On Stochastic Equations

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Liouville equation

- Classical system: N particles, Hamiltonian $H(\{\vec{q}_i, \vec{p}_i\})$, with $\vec{q}_i = (x_i, y_i, z_i)$ and $\vec{p}_i = (p_{x,i}, p_{y,i}, p_{z,i})$
- Equations of motion

$$\begin{aligned} \dot{\vec{q}}_i &= \frac{\partial H}{\partial \vec{p}_i} \\ \dot{\vec{p}}_i &= -\frac{\partial H}{\partial \vec{q}_i} \end{aligned}$$

- Density of particles at position $\vec{q}$ is proportional to the particle number

$$n(\vec{q}, t) = \sum_{i=1}^{N} \delta(\vec{q} - \vec{q}_i(t))$$

particle conservation $\int \mathrm{d}\vec{q}\, n(\vec{q}, t) = N$

Liouville equation II

- Joint probability distribution function of finding the particle 1 at position $\vec{q}_1$ with momentum $\vec{p}_1$, … particle i at position $\vec{q}_i$ with momentum $\vec{p}_i$, at time t

$$P(\{\vec{q}_i\},\{\vec{p}_i\},t) \propto \sum_i \delta(\vec{q}_i - \vec{q}_i(t))\delta(\vec{p}_i - \vec{p}_i(t))$$

- Time evolution

$$\begin{aligned}\frac{\partial P(\{\vec{q}_i\},\{\vec{p}_i\},t)}{\partial t} &= -\Bigg\{\sum_i \frac{\partial}{\partial \vec{q}_i}\left[\delta(\vec{q}_i - \vec{q}_i(t))\right]\frac{\partial \vec{q}_i}{\partial t}\delta(\vec{p}_i - \vec{p}_i(t)) \\ &\quad + \frac{\partial}{\partial \vec{p}_i}\left[\delta(\vec{p}_i - \vec{p}_i(t))\right]\frac{\partial \vec{p}_i}{\partial t}\delta(\vec{q}_i - \vec{q}_i(t))\Bigg\}\end{aligned}$$

- Plug the Hamilton's equations into the previous equation

$$\frac{\partial P(\{\vec{q}_i\},\{\vec{p}_i\},t)}{\partial t} = \sum_i -\frac{\partial}{\partial \vec{q}_i}\left[P(\{\vec{q}_i\},\{\vec{p}_i\},t)\frac{\partial H}{\partial \vec{p}_i}\right] + \frac{\partial}{\partial \vec{p}_i}\left[P(\{\vec{q}_i\},\{\vec{p}_i\},t)\frac{\partial H}{\partial \vec{q}_i}\right]$$

normalization is conserved $\int \prod_i \mathrm{d}\vec{q}_i \mathrm{d}\vec{p}_i \, P(\{\vec{q}_i\},\{\vec{p}_i\},t) = 1, \quad \forall t.$

Stochastic system

- Canonical ensemble ($T = const.$), prepare you system with any initial condition $P(\{\vec{q}_i\}, \{\vec{p}_i\}, 0)$
- at $t \to \infty$ you expect the system to be in equilibrium

$$P(\{\vec{q}_i\}, \{\vec{p}_i\}, t) = P_{eq}(\{\vec{q}_i\}, \{\vec{p}_i\}) = \frac{\mathrm{e}^{-\beta H(\{\vec{q}_i, \vec{p}_i\})}}{Z}$$

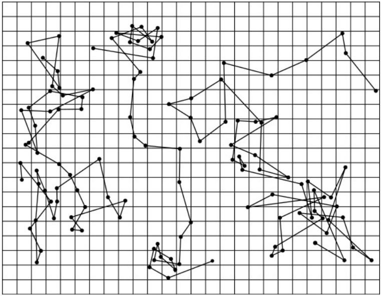
- Extension of the Liouville equation

$$\frac{\partial P(\{\vec{q}_i\}, \{\vec{p}_i\}, t)}{\partial t} = \sum_i -\frac{\partial}{\partial \vec{q}_i}\left[P(\{\vec{q}_i\}, \{\vec{p}_i\}, t)\frac{\partial H}{\partial \vec{p}_i}\right] + \frac{\partial}{\partial \vec{p}_i}\left[P(\{\vec{q}_i\}, \{\vec{p}_i\}, t)\frac{\partial H}{\partial \vec{q}_i}\right] + \boxed{?}$$

Additional terms such that we obtain again the Liouville equation when we eliminate the source of stochasticity?

