** next weeks theory colloquium is about Large-deviation. **

Attend it

Q. from previous lecture.

~~the~~ In our derivation for FP-equation when we expand $\omega(x,y)$, how is $\sum_x W(x,y) = 0$ taken care of?

Note the difference:

$$\frac{dP(x)}{dt} = \sum_y W_{x,y} \, P(y)$$

① Here entries of W-matrix is

$$W_{x,y} = \begin{cases} \omega(x,y) & \text{for } x \neq y \\ -\sum_{z \neq y} \omega(z,y) & \text{for } x = y \end{cases}$$

There is no condition on $\omega(x,y)$. Infact we donot even specif $\omega(x,x)$.

② To go to continuous configuration space we write

$$\frac{dP_t(x)}{dt} = \sum_{y \neq x} \{\omega(x,y) P(y) - \omega(y,x) P(x)\}$$

noting $\{\,\} = 0$ for $y = x$, we can also include $y = x$.

$$\rightarrow \int dy \, \{\omega(x,y) P(y) - \omega(y,x) P(x)\}$$

This way we can define $\omega(x,x)$ as smooth continuation of $\omega(x,y)$ as $y \to x$.

FP equation $\longrightarrow$ Schrödinger equation.

$$\boxed{\frac{d}{dt}P_t(x) = \frac{d}{dx}U'(x)P_t(x) + K_BT\frac{d^2}{dx^2}P_t(x)}$$

most commonly used FP-equation.
A Brownian particle in potential $U(x)$.

Define $P_t(x) = e^{-\frac{1}{2K_BT}U(x)}\,\psi_t(x)$

Do the algebra and show that

$$-\frac{d}{dt}\psi_t(x) = \left\{-K_BT\frac{d^2}{dx^2}\psi_t + V(x)\psi_t\right\}$$

with effective potential

$$V(x) = \frac{1}{4K_BT}\left(U'(x)\right)^2 - \frac{U''(x)}{2}$$

Remark: what does it mean for $\mathcal{L}$-operator?

$$H = -\left(P_{eq}(x)\right)^{\frac{1}{2}}\mathcal{L}\left(P_{eq}(x)\right)^{-1/2} \qquad \left[P_{eq}(x) = e^{-\frac{U(x)}{K_BT}}\right]$$

a choice

$$= -K_BT\frac{d^2}{dx^2} + V(x) \quad \text{is Hermitian.}$$

This makes thing easy.

① For H, both left and right eigenvectors are same.

② $\mathcal{L}\cdot r_\lambda = \lambda r_\lambda \Longrightarrow H\psi_\lambda = -\lambda\psi_\lambda$ with $r_\lambda(x) = \sqrt{P_{eq}(x)}\cdot\psi_\lambda(x)$

$\mathcal{L}^{+}\cdot l_\lambda = \lambda l_\lambda \longrightarrow l_\lambda(x) = \frac{1}{\sqrt{P_{eq}(x)}}\psi_\lambda(x)$

③ Eigenvalues λ are real.

④ Eigenvalue of $\mathcal{L}$ is ~~as~~ minus of eigenvalue of H.

$\Rightarrow$ Steady state for $\mathcal{L}$ $\Leftrightarrow$ ground state of H.

This has important meaning:

Generalization of Perron-Frobenius, which essentially means that there is spectral gap between largest and second largest eigenvalues (non-degeneracy) $\Leftrightarrow$ question of spectral gap for H in QM $\Leftrightarrow$ existence of Bound states.

[Bound states in QM: ① Brownstein, Am. J. Phys. 68 (2000), 160
② Landau & Lifshitz]

An explicit solution

Ornstein-Uhlenbeck Process: Brownian particle in a harmonic potential. $U(x) = \frac{1}{2}x^2$

QM-potential

$$V(x) = \frac{x^2}{4k_BT} - \frac{1}{2}$$

Harmonic oscillator problem.

Eigenvalues $\lambda_n = -n$ with $n = 0, 1, 2, \ldots$

Eigen functions

$$\Psi_n(x) = \left[\frac{1}{2\pi k_BT}\right]^{1/4} \cdot \frac{1}{\sqrt{2^n n!}} \cdot H_n\left(\frac{x}{\sqrt{2k_BT}}\right) e^{-\frac{x^2}{4k_BT}}$$

Hermit polynomial.

$$\Rightarrow r_n(x) = \Psi_n(x) \cdot e^{-\frac{x^2}{4k_BT}}, \quad l_n(x) = \Psi_n(x)\, e^{+\frac{x^2}{4k_BT}}$$

Show: $r_0(x) = P_{st}(x) \propto e^{-\frac{x^2}{2k_BT}}$ and $l_0(x) = 1$ (after trivial re-scaling)

