_1(t+dt)\, \eta(t+dt) \rangle = \underset{=0}{\langle\rangle \cdot \langle\rangle}$

But $x_2(t+dt) = x_2(t) + dt\, \frac{\eta(t) + \eta(t+dt)}{2}$ looks also ok at order dt (semi-implicit scheme). This time $x_2(t+dt)$ and $\eta(t+dt)$ are not independent.

a) Choice of Itô $\langle x(t)\eta(t)\rangle = \langle x(t)\rangle\langle \eta(t)\rangle$ simple but we need to learn how to do calculus again: $\frac{d}{dt}x^2 \neq 2x\dot{x}$

b) Choice of Stratonovich $\Rightarrow$ standard calculus applies but computing $\langle x(t)\eta(t)\rangle$ is painful.

II Itô formula

How does $f(x(t))$ evolve when $x(t)$ is solution of $\dot{x} = F(x) + \eta$ (*) where $\eta(t)$ is a Gaussian white noise with $\langle \eta(t)\rangle = 0$; $\langle \eta(t)\,\eta(t')\rangle = \sigma\,\delta(t-t')$

(or equivalently $\dot{x} = F(x) + \sqrt{\sigma}\,\xi(t)$ with $\langle \xi(t)\,\xi(t')\rangle = \delta(t-t')$)

Comment: Naive solution of (*) $x(t+dt) = x(t) + \underbrace{\int_t^{t+dt} F(x(s))ds}_{\simeq dt\,F(x(t)) + \mathcal{O}(dt^2)} + \underbrace{\int_t^{t+dt} \eta(s)ds}_{d\xi}$

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

$d\xi \sim \sqrt{dt}$! unusual $\to$ this will alter the chain rule.

Comment: To simulate (*), use $x(t+dt) = x(t) + dt\,F(x(t)) + \sqrt{2\sigma dt}\,u$ where u is chosen from a unit-variance, zero mean Gaussian distribution $P(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{u^2}{2}}$

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

$$x(t+dt) = x(t) + F(x(t))\,dt + d\xi(t) + \mathcal{O}(dt^2) \quad ; \quad d\xi(t) = \int_t^{t+dt} \eta(t')\,dt'$$

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

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

Idea: N large, dt small $\Rightarrow$ expand $f(x(t_{j+1})) - f(x(t_j)) \simeq \frac{\partial f}{\partial x}(x(t_j))dx_j + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}(x(t_j))dx_j^2$

where $dx_j = x(t_{j+1}) - x(t_j) \simeq F(x(t_j))dt + d\xi(t_j)$ and $d\xi(t_j) = \int_{t_j}^{t_{j+1}} \eta(s)\,ds$

Then identify $f(x(t)) - f(x(0)) = \int_0^t \frac{df}{dt}(x(s))\,ds$

$$f(x(t)) - f(x(0)) = \sum_{j=0}^{N-1} \frac{\partial f}{\partial x} dx_j + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}\left[F^2 dt^2 + 2F\,dt\,d\xi + d\xi^2\right]$$

Analyse term by term

$$\sum_{j=0}^{N-1} \frac{\partial f}{\partial x} dx_j = \sum_{j=0}^{N-1} \frac{\partial f}{\partial x} \frac{dx_j}{dt} dt \underset{dt\to 0}{\sim} \int_0^t ds \frac{\partial f(x(s))}{\partial x} \dot{x}(s)\,ds = \int_0^t ds \frac{\partial f(x(s))}{\partial x}\left[F(x(s)) + \eta(s)\right]$$

$$\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2} F^2 dt^2 = dt \sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j)) F^2[x(t_j)]\,dt \underset{dt\to 0}{\sim} dt \int_0^t \frac{\partial^2 f}{\partial x^2}(x(s))\, F^2(x(s))\,ds \xrightarrow[dt\to 0]{} 0$$

$$\cancel{\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(s))\, F(x(s))\,dt}$$

$$\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))\, F(x(t_j))\, d\xi(t_j)\, dt = \sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))\, F(x(t_j))\, dt \int_{t_j}^{t_{j+1}} \eta(s)\,ds \equiv A \text{ random variable}$$

$$\langle A \rangle = \sum_{j=0}^{N-1} dt \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))\, F(x(t_j)) \int_{t_j}^{t_{j+1}} \eta(s)\,ds \right\rangle$$

$$\underset{\text{Itô}}{=} \sum_{j=0}^{N-1} dt \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))\, F(x(t_j))\right\rangle \underbrace{\left\langle \int_{t_j}^{t_{j+1}} \eta(s)\,ds \right\rangle}_{=0} \Rightarrow \langle A \rangle = 0$$

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$$\langle A^2\rangle = \sum_{j,k=0}^{N-1} dt^2 \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j)) \frac{\partial^2 f}{\partial x^2}(x(t_k)) F(x(t_j)) F(x(t_k))\, d\xi(t_j)\, d\xi(t_k)\right\rangle$$

if $t_j < t_k$, $d\xi(t_k)$ is independent of the rest $\Rightarrow \langle \ldots d\xi(t_k)\rangle = \langle \ldots\rangle \underbrace{\langle d\xi(t_k)\rangle}_{=0}$

if $t_j = t_k$, $d\xi^2(t_k)$ ________________

$$\langle A^2\rangle = \sum_{j=0}^{N-1} dt^2 \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))^2 F(x(t_j))^2\right\rangle \underbrace{\langle d\xi(t_j)^2\rangle}_{=\sigma\, dt}$$

$$\sim \sigma\, dt^2 \int_0^t \left\langle \left(\frac{\partial^2 f}{\partial x^2}(x(s)) F(x(s))\right)^2\right\rangle ds \xrightarrow[dt\to 0]{} 0$$

same for all the higher moments.

