

Theoretical Analysis of Complex Systems

University: 00886 + 9105.

Course 2:

- * Comp. Phys. course.
- * French Phys. ...
- * Course on ...
- MAT 432, MAP Malent,
- PHY Comp. Systems
- * Aff. immersion, gener. F. Plan

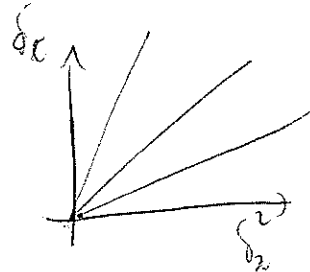
20th Sept, Friday
9h - 12h
wks of knowledge.

Conclusion:

If speed is zero (δt) a scale is still not more?

as in diffuse living cells

(see next page)



if not on line

↳ best macro scale to see sg.

Universality of description \rightarrow asymptotic.

2. Asymmetric. Equation is $\partial_t P + \mathcal{E} \partial_x P = D \partial_x^2 P$
drift + field of force?

$$-\frac{\partial \mathcal{E}}{\partial x} \Rightarrow \text{etc.}$$

"Drift" term.

if going $\rightarrow 0$, neglect the drift.

$$\mathcal{E} \sim \epsilon, \partial_x \sim \epsilon, \partial_t \sim \epsilon^2$$

∂ and \mathcal{E} do not scale in the same way.

Are the two described by same scaling function?

$$\tilde{x} = x_0 + v \cdot t$$

$$P(x, t) = P(x_0 + v \cdot t, t) = P_0(x_0, t) = P_0(x - v \cdot t, t)$$

$$\partial_t P(x, t) = \partial_t P_0 - v \cdot \partial_x P_0$$

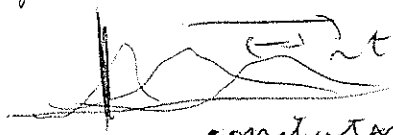
eg. verified by P_0 :

$$\partial_t P_0 - v \partial_x P_0 + \mathcal{E} \partial_x P_0 = D \partial_x^2 P_0$$

take $v = \mathcal{E}$.

$$\partial_t P_0 = D \partial_x^2 P_0$$

In general, such transformation is not possible.



constant velocity $v = \mathcal{E}$

if limit don't depend on $\delta x, \delta t$.

↳ forget about micro-scale.

Goal: How can we describe systems with noise?
what type of noise?

$$x_{t+\delta t} = x_t + \dot{\eta}_t \delta t \quad \text{with } \dot{\eta}_t = \begin{cases} \delta x & \delta \\ -\delta x & \delta \\ 0 & 1-2\delta \end{cases}$$

$$\left| \begin{array}{l} \delta x \rightarrow 0 \\ \delta t \rightarrow 0 \end{array} \right. \quad \delta \frac{\delta x^2}{\delta t} \rightarrow D$$

$$\boxed{\partial_t P = D \partial_x^2 P} \quad \eta(t) = \frac{\delta x}{\delta t}$$

continuous space.

$\dot{x}(t) = \eta(t)$ white noise.

$x(t)$: Brownian motion.

$$P(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{1}{2} \frac{x^2}{2Dt}\right) \quad \text{with } x(0)=0$$

Properties of Brownian and White Noise.

$$\left[\begin{array}{l} \langle [x(t_2) - x(t_1)]^2 \rangle = 2D|t_2 - t_1| \\ \langle \eta(t_2) \eta(t_1) \rangle = 2D \delta(t_2 - t_1) \end{array} \right]$$

Fully describe Brownian
because Gaussian process.

Now more general tool to describe stochastic processes -

Remark: (from micro description)

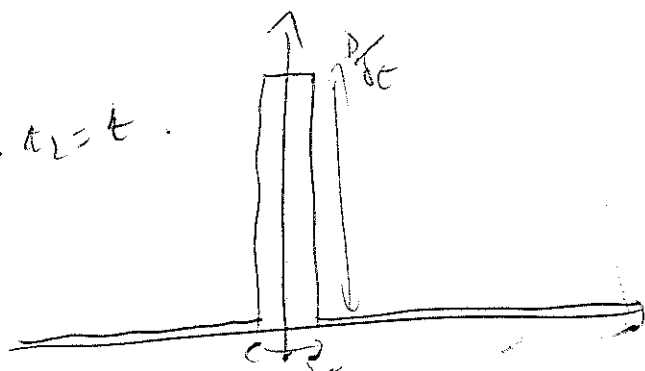
$$t_1 \neq t_2: \langle \eta(t_2) \eta(t_1) \rangle = 0$$

independent

$$t_1 = t_2 = t = \frac{1}{\delta t} \langle \dot{\eta}^2 t \rangle = \frac{1}{\delta t} \left(\delta x^2 \delta + \delta x^2 \delta + 0 \right)$$

$$= 2\delta \frac{\delta x^2}{\delta t} = \boxed{\frac{2D}{\delta t}}$$

$$t_1=0, t_2=t$$



$$\xrightarrow{\delta t \rightarrow 0} 2D \delta(t_2 - t_1)$$

is brownian width.

other way
to obtain
the result.

