Theoretical Analysis of Complex Systems.
Lecture 1.

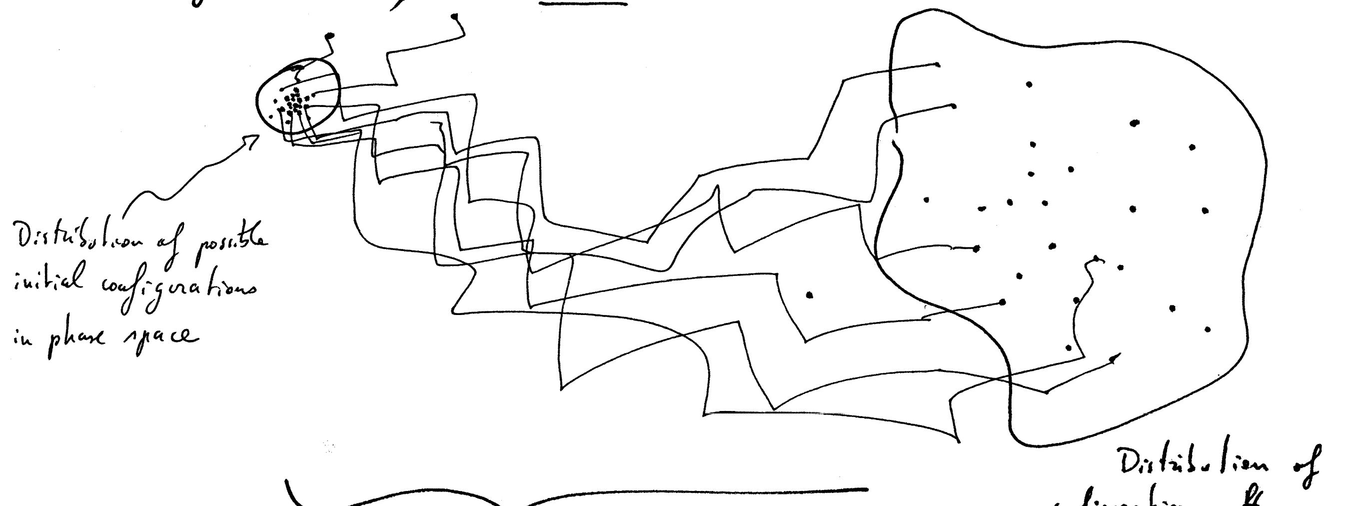
INTRODUCTION TO STOCHASTIC PROCESSES

1. From microscopic to macroscopic: role of fluctuations and randomness.

- Microscopic classical system: N particles of positions $\{\vec{x}_i^{\,mic}\}$ $1 \leq i \leq N$
  - × Evolution in time: Newton's law $m_i \ddot{\vec{x}}_i^{\,mic} = \underbrace{\vec{F}_i(\{\vec{x}_j^{\,mic}\})}$

    forces ruling interactions between particles and with the environment

    Deterministic equations
  - × Very difficult to solve in general. Yet one would like to understand how things work!
  - × Even if a solution is available
    - high sensitivity to initial conditions (Chaos) (Think of billiards or of the baker transformation)
    - high sensitivity to noise



possible evolutions (each trajectory represents the evolution of all $\{\vec{x}_i^{\,mic}\}$) depending on initial conditions and/or different noise realisations.

→ Idea: Focus on distributions rather than on individual trajectories (which also helps to smooth out microscopic details)

- **1st solution**: equilibrium thermodynamics (Boltzmann, Gibbs)

  × microcanonical ensemble: all configurations with the same energy are equiprobable
  (or other global conserved quantity)

  × canonical ensemble: equilibration with a thermostat of temperature β^{-1}

  $$\text{Prob}(\text{configuration}) \propto \exp\{-\beta\, \text{Energy}(\text{configuration})\}$$

↳ Applies
× to determine the mean value of observables
× in the limit of very large system size
× at equilibrium (no currents) and for static properties

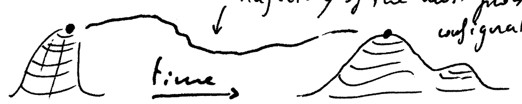
This provide a very generic framework, but is unsuitable to catch
× full distribution of observables (not only the mean value)
× non-equilibrium (currents or time evolutions) dynamics
× generic effects of finite system size

