Models of Theoretical Physics

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Contents

Introduction

This is a humble attempt to collect all the handwritten notes of the 2021/22 academic year and complete all the missing or differently treated parts mainly respect to the 2020/2021 notes of the powerful Francesco Manzali and Andrea Nicolai, that I have to sincerely thank.
There are some miscalculations and imprecision here and there which have not been corrected, nevertheless I hope this notes will be useful on your course of studies. Bon voyage.

Filippo Festa, 20/02/2022

⚠User Guide

- Essentially almost all the notes, except the final chapters treated by Maritan, are partial and refer to other material (Manzali-Nocolai Notes 2020/2021 https://goldshish.it/notes/models-of-theoretical-physics/full-notes-19-20 and the professors' notes uploaded in the moodle).
- In all the notes you will find a initial section with the topic treated and the corresponding reference (pages/chapters...) to the followed material.

Take a look and good luck!

Part I
Maritan's Lectures

1 The Diffusion problem

1.1 Solution of the Diffusion Equation

See Manzali-Nicolai's Notes:

- pag.11/12 - **Example 1** (Particle diffusing in **d=1**)
- pag.24 - ch1.5 Solution of the Diffusion Equation

(*) Now if we have $N=1$ (one particle):

$$\int_{\mathbb{R}^d} \rho_1(x,t)\, d^dx = 1 \qquad \text{Prob. to find the particle in } V \equiv \int_V \rho_1(x,t)\, d^dx \qquad (\rho_1 = \rho)$$

$$\langle f(x)\rangle_t = \int_{\mathbb{R}^d} d^dx\, f(x)\, \rho(x,t)$$

$$\frac{d}{dt}\langle f(x)\rangle_t = \int_{\mathbb{R}^d} d^dx\, f(x)\frac{d\rho(x,t)}{dt} = \int_{\mathbb{R}^d} d^dx\, f(x)\, \nabla(D\cdot\nabla\rho(x,t))$$

$$\overset{!}{=} D\int_{\mathbb{R}^d} d^dx\, f(x)\, \nabla^2\rho(x,t) \overset{\circ}{=} D\int_{\mathbb{R}^d} d^dx\, \rho(x,t)\, \nabla^2 f(x)$$ (*) see pag. 11

If we are in $d=1$ (Pag. 11):

$$\langle x\rangle_t = \int_{\mathbb{R}} \rho(x,t)\, x\, dx \qquad \langle \dot{x}\rangle_t = D\int_{\mathbb{R}} \rho(x,t)\frac{d^2}{dx^2}x = 0\,!$$

and $\langle x\rangle_{t=0} = \int dx\, \rho(x,0)\, x$ .... see pag. 11

Solution of the Diffusion Equation in $d=1$

$$\frac{d}{dt}\rho(x,t) = D\frac{d^2}{dx^2}\rho(x,t)$$

Like the Schrodinger equation, we exploit the separation of variables:

$$\rho(x,t) = \varphi(x)\, c(t)$$

$$\Rightarrow \frac{d/dt\, c(t)}{c(t)} = D\,\frac{d^2/dx^2\, \varphi(x)}{\varphi(x)}$$

This equality to hold must have both the sides equal to a constant: $-Dk^2$ where $k\in\mathbb{R}$

$$\Rightarrow \frac{d^2}{dx^2}\varphi(x) = -k^2\varphi(x)$$

So the solution: $\varphi_k(x) \propto e^{\pm ikx}$ These are eigenfunctions of the Laplacian (free particle?)

$\propto e^{ikx}$ & k absorbs the $\pm$ signs

Moreover: $\int_{\mathbb{R}} dx\, \varphi_k^*(x)\, \varphi_{k'}(x) = \int_{\mathbb{R}} dx\, e^{ix(k-k')} = 2\pi\,\delta(k-k')$ ⊙

and $\int_{\mathbb{R}} dk\, \varphi_k^*(x)\, \varphi_k(x') = \int_{\mathbb{R}} dk\, e^{ik(x'-x)} = 2\pi\,\delta(x-x')$

(orthogonality relations)