Let see how related to irregularity of Brownian?

if $x(t)$ was a regular function of t .

$$x(t_2) - x(t_1) \stackrel{c_1 \approx c_2}{\sim} (t_2 - t_1) x'(t).$$

$$\text{then } \langle [x(t_2) - x(t_1)]^2 \rangle \sim (t_2 - t_1)^2.$$

BUT in fact: $|x(t_2) - x(t_1)| \sim \sqrt{t_2 - t_1} \gg |t_2 - t_1|.$

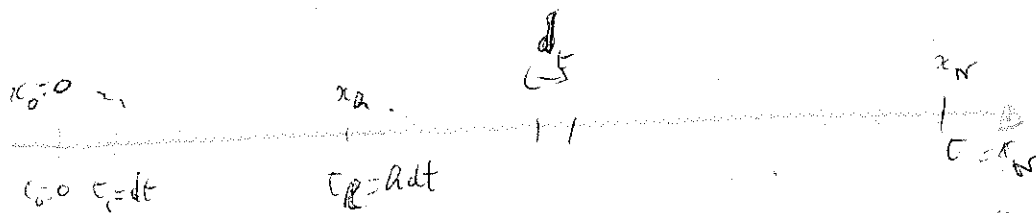
→ Use of Brownian in a physical way.

Distribution of the full trajectories?

$$[x(t')]_{0 \leq t' \leq t}, \quad [\eta(t')]_{0 \leq t' \leq t}$$

$$x(t) = \eta(t) \rightarrow x(t) = \int_0^t dt' \eta(t') \quad \text{Ito Integral}$$

$$(dx = \mu(x) + dB_x)$$



if slice of time $dt = \frac{t}{N} \rightarrow dt \gg \delta_t$ so as to keep a continuous space. (discrete description)

$$P(x_h, t_h | x_{h-1}, t_{h-1}) = \frac{1}{\sqrt{4D(t_h - t_{h-1})}} e^{-\frac{1}{2} \frac{(x_h - x_{h-1})^2}{4D(t_h - t_{h-1})}}$$

* Gaussian growth rates of the Brownian

→ Full trajectory

$$P(x_N, t_N | x_{N-1}, t_{N-1} | \dots | x_0, t_0) = [4D\Delta t]^{-N/2} \exp \left[-\frac{1}{2} \sum_{k=1}^N \frac{(x_k - x_{k-1})^2}{4D\Delta t} \right]$$

observable

$$\langle O(x_0, t_0; \dots; x_N, t_N) \rangle = \int dx_0 \dots dx_N P(x_N, t_N | \dots | x_0, t_0) P(x_0)$$

prob. density of the trajectory of the initial position.

How depends on the discretisation we took?

in the limit:

$$\lim_{h \rightarrow 0} \sum_{k=1}^N dt \left(\frac{x_k - x_{k-1}}{dt} \right)^2 \xrightarrow{dt \rightarrow 0} \int_0^t dt' (\partial_{t'} x)^2$$

(Riemann Sum).

Pre-factor? \rightarrow both \hbar and \hbar^2 of normalisation.

Continuous Time notations:

$$\int \frac{dx_0 \dots dx_N}{[4\pi D dt]^{N/2}} \stackrel{(\text{def})}{=} \int Dx \quad \leftarrow \text{path integral over all possible paths}$$

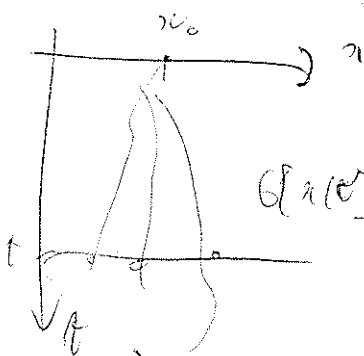
$$\langle G[x(t')] \rangle = \int Dx \cdot G[x(t')] e^{-\frac{1}{2} \int_0^t dt' \frac{(\partial_{t'} x)^2}{2D}} P(x_0)$$

depends not of the discretisation. (if G reasonable!).