Those effects are less generic (they depend one some microscopic features)

- **2nd solution**: adopt a mesoscopic point of view (i.e. including fluctuations)

Focus one some mesoscopic degrees of freedom $\{\vec{x}_i\}$
Two complementary descriptions:

× evolution of the distribution $P(\{\vec{x}_i\}, t)$

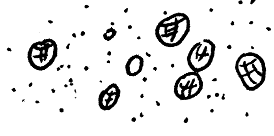


× (effective) evolution of stochastic trajectories

e.g. $$\boxed{m_i \ddot{\vec{x}}_i = \underbrace{-\gamma_i \dot{\vec{x}}_i}_{\text{friction}} + \vec{F}_i(\{\vec{x}_j\}, t) + \underbrace{\vec{\eta}_i}_{\text{noise}}}$$

Both effectively accounting for the effect of microscopic degrees of freedom

→ traditional example: particles in a fluid



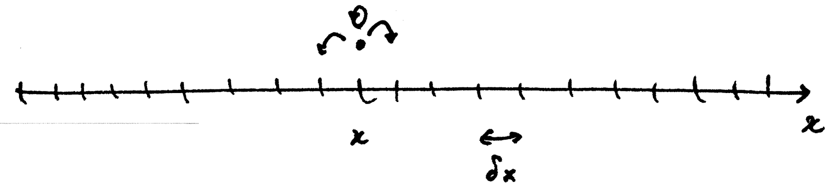
molecules of the fluid induce friction and noise on the mesoscopic particles

However: much more general framework

2 - Archetypal Example : Random Walk and Diffusion in 1D

Between t and $t+\delta t$ a particle can jump symetrycally to its left or its right on a lattice, or stay at the same place

$\mathring{D} < 1/2$



↷ with prob $\mathring{D}$
↶ — $\mathring{D}$
stay — $1-2\mathring{D}$

sum = 1 : conservat° of probability

• Point of view of trajectories :

× initial condition : $x_0 = 0$

× evolution : $\boxed{x_{t+\delta t} = x_t + \mathring{\eta}_t}$, noise $\mathring{\eta}_t = \begin{cases} +\delta x & \text{with prob. } \mathring{D} \\ -\delta x & — \quad \mathring{D} \\ 0 & — \quad 1-2\mathring{D} \end{cases}$

Each occurence of the noise $\mathring{\eta}_t$ is independent of the previous and following ones

This describes the distribution of probability of the noise (The distribution does not depend on time)

How can one take a continuum space limit ? $(\delta t \to 0,\ \delta x \to 0)$

this is not a trivial question : indeed, the instantaneous velocity writes

$$\frac{x_{t+\delta t} - x_t}{\delta t} = \frac{\mathring{\eta}_t}{\delta t}$$

⚠ → depending on how $\delta t \to 0$ & $\delta x \to 0$ it is not obvious to catch how $\mathring{\eta}$ (i.e. $\mathring{D}$) should be tuned so as the limit to be well-defined (i.e. not vanishing nor exploding)

• Point of view of distributions :

$\mathring{P}(x,t)$ = $\underbrace{\text{probability}}$ that the particle is in x at time t
↳ over all possible realizations of the noise $\mathring{\eta}$

⚠ x in $\mathring{P}(x,t)$ is a dummy variable (do not write $\mathring{P}(x_t)$)

× normalisation : $\forall t, \quad \sum_x \mathring{P}(x,t) = 1$

× initial condition : $\mathring{P}(x,0) = \delta_{x0} = \begin{cases} 1 & x=0 \\ 0 & \text{otherwise} \end{cases}$

× evolution :

"Master equation"

$$\boxed{\mathring{P}(x, t+\delta t) = \underbrace{\mathring{D}\,\mathring{P}(x-\delta x,t) + \mathring{D}\,\mathring{P}(x+\delta x,t)}_{\text{one was in } x\mp\delta x \text{ at time } t} + \underbrace{(1-2\mathring{D})\,\mathring{P}(x,t)}_{\text{one was already in } x \text{ at time } t.}}$$