So from the other side of ✱: $\dfrac{\partial_t C_k(t)}{C_k(t)} = -Dk^2$ separation of variables

$$\Rightarrow C_k(t) = e^{-Dk^2 t}\, C_k(0)$$

So then: $\rho(x,t) = \int_{R} dk\, C_k(t)\, \varphi_k(x) = \int_{R} dk\, e^{-Dk^2 t}\, C_k(0)\, e^{ikx}$

where the i.c. is $\rho(x,0) = \int_{R} dk\, C_k(0)\, e^{ikx}$

If we integrate both side respect to x and multiplicate by $e^{-ik'x}$ factor:

$$\int_{\mathbb{R}} dx\, e^{-ik'x} \rho(x,0) = \int_{\mathbb{R}} dx\, e^{-ik'x} \int_{\mathbb{R}} dk\, C_k(0)\, e^{ikx}$$

swich

$$\overset{!}{=} \int_{\mathbb{R}} dk\, C_k(0) \int_{R} dx\, e^{ix(k-k')} \overset{⊙}{=} \int_{R} dk\, C_k(0)\, 2\pi\,\delta(k-k') = 2\pi\, C_{k'}(0)$$

$$\Rightarrow C_k(0) = \frac{1}{2\pi} \int_{R} dx\, e^{-ikx} \rho(x,0)$$

So: $\rho(x,t) = \int_{\mathbb{R}} dx' \underbrace{\int_{\mathbb{R}} \frac{dk}{2\pi} e^{ik(x-x')-k^2Dt}}\rho(x',0)$

$= \int dx' \underbrace{W(x,t|x',0)}_{\text{Propagator}} \rho(x',0)$

Reminder - Gaussian Integrals ($a>0$)

$\int_{\mathbb{R}} dx\, e^{-x^2} = \sqrt{\pi}$ $\qquad \int_{\mathbb{R}} dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}}$ change of variables: $\sqrt{a}\,x = y$

$\int_{\mathbb{R}} dx\, e^{-ax^2+bx} = \int_{\mathbb{R}} dx\, e^{-a(x-\frac{b}{2a})^2} e^{b^2/4a}$

$\sqrt{a}\left(x-\frac{b}{2a}\right) = y$ $\qquad = \int_{\mathbb{R}} dy\, \frac{e^{-y^2}}{\sqrt{a}} e^{b^2/4a} = \sqrt{\frac{\pi}{a}}\, e^{b^2/4a}$

↳ holds also if b is constant ($b \in \mathbb{C}$)

$$\Rightarrow W(x,t|x',0) = \frac{e^{-\frac{(x-x')^2}{4Dt}}}{\sqrt{4\pi Dt}}$$

If the initial condition i.c. was at time $t = t_0$:

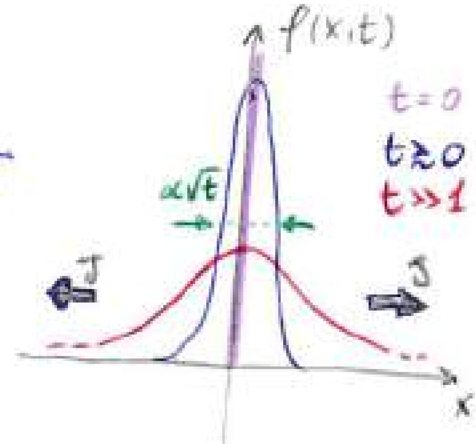
$W(x,t|x',t_0) = W(x,t-t_0|x',0) = W(x-x',t-t'|0,0)$

$= \frac{1}{\sqrt{4\pi D(t-t_0)}} e^{-\frac{(x-x')^2}{4D(t-t_0)}}$

This is because the problem is invariant under spatial translation and do not care of the origin of time!

and $\rho(x,t) = \int dx_0\, W(x,t|x_0,t_0)\, \rho(x_0,t_0)$

Ex Let's take the i.c. $\rho(x,0) = \delta(x)$



$$\Rightarrow \rho(x,t) = W(x,t|0,0) = \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}}$$

Notice that: $\int dx\, \rho(x,t) = 1$

→ We haven't impose this condition to solve the differential equation! The normalization condition derive directly from the characteristics of the continuity equation: in particular the flux J at infinity has to be zero!

$$J = -D\frac{\partial}{\partial x}\rho = \frac{D}{\sqrt{4Dt}}\frac{2x}{4Dt}\, e^{-x^2/4Dt} \to 0 \text{ when } |x|\to\infty$$

↳ It's odd in x, while $\rho(x,t)$ it's even! Notice that the oddness of J suggest that J goes away from high ρ concentration (in our example), as we expected!