One term left $\frac{1}{2}\sum_{j=0}^{N-1} \frac{\partial^2 f}{\partial x^2}(x(t_j))\, d\xi^2(t_j)$

$d\xi^2(t_j)$ is a random variable such that $\langle d\xi^2\rangle = \sigma\, dt$.
Its higher moments scale as dt^n, $n>1$. Let us show that to compute $f(x(t)) - f(x(0))$ we can simply replace $d\xi^2$ by $\sigma\, dt$ (Note the absence of $\langle\ldots\rangle$).

$$\Rightarrow B \equiv \sum_j \frac{\partial^2 f}{\partial x^2}(d\xi^2 - \sigma\, dt)$$

$$\langle B\rangle = \sum_j \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j)) \left(d\xi^2_{(t_j)} - \sigma\, dt\right)\right\rangle \underset{\text{Itô}}{=} \sum_j \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))\right\rangle \underbrace{\left\langle d\xi^2(t_j) - \sigma\, dt\right\rangle}_{=0}$$

$$= 0$$

$$\langle B^2\rangle = \sum_{j,k} \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j)) \frac{\partial^2 f}{\partial x^2}(x(t_k)) \left(d\xi^2(t_j) - \sigma\, dt\right)\left(d\xi^2(t_k) - \sigma\, dt\right)\right\rangle$$

if $t_j < t_k$, then $d\xi^2(t_k) - \sigma\, dt$ is independent from the rest and
$\langle\ldots\rangle = \langle\ldots\rangle\cdot\langle d\xi^2(t_k) - \sigma\, dt\rangle = 0 \Rightarrow$ only $j=k$ matters.

$$\langle B^2\rangle \underset{\text{Itō}}{=} \sum_{j=0}^{N-1} \left\langle \frac{\partial^2 f}{\partial x^2}(t_j)^2\right\rangle \cdot \left\langle d\xi^4(t_j) - 2\sigma dt\, d\xi^2(t_j) + \sigma^2 dt^2\right\rangle$$

$\langle d\xi^4(t_j)\rangle \overset{?}{=}$ $\Rightarrow$ $d\xi$ is a Gaussian random variable $\Rightarrow$ $\langle d\xi^4\rangle = 3\langle d\xi^2\rangle^2$
(fourth cumulant $C_4 = \langle x^4\rangle - 3\langle x^2\rangle^2 = 0$)

<u>Proof</u>: $$\langle x^4\rangle = \frac{1}{\sqrt{2\pi\sigma}}\int_{-\infty}^{+\infty} dx\, x^4 e^{-\frac{1}{2}\frac{x^2}{\sigma}} = \frac{\sigma}{\sqrt{2\pi\sigma}}\int_{-\infty}^{+\infty} dx\, x^3 \frac{x}{\sigma} e^{-\frac{1}{2}\frac{x^2}{\sigma}}$$

$$= \frac{\sigma}{\sqrt{2\pi\sigma}}\left[-x^3 e^{-\frac{1}{2}\frac{x^2}{\sigma}}\right]_{-\infty}^{+\infty} + \sigma\cdot\frac{3}{\sqrt{2\pi\sigma}}\int dx\, x^2 e^{-\frac{1}{2}\frac{x^2}{\sigma}}$$

$$= 0 + 3\sigma^2 = 3\langle x^2\rangle^2$$

<u>Thus</u>: $\langle d\xi^4\rangle = 3\langle d\xi^2\rangle^2 = 3\sigma^2 dt^2$

$$\langle B^2\rangle = \sum_j \left\langle \frac{\partial^2 f}{\partial x^2}(x(t_j))^2\right\rangle 2\sigma^2 dt^2 \sim 2\sigma dt \int_0^t ds \left\langle \frac{\partial^2 f}{\partial x^2}(s)\right\rangle \xrightarrow[dt\to 0]{} 0$$

Higher moments also vanish and in practice we take $B=0$ in the limit $dt\to 0$

<u>All in all</u>

$$f(x(t)) - f(x_0) = \int_0^t ds \left[\frac{\partial f}{\partial x}(x(s))\,\dot{x}(s) + \frac{\sigma}{2}\frac{\partial^2 f}{\partial x^2}(x(s))\right]$$

Itō lemma: $$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial x}\dot{x} + \frac{\sigma}{2}\frac{\partial^2 f}{\partial x^2}}$$

(β) Generalisation to $f(x(t),t)$

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\sigma}{2}\frac{\partial^2 f}{\partial x^2}}$$

(γ) <u>N-dimensional Itō formula</u>

$\dot{x}_i = F_i(x_1, \dots, x_N) + \eta_i$; $\langle \eta_i\rangle = 0$; $\langle \eta_i(t)\eta_j(t')\rangle = \sigma_{ij}\,\delta(t-t')$

$$\boxed{\frac{df(x_1(t), \dots, x_N(t))}{dt} = \sum_i \frac{\partial f}{\partial x_i}\dot{x}_i + \frac{1}{2}\sum_{ij}\sigma_{ij}\frac{\partial^2 f}{\partial x_i \partial x_j}}$$

Let us come back to $\langle x^2(t)\rangle$

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

$\dot{x}=\sqrt{2D}\,\eta(t) \iff \dot{x}=\xi(t)$

$\langle\eta(t)\rangle=0 \qquad \langle\xi(t)\rangle=0$

$\langle\eta(t)\eta(t')\rangle=\delta(t-t') \qquad \langle\xi(t)\xi(t')\rangle=2D\delta(t-t')$

Itō: $\dfrac{df(x(t))}{dt}=\dfrac{\partial f}{\partial x}\dot{x}+D\dfrac{\partial^2 f}{\partial x^2}=2x\xi+2D \Rightarrow \dfrac{d}{dt}\langle x^2(t)\rangle=2\underbrace{\langle x\xi\rangle}_{\text{Itō}\to 2\langle x\rangle\langle\xi\rangle=0}+2D$

$\Rightarrow \langle x^2(t)\rangle=2Dt$

Comment: can now do better $\dfrac{d}{dt}x^2(t)=2D+\underbrace{2x(t)\xi(t)}$ characterizes the fluctuations of x^2.

Also works for higher moments

$\dfrac{d}{dt}\langle x^4\rangle=4\langle x^3\dot{x}\rangle+D\,12\langle x^2\rangle \underset{\text{Itō}}{=} 4\langle x^3\rangle\underbrace{\langle\dot{x}\rangle}_{=0}+24D^2t$

$\Rightarrow \langle x^4\rangle=12D^2t^2=3\cdot(2Dt)^2=3\langle x^2(t)\rangle^2$

You can now compute moments of $x(t)$ without knowing $P(x,t)$

Comment: the $\xi(t)$ form a set of correlated Gaussian variables.
What is their joint probability distribution?

$$P[\xi(t)]=Z^{-1}\exp\left[-\frac{1}{2}\int_0^t\xi^2(s)ds\right]$$

$\Rightarrow$ weight in trajectory space; can be used to construct path-integral representation of a stochastic process.