• The continuum limit is now easier to tackle: the master equation rewrites:

$$\frac{\mathring{P}(x,t+\delta t)-\mathring{P}(x,t)}{\delta t} = \frac{\mathring{D}}{\delta t}\left[\mathring{P}(x-\delta x,t)+\mathring{P}(x+\delta x,t)-2\mathring{P}(x,t)\right] \quad (*)$$

One introduces a probability density $P(x,t)$ of the continuous variables x,t

$$\boxed{P(x,t) = \frac{1}{\delta x}\mathring{P}(x,t)}$$ in the limit $\delta x \to 0$, $\delta t \to 0$

with normalisation condition $\int dx\, P(x,t) = 1 \;\; \forall t$ (arising from $\sum_x \overbrace{\mathring{P}(x,t)}^{\delta x \cdot P(x,t)} = 1$)

and initial condition $P(x,0) = \delta(x)$ (Dirac delta; arising from $P(x,0) = \lim_{\delta x \to 0} \frac{\delta_{0x}}{\delta x} = \delta(x)$)

[Remark: normalizing probabilities is very important!]

Expanding $(*)$ for small δt and small δx one obtains:

$$\partial_t P(x,t) = \frac{\mathring{D}}{\delta t}\Big[\underbrace{P(x,t)+P(x,t)-2P(x,t)}_{=0 \text{ (conservation of probability)}} + \underbrace{(-\partial_x P + \partial_x P)\delta x}_{=0 \text{ (symmetry of the noise)}} + \underbrace{(\tfrac{1}{2}+\tfrac{1}{2})\delta x^2\, \partial_x^2 P(x,t)}_{\text{first non-trivial term of the expansion}}\Big]$$

$$\partial_t P(x,t) = \frac{\mathring{D}\,\delta x^2}{\delta t}\,\partial_x^2 P(x,t)$$

One thus obtains a non-trivial and well defined limit provided $\boxed{D = \frac{\mathring{D}\,\delta x^2}{\delta t}}$ is finite

$$\boxed{\partial_t P(x,t) = D\,\partial_x^2 P(x,t)} \quad (**)$$

This is the $\boxed{\text{diffusion equation}}$. (Occurs in a lot of contexts!)

Solution by scaling: $P(x,t) \overset{?}{=} t^{-\zeta}\hat{P}(x t^{-\zeta})$ with $1 = \int dx\, P(x,t) = \int d(xt^{-\zeta})\,\hat{P}(xt^{-\zeta}) = \int d\hat{x}\,\hat{P}(\hat{x})$ ($\hat{P}$ normalized to 1)

with $\hat{x} = x t^{-\zeta}$, $(**) \iff -\zeta \underbrace{t^{-1-\zeta}}\left(\hat{P}(\hat{x}) + \hat{x}\,\hat{P}'(\hat{x})\right) = D\underbrace{t^{-3\zeta}}\,\hat{P}''(\hat{x})$

meaningful only provided $-1-\zeta = -3\zeta$ ie $\boxed{\zeta = 1/2}$

The Partial Differential Equation (PDE) then reduces to an Ordinary Differential Equation (ODE)

$$\hat{P}(\hat{x}) + \hat{x}\,\hat{P}'(\hat{x}) + 2D\,\hat{P}''(\hat{x}) = 0$$

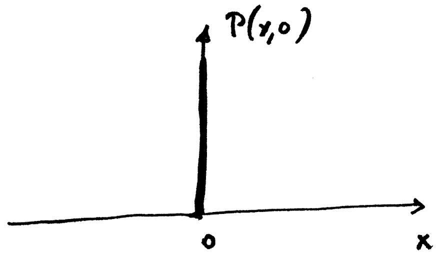
A (normalized) solution is $$\boxed{\hat{P}(\hat{x}) = \frac{1}{\sqrt{4\pi D}}\, e^{-\frac{1}{2}\frac{\hat{x}^2}{2D}}}$$

3. Analysis of the solution and continuum limit for trajectories:

Lecture on Complex Systems (15)