In a quantum system \rightarrow "path integral".

Describe which depends on the full trajectory.

e.g. $G[x] = \int_0^t dt' x^2(t') \dots$



$$G[x(t)] = \int_0^t dt' E(x(t'), t')$$

Wiener Integration...

What about the white noise?

$$\eta(t_2) = \eta_R$$

$$P(\underbrace{\eta_1, \dots, \eta_N}_{N+1}, t_0) = \frac{1}{(\sqrt{4\pi D} dt)^{N+1/2}} e^{-\frac{1}{2} \sum_{k=0}^N \frac{\eta_k^2}{2D} dt}$$

$$\text{because } (x_0, \dots, x_N) \Rightarrow (x_0, \eta_0, \dots, \eta_{N-1}) \quad x_2 = x_{2-1} + \eta_{2-1}$$

In the continuous limit,

$$P(\dots) = \prod_{k=0}^N \left[\frac{1}{\sqrt{4\pi D} dt} \cdot \exp\left(-\frac{1}{2} \frac{\eta_k^2}{2D} dt\right) \right]$$

$$-\frac{1}{2} \sum_{k=0}^N \frac{\eta_k^2}{2D} dt$$

$$-\frac{1}{2} \int_0^t dt' \frac{\eta^2(t')}{2D}$$

Quadratic form on the coordinate for x_k, η_k .

↳ Generalization possible → Gaussian Integrals.

- Use of Brownian with forces and interactions.

In many systems, phase transition between 2 kinds of trajectories, phase coexistence.

Use of white noise and Brownian motion to describe the evolution of a particle in a force:

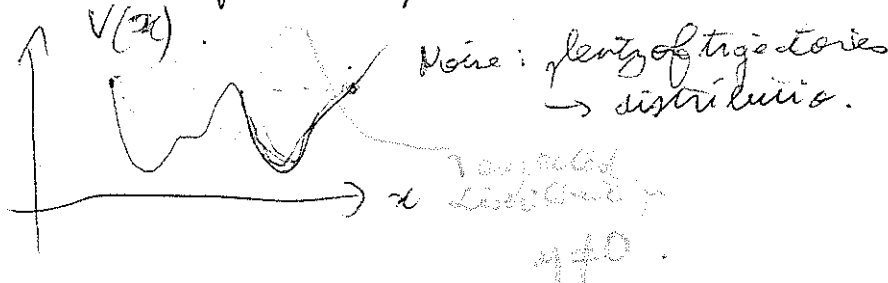
The equation $\partial_t x = \eta(t)$ can be seen as a particular case.

$$\underbrace{m}_{\text{mass}} \partial_t^2 x = \underbrace{-\gamma \partial_t x}_{\text{friction}} + \underbrace{F(x(t), t)}_{\text{deterministic force}} + \underbrace{\eta(t)}_{\text{noise}}.$$

$$\begin{matrix} m=0 \\ F=0 \end{matrix}$$

e.g. $F(x, t) = -V'(x)$.

Forces derive from a potential.



Point of view of trajectories:

$$\partial_t x = F(x(t), t) + \eta(t) \quad \begin{cases} n=0 \\ \neq 0 \end{cases}$$

other method without discretizing space.

(\rightarrow Fokker-Planck - generalized F.P. from Langevin eq.)
[Kramers Eq.]

Let's discretize time & keep x continuous:

$$\int_t^{t+\delta t} \dots$$

$$x_{t+\delta t} - x_t = \underbrace{\int_t^{t+\delta t} dt' F(x(t'), t')}_{\approx \delta t F(x_t, t)} + \underbrace{\int_t^{t+\delta t} dt' \eta(t')}_{\eta_t}$$

"local mean field" \approx η_t

approx. $\approx O(\delta t)$ $O(\sqrt{\delta t})$

$$\eta_t = B(t+\delta t) - B(t)$$

$$\rightarrow B(t) = \int_0^t dt' \eta(t') : \text{Brownian motion}$$

$$\langle \eta_t \rangle = 0$$

$$\langle \eta_t \eta_t \rangle = \langle (B(t+\delta t) - B(t))^2 \rangle = C(\delta t) = 2D \delta t$$

$$\rightarrow \eta_t = O(\sqrt{\delta t}) \quad \because \text{time increments of } B \text{ scales as } \sqrt{\delta t}$$

why important to have this scale property? \rightarrow see flier

Evaluation of $P(x, t)$ - 1st try:

$$P(x, t+\delta t) = \int dx_1 P(x_1, t) P(x, t+\delta t | x_1, t)$$

So we get:

$$\frac{P(x, t + \delta t) - P(x, t)}{\delta t} = \frac{1}{\delta t} \int dx_1 P(x_1, t) \left[P(x, t + \delta t | x_1, t) - \delta(x - x_1) \right]$$

small δt : expansion around $\delta(x - x_1)$.

difficult \rightarrow singularities (small & large values)

From trajectories to distrib for more regularity.