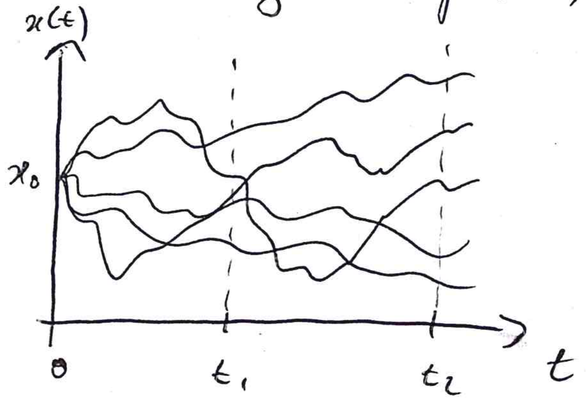
Bibliography: Oksendal, "Stochastic differential equations", Springer

⚠ Remember that $\dot{x}(t)=\sqrt{2D}\,\eta(t)$ is not defined, only ~~$x(t)-x(0)=\int$~~ $x(t)-x(0)=\int_0^t\eta(s)\sqrt{2D}\,ds$ is well defined. The same holds for Itō formula, only $f(t)-f(0)=\int_0^t ds\left[\frac{\partial f}{\partial x}\dot{x}+\frac{\partial^2 f}{\partial x^2}\frac{\Gamma}{2}\right]$ has been proven. Do not start to play with, say, $\exp[\dot{f}(t)]$ and use Itō formulae.

Chapter IV : The Fokker-Planck Equation.

Risken: The Fokker-Planck equation, Springer

$x(t)$ stochastic process solution of $x(0) = x_0$ and $\dot{x}(t) = F(x) + \xi(t)$ $(*)$ where $\xi(t)$ is a Gaussian white noise with zero mean $\langle \xi(t) \rangle = 0$ and variance $\langle \xi(t)\, \xi(t') \rangle = 2D\, \delta(t-t')$. Let us consider several realizations of $x(t)$:



Let us call $P(x(t) = \bar{x}, t \mid x_0, 0)$ the probability density that the process $x(t)$ is at $\bar{x}$ at time t, given that it was at x_0 at time 0. We write more concisely $P(\bar{x}, t \mid x_0, 0)$. Note that, here, $\bar{x}$ and x_0 are simple real numbers and not stochastic processes.

Clearly, $P(x, t_1 \mid x_0, 0)$ and $P(x, t_2 \mid x_0, 0)$ are different

$\rightarrow$ Q: what is the time evolution of $P(x, t \mid x_0, 0)$?

I/ The Fokker-Planck equation

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a C^2 function. By definition

$$\langle f(x(t)) \rangle = \int dx\, f(x)\, P(x, t \mid x_0, 0)$$

and thus

$$\left\langle \frac{df}{dt} \right\rangle = \int dx\, f(x)\, \frac{dP(x, t \mid x_0, 0)}{dt} \qquad (1)$$

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Itō formula: $\frac{df}{dt} = \frac{\partial f}{\partial x}\dot{x} + D\frac{\partial^2 f}{\partial x^2}$ $\quad \underset{\text{Itō}}{=} \langle \frac{\partial f}{\partial x}\rangle \langle \xi(t)\rangle = 0$

$$\Rightarrow \langle \frac{df}{dt}\rangle = \langle \frac{\partial f}{\partial x}F(x)\rangle + \langle D\frac{\partial^2 f}{\partial x^2}\rangle + \langle \frac{\partial f}{\partial x}\xi(t)\rangle$$

$$= \int dx\, \frac{\partial f}{\partial x}F(x)P(x,t|x_0,0) + \frac{\partial^2 f}{\partial x^2}D\,P(x,t|x_0,0)$$

$$\underset{\text{IBP}}{=} \Big[f(x)F(x)P(x,t|x_0,0) + \frac{\partial f}{\partial x}D\,P(x,t|x_0,0)\Big]_{\text{boundary 1}}^{\text{boundary 2}} - \int dx \Big\{ f(x)\frac{\partial}{\partial x}[F(x).P] + f'(x)\frac{\partial}{\partial x}[DP]\Big\}$$

Case 1: periodic boundary conditions $\quad [-]_{\text{boundary 1}}^{\text{boundary 1}} = 0$

Case 2: closed box $x \in [x_1, x_2]$ $\quad P(x<x_1, t|x_0,0) = P(x>x_2, t|x_0,0) = 0$

$\Rightarrow [-] = 0$

Case 3: infinite system, for finite time $P(x=\pm\infty, t|x_0,0) = 0$

$\Rightarrow$ in all cases, we can neglect the boundary terms.

$$\langle \frac{df}{dt}\rangle \underset{\text{IBP}}{=} \int dx\, f(x)\Big[\frac{\partial^2}{\partial x^2}(D\,P(x,t|x_0,0)) - \frac{\partial}{\partial x}(F(x)\,P(x,t|x_0,0))\Big] \quad (2)$$

(1) and (2) hold for any test function f so that

$$\frac{dP(x,t|x_0,0)}{dt} = \frac{\partial}{\partial x}\Big[\frac{\partial}{\partial x}D - F(x)\Big]P(x,t|x_0,0)$$

where $\frac{\partial}{\partial x}$ is an operator that acts on everything on its right

Comment: In (*), the statistics of $\xi(t)$ do not depend on the position of $x(t)$. This is called an <u>additive</u> noise.

On the contrary, in $\dot{x} = F(x) + \sqrt{2D(x)}\,\xi(t)$, with $\langle \xi \rangle = 0$, $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$ (**)

$\sqrt{2D(x)}\,\xi(t)$ is called a <u>multiplicative</u> noise.