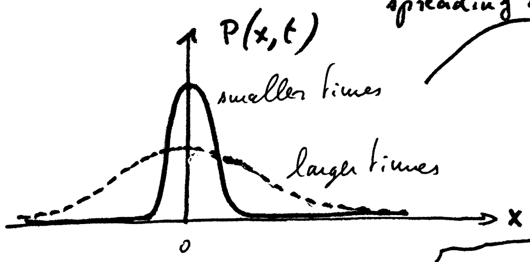
One thus finds
$$\boxed{P(x,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{1}{2}\frac{x^2}{2Dt}}}$$

this describes the spreading of trajectories as time increases in a space-time representation

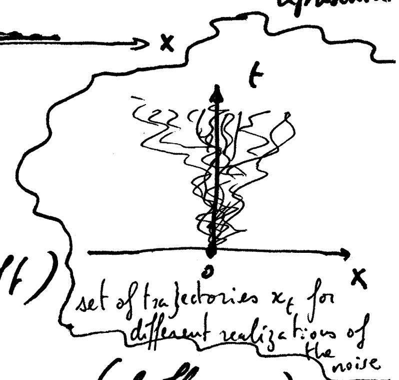


$t = 0$

$\underset{t>0}{\leadsto}$



$t > 0$



The average $\langle x(t)\rangle = 0$ is always zero (no drift)

The variance $\langle x^2(t)\rangle = 2Dt$ is increasing linearly with time (diffusion)

$\boxed{\text{What is the continuum limit of the noise ?}}$ What distribution does it have?

↳ let's first determine the mean & variance.

Let us recall the discrete evolution
$$\frac{x_{t+\delta t} - x_t}{\delta t} = \frac{\mathring{\eta}_t}{\delta t} \qquad \text{with} \qquad \mathring{\eta}_t = \begin{cases} +\delta x & \text{prob. } \mathring{D} \\ -\delta x & \text{prob. } \mathring{D} \\ 0 & \text{prob. } 1-2\mathring{D} \end{cases}$$

one has found that: keeping $D = \frac{\mathring{D}\,\delta x^2}{\delta t}$ finite yields the "correct" continuum limit.
Our aim is to give a meaning to the equation $\boxed{\partial_t x = \eta(t)}$

× average of the noise: where $\eta(t) = \frac{\mathring{\eta}_t}{\delta t}$ the "correct" limit of the noise.

$$\langle \eta(t)\rangle = \langle \partial_t x\rangle = \partial_t \langle x\rangle = \partial_t \int dx\, x\, P(x,t) = 0$$

jump from averaging on trajectories to averaging with the distribution $P(x,t)$

Hopefully, this is compatible with the discrete-time
$$\langle \mathring{\eta}_t\rangle = \delta x\,\mathring{D} - \delta x\,\mathring{D} + 0\times(1-2\mathring{D}) = 0$$

× variance of the noise: determining $\langle \eta(t_1)\eta(t_2)\rangle$ requires to know the two-point distribution $P(x_1 t_1 ; x_2 t_2)$.

One has in fact:
$$\boxed{P(x_2 t_2 \,|\, x_1 t_1) = \frac{1}{\sqrt{4\pi D(t_2-t_1)}}\, e^{-\frac{1}{2}\frac{(x_2-x_1)^2}{2D(t_2-t_1)}}} \qquad \text{for } t_2 > t_1$$

The demonstration is the same as previously (it amounts to change the origins of time and space)

Let's first determine the correlator $C_2(t_1,t_2) = \langle (x(t_2) - x(t_1))^2\rangle$ of the integral $x(t) = \int_0^t d\tau\, \eta(\tau)$
which is a more regular quantity than $\eta(t)$.

[Indeed determining $\langle \eta(t_1)\eta(t_2)\rangle$ directly may lead to inconsistencies.]

One has: for $t_2 > t_1$

$$C_2(t_1,t_2) = \langle (x(t_2)-x(t_1))^2 \rangle = \int dx_1 dx_2 \, (x_2-x_1)^2 \underbrace{P(x_2\, t_2 \,|\, x_1\, t_1)} \, \underbrace{P(x_1\, t_1)}$$

allows to sample the position $x_2 = x(t_2)$ at time $t_2 > t_1$, knowing that one had $x(t_1) = x_1$

allows to follow the evolution of the distribution up to time t_1 and to sample $x_1 = x(t_1)$

The computation is a matter of Gaussian integrals. One finds:

$C_2(t_1,t_2) = 2D\,(t_2-t_1)$ and similarly if $t_1 > t_2$ $C(t_1,t_2) = 2D(t_1-t_2)$

Finally: $$\boxed{C_2(t_1,t_2) = \langle (x(t_2)-x(t_1))^2 \rangle = 2D\,\underbrace{|t_2-t_1|}} \quad (*)$$

This absolute value is (although unnoticeably) extremely important.