- We know from QM

$$\int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, \psi_m(x) = \delta_{n,m} \qquad \text{Orthonormal.}$$

$$\sum_{n\geq 0}^{\infty} \psi_n^*(x)\, \psi_n(y) = \delta(x-y) \qquad \text{completeness.}$$

Then, solution of F-P equation for OU-process is

$$P_t(x) = \sum_{n\geq 0}^{\infty} e^{-nt}\, r_n(x) \langle l_n | P_0 \rangle$$

$$= \sum_{n\geq 0}^{\infty} e^{-nt} \frac{\psi_n(x)\, e^{-\frac{x^2}{4K_BT}}}{(2\pi K_BT)^{1/4}} \cdot a_n$$

$\leftarrow$ prefactor pulled from $l_n(x)$. ~~[illegible]~~ to make $l_0 = 1$

where

$$a_n = \int_{-\infty}^{\infty} dx\, (2\pi K_BT)^{1/4} \cdot \psi_n(x) \cdot e^{\frac{x^2}{4K_BT}} \cdot P_0(x)$$

<u>Remark</u>: note that e^{-nt}-term in $P_t(x)$ does not depend on K_BT. This means the the spectral gap is one, which gives the time scale to reach steady state. Then this time-scale is independent of K_BT !! Check if this is correct.

Other examples: (A) Free Brownian particle $(U(x)=0)$ on infinite line.

- corresponding QM potential $V(x)=0$:

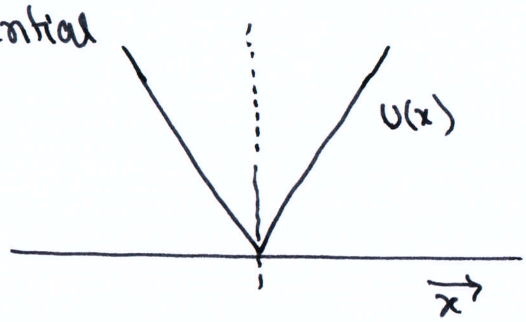
It has only propagating solutions $e^{\pm ikx}$ with eigenvalues of $\mathcal{L}$-operator is continuous and given by

$$\lambda = -k^2 \cdot K_B T \quad \text{for} \quad k \geq 0.$$

- There is no gap in eigen-spectrum, and this means the Brownian particle takes infinite time to reach the uniform distribution, which is zero.

Remark: do the same excercise on a ring,  and show that the spectrum is discrete.

(B) Brownian particle in a linear potential



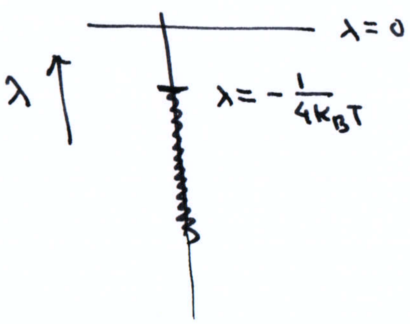
$$U(x) = |x|$$

$\Rightarrow$ QM potential

$$V(x) = \frac{1}{4K_BT} - \delta(x)$$

There is only one bound-state, and that is the stationary state.

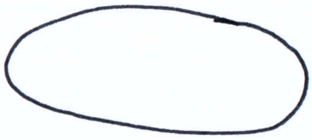
Spectral gap $= \frac{1}{4K_BT}$



Remark: unlike in OU-process, the spectral gap depends on K_BT. This means the time scale $\tau = 4K_BT$ to reach the stationary state depends on K_BT. Check this!

Remark: FP $\rightarrow$ Sch map works when in a potential, meaning when force $= -U'(x)$. This is called a gradient force.

There are examples where force is not gradient.



Brownian in a periodic potential with constant ~~driving~~ Electric field (f)

$$F(x) = \text{Force} = -\underset{\substack{\uparrow \\ \text{Periodic} \\ [U(x+1) = U(x)]}}{U'(x)} + \underset{\substack{\uparrow \\ \text{constant}}}{f}$$

Because of periodicity it is not possible to write $F(x)$ as $-V'(x)$.

~~Show that the stationary st.~~

corresponding Fokker-Planck equation

$$\frac{d}{dt} P_t(x) = -\frac{d}{dx} F(x) P_t(x) + K_B T \frac{d^2}{dx^2} P_t(x)$$

Show that the stationary state

$$P_{st}(x) = P_1(x) + P_2(x) \; ; \quad P_1(x) = \int_0^x dy\, e^{-\frac{1}{K_BT}\left(V(x)-V(y)\right) + \frac{f}{K_BT}(x-y)}$$

$$P_2(x) = e^{\frac{f}{K_BT}} \int_x^1 dy \ldots \underset{\uparrow}{\text{same}} \ldots$$

If driving force $f = 0$, then $P_{st}(x) = P_{eq}(x) = e^{-\frac{U(x)}{K_BT}}$

for $f \neq 0$, system is in non-equilibrium stationary state.