Let us now construct the Fokker Planck equation for (**), proceeding in a "dirty" physics way.

$$P(x,t\,|\,x_0,0) = \int d\bar{x}\; P(\bar{x},t\,|\,x_0,0)\,\delta(x-\bar{x}) = \langle \delta(\overset{\text{real number}}{x} - \bar{x}) \rangle_{\bar{x}(t)\ \leftarrow\ \text{stochastic process}}$$

$$\frac{dP}{dt} = \left\langle \frac{d}{dt}\,\delta(x-\bar{x}(t)) \right\rangle \overset{\text{Itō}}{=} \left\langle \frac{d\delta(x-\bar{x})}{d\bar{x}}\,\dot{\bar{x}} + D(\bar{x})\,\frac{d^2}{d\bar{x}^2}\,\delta(x-\bar{x}) \right\rangle$$

$$= \left\langle \frac{d\delta(x-\bar{x})}{d\bar{x}}\,F(\bar{x}) \right\rangle + \underbrace{\left\langle \frac{d\delta(x-\bar{x}(t))}{d\bar{x}}\,\sqrt{2D(\bar{x}(t))}\,\xi(t) \right\rangle}_{\underset{\text{Itō}}{=} \left\langle \frac{d\delta(x-\bar{x}(t))}{d\bar{x}}\sqrt{2D(\bar{x}(t))} \right\rangle \langle \xi(t) \rangle = 0} + \left\langle D(\bar{x})\,\frac{d^2}{d\bar{x}^2}\,\delta(x-\bar{x}) \right\rangle$$

$$\Rightarrow \frac{dP}{dt} = \int d\bar{x}\; \frac{d\delta(x-\bar{x})}{d\bar{x}} \cdot F(\bar{x})\,P(\bar{x},t\,|\,x_0,0) + \frac{d^2\delta(x-\bar{x})}{d\bar{x}^2}\,D(\bar{x})\,P(\bar{x},t\,|\,x_0,0)$$

$$\underset{\text{IBP}}{=} \int d\bar{x}\; \delta(x-\bar{x}) \left[-\frac{\partial}{\partial\bar{x}} \cdot F(\bar{x})\,P(\bar{x},t\,|\,x_0,0) + \frac{\partial^2}{\partial\bar{x}^2} \cdot D(\bar{x})\,P(\bar{x},t\,|\,x_0,0) \right]$$

$$\frac{dP(x,t\,|\,x_0,0)}{dt} = \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}\,D(x) - F(x) \right] P(x,t\,|\,x_0,0)$$

Intuition: ① $F=0$; $\dot{x}=\sqrt{2D}\,\eta \to$ diffusion $\Rightarrow \frac{dP}{dt} = D\Delta P$ diffusion equation.

② $D=0$; $\dot{x}=F(x) \to$ advection $\frac{dP}{dt} = -\operatorname{div}(FP) = -\frac{\partial}{\partial x}[FP]$

①+② $\Rightarrow$ Fokker-Planck equation $\partial_t P = \partial_{xx}(DP) - \partial_x(FP)$

Comment: FPE $\Leftrightarrow \frac{dP}{dt} = -\partial_x (J(x))$ which is a conservation equation for the probability; $J(x)$ is called a probability current.

Example:

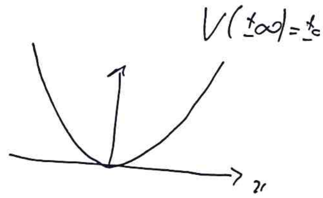
$\dot{x} = -\mu m g + \sqrt{2\mu k T}\,\eta$; FPE: $\partial_t P = +\frac{\partial}{\partial x}\left[\mu m g P + \mu k T \partial_x P\right]$

Steady-state $\Rightarrow P = Z^{-1} \exp\left[-\frac{mgx}{kT}\right]$

This exponential atmosphere is called a Perrin Profile.

Comment: Here the steady-state is given by $J = C^{st}$; the wall at $x=0$ imposes $J=0$, otherwise $\to$ free fall & no steady-state. Boundary conditions are very important.

More general: $\dot{x} = -\mu V'(x) + \sqrt{2kT}\,\eta(t)$ (*) ; $V(x)$ a binding / confining potential



$\partial_t P = \frac{\partial}{\partial x}\left[\mu k T \partial_x P + \mu V'(x) P\right] \Rightarrow P(x) = Z^{-1} e^{-\beta V(x)} \Rightarrow$ Boltzmann weight

The steady-state solution of (1) is the canonical equilibrium. The solvent acts like a thermostat: an equilibrated fluid drives an inert particle into an equilibrated steady-state.

Object in equilibrated bath $\xrightarrow{\text{coarse graining}}$ Langevin equation $\xrightarrow{\text{steady state}}$ Canonical measure

Comment: For P to be normalizable, we need $\int dx\, e^{-\beta V(x)}$ finite $\Rightarrow V(x)$ has to diverge fast enough. $V(x) \underset{x\to\pm\infty}{\sim} \log|x| \Rightarrow$ problem $e^{-\beta V(x)} \sim \frac{1}{|x|^\beta}$ not integrable in $\pm\infty$ for $\beta \leq 1$.

II N-dimensional Fokker-Planck equation

$\dot{x}_i = F_i(\underbrace{x_1, \dots, x_N}_{\equiv \vec{x}}) + \eta_i$ where the η_i's are GWN s.t. $\langle \eta_i \rangle = 0$ & $\langle \eta_i(t)\eta_j(t') \rangle = B_{ij}\,\delta(t-t')$

$$P(x_1, \dots, x_N, t) = \left\langle \prod_i \delta(x_i - x_i^0) \right\rangle_{\vec{x}^0}$$

$$\frac{dP}{dt} = \sum_j \underbrace{\left\langle \prod_{i\neq j} \delta(x_i - x_i^0)\, \frac{\partial \delta(x_j - x_j^0)}{\partial x_j^0}\, \dot{x}_j^0 \right\rangle}_{\overset{=}{\text{Itō}} \left\langle \prod_{i\neq j} \delta(x_i - x_i^0) \frac{\partial \delta(x_j - x_j^0)}{\partial x_j^0} F_j \right\rangle} + \frac{1}{2}\sum_{i,j} \left\langle \frac{\partial^2}{\partial x_i^0 \partial x_j^0}\left[\prod_k \delta(x_k - x_k^0)\right] \times B_{ij} \right\rangle$$

$$= \int \left(\prod_j dx_j^0\right) \left\{ \sum_j \frac{\partial}{\partial x_j}\left[\prod_i \delta(x_i - x_i^0)\right] F_j(\vec{x}^0) P(\vec{x}^0) + \frac{1}{2}\sum_{i,j} \frac{\partial^2 \prod_k \delta(x_k - x_k^0)}{\partial x_i^0 \partial x_j^0} \cdot B_{ij}(\vec{x}^0) P(\vec{x}^0) \right\}$$

$$\overset{\text{IBP}}{=} \int \left(\prod_j dx_j^0\right) \prod_i \delta(x_i - x_i^0) \left\{ -\sum_j \frac{\partial}{\partial x_j^0}\left[F_j(\vec{x}^0) P(\vec{x}_0)\right] + \frac{1}{2}\sum_{i,j} \frac{\partial^2}{\partial x_i^0 \partial x_j^0} B_{ij}(\vec{x}^0) P(\vec{x}^0) \right\}$$

$$\frac{dP}{dt} = \frac{1}{2}\sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j}(B_{ij} P) - \sum_j \frac{\partial}{\partial x_j}(F_j P) = -\sum_j \frac{\partial}{\partial x_j} \cdot J_j(P)$$

$$J_j(P) = \underbrace{-\frac{1}{2}\sum_k \frac{\partial}{\partial x_k}(B_{jk} P)}_{\text{diffusive current}} + \underbrace{F_j P}_{\text{drift term}}$$