Ex Reflecting Boundary Condition

$\Rightarrow$ flux $= 0$ at $x = 0$

$$\Rightarrow -D\frac{\partial}{\partial x}\rho(x,t)\Big|_{x=0} = 0 \quad \forall t$$

Hint to solve the Exercise

So then: $\frac{\partial^2}{\partial x^2}\varphi_k(x) = -k^2\varphi_k(x)$ $\quad \frac{\partial}{\partial x}\rho = \int dk \frac{\partial \varphi_k}{\partial x} c_k(t)$

$\Rightarrow \frac{\partial}{\partial x}\varphi_k(x) = 0$ at $x=0$ $\Rightarrow$ $\varphi_k(x)$ must be a combination of $e^{\pm ikx}$

$\Rightarrow \underline{k>0}$ $\quad \varphi_k(x) = \cos(kx)$ $\Rightarrow$ Find the orthogonality relation ...

Ex Absorbing b.c. $(x=0)$ $\Rightarrow \rho(x=0,t) = 0 \quad \forall t$

.... $\Rightarrow \varphi_k(x) = \sin(kx)$

Initial condition: $\rho(x,t=0) = \delta(x-x_0)$ for example

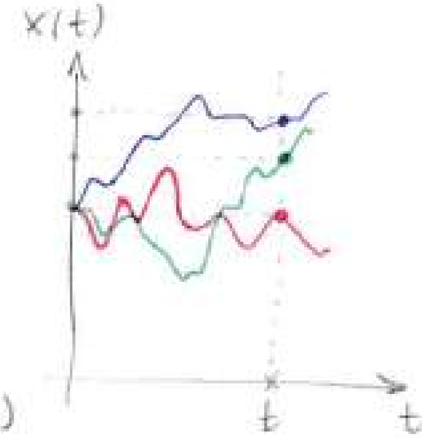
1.2 Microscopical-Modelistic approach

See Manzali-Nicolai's Notes :

- pag.13/14 - ch1.3 Microscopical approach
- pag.16 - ch1.3.2 Moments of the diffusion distribution

Remark on the relation between $\langle f(x(t))\rangle$ and $\langle f\rangle_\rho$

$$\boxed{\underset{①}{\langle f(x(t))\rangle} = \int dx \, \overset{②}{\rho(x,t)} f(x)}$$



① $\langle f(x(t))\rangle \equiv$ Average of the observable f over $n \to \infty$ trajectories $x(t)$ ~ stocastic variable at time t

generating n-indipendent trajectories $x_i(t)$ with $i = 1, \dots, n$

$$= \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} f(x_i(t)) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \int dx \, \delta(x - x_i(t)) f(x)$$

$$= \int dx \, f(x) \underbrace{\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \delta(x - x_i(t))} = \int dx \, f(x) \underbrace{\rho(x,t)} \quad ②$$

So then we can define: $\boxed{\rho(x,t) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \delta(x - x_i(t))}$

... see pag. 13-14 Manzoli ~ Modelistic approach to Diffusion

Let's take $P_0 = 0 \Rightarrow P_+ + P_- = 1$ so the particles move at each time step without a preferred direction

Furthermore let's suppose that at time $t = 0$ the particle is at the origin of the discrete lattice, that is at site $i = 0$ (Initial condition):

$$w_i(0) = \delta_{i,0}$$

So, starting from the zero site $i=0$ at time $t_0 = 0$ ($t_n = \varepsilon n \Rightarrow n=0$), the prob. to find the particle at site i at time t_n (so after n timesteps) is given by a binomial distribution:

$a+b=2c$	$a+b=2c+1$
$a-b=2(c-b)$ even!	$a-b=2(c-b)+1$ odd!

$$\underline{w_i(t_n)} = \begin{cases} \binom{n}{n_+} P_+^{n_+} P_-^{n_-} & \text{where } n \text{ and } i \text{ have the same parity} \\ 0 & \text{otherwise} \end{cases}$$

math way

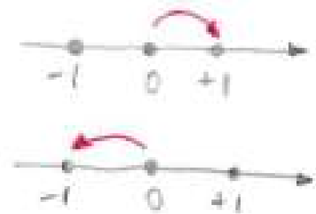
intuitive way

In fact notice that if $n=1$ we can visit only odd indexed sites:

$t_0 = 0$

Two possibilities:

$t_1 = \varepsilon$



If $n=2$ we have three possibilities (only even indexed arrival states):

In particular we have:

$$\begin{cases} n_+ - n_- = i \\ n_+ + n_- = n \end{cases}$$

where:

$n_+ \equiv$ total number of step to the right from the beginning

$n_- \equiv$ ... left ...