However, still singul. \rightarrow average of an observable to more reg

2nd try: evolutⁿ of an observable $\varphi(x)$.

$$\langle \varphi(x) \rangle_{t+\delta t} = \int dx_1 P(x_1, t) \varphi(x_1)$$

mean value of φ at time $t + \delta t$

variables x_1 at time t .

$$x = x_1 + \delta t F(x, t) + \overset{\circ}{\eta}_t + \mathcal{O}(\delta t^{3/2})$$

\uparrow \uparrow
 $x + \delta t$ x
 $\mathcal{O}(\sqrt{\delta t})$

$$\langle \varphi(x) \rangle_{t+\delta t} = \int dx_1 P(x_1, t) \int d\overset{\circ}{\eta}_t P(\overset{\circ}{\eta}_t) \varphi(x_1 + \delta t F(x, t) + \overset{\circ}{\eta}_t)$$

\rightarrow expansion of φ .

small δt :

$$\varphi(\dots) = \varphi(x_1) + \delta t F(x, t) \varphi'(x_1) + \overset{\circ}{\eta}_t \varphi'(x_1) + \frac{1}{2} \overset{\circ}{\eta}_t^2 \varphi''(x_1) + \mathcal{O}(\delta t^{3/2})$$

$\mathcal{O}(\delta t)$ $\rightarrow \langle \overset{\circ}{\eta}_t^2 \rangle \propto \delta t$

\rightarrow operation of the 2nd derivative thanks to order of $\overset{\circ}{\eta}_t$ in $\sqrt{\delta t}$.

$$= \int dx_1 P(x_1, t) [\varphi(x_1) + \delta t (F(x, t) \varphi' + D \varphi'')]]$$

$$\langle \varphi(x) \rangle_t$$

So we get .

F supposed regular to have mean (no) but one can think to $\langle \dot{x}(t) \rangle = 0$.

$$\frac{\langle \varphi(x) \rangle_{t+\delta t} - \langle \varphi(x) \rangle_t}{\delta t} = \langle F(x, t) \varphi'(x) + D \varphi''(x) \rangle_t$$

(if F not regular, more complicated: no Brownian motion - only solved recently . . .)

eq:

$$\langle F(x, t) \varphi'(x) + D \varphi''(x) \rangle_t = \delta t \langle \varphi(x) \rangle_t$$

math. : φ is a test function - (if distrib.) due to the noise - what does it mean? (going back for observable to try?)

3rd try: $\partial_t x_t = \eta + F$

informally:

$$\partial_t \varphi(x_t) = \varphi'(x_t) \partial_t x_t$$

$$\partial_t \langle \varphi(x) \rangle = \langle F(x, t) \varphi'(x) \rangle + \langle \eta \varphi'(x) \rangle$$

↳ PB to determine

= $D \langle \varphi''(x) \rangle$ from precedent calculation

NOT OBVIOUS -

Equation obtained by Ito formula.

Equation eq to diffusion with Force? \rightarrow Fokker-Planck

By: δ_t not along trajectory, but as time end?

Time derivative of averages:

Correspondence between -trajectories
-distributions.

$$\frac{\langle \varphi(x_{t+\delta t}) - \varphi(x_t) \rangle}{\delta t} = \int dx \frac{P(x, t+\delta t) - P(x, t)}{\delta t} \varphi(x)$$

$\delta t \rightarrow 0$ x as a state variable: not along trajectory, but all distribution.

$$\boxed{\partial_t \langle \varphi(x) \rangle_t = \int dx \partial_t P(x, t) \varphi(x)}$$

Hence -

$$\int dx \partial_t P(x, t) \varphi(x) = \int dx \left[P(x, t) F(x, t) \varphi'(x) + P(x, t) D \varphi''(x) \right]$$

Integrating by part $\varphi \in \mathcal{D}(\mathbb{R})$ [if does for $\varphi \rightarrow$ distributions?]

$$= \int dx \left\{ -\varphi(x) \partial_x [P(x, t) F(x, t)] + D \varphi(x) \partial_x^2 P(x, t) \right\}$$

$$= \int dx \varphi(x) \left\{ \partial_x \left[-F(x, t) P(x, t) + D \partial_x P \right] \right\}$$

$\forall \varphi$

So (...) is $\partial_t P(x)$, we obtain the Fokker-Planck eq.