Application: The Kramers equation

$\dot{q} = p\ ;\ \dot{p} = -\gamma p - V'(q) + \sqrt{2\gamma k T}\,\eta\ ;\ \langle \eta \rangle = 0\ ;\ \langle \eta(t)\eta(t') \rangle = \delta(t-t')$

$(\sigma_{qq} = 0,\ \sigma_{qp} = 0,\ \sigma_{pp} = 1)$

Itō formula $\quad \dfrac{d}{dt}\left[f(q(t), p(t))\right] = \dfrac{\partial f}{\partial q}\dot{q} + \dfrac{\partial f}{\partial p}\dot{p} + \gamma k T \dfrac{\partial^2 f}{\partial p^2} + \dfrac{1}{2}\cdot 0 \cdot \dfrac{\partial^2 f}{\partial p \partial q} + \dfrac{1}{2}\cdot 0 \cdot \dfrac{\partial^2 f}{\partial q \partial q}$

Fokker-Planck equation: $\boxed{\partial_t P(q,p;t) = -\frac{\partial}{\partial q}(pP) + \frac{\partial}{\partial p}\left(\left[\gamma p + V'(q)\right]P\right) + \gamma k T \frac{\partial^2 P}{\partial p^2}}$

Steady-state under confining potential $H = \frac{p^2}{2} + V(q)$

Show that in steady-state $P_s(q,p) = Z^{-1} e^{-\beta H(q,p)}$

$$Z \partial_t P_s = -\partial_q \left(p e^{-\beta H}\right) + \partial_p \left([\gamma p + V'(q)] e^{-\beta H} \right) + \gamma k T \partial_{pp} e^{-\beta H}$$

$$= \beta p V'(q) e^{-\beta H} + \partial_p \left(\gamma p e^{-\beta H}\right) - \beta p V'(q) e^{-\beta H} + \gamma k T \left(-\beta \partial_p p e^{-\beta H}\right)$$

$$= \gamma \partial_p \left(p e^{-\beta H}\right) - \gamma \partial_p \left(p e^{-\beta H}\right) = 0$$

The steady-state is the same with inertia. Great because γ is a kinetic parameter which does not impact the steady-state. The computation also holds for $\gamma(x)$.

III The Fokker-Planck operator

$\partial_t P = \frac{\partial}{\partial x} \left[kT \frac{\partial}{\partial x} + V'(x) \right] P(x,t)$ (1) $\Leftrightarrow$ $\partial_t P = -H_{FP} P$ where H_{FP} is the operator $H_{FP} = -\frac{\partial}{\partial x} \left[kT \frac{\partial}{\partial x} + V'(x) \right]$ which acts on the Hilbert space of functions $\mathcal{H}(P)$ that depends on the dimensions and boundary conditions of the problem.

The study of H_{FP} contains a lot of information on the dynamics of the system

III.1) Relaxing towards equilibrium

Has the system a typical relaxation time scale? Look for $P(x,t) = e^{-\lambda t} P_0(x)$

$(1) \Rightarrow \partial_t P = -\lambda P_0 e^{-\lambda t} = -H_{FP} P_0 e^{-\lambda t}$ $\Rightarrow$ $H_{FP} P_0 = \lambda P_0$; $P_0(x)$ is an eigenvector of H_{FP}.

If H_{FP} is diagonalisable in $\mathcal{H}(P)$, there exists a basis $\varphi_\alpha(x)$ of $\mathcal{H}(P)$ made of eigenvectors of H_{FP} : $H_{FP} \varphi_\alpha(x) = \lambda_\alpha \varphi_\alpha(x)$.

All initial distributions $P(x,t)$ can be split as $P(x,t) = \sum_\alpha c_\alpha(t) \varphi_\alpha(x)$

One then has

$$\partial_t P = \sum_\alpha \dot{c}_\alpha(t)\,\varphi_\alpha(x) = -H_{FP}\sum_\alpha c_\alpha \varphi_\alpha(x) = -\sum_\alpha c_\alpha(t)\,H_{FP}\,\varphi_\alpha(x) = -\sum_\alpha \lambda_\alpha c_\alpha \varphi_\alpha(x)$$

$\{\varphi_\alpha\}$ is a free family so that $\dot{c}_\alpha = -\lambda_\alpha c_\alpha \Rightarrow c_\alpha(t) = c_\alpha(0)\,e^{-\lambda_\alpha t}$

$$\Rightarrow \boxed{P(x,t) = \sum_\alpha c_\alpha(0)\,e^{-\lambda_\alpha t}\,\varphi_\alpha(x)} \Rightarrow \text{solution (1) } \forall (x,t)\,!$$

Comments: · $\mathrm{Re}(\lambda_\alpha) > 0$, otherwise $P(x,t) \xrightarrow[t\to\infty]{} +\infty \Rightarrow$ normalisation problem...

· $\mathrm{Inf}(\lambda_\alpha) = 0$: $\varphi_0(x) = Z^{-1}\exp[-\beta V(x)]$; $H_{FP}\varphi_0 = 0 \Rightarrow \lambda_0 = 0$

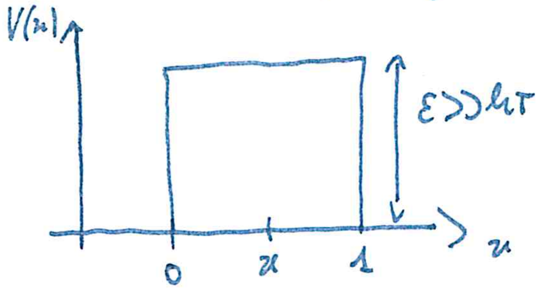
· $P(x,0) = c_1\varphi_1 + c_2\varphi_2$ with $\mathrm{Re}(\lambda_1) < \mathrm{Re}(\lambda_2)$

then $P(x,t) = c_1\varphi_1 e^{-\lambda_1 t} + c_2\varphi_2 e^{-\lambda_2 t} = c_1 e^{-\lambda_1 t}\Big[\varphi_1 + \underbrace{\frac{c_2}{c_1}\varphi_2 e^{-(\lambda_2-\lambda_1)t}}_{\xrightarrow[t\to+\infty]{} 0}\Big]$

φ_2 is "forgotten" exponentially fast, with a typical time-scale given by the gap $\dfrac{1}{\mathrm{Re}(\lambda_2-\lambda_1)}$

$\Rightarrow$ The typical timescale can be read in the spectrum of H_{FP}. (See appendix on metastability)

III.2) Example of diagonalisation of H_{FP}: diffusion with absorbing boundaries



If $x(t)$ exits $[0,1]$, the particle cannot come back $\Rightarrow$ absorbing boundary condition.