P.S.

- Each step is indipendent from the others! $P_+^{n_+}$ = Prob. to take n_+ steps to the right
- The order each step is taken doesn't count: for example if $n=4$ and $n_+=3$ $\rightsquigarrow$ $i = n_+ - n_- = n_+ - (n - n_+) = 2n_+ - n = 2$ we have 4 possible path followed by the particle:

$+++-$ $\quad +-++ \quad ++-+ \quad -+++$ } Taken into account by the binomial factor: $\binom{n}{n_+}$

Moreover notice that at a fixed time t_n generic the particle must be in one of $\mathbb{Z}$ lattice's sites as the particle cannot escape from the system, so then:

$$\sum_{i\in\mathbb{Z}} w_i(t_n) = 1 \qquad \left(\sum_{i\in\mathbb{Z}} w_i(t_{n+1}) = \sum_{i\in\mathbb{Z}} w_i(t_n) = \dots = \sum_{i\in\mathbb{Z}} w_i(0)\right)$$

$$\sum_{i=-\infty}^{+\infty} w_i(t_n) = \sum_{i=-n}^{n} w_i(t_n) = \sum_{n_+=0}^{n} \binom{n}{n_+} P_+^{n_+} P_-^{n-n_+} = (P_+ + P_-)^n = 1^n = 1$$

Binomial theorem

All others terms are zero, after n timesteps the particle can reach at most sites $\pm n$

$i = n_+ - n_- = 2n_+ - n \rightsquigarrow n_+ = \frac{i+n}{2}$

$P_+ + P_- = 1$ ($P_0 = 0$)

The motion of the particle in the lattice can be seen as a Bernoulli process (Remember that the Binomial distribution describe a stocastic variable that is the sum of n indipendent Bernoulli distributed stocastic variables: in our case we have n_+ successes and $n-n_+=n_-$ failures in n trials with probabilities P_+ and P_- respectively ④ The Bernoulli distribution describe a stocastic variable that can take only two values $\{0,1\}$: failure or success) so we have:

(4)

$$\langle x_i\rangle_n = \langle i\ell\rangle_n = \ell\langle i\rangle_n = \ell\langle n_+ - n_-\rangle_n = \ell\langle 2n_+ - n\rangle_n$$

$$= \ell(2\langle n_+\rangle_n - n) \underset{*}{=} \ell\left[2(nP_+) - n\right] = \ell\left[2P_+ - 1\right]n$$

$$= \ell\left[2P_+ - (P_+ + P_-)\right]n = \ell\left[P_+ - P_-\right]n$$

where $^*\langle n_+\rangle = nP_+$ Comes from the Bernoulli distribution!

$$\hat{S} = \sum_{n_+=0}^{n}\binom{n}{n_+}P_+^{n_+}P_-^{n_-} = 1$$

$$\Rightarrow \frac{\partial}{\partial P_+}\hat{S} = n_+\sum\binom{n}{n_+}P_+^{n_+-1}P_-^{n-n_+} +$$

$$-\sum\binom{n}{n_+}P_+^{n_+}(n-n_+)(1-P_+)^{n-n_+-1}$$

$$= \frac{\langle n_+\rangle}{P_+} - \frac{1}{1-P_+}\sum\binom{n}{n_+}P_+^{n_+}(1-P_+)^{n-n_+}(n-n_+)$$

$$= \frac{\langle n_+\rangle}{P_+} - \frac{1}{1-P_+}\langle n-n_+\rangle$$

$$= \frac{\langle n_+\rangle - P_+\langle n_+\rangle - P_+ n + P_+\langle n_+\rangle}{P_+(1-P_+)}$$

$$\Rightarrow \frac{\partial}{\partial P_+}\hat{S} = 0 = \frac{\langle n_+\rangle - P_+ n}{P_+(1-P_+)}$$

$$\Rightarrow \langle n_+\rangle = nP_+$$

Ex $P_+ = P_- = 1/2$ and $P_0 = 0$

$\rightsquigarrow$ In this case ($P_+ = P_-$) we have the smallest possible entropy: it's like if the drop of ink that is diffusing it's spherical! (a sort of "ordered" random motion)