Fokker-Planck
eq. of evolution

$$\boxed{\partial_t P(x, t) = \partial_x \left[-F(x, t) P(x, t) + D \partial_x P(x, t) \right]}$$

force term diffusion term

Physical interpretation for φ ?

$\varphi \in \mathcal{D}(\mathbb{R})$?

\rightarrow System finite, proba conserved: boundary conditions.

Use of systems at equilibrium.
How related to that?

Steady state $P_{st}(x)$:

\rightarrow $t \rightarrow \infty$ if exists, will converge to it.

$$\partial_x [-F(x, t) P_{st}(x) + D \partial_x P_{st}(x)] = 0.$$

Ex: 1 particle on \mathbb{R} $F=0$:

$$P(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{1}{2} \frac{x^2}{Dt}\right) \xrightarrow{t \rightarrow \infty} 0$$

No steady state

② 1 particle on $[a, b]$, isolated.

$$\partial_x^2 P_{st}(x) = 0 \rightarrow \boxed{P_{st}(x) = \frac{1}{b-a}} \quad \left| \begin{array}{l} \text{uniform} \\ \text{distrib.} \end{array} \right.$$

• Current of probabilities $J[P]$: FPEq:

$$\partial_t P = -\partial_x J[P]. \quad \text{with } J[P] = -[-FP + D \partial_x P].$$

• steady state: $\partial_x J[P_{st}] = 0$

• by def. on equilibrium steady state P_{eq} verifies:

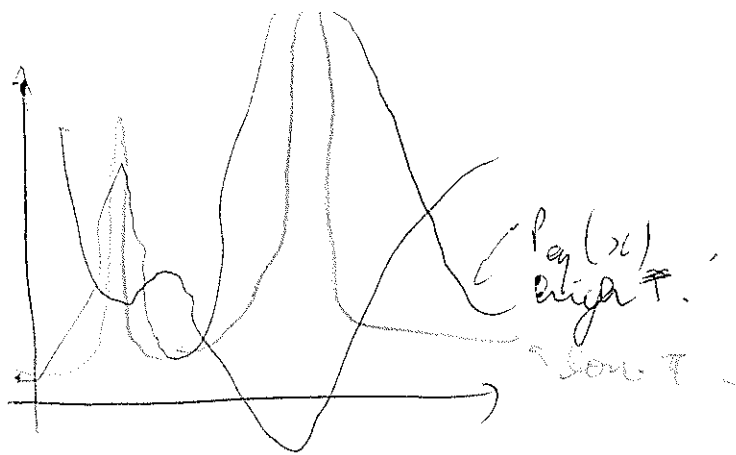
$$J[P_{eq}] = 0, \text{ i.e. } F(x, t) P_{eq}(x) = + D \partial_x P_{eq}(x).$$

1D: $F(x) = -V'(x)$

$$V'(x) P_{eq}(x) = D \partial_x P_{eq}(x)$$

$$\boxed{P_{eq}(x) = \exp\left(-\frac{1}{D} V(x)\right)}$$

Boltzmann distribution in a potential V at "temperature" D .
 Thermodyn. results at long time.



Temperature: How distributed around minimum -
 Case with a current? \rightarrow Project.

Meaning of the current?

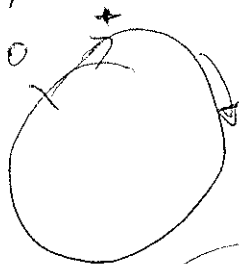
example out of equil.

$$F(x) = f$$

$$\partial_t x = f + \eta$$

average: $\partial_t \langle x \rangle = f \Rightarrow$ mean velocity v is $\boxed{v = f}$.

space is periodic: $[0; 1]$.



$$J(x) = fP + D\partial_x P$$

$$v = \partial_t \langle x \rangle = \langle \partial_t x \rangle = \int dx \partial_t P(x, t) x$$

$$= \int dx (-\partial_x J) x = \int dx J[x]$$

long t.

$$v = \int_0^1 dx J[P_{st}] = \int_0^1 dx j = \bar{j}$$

$$\partial_x J[P_{st}] = 0 \Rightarrow \boxed{J[P_{st}] = \bar{j}}^{2D}$$

$\boxed{\bar{j} = v}$ in that particular case!

$v = f \rightarrow$ coherent eq. steady state: no force!

$$J[P_{eq}] = 0$$

\Rightarrow Reversibility .

[impossible to distinguish between a trajectory and its time reverse]

(explained next time) .