Q°: how does $P(x,t)$ evolves for $x \in [0,1]$?

$\rightarrow$ solve $\partial_t P = D\,\partial_{xx}P$ with $P(x=0,t) = P(x=1,t) = 0$

Then $\int_0^1 dx\, P(x,t)$ is the probability that the system is still in $[0,1]$ at time t, this is called a survival probability.

$H_{FP} = -D\frac{\partial^2}{\partial x^2}$; Look for a basis of functions satisfying the boundary conditions and such that $H_{FP}\varphi_\alpha = \lambda_\alpha \varphi_\alpha \Rightarrow \varphi_\alpha''(x) = -\frac{\lambda_\alpha}{D}\varphi_\alpha$; $\varphi_\alpha = Ae^{i\sqrt{\frac{\lambda_\alpha}{D}}x} + Be^{-i\sqrt{\frac{\lambda_\alpha}{D}}x}$

Boundary-conditions: $\varphi_\alpha(0) = 0 \Rightarrow A = -B$ & $\varphi_\alpha(x) = 2iA\sin\left(\sqrt{\frac{\lambda_\alpha}{D}}\,x\right)$

$\varphi_\alpha(1) = 0 \Rightarrow \sqrt{\frac{\lambda_\alpha}{D}} = k_\alpha \pi$ with $k \in \mathbb{Z}^+$

$\Rightarrow \varphi_\alpha(x) = \sin(k_\alpha \pi D)$ and $\lambda_\alpha = D k_\alpha^2 \pi^2$

$t=0$ $P(x,0) = \sum_{k=1}^{\infty} c_k \sin(k\pi x)$ where $c_k = 2\int_0^1 dx \sin(k\pi x) P(x,0)\,dx$

Example: $P(x,0) = \delta(x-x_0) \Rightarrow P(x,t) = \sum_{k=1}^{\infty} 2\sin(k\pi x_0)\sin(k\pi x)\,e^{-Dk^2\pi^2 t}$

$P(x,t) \underset{t\to+\infty}{\sim} 2\sin(\pi x_0)\sin(\pi x)\,e^{-D\pi^2 t}$

$P(x\in[0,1],t) \approx \int_0^1 dx\, P(x,t) \underset{t\to\infty}{\approx} \frac{4}{\pi}\sin \pi x_0\, e^{-D\pi^2 t}$

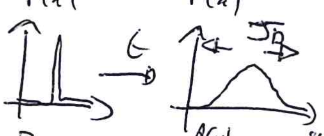
IV Time-reversability

As we shall see, equilibrium system are often associated with the idea of reversibility or with the absence of a clear arrow of time, let us see how this can be rationalized.

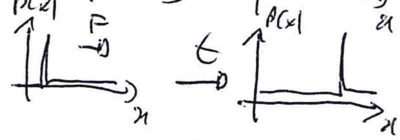
IV.1 Probability current

Fokker-Planck equation: $\partial_t P + \partial_x J = 0$; $J = -D\partial_x P + F(x)P$

$J_D(x) = -D\partial_x P$ diffusive current, spread out the probability



$J_A(x) = F(x)P(x)$ advective current, the force "pushes" the proba



In equilibrium, $J(P) = -kT\partial_x P - V'P = -kT\partial_x[e^{-\beta V}] - V'e^{-\beta V} = 0$

$J(P_{eq}) = 0 \Rightarrow$ no probability flux, there is no preferred direction for the transfer of probability.

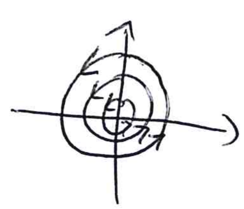
Kramers equation $\partial_t P(q,p) = -\operatorname{div}\vec{J}$; $\vec{J} = (J_q, J_p)$

$J_q = p\,P$; $J_p = -[\gamma p + V'(q)]\,P - \gamma kT \frac{\partial P}{\partial p}$

Equilibrium steady-state: $P \propto \exp[-\beta \mathcal{H}]$

$J_q = p \exp[-\beta\mathcal{H}]$; $J_p = -V'(q)\exp[-\beta\mathcal{H}]$ $\quad \vec{J} \neq \vec{0}$

harmonic oscillator



Rq: $\tilde{\vec{J}}(P) = \vec{J}(P) + \vec{\mathrm{rot}}\,\vec{A}$ then $\operatorname{div}\tilde{\vec{J}}(P) = \operatorname{div}\vec{J}(P) + \operatorname{div}\vec{\mathrm{rot}}\,\vec{A}$

$\vec{\nabla}\cdot\vec{\nabla}\times\vec{A} = 0$

$\partial_t P = -\operatorname{div} J = -\operatorname{div}\tilde{J} \Rightarrow$ which J should vanish!

Reduced current: $(J_q^{\wedge}, J_p^{\wedge}) = (J_q, J_p) + kT\,(\partial_p P, -\partial_q P)$

$\operatorname{div}\vec{J}^{\wedge} = \operatorname{div}\vec{J}$

Equilibrium steady-state $(J_q^{\wedge}, J_p^{\wedge}) = \vec{0}$

$\Rightarrow$ The connection between probability current and equilibrium system and time-reversibility is complex. Is it important? Yes at a fundamental level, no in practice.

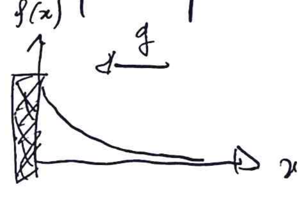
$P(R) = \int dq\,dp\, P(q,p)$; $\partial_t P(R) = -\int dq\,dp\,\operatorname{div}\vec{J}$

$= -\oint d\vec{S}\cdot\vec{J}$

$\Rightarrow$ only | $\operatorname{div}\vec{J}$ matters
| flux of $\vec{J}$ through surfaces.