In this case: $\langle x_i \rangle_n = \ell [P_+ - P_-] n = 0$

While: $\langle (x_i - \langle x_i \rangle_n)^2 \rangle = \langle x_i^2 \rangle_n - \cancel{\langle x_i \rangle_n^2} = \langle x_i^2 \rangle_n \equiv (\mathrm{Var}\, x_i)_n$

$\rightsquigarrow \langle x_i^2 \rangle_n = \langle i^2 \ell^2 \rangle_n = \langle i^2 \rangle_n \ell^2 = \langle (n_+ - n_-)^2 \rangle_n \ell^2$ where $n = n_+ + n_-$, $n_- = n - n_+$

$= \langle (2n_+ - n)^2 \rangle_n \ell^2 = \langle 4n_+^2 - 4n_+ n + n^2 \rangle_n \ell^2$ where $\langle n_+ \rangle_n = P_+ n$

$= \ell^2 (4 \langle n_+^2 \rangle_n - 4n \langle n_+ \rangle_n + n^2) = \ell^2 (4 \langle n_+^2 \rangle_n - 4n^2 P_+ + n^2)$

Recall that the k-th moment is: $\langle x_i^k \rangle_n = \sum_i w_i(t_n) x_i^k$

So to compute $(\mathrm{Var}\, x_i)_n$ we need to have $\langle n_+^2 \rangle_n$: let's develop a strategy to calculate in general $\langle n_+^J \rangle_n$:

$$\langle n_+^J \rangle_n = \sum_{i \in \mathbb{Z}} w_i(t_n) n_+^J = \sum_{n_+ = 0}^{n} \binom{n}{n_+} P_+^{n_+} P_-^{n_-} n_+^J$$

Let's introduce $\hat{\omega}(z, n) = \sum_{n_+ = 0}^{n} \binom{n}{n_+} P_+^{n_+} P_-^{n - n_+} z^{n_+}$

$= \sum_{n_+ = 0}^{n} \binom{n}{n_+} (P_+ z)^{n_+} P_-^{n - n_+} = (P_+ z + P_-)^n$ where we use the Binomial theorem $(a+b)^n = \binom{n}{k} a^k b^{n-k}$

Notice that: $\left(z \frac{\partial}{\partial z}\right) \hat{\omega}(z, n) = \sum_{n_+ = 0}^{n} \binom{n}{n_+} P_+^{n_+} P_-^{n - n_+} z \frac{\partial}{\partial z} (z^{n_+})$

$= \sum_{n_+ = 0}^{n} \binom{n}{n_+} P_+^{n_+} P_-^{n - n_+} z (n_+ z^{n_+ - 1}) = \sum_{n_+ = 0}^{n} \binom{n}{n_+} P_+^{n_+} P_-^{n - n_+} (n_+ z^{n_+})$

$$\Rightarrow \left(z\frac{\partial}{\partial z}\right)\hat{\omega}(z,n)\Big|_{z=1} = \sum_{n_+=0}^{n}\binom{n}{n_+}P_+^{n_+}P_-^{n-n_+}n_+ = \langle n_+\rangle_n$$

In general: $\left(z\frac{\partial}{\partial z}\right)^J\hat{\omega}(z,n) = \sum_{n_+=0}^{n}\binom{n}{n_+}P_+^{n_+}P_-^{n-n_+}\left(n_+^J z^{n_+}\right)$

$$\Rightarrow \left(z\frac{\partial}{\partial z}\right)^J\hat{\omega}(z,n)\Big|_{z=1} = \langle n_+^J\rangle_n$$

So then in our case we want $\langle n_+^1\rangle_n$, we have:

$$\langle n_+\rangle_n = \left(z\frac{\partial}{\partial z}\right)\hat{\omega}(z,n)\Big|_{z=1} = \left(z\frac{\partial}{\partial z}\right)(P_+z+P_-)^n\Big|_{z=1}$$

$$= z\left(n(P_+z+P_-)^{n-1}P_+\right)\Big|_{z=1} = nP_+(P_++P_-)^{n-1}$$

$$= nP_+(P_++(1-P_+))^{n-1} = nP_+ \quad \text{where } P_++P_-=1$$

$\Rightarrow \langle n_+\rangle_n = nP_+$ that's the general case we obtained before