Brownian motion

A micron-sized particle in solution performs a *random walk*, as an effect of the large number of random collisions with the solvent molecules



Jean Baptiste Perrin, *Les Atomes (1914)*
mastic particle $r = 0.53\,\mu$m, mesh size $3.2\,\mu$m

Langevin equation

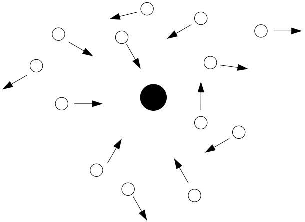
For a single particle in 1D

$$\begin{aligned} \dot{x} &= \frac{p}{m} \\ \dot{p} &= -U'(x) - \gamma \frac{p}{m} + \eta(t) \end{aligned}$$

$\eta(t)$ is called *Gaussian noise*

$$\langle \eta(t) \rangle = 0; \qquad \langle \eta(t)\eta(t') \rangle = 2k_B T \gamma \delta(t - t')$$

Gaussian noise?



- The noise mimics the effect of the large number of random collisions with the solvent molecules
- Central limit theorem $\Rightarrow$ in a small interval δt

$$\mathscr{P}(\eta_t) = \mathrm{e}^{-\delta t \frac{\eta_t^2}{4\gamma k_B T}} \sqrt{\frac{\delta t}{4\pi\gamma k_B T}} \Rightarrow \langle \eta_t \rangle = 0 \quad \text{AND} \quad \langle \eta_t \eta_{t'} \rangle = \frac{2\gamma k_B T}{\delta t} \delta_{t,t'}$$

with $\langle \eta_t \rangle = \int \mathrm{d}\eta_t \, \eta_t \mathscr{P}(\eta_t)$, $\langle \eta_t \eta_{t'} \rangle = \int \mathrm{d}\eta_t \mathrm{d}\eta_{t'} \, \eta_t \eta_{t'} \mathscr{P}(\eta_t) \mathscr{P}(\eta_{t'})$

Liouville eq. $\rightarrow$ Fokker-Planck eq.: quick and dirty

- $$\dot{x} = \frac{p}{m}; \qquad \dot{p} = -U'(x) - \gamma \frac{p}{m} + \eta(t)$$

- $$\frac{\partial P(x,p,t)}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{p}{m}P(x,p,t)\right] + \frac{\partial}{\partial p}\left[\left(U'(x) + \boxed{\gamma \frac{p}{m}}\right)P(x,p,t)\right] + \boxed{?}$$

- we want that $P_{eq}(\{\vec{q}_i\},\{\vec{p}_i\}) = \frac{\mathrm{e}^{-\beta H(\{\vec{q}_i,\vec{p}_i\})}}{Z}$, with $\partial_t P_{eq}(\{\vec{q}_i\},\{\vec{p}_i\}) = 0$

- $$\frac{\partial P(x,p,t)}{\partial t} = -\frac{\partial}{\partial x}\left[\frac{p}{m}P(x,p,t)\right] + \frac{\partial}{\partial p}\left[\left(U'(x) + \boxed{\gamma \frac{p}{m}}\right)P(x,p,t)\right]$$
$$\boxed{+\gamma k_B T \frac{\partial^2}{\partial p^2} P(x,p,t)}$$

$P_{eq}(\{\vec{q}_i\},\{\vec{p}_i\})$ is the stationary solution of the Fokker-Planck equation

Langevin eq. $\to$ Fokker-Planck eq.

- Let's consider a free particle $U(x) = 0 \Rightarrow \dot{p} = -\gamma p/m \Rightarrow$

$$p(t + \delta t) = p(t) - \delta t\, \gamma \frac{p(t)}{m} + \delta t\, \eta(t)$$

with no assumption on the noise variance

$$\mathscr{P}(\eta_t) = \mathrm{e}^{-\delta t \frac{\eta_t^2}{2A}} \sqrt{\frac{\delta t}{2\pi A}} \Rightarrow \langle \eta_t \rangle = 0 \qquad \text{AND} \qquad \langle \eta_t \eta_{t'} \rangle = \frac{A}{\delta t} \delta_{t,t'} \ (*)$$

- Conditional probability of finding momentum p' given that you start from p

$$P(p', t + \delta t | p, t) = \langle \delta(p' - p(t + \delta t)) \rangle_{\text{noise}}$$

where $\langle \ldots \rangle_{\text{noise}}$ is an average over $\mathscr{P}(\eta_t)$