Comment: even in the simple overdamped case where $J=0$, the vanishing of the current is statistical, it does not mean that a particle at x has equal probability to go right or left.

Example:



$\dot{x} = -\mu m g + \sqrt{2\mu kT}\,\eta$

$\langle \dot{x} \rangle = -\mu m g < 0$

What makes $J=0$ is that the mean fall of particles $J = -\mu m g P$ is balanced by the diffusive drift $-kT\partial_x P$: since $P(x)$ decreases, more particles hop at random from x to $x+dx$ than conversely.

IV.2 Detailed balance

Statistical reversibility means that observing a succession of events, say the system is at x' at time t and at x at time t', is equally likely to observe the reversed ~~succession~~ sequence (x,t) and then (x',t'). This can be written as

$$P(x,t';x',t) = P(x',t';x,t) \qquad (*)$$

Using Bays formula $P(A,B) = P(A|B)\,P(B)$, this becomes in steady-state

$$P(x,t'|x',t)\,P_{st}(x') = P(x',t'|x,t)\,P_{st}(x) \qquad (2)$$

What is the requirement on the evolution operator H_{FP}? Use $t'=t+dt$ and Taylor expand (2)

$$\left[P(x,t|x',t) + dt\,\partial_t P(x,t|x',t)\right] P_{st}(x') = \left[P(x',t|x,t) + dt\,\partial_t P(x',t|x,t)\right] P_{st}(x) \qquad (3)$$

But $P(x,t|x',t) = \delta(x-x')$ as can be checked by computing $\langle f(x(t))\rangle = f(x')$

and $\partial_t P(x,t|x',t) = -H_{FP}(x)\,P(x,t|x',t)$ when the dependency of H_{FP} on x has been made explicit

$$(3) \Leftrightarrow \left[1 - dt\,H_{FP}(x)\right]\delta(x-x')\,P_{st}(x') = \left[1 - dt\,H_{FP}(x')\right]\delta(x-x')\,P_{st}(x) \qquad (4)$$

Since $\delta(x-x')\,f(x') = \delta(x-x')\,f(x)$ for any function f, (4) implies

$$H_{FP}(x)\,\delta(x-x')\,P_{st}(x') = H_{FP}(x')\,\delta(x-x')\,P_{st}(x) \qquad (5)$$

Let us show that for any operator A, one has $A(x)\,\delta(x-x') = A^{+}(x')\,\delta(x-x')$ when the underlying scalar product is $\langle f, g\rangle = \int dx\, f(x)\,g(x)$.

2017 | Take a function $f(x)$ 4.11

$$A(x) f(x) = A(x) \int dx'\, \delta(x-x') f(x') = \int dx'\, f(x') A(x)\, \delta(x-x')$$ since $A(x)$ does not act on functions of x'

$$= \int dx'\, \delta(x-x') A(x') f(x') = \langle \delta(x-x'), A(x') f(x') \rangle = \langle A^{+}(x')\delta(x-x'), f(x') \rangle$$

$$= \int dx'\, f(x') A^{+}(x')\, \delta(x-x')$$

so that $\int dx'\, f(x') \left[A^{+}(x')\delta(x-x') - A(x)\delta(x-x') \right] = 0$

Hence $A^{+}(x')\delta(x-x') = A(x)\delta(x-x')$

(S) can be rewritten

$$H_{FP}(x) P_{st}(x)\, \delta(x-x') = P_{st}(x) H_{FP}(x')\, \delta(x-x') = P_{st}(x) H^{+}_{FP}(x)\, \delta(x-x')$$

so that $\left[H_{FP}(x) P_{st}(x) - P_{st}(x) H^{+}_{FP}(x) \right] \delta(x-x') = 0$

$\Rightarrow H_{FP}(x) P_{st}(x) = P_{st}(x) H^{+}_{FP}(x)$ and $\boxed{H^{+}_{FP}(x) = P_{st}^{-1}(x) H_{FP}(x) P_{st}(x)}$ (**)

Let us check what happens for $H_{FP} = \frac{\partial}{\partial x}\left[T\frac{\partial}{\partial x} + V' \right]$ and $P_{st} = e^{-\beta V}$

$$P_{st}^{-1} \frac{\partial}{\partial x}\left[T \frac{\partial}{\partial x} e^{-\beta V} + V' e^{-\beta V} \right] = P_{st}^{-1} \frac{\partial}{\partial x}\left[T\left(-\beta V' e^{-\beta V} + e^{-\beta V} \frac{\partial}{\partial x} \right) + V' e^{-\beta V} \right]$$

$$= e^{\beta V} \frac{\partial}{\partial x} T e^{-\beta V} \frac{\partial}{\partial x} = e^{\beta V}\left[-\beta V' T e^{-\beta V} + T e^{-\beta V} \frac{\partial}{\partial x} \right] \frac{\partial}{\partial x} = \left(V' - T\frac{\partial}{\partial x} \right)\left(-\frac{\partial}{\partial x} \right) = H^{+}_{FP}$$

$\Rightarrow$ the Fokker-Planck equation satisfies detailed balance

Comment: (**) $\Rightarrow H^{h} = P_{st}^{-1/2} H_{FP} P_{st}^{1/2}$ is hermitian. Indeed

$(H^{h})^{+} = P_{st}^{1/2} H^{+}_{FP} P_{st}^{-1/2} = P_{s}^{-1/2} H_{FP} P_{st}^{1/2} = H^{h} \Rightarrow$ real spectrum and diagonalisable in orthonormal basis.

$\Rightarrow H_{FP}$ also has a real spectrum.

IV.3) The bra-ket notation & linear response

Remember quantum mechanics $|x\rangle$ such that $\hat{x}\,|x\rangle = x\,|x\rangle$

"~~bra~~" "ket" — position operator

$P(x)$ can then be represented by $|P\rangle = \int dx\, P(x)\, |x\rangle$

and $\langle x'|P\rangle = \int dx\, \underbrace{\langle x'|x\rangle}_{\delta(x-x')} P(x) = P(x')$

"bra"

Flat measure $\langle -| = \int dx\, \langle x|$

Average $\langle O(x)\rangle = \int dx\, O(x) P(x) = \langle -|O|P\rangle$

Fokker-Planck $\partial_t |P(t)\rangle = \int dx\, \partial_t P(x,t)\, |x\rangle = -\int dx\, H_{FP}\, P(x,t)\, |x\rangle$

$$\text{“}=\text{”} -H_{FP}\, |P\rangle$$

Solution $|P(t)\rangle = e^{-tH_{FP}}\, |P(0)\rangle$

(Transition probability $P(x,t;x_0,t_0) = \langle x|e^{-(t-t_0)H_{FP}}|x_0\rangle$) later

Diagonalisation: $H_{FP}\, |\psi_\alpha^R\rangle = \lambda_\alpha |\psi_\alpha^R\rangle$; $\langle \psi_\alpha^L| H_{FP} = \lambda_\alpha \langle \psi_\alpha^L|$

$H_{FP} \neq$ hermitian $\Rightarrow |\psi_\alpha^R\rangle$ and $\langle \psi_\alpha^L|$ not transpose of each other.