$\Rightarrow$ If $P_+=P_-=1/2$: $\langle n_+\rangle_n = n/2$ so half of the step done by the particle goes from the right in average!

$$\langle n_+^2\rangle_n = \left(z\frac{\partial}{\partial z}\right)^2\hat{\omega}(z,n)\Big|_{z=1} = \left(z\frac{\partial}{\partial z}\right)\left(nzP_+(P_+z+P_-)^{n-1}\right)\Big|_{z=1}$$

$$= nzP_+(P_+z+P_-)^{n-1} + nz^2P_+(n-1)(P_+z+P_-)^{n-2}P_+\Big|_{z=1}$$

$$= nP_+(P_++P_-)^{n-1} + nP_+(n-1)(P_++P_-)^{n-2}P_+ \quad \text{where } P_++P_-=1$$

$$= nP_+ + n(n-1)P_+^2$$

$\Rightarrow \langle n_+^2 \rangle_n = n(n-1)P_+^2 + nP_+$ (Holds in general, also for $P_+ \neq P_-$!)

Now we can finally compute $(\mathrm{Var}\, x_i)_n$, in particular:

$x_i = i\ell = (n_+ - n_-)\ell = (2n_+ - n)\ell \Rightarrow (\mathrm{Var}\, x_i)_n = 4(\mathrm{Var}\, n_+)_n \ell^2$

$$(\mathrm{Var}\, x_i)_n = (\mathrm{Var}(2n_+\ell - n\ell))_n = \langle (2n_+\ell - n\ell)^2 \rangle_n - \langle 2n_+\ell - n\ell \rangle_n^2$$

$$\stackrel{!}{=} \langle 4n_+^2\ell^2 - 4n\ell^2 n_+ + n^2\ell^2 \rangle_n - (2\ell\langle n_+\rangle_n - n\ell)^2$$

$$\stackrel{!}{=} 4\ell^2\langle n_+^2\rangle_n - \cancel{4n\ell^2\langle n_+\rangle_n} + \cancel{n^2\ell^2} - (4\ell^2\langle n_+\rangle_n^2 - \cancel{4n\ell^2\langle n_+\rangle_n} + \cancel{n^2\ell^2})$$

$$\stackrel{!}{=} 4\ell^2(\langle n_+^2\rangle_n - \langle n_+\rangle_n^2) = 4\ell^2(\mathrm{Var}\, n_+)_n$$

$$\Rightarrow (\mathrm{Var}\, n_+)_n = \langle n_+^2\rangle_n - \langle n_+\rangle_n^2$$

$$\stackrel{!}{=} n(n-1)P_+^2 + nP_+ - (nP_+)^2 = \cancel{n^2P_+^2} - nP_+^2 + nP_+ - \cancel{n^2P_+^2}$$

$$\stackrel{!}{=} nP_+(1-P_+) = nP_+P_-$$

$$\Rightarrow (\mathrm{Var}\, x_i)_n = \langle x_i^2\rangle_n - \langle x_i\rangle_n^2 = 4\ell^2 n P_+ P_-$$

In particular in our case $P_+ = P_- = \frac{1}{2}$ we get: $(\mathrm{Var}\, x_i)_n = \ell^2 n$

---- Continuum limit (Manzoli pag. 19)

1.3 A more General Case

- $\star$ **New material** $\star$ done after ch1.4 and before ch1.5.1 of Manzali-Nicolai's Notes
- Professors' notes - Scale invariance of the diffusion pag.17 ch2.2.3

$\boxed{\text{Ex}}$ A More General Case (Not only nearest neighbours jumps)

We start from the Master Equation for a particle diffusing in a 1D lattice:

$$w_i(t_{n+1}) = \sum_{j \in \mathbb{Z}} W_{ij}\, w_j(t_n)$$

⇝ Now we suppose (Ansatz) that the probability to jump from j to sites i depends only on the distance between sites i and j:

$$\underline{W_{ij} = p(i-j)} \; \} \text{ prob. to jump of a lenght } k = i-j$$

Notice that: $\underline{\sum_i W_{ij} = 1}$ $\forall j \in \mathbb{Z}$ (= Probability Conservation)

⇝ In fact if we start from a sites fixed j, after a timestep we will surely be in one of the other $i \in \mathbb{Z}$ sites of the lattice: so the sum of the transition rates from j fixed to $i \in \mathbb{Z}$ makes fully explicit all possible final position that the particle can assume!