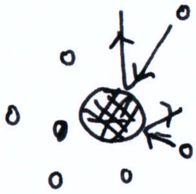
and <u>can not</u> be written as $P_{st}(x) \propto e^{-\frac{1}{K_BT}\phi(x)}$

with a local function $\phi(x)$.

* **Langevin description:** ~~[illegible]~~

A mechanical description of Brownian particle.

$$m\ddot{x} = F(x) - \frac{1}{\mu}\dot{x} + \eta(t) \qquad \text{[Newtons eq}^n\text{]}$$



with

① $\frac{1}{\mu}\dot{x}$ term is due to viscosity in the fluid medium.

For a sphere $\mu = \frac{1}{6\pi\eta R}$, R is the radius, η is viscosity.

μ is called mobility. [Ref. Kardar, vol2, ch6]

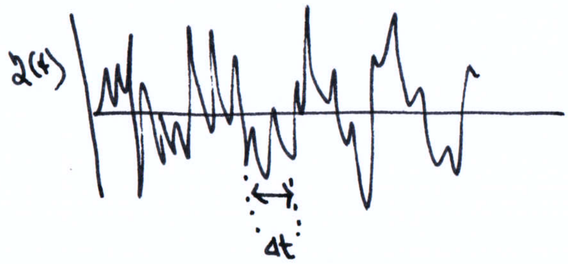
② $\eta(t)$ is a random noise due to kicks from fluid particles.

$$\left.\begin{array}{l}\langle \eta(t)\rangle = 0 \\ \langle \eta(t)\eta(t')\rangle = 2\Gamma\,\delta(t-t')\end{array}\right\}$$ Gaussian noise. All higher cumulant's vanish.

Remark: Mathematically $\eta(t)$ is not a "nice" function to deal.

A better function

$$dW_t = \int_t^{t+\Delta t} ds\, \eta(s)$$



dW_t is continuous everywhere, but nowhere differentiable.

$$P(dW_t) = \frac{1}{\sqrt{4\pi\Gamma\Delta t}}\, e^{-\frac{dW_t^2}{4\Gamma\Delta t}} \iff \langle dW_t\rangle = 0$$

$$\langle (dW_t)^2\rangle = \Delta t\cdot 2\Gamma$$
(from CLT)

dW_t is called a Wiener process.

Remark: Brownian particle gets energy from fluid by the $\eta(t)$ term. and it dissipates energy back to fluid by the $\frac{1}{\mu}\dot{x}$ term.

There is a balance between the two, which gives

$$\boxed{\Gamma\cdot\mu = k_B T}$$

T = temp of the fluid.

Fluctuation dissipation relation.
[Einstein-Smoluchowski relation.]

Jean Perrin confirmed this relation in an experiment.

Gave a conclusive evidence for atomistic world.

Perrin got Nobel prize for this work.

Relation to Fokker-Planck equation:

$$\boxed{\begin{aligned} m\dot{v} &= F(x) - \frac{1}{\mu}v + \eta(t) \\ \dot{x} &= v \end{aligned}}$$

evolution of probability on (x,v)-plane is described by a F-P equation

$$\frac{\partial}{\partial t}P_t(x,v) = \mathcal{L}\cdot P_t(x,v)$$

$$= \frac{\Gamma}{m^2}\frac{\partial^2 P_t}{\partial v^2} + \frac{\partial}{\partial v}\left(\frac{\frac{1}{\mu}v - F(x)}{m}\cdot P_t\right) - v\frac{\partial}{\partial x}P_t$$

How does one show? [see next page]

✡ Overdamped limit:

A simpler limit when inertial term $(m\dot{v})$ can be ignored. This is justified in a highly viscous fluid OR ~~for~~ low Raynold's number. This is often the case in mesoscopic length scale, for example, inside biological cells.

Then, $$m\ddot{x} = F(x) - \frac{1}{\mu}\dot{x} + \eta(t)$$

$$\longrightarrow \quad \dot{x} = \mu\cdot F(x) + \mu\,\eta(t)$$

$$= \mu F(x) + \xi(t) \qquad \text{where } \xi(t) = \mu\,\eta(t)$$

Equivalently: $\langle \xi(t)\rangle = 0$

$$\langle \xi(t)\xi(t')\rangle = 2\Gamma\mu^2\,\delta(t-t')$$