- Let's define $\epsilon = \delta t(-p/m + \eta(t))$, and $p = p(t)$, we have

$$\delta(p' - p - \epsilon) \simeq \delta(p' - p) + \epsilon \frac{\partial}{\partial p} [\delta(p' - p)] + \frac{\epsilon^2}{2} \frac{\partial^2}{\partial p^2} [\delta(p' - p)]$$

Langevin eq. $\to$ Fokker-Planck eq. II

- Consider eq. (*) in the previous slide, and keep the terms up to the first order in δt ($\eta(t) \sim \sqrt{A/\delta t}$)

$$P(p', t{+}\delta t|p,t) = \langle \delta(p' - p - \epsilon)\rangle_{\text{noise}} = \left[1 - \frac{p}{m}\delta t \gamma \frac{\partial}{\partial p} \cdot + \delta t \frac{A}{2}\frac{\partial^2}{\partial p^2}\cdot\right]\delta(p'{-}p)$$

- Use $P(p', t+\delta t) = \int \mathrm{d}p \, P(p', t+\delta t|p,t)P(p,t)$

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

- We want $P(p, t \to \infty) = P_{eq}(p) = \exp\left[-\beta p^2/2m\right]/Z$, with $\partial_t P_{eq}(p) = 0 \Rightarrow$

$$\boxed{A = 2\gamma k_B T}$$

Fluctuation-dissipation relation: the noise (A) and the friction force ($-\gamma p/m$) have the same physical origin

Fokker-Planck $\rightarrow$ Smoluchowski eq.

- in the Langevin eq.

$$m\dot{v} = -U'(x) - \gamma v + \eta(t)$$

  let's assume that the relaxation time $\tau = m/\gamma \ll 1$ is much smaller than any natural time scale associated with the motion in the potential $U(x)$: *overdamped regime*
  Neglect the inertial contribution $m\dot{v}/\gamma$

- The Langevin equation becomes

$$\dot{x} = -\Gamma U'(x) + \tilde{\eta}(t), \qquad \text{with}\, \Gamma = 1/\gamma, \qquad \langle \tilde{\eta}_t \tilde{\eta}_{t'} \rangle = 2\Gamma k_B T \delta(t - t')$$

- With a procedure similar to the one described above one obtains the Smoluchowski equation

$$\frac{\partial P(x,t)}{\partial t} = \Gamma \frac{\partial}{\partial x} \left[U'(x) P(x,t) \right] + \Gamma k_B T \frac{\partial^2}{\partial x^2} P(x,t)$$

Einstein relation

Smoluchowski equation with $U(x) = 0$

$$\frac{\partial P(x,t)}{\partial t} = \Gamma k_B T \frac{\partial^2}{\partial x^2} P(x,t)$$

with stationary solution $P_{st}(x) = \exp(-x^2/(4Dt))/\sqrt{4\pi Dt}$

$$\boxed{D = \Gamma k_B T}$$

$$\left\langle \Delta x^2 \right\rangle_t = 2Dt$$

Generalized Brownian motion

Evolution of an observable: $m(x,p)$ takes values m

$$P_{eq}(m) = \int \mathrm{d}x\mathrm{d}p\, \delta(m(x,p) - m) \frac{\mathrm{e}^{-\beta H(x,p)}}{Z} \equiv \frac{\mathrm{e}^{-\beta \mathcal{F}(m)}}{Z}$$

A SDE for m

$$\frac{dm}{dt} = \mathcal{V}(m) + \eta_m(t),$$

assumptions:

- m varies over time scales which are longer than those for $\eta_m(t)$
- $\eta_m(t)$ is the result of many independent processes
  $\Rightarrow \eta_m$ Gaussian with $\langle \eta_m \eta_m' \rangle = 2\lambda\delta(t - t')$
- m is independent of the instantaneous value of m (this requirement can be relaxed)

Generalized Brownian motion (cont.)