Using the master equation we derive that:

$$\sum_i w_i(t_{n+1}) = \sum_j \underbrace{\sum_i W_{ij}}_{\overset{!}{=}1} w_j(t_n) = \sum_j w_j(t_n)$$

$$= \dots \text{ Iterating the procedure } \dots = \sum_j w_j(0) = 1$$

$$\Rightarrow \sum_i w_i(t_{n+1}) = \sum_i w_i(t_n) = \dots = \sum_i w_i(0) = 1$$

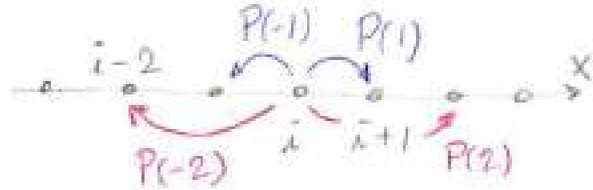
So the probability is conserved! The particle is always somewhere in the lattice $\mathbb{Z}$ and cannot disappear: in fact we have not considered the case in which this happen (the disappereance of the particle) like for example chemical reaction (some substance disappear in order to create new one)

In this ansatz our <u>Master Equation</u> becomes:

$$\underline{w_i(t_{n+1})} = \sum_{j\in\mathbb{Z}} P(i-j)\, w_j(t_n) = \sum_{k\in\mathbb{Z}} P(k)\, w_{i-k}(t_n) \quad \text{where } k = i-j$$

And for simplicity let's take:

$$\underline{P(k) = P(-k)} \quad \forall k \in \mathbb{Z}$$



↳ So we are interested only on the distance made by the jump (the modulous) and not by the direction taken!

$\Rightarrow$ By the previous observation: $\sum_i P(i-j) = \sum_i W_{ij} = 1 \Rightarrow \underline{\sum_k P(k) = 1}$

Remember that our discretized diffusion is such $x = i\ell$ and $t_n = n\varepsilon$ and from the continuum limit section that we can define a prob. density $\omega(x,t)$ such that $w_i(t_n) = \ell\,\omega(x,t)$. Let's rewrite our ME:

$$w_i(t_{n+1}) = \sum_{k\in\mathbb{Z}} P(k) w_{i-k}(t_n) \rightsquigarrow \cancel{\ell}\,\omega(x,t+\varepsilon) = \sum_{k\in\mathbb{Z}} P(k)\,\cancel{\ell}\,\omega(x-k\ell,t)$$

$$\omega(x,t+\varepsilon) = \sum_{k\in\mathbb{Z}} P(k)\,\omega(x-k\ell,t)$$

Now we can expand the left and right side of the equation respectively when $\varepsilon = 0$ and $-k\ell = 0$ so $t+\varepsilon = t$ and $x - k\ell = x$ points

$$\omega(x,t) + \varepsilon\,\dot{\omega}(x,t) + \frac{\varepsilon^2}{2}\ddot{\omega}(x,t) + \cdots = \sum_{k\in\mathbb{Z}} P(k) \sum_{m=0}^{\infty} \frac{(-k\ell)^m}{m!}\,\omega^{(m)}(x,t)$$

$$\overset{!}{=} \overbrace{\sum_k P(k)}^{=1}\,\omega(x,t) - \ell\,\cancel{\sum_{k\in\mathbb{Z}} P(k)k}\,\omega'(x,t) + \frac{\ell^2}{2}\sum_k P(k)k^2\,\omega''(x,t) +$$

$$- \frac{\ell^3}{3!}\cancel{\sum_k P(k)k^3}\,\omega'''(x,t) + \cdots$$

where $\sum_k k\,P(k) = 0$ and $\sum_k k^3 P(k) = 0$ because $P(k)$ is even $(P(k) = P(-k))$ and k, k^3 are odd!

$$\cancel{\omega(x,t)}+\varepsilon\dot{\omega}(x,t)+\frac{\varepsilon^2}{2}\ddot{\omega}(x,t)+\mathcal{O}(\varepsilon^3)=\cancel{\omega(x,t)}+\frac{\ell^2}{2}\omega''(x,t)\langle k^2\rangle_p+ +\mathcal{O}(\ell^4)$$ (7)

$$\dot{\omega}(x,t)+\frac{\varepsilon}{2}\ddot{\omega}(x,t)+\mathcal{O}(\varepsilon^3)=\frac{\ell^2}{2\varepsilon}\omega''(x,t)\langle k^2\rangle_p+\mathcal{O}(\ell^4)$$