- Formal Remark: link between $\underbrace{\langle (x(t_2)-x(t_1))^2 \rangle}_{\equiv C_2(t_1,t_2)\equiv C(t_2-t_1)}$ and $\underbrace{\langle \eta(t_2)\,\eta(t_1)\rangle}_{\equiv R_2(t_1,t_2)\equiv R(t_2-t_1)}$:

Using $x(t)-x(0) = \int_0^t dt'\,\eta(t')$

One has: $C''(t) = \partial_t^2 \langle [x(t)-x(0)]^2 \rangle = \partial_t^2 \int_0^t dt_1 \int_0^t dt_2 \underbrace{\langle \eta(t_2)\,\eta(t_1)\rangle}_{R(t_2-t_1)} = \dots = R(t) + R(-t)$

Thus, using the parity $R(t) = R(-t)$ [arising from $\langle \eta(t)\eta(0)\rangle = \langle \eta(0)\eta(-t)\rangle$ by invariance of the distribution of η by translation along time]

One finally gets: $\boxed{R(t) = \frac{1}{2}\, C''(t)}$ i.e $\boxed{\langle \eta(t)\eta(0)\rangle = \partial_t^2 \langle (x(t)-x(0))^2 \rangle}$

- Finally: one gets the variance of $\eta(t)$ from (*)

$$\boxed{\langle \eta(t_2)\,\eta(t_1)\rangle = 2D\,\delta(t_2-t_1)}$$ Dirac-delta correlations

- Remark: this corresponds to a naive argument on $\mathring{\eta}_t$: (with $\eta(t) = \frac{\mathring{\eta}_t}{\delta t}$)

indiscrete time

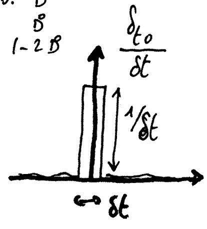
if $t_2 \neq t_1$, $\langle \eta(t)\,\eta(t_2)\rangle = \frac{1}{\delta t^2}\langle \mathring{\eta}_{t_1}\mathring{\eta}_{t_2}\rangle = 0$ since for $t_1 \neq t_2$, $\mathring{\eta}_{t_1}$ and $\mathring{\eta}_{t_2}$ are uncorrelated

if $t_1 = t_2 = t$, $\langle \eta(t)\,\eta(t)\rangle = \frac{1}{\delta t^2}\langle \mathring{\eta}_t^2\rangle = \frac{1}{\delta t^2}\underbrace{\left(\delta x^2\,\mathring{D} + \delta x^2\,\mathring{D} + 0\cdot(1-2\mathring{D})\right)}$

since $\mathring{\eta}_t = \begin{cases} \delta x & \text{with prob. } \mathring{D} \\ -\delta x & \quad = \quad \mathring{D} \\ 0 & \quad = \quad 1-2\mathring{D} \end{cases}$

$$= 2\,\frac{\mathring{D}\,\delta x^2}{\delta t}\,\frac{1}{\delta t} \quad \text{where } D = \frac{\mathring{D}\,\delta x^2}{\delta t}$$

Hence: $$\langle \eta(t_1)\,\eta(t_2)\rangle = 2D\,\frac{\delta_{t_1 t_2}}{\delta t} \xrightarrow[\delta t\to 0]{} 2D\,\delta(t_2-t_1)$$



• Remark : regularity of the function $x(t)$

One has $\left\langle \left(x(t+\delta t) - x(t)\right)^2 \right\rangle = \delta t$

Hence $\boxed{|x(t+\delta t) - x(t)| \sim \sqrt{\delta t}}$ which is much larger than δt

(one would have $x(t+\delta t)-x(t) \sim \delta t$ for a differentiable / regular-enough function)

⚠ Note that from the discrete equation $x_{t+\delta t} = x_t + \eta_t$ this behavior is not obvious as long as one has not determined the correct $\delta x \to 0$, $\delta t \to 0$ limit.