Write a FP equation

$$\frac{\partial P(m,t)}{\partial t} = -\partial_m \left[\mathcal{V}(m) P(x,t)\right] + \lambda \frac{\partial^2}{\partial m^2} P(m,t)$$

and require $P_{eq}(m)$ to be the steady state solution

$$\Rightarrow \mathcal{V}(m) = -\frac{\lambda}{k_B T} \partial_m \mathcal{F}(m)$$

and defining $\Gamma = \lambda / k_B T$ we obtain

$$\frac{dm}{dt} = -\Gamma \partial_m \mathcal{F}(m) + \eta_m(t), \qquad \langle \eta_m \eta'_m \rangle = 2 k_B T \Gamma \delta(t - t')$$

Construction of a field theory

Fields $\phi_{\mathbf{l}}$ defined on N sites of a d-dimensional regular lattice with position $\mathbf{x}_{\mathbf{l}}$

$$H(\{\phi_{\mathbf{l}}\}) = \sum_{\mathbf{l}} G(\phi_{\mathbf{l}}) + \frac{1}{2} \sum_{\mathbf{l},\mathbf{l}'} K_{\mathbf{l},\mathbf{l}'} (\phi_{\mathbf{l}} - \phi_{\mathbf{l}'})^2$$

with $G(\phi)$ a power series expansion about $\phi = 0$ and $K_{\mathbf{l},\mathbf{l}'}$ a finite range coupling matrix.

The partition function and the (overdamped) Langevin equation are well defined

$$\begin{aligned} Z &= \int \prod_{\mathbf{l}} \mathrm{d}\phi_{\mathbf{l}} \, \mathrm{e}^{-\beta H(\{\phi_{\mathbf{l}}\})} \\ \frac{d\phi_{\mathbf{l}'}}{dt} &= -\frac{\partial H(\{\phi_{\mathbf{l}}\})}{\partial \phi_{\mathbf{l}'}} + \eta_{\mathbf{l}'}(t), \qquad \langle \eta_{\mathbf{l}}(t) \eta_{\mathbf{l}'}(t') \rangle = 2 k_B T \delta_{\mathbf{l},\mathbf{l}'} \delta(t - t') \end{aligned}$$

Construction of a field theory (cont.)

continuum limit

- volume per lattice site $\mathbb{v} \to 0$ and keep the total volume $V = N\mathbb{v}$ constant
- $\mathbf{x}_\mathbf{l} \to \mathbf{x}$ continuous variable
- $\sum_\mathbf{l} \to \int \mathrm{d}\mathbf{x}/\mathbb{v}$ (d-dim)
- $$\sum_\mathbf{l} G(\phi_\mathbf{l}) \to \int \mathrm{d}\mathbf{x}\, g\left[\phi(x)\right], \quad g = G/\mathbb{v}$$
- $$\frac{1}{2}\sum_{\mathbf{l},\mathbf{l}'} K_{\mathbf{l},\mathbf{l}'}(\phi_\mathbf{l} - \phi_{\mathbf{l}'})^2 \to \frac{1}{2}\int \mathrm{d}\mathbf{x}\, k(\nabla\phi(\mathbf{x}))^2, \quad k = \frac{1}{d\mathbb{v}}\sum_\mathbf{l} \mathbf{x}_\mathbf{l}^2 K_{\mathbf{l},0}$$

$$\begin{aligned} H\left[\phi(\mathbf{x})\right] &= \int \mathrm{d}\mathbf{x}'\, g\left[\phi(\mathbf{x}')\right] + \frac{1}{2}k(\nabla\phi(\mathbf{x}'))^2 \\ Z &= \int \mathcal{D}\phi(\mathbf{x})\, \mathrm{e}^{-\beta H[\phi(\mathbf{x})]} \end{aligned}$$

Time dependent Landau-Ginzburg equation

$$\frac{d\phi(\mathbf{x})}{dt} = -\frac{\delta H\left[\phi(\mathbf{x})\right]}{\delta\phi(\mathbf{x})} + \eta(\mathbf{x},t),$$
$$\langle\eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle = 2k_B T\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

Taking, e.g., $g\left[\phi(\mathbf{x})\right] = r\phi^2/2 + u\phi^4/4$ one obtains

$$H\left[\phi(\mathbf{x})\right] = \int \mathrm{d}\mathbf{x}'\,\frac{r}{2}\phi^2(\mathbf{x}') + \frac{u}{4}\phi^4(\mathbf{x}') + \frac{1}{2}k(\nabla\phi(\mathbf{x}'))^2$$
$$\frac{d\phi(\mathbf{x})}{dt} = -r\phi(\mathbf{x}) - u\phi(\mathbf{x})^3 + \eta(\mathbf{x},t)$$