Conservation of probability: $\int dx\, P(x,t) = 1 \Rightarrow \langle -|P\rangle = 1$

$$\partial_t \langle -|P\rangle = -\langle -|H_{FP}|P\rangle = 0 \Rightarrow \langle -|H_{FP} = 0$$

Steady-state: $\partial_t |P_{stat}\rangle = 0 = -H_{FP}\, |P_{stat}\rangle \Rightarrow H_{FP}\, |P_{stat}\rangle = 0$

Transition proba here

$$P(x,t|x_0,t_0) = \langle x| e^{-(t-t_0)H_{FP}} |x_0\rangle \in \mathbb{R} \Rightarrow P(x,t|x_0,t_0) = \langle x| \dots |x_0\rangle^+$$
$$= \langle x_0| e^{-(t-t_0)H_{FP}^+} |x\rangle$$

$$P^{-1}HP = H^+ \Rightarrow (H^+)^k = P^{-1}HP.P^{-1}HP. \dots P^{-1}HP = P^{-1}H^kP$$

$$\Rightarrow e^{-(t-t_0)H_{FP}^+} = \sum_k [-(t-t_0)]^k \frac{(H_{FP}^+)^k}{k!} = P^{-1}\sum_k [-(t-t_0)]^k \frac{H_{FP}^k}{k!}P = P^{-1}e^{-(t-t_0)H}P$$

$$P(x,t|x_0,t_0) = \langle x_0|P^{-1}e^{-(t-t_0)H_{FP}}P|x\rangle = \frac{P(x)}{P(x_0)}\langle x_0|e^{-(t-t_0)H_{FP}}|x\rangle$$

$$\Rightarrow P(x_0)\,P(x,t|x_0,t_0) = P(x)\,P(x_0,t|x,t_0) \quad \text{detailed balance!}$$

Reciprocity relation

$$C_{AB}(t,t') = \langle -|A\,e^{-(t-t')H}B\,e^{-t'H}|P_{initial}\rangle$$

take $t > t' \to \infty$ $\quad e^{-t'H}|P_{initial}\rangle = |P_{GB}\rangle$

$$C_{AB}(t,t') = C_{AB}(t-t') = \langle -|A\,e^{-(t-t')H}B|P_{GB}\rangle$$
$$= \langle P_{GB}|B^+ e^{-(t-t')H^+}A^+|-\rangle$$
$$= \langle -|e^{-\beta\mathcal{H}}B\,e^{\beta\mathcal{H}}\,e^{-(t-t')H}\,e^{-\beta\mathcal{H}}A|-\rangle$$
$$= \langle -|B\,e^{-(t-t')H}A|-\rangle = C_{BA}(t,t')$$

Measuring A and then B leads to the same correlations as measuring B and then A $\Rightarrow$ signature of time reversal symmetry.

Fluctuation-dissipation relation:

Small perturbation of the energie of the system

$E(t) = E - h(t)\, A(x)$

Impact on observable $B(x)$ for "weak" field

$$\langle B(t)\rangle_h \simeq \langle B(t)\rangle_{h=0} + \text{"}\sum_{t'} \frac{\partial\langle B(t)\rangle}{\partial h(t')} \cdot h(t')\text{"} \quad (\text{Taylor})$$

$$\simeq \langle B(t)\rangle_{h=0} + \int dt'' \frac{\delta\langle B(t)\rangle}{\delta h(t')} h(t') \quad (\text{Functional derivative})$$

$$+ \mathcal{O}(h^2) \to \text{neglect} \to \underline{\text{Linear response}} \quad \frac{\delta\langle B(t)\rangle}{\delta h(t')} \equiv R(t-t')$$

* Take $h(t) = h_0$ for $t < t'$

$\qquad\quad = 0$ for $t > t'$

$\to$ Large t', system equilibrates at $P_{st} = Z_{h_0}^{-1} e^{-\beta[E - h_0 A]}$

$$P_{st}^{h_0} \simeq \frac{1}{Z_{h_0}} (1+\beta h_0 A)\, e^{-\beta E} \;;\; Z_{h_0} = \int dx\, e^{-\beta(E-h_0A)} \simeq \int dx\, (1+\beta h_0 A) e^{-\beta E}$$

$$= Z(1+\beta h_0 \langle A\rangle_{h_0=0})$$

$$P_{st}^{h_0} \simeq \frac{1}{Z} (1+\beta h_0 A)(1-\beta h_0\langle A\rangle)\, e^{-\beta E}$$

$$\simeq \frac{1}{Z} (1 - \beta h_0\langle A\rangle + \beta h_0 A)\, e^{-\beta E}$$

$$\to \langle B(t)\rangle_h \simeq \langle B(t)\rangle_{h=0} + \int_{-\infty}^{t'} dt''\, h_0\, R(t-t'') = \langle -|B\, e^{-(t-t')H} |P_{st}^{h_0}\rangle$$

$$= \langle -|B\, e^{-(t-t')H} (1-\beta h_0\langle A\rangle + \beta h_0 A)\, |P_{st}^{h=0}\rangle$$

$$= \langle B(t)\rangle_{h=0} + \beta h_0 \{ \underbrace{\langle -|B\, e^{-(t-t')H} A\, |P_{st}^{h=0}\rangle}_{C_{BA}(t-t')} - \beta h_0 \langle A\rangle\langle B\rangle \}$$

$$\frac{\partial}{\partial t'} \Rightarrow h_0 R(t-t') = \beta h_0 \frac{\partial}{\partial t'} C_{BA}(t-t') \Rightarrow \boxed{R(t) = -\beta \frac{d}{dt} C_{BA}(t)} = -\beta\langle \dot{B}(t) A(

The response of B to an external perturbation $E \to E - hA$ is given by the correlations between A & B in the absence of the field. 4.15