◐ - the evolution of the distribution is very simple (a Gaussian)
- the trajectories are non-trivial 'processes'.

4. Determination of the distribution of trajectories : the Brownian motion

• After having determined $\langle \eta(t) \rangle = 0$, $\langle \eta(t)\eta(t') \rangle = 2D\,\delta(t-t')$

or equivalently $\langle x(t) \rangle = 0$, $\langle [x(t)-x(t')]^2 \rangle = 2D\,|t-t'|$

through $x(t) = \int_0^t dt'\,\eta(t')$

let us now determine the full distribution of the processes $[\eta(t)]_{0\le t'\le t}$, $[x(t')]_{0\le t'\le t}$

• This is not direct, since $P(x,t) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{1}{2}\frac{x^2}{2Dt}}$ gives only the distribution at final time.

• Let us discretize time, keeping x continuous

values of the positions $x_k = x(t_k)$ at different times t_k.

$x_0 = 0$, x_1, x_2 ...

dt $\qquad (dt \gg \delta t)$

time

$t_0 = 0$, t_1, t_2 ... $\qquad t = \mathcal{N} dt = t_{\mathcal{N}}$ $\qquad dt = \frac{t}{\mathcal{N}}$ $\qquad t_k = k\,dt$

One uses $P(x_k t_k | x_{k-1} t_{k-1}) = \frac{1}{\sqrt{4\pi D\, dt}} \exp\left(-\frac{1}{2}\frac{(x_k - x_{k-1})^2}{2D\,dt}\right)$

to write
$$\boxed{P(x_{\mathcal{N}} t_{\mathcal{N}} | x_{\mathcal{N}-1} t_{\mathcal{N}-1} | \dots | x_0 t_0) = (4\pi D\,dt)^{-\frac{\mathcal{N}}{2}} \exp\left(-\frac{1}{2}\sum_{k=1}^{\mathcal{N}} \frac{(x_k - x_{k-1})^2}{2D\,dt}\right)}$$

This represents the probability (density) of the history $x_0 t_0 \dots x_{\mathcal{N}} t_{\mathcal{N}}$, allowing to compute any mean-value of observable $\mathcal{O}(x_0 \dots x_{\mathcal{N}})$ as

$$\langle \mathcal{O}(x_0 \dots x_N) \rangle = \int dx_0 \dots dx_N \, \mathcal{O}(x_0 \dots x_N) P(x_N t_N | x_{N-1} t_{N-1} | \dots | x_0 t_0) \underbrace{P_0(x_0)}_{\text{(arbitrary) initial distribution at time } t_0}$$

Going to continuum notations, $\sum_{k=1}^{N} \frac{(x_k - x_{k-1})^2}{2D\,dt} = \sum_{k=1}^{N} dt \frac{1}{2D}\left(\frac{x_k - x_{k-1}}{dt}\right)^2 \underset{dt \to 0}{\simeq} \int_0^t d\tau \frac{(\partial_\tau x)^2}{2D}$

square braquets ↓

and denoting : $\mathrm{Prob}[x]$ the probability density of the history $[x(\tau)]_{0 \le \tau \le t}$

$\mathcal{O}[x]$ the observable depending on the whole history

$\mathcal{D}x = \dfrac{dx_0 \dots dx_N}{(4\pi D\, dt)^{N/2}}$ the precise weighted measure on trajectories

One may write: Represents an integration over trajectories. distribution of $x(0)$ @ initial time $t=0$

note : $x = x$
sorry for the variation of notation

$$\boxed{\begin{aligned} \langle \mathcal{O}[x] \rangle &= \int \mathcal{D}x \; \mathcal{O}[x] \; \mathrm{Prob}[X] \; P_0(x(0)) \\ \mathrm{Prob}(x) &= \exp\left\{ -\frac{1}{2} \int_0^t d\tau \frac{(\partial_\tau x)^2}{2D} \right\} \end{aligned}}$$

→ Note that the normalization is hidden in $\mathcal{D}x$ through $\int \mathcal{D}x \; \mathrm{Prob}[X] \; P_0(x(0)) = 1$

- With the notation above, $\langle 1 \rangle = 1$: the integral $\int \mathcal{D}x$ is normalized.

