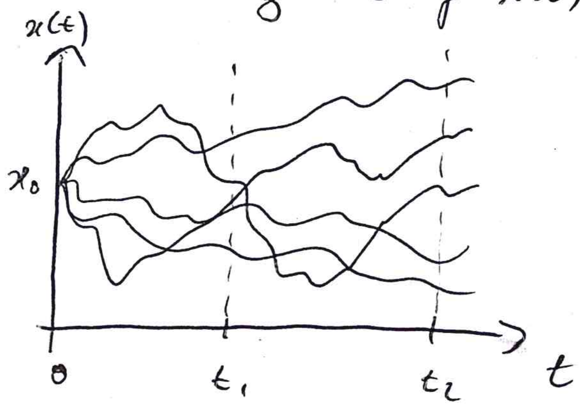
Chapter IV : The Fokker-Planck Equation.

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 $P(x(t) = \bar{x}, t | x_0, 0)$ 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 $P(\bar{x}, t | x_0, 0)$. Note that, here, $\bar{x}$ and x_0 are simple real numbers and not stochastic processes.

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

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

I / The Fokker-Planck equation

Let $f : \mathbb{R} \to \mathbb{R}$ be a C^2 function. By definition ~~$\langle f(x(t)) \rangle$~~

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

and thus

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

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

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

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

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

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

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.

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

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

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

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.

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

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

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

$$\underset{\text{Itô}}{=} \left\langle \frac{d\delta(x-\bar{x}(t))}{d\bar{x}} \sqrt{2D(\bar{x}(t))} \right\rangle \langle \xi(t) \rangle = 0$$

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

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

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

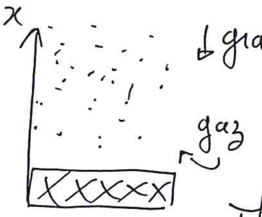
Intuition: ① $F=0$; $\dot{x}=\sqrt{2D}\,\eta \to$ diffusion $\Rightarrow \frac{dP}{dt} = D\Delta P$ diffusion equation.

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:



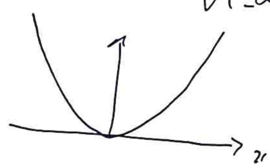
$\dot{x} = -\mu m g + \sqrt{2\mu kT}\,\eta$; FPE: $\partial_t P = +\frac{\partial}{\partial x}\left[\mu m g P + \mu kT \partial_x P\right]$

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



$\partial_t P = \frac{\partial}{\partial x}\left[\mu kT \partial_x P + \mu V'(x) P\right] \Rightarrow P(x) = Z^{-1} e^{-\beta V(x)} \Rightarrow$ 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 $\beta \le 1$.

II N-dimensional Fokker-Planck equation

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

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

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

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

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

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

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

Application: The Kramers equation

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

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

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

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 $P_s(q,p) = Z^{-1} e^{-\beta \mathcal{H}(q,p)}$

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

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

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

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

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

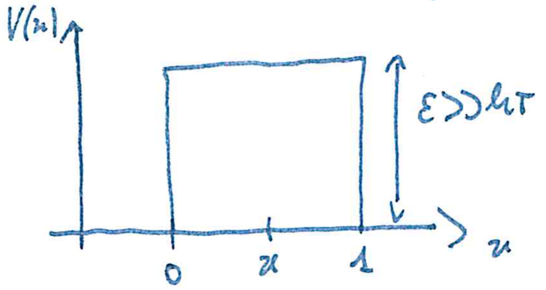
. $P(x,0) = c_1\varphi_1 + c_2\varphi_2$ with $Re(\lambda_1) < Re(\lambda_2)$

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 $\frac{1}{Re(\lambda_2-\lambda_1)}$

$\Rightarrow$ 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 $H_{FP}\varphi_\alpha = \lambda_\alpha \varphi_\alpha \Rightarrow \varphi_\alpha''(x) = -\frac{\lambda_\alpha}{D}\varphi_\alpha$; $\varphi_\alpha = A e^{i\sqrt{\frac{\lambda_\alpha}{D}}x} + B e^{-i\sqrt{\frac{\lambda_\alpha}{D}}x}$

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

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

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

IV Time-reversability

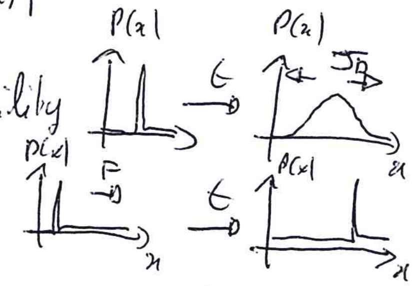
As we shall see, equilibrium system are often associated with the idea of reversibility or with the absence of a clear arrow of time, let us see how this can be rationalized.

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 prefered direction for the transfer of probability.

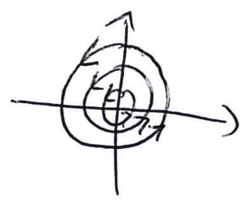
2017 <u>Kramers equation</u> $\partial_t P(q,p) = -\operatorname{div}\vec{J}$; $\vec{J} = (J_q, J_p)$

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

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



<u>Rq:</u> $\tilde{\vec{J}}(P) = \vec{J}(P) + \vec{\mathrm{rot}}\,\vec{A}$ 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!

<u>Reduced current:</u> $(J_{\hat{q}}, J_{\hat{p}}) = (J_q, J_p) + kT\,(\partial_p P, -\partial_q P)$

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

Equilibrium steady-state $(J_{\hat{q}}, J_{\hat{p}}) = \vec{0}$

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

<u>Comment:</u> 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 $\partial_t P(x,t|x',t) = -H_{FP}(x)P(x,t|x',t)$ where 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 $A(x)\,\delta(x-x') = A^{+}(x')\,\delta(x-x')$ where the underlying scalar product is $\langle f,g\rangle = \int dx\, f(x)g(x)$.

2017 Take a function $f(x)$

$$A(x) f(x) = A(x) \int dx' \, \delta(x-x') f(x') = \int dx' f(x') A(x) \delta(x-x')$$ 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" ← $|x\rangle$; $\hat{x}$ ← 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" ← $\langle x'|$

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

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

$$= \langle x_0 | e^{-(t-t_0)H_{FP}^+} | x \rangle$$

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

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

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

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

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 $P_{st} = Z_{h_0}^{-1}\, e^{-\beta[E - h_0 A]}$

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

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

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

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

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

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

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

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

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

4.15