<u>Remark</u>: in most cases, this integration over trajectories does <u>not</u> depend on the number of time slices N as $N \to \infty$. In case of doubt: check explicitly!

In the limit $N \to \infty$, the process $[x(\tau)]_{0 \le \tau \le t}$ is called a <u>Brownian motion</u>.

- it has zero mean and variance $\langle [x(t_2) - x(t_1)]^2 \rangle = 2D\,|t_2 - t_1|$
- it has a Gaussian distribution

- <u>In terms of η : the white noise</u> in discrete: $x_{k+1} - x_k = \eta_k \, dt$

Similarly :

$$\boxed{\begin{aligned} &\text{in discrete time } P(\eta_N t_N | \dots | \eta_0 t_0) = \exp\left(-\frac{1}{2}\frac{1}{2D}\sum_{k=0}^{N} dt\, \eta_k^2\right) \times (4\pi D\, dt)^{-\frac{(N+1)}{2}} \\ &\text{in continuous time } \mathrm{Prob}[\eta] = \exp\left(-\frac{1}{2}\frac{1}{2D}\int_0^t d\tau\, \eta^2(\tau)\right) \end{aligned}}$$

$\eta(\tau)$ has zero mean and variance $\langle \eta(t_1)\eta(t_2) \rangle = 2D\,\delta(t_2 - t_1)$

Its distribution is Gaussian.

Rq: note the difference of indexation. The amount of information in $(x_N \dots x_0)$ is the same as in $(\eta_{N-1} \dots \eta_0 ; x_0)$.

<u>Remark</u>: the writing

$$P(\eta_N t_N | \dots | \eta_0 t_0) = \prod_{k=0}^{N} \frac{1}{\sqrt{4\pi D dt}} e^{-\frac{1}{2}\frac{\eta_k^2}{2Ddt}}$$

makes it clear that the η_i's are independent and uncorrelated.

<u>Remark</u>: the generalisation to other correlators writes:

× <u>for a $N \times N$ invertible matrix, if</u>: A with $A^T = A$

$$P(\eta_0 \dots \eta_N) = \sqrt{\det \frac{A}{2\pi}}\; e^{-\frac{1}{2}\eta A \eta}$$

(For η, $A = \frac{1}{2D}\mathbb{1}$, where $\mathbb{1}$ is the identity matrix)

then $\langle \eta_i \eta_j \rangle = (A^{-1})_{ij}$

× <u>for a functional operator $\mathcal{A}(t_1, t_2)$</u>: (which is symmetric: $\mathcal{A}(t_1,t_2) = \mathcal{A}(t_2,t_1)$)

$$\text{Prob}[\eta] = \exp\left(-\frac{1}{2}\int dt_1 dt_2\, \eta(t_1)\mathcal{A}(t_1,t_2)\eta(t_2)\right)$$

$$\langle \eta(t_1)\eta(t_2)\rangle = \mathcal{A}^{-1}(t_1,t_2)$$

$\mathcal{A}^{-1}$ = functional inverse of $\mathcal{A}$

$$\int dt\; \mathcal{A}^{-1}(t_1,t)\mathcal{A}(t,t_2) = \delta(t_1-t_2)$$

5. Physical interpretation and generalizations

• <u>Overdamped dynamics</u>: $\dot{x} = \eta$ rewrites as

$$\underbrace{m\ddot{x}}_{\text{with zero mass}} = \underbrace{-\gamma\dot{x}}_{\text{friction}}\; \underbrace{- V'(x)}_{\text{and no potential}} + \underbrace{\eta(t)}_{\text{noise}}$$

with friction coefficient $\gamma = 1$

As a first generalization, one may consider the overdamped Langevin dynamics

$$\boxed{\dot{x} = -V'(x) + \eta(t)}$$

$V(x)$ being a potential of corresponding force $-V'(x)$

in details: $\partial_t x(t) = -V'(x(t)) + \eta(t)$

or: $\boxed{\dot{x} = F(x) + \eta(t)}$ for a generic force