$\Rightarrow$ If we take $\ell\to 0$ and $\varepsilon\to 0$: $\underline{\dot{\omega}(x,t)=D\omega''(x,t)}$ where $D=\frac{\ell^2}{2\varepsilon}\langle k^2\rangle_p$

So we get again the differential equation $\dot{\omega}=D\omega''$ for the diffusion in the continuum limit ($\ell\to 0, \varepsilon$), even if we allow jumps greater than 1 site! In some sense we can appreciate the "universality" of the model and so the indipence of the result from the microscopic details. Notice that the second moment $\langle k^2\rangle_p$ is the only one that is part of D (the constant that governs the diffusion process), so it's the only carrier of the important details, in other words it characterizes the details that really matters for the model!

<u>Weakness of the model</u>: Everything works in this model until $\langle k^2\rangle_p=\sum_k k^2 p(k)$ is finite but this is not always the case and depends on the choice of the transition rates $p(k)$! The finiteness it's necessary for the universality of the model, otherwise everything go down the drain! (va in malora)

$\rightsquigarrow$ For example if we choose $p(k)$ as a gaussian everything works well and $\langle k^2\rangle_p$ exists and it's finite

Ex • $P(k)=\dfrac{e^{-\alpha|k|}}{Z(\alpha)}$ Decreasing exponential $(\alpha>0)$ $\boxed{\sum_{n=0}^{\infty}x^n=\frac{1}{1-x}}$

Normalization $\displaystyle\sum_{k\in\mathbb{Z}}e^{-\alpha|k|}=\sum_{k=-\infty}^{-1}e^{-\alpha|k|}+\sum_{k=0}^{+\infty}e^{-\alpha|k|}=\sum_{k=-1}^{-\infty}e^{\alpha k}+\sum_{k=0}^{+\infty}e^{-\alpha k}$

$J=-k-1$
$J=0\rightsquigarrow k=-1$
$J=\infty\rightsquigarrow k=-\infty$

$$=\sum_{J=0}^{+\infty}e^{-\alpha k-\alpha}+\sum_{k=0}^{+\infty}e^{-\alpha k}=e^{-\alpha}\sum_{k=0}^{+\infty}e^{-\alpha k}+\sum_{k=0}^{+\infty}e^{-\alpha k}$$

$$=e^{-\alpha}/(1-e^{-\alpha})+1/(1-e^{-\alpha})=\frac{1+e^{-\alpha}}{1-e^{-\alpha}}\equiv Z(\alpha) \iff |e^{-\alpha}|<1$$

$\langle k^2 \rangle = \sum_k P(k) k^2 = \frac{\partial^2}{\partial \alpha^2} \ln Z(\alpha)$

$$\langle k^2 \rangle = \sum_{k \in \mathbb{Z}} \frac{e^{-\alpha|k|}}{Z(\alpha)} k^2 = \frac{\partial^2}{\partial \alpha^2} \ln Z(\alpha) = \frac{1}{Z(\alpha)} \frac{\partial^2}{\partial \alpha^2} Z(\alpha)$$

$$\stackrel{!}{=} \frac{1}{Z(\alpha)} \frac{\partial^2}{\partial \alpha^2} \left[\sum_{k \in \mathbb{Z}} e^{-\alpha|k|} \right] = \sum_{k \in \mathbb{Z}} \frac{|k||k|}{Z(\alpha)} e^{-\alpha|k|} = \sum_{k \in \mathbb{Z}} \frac{k^2 e^{-\alpha|k|}}{Z(\alpha)}$$

$$\stackrel{!}{=} \sum_k P(k) k^2$$

- $P(k) = \frac{1}{k^2 + |\alpha|}$ Cauchy Distribution

$\langle k^2 \rangle = \sum_k P(k) k^2 = +\infty$ diverges because $P(k) k^2 \xrightarrow[k \to \infty]{} 1$

- $P(k) = \frac{1}{|k|^\alpha} \frac{\mathbb{1}_{k \geq 1}}{Z(\alpha)}$ where $\alpha > 1$ ⊛

$\boxed{\mathbb{1}_A(x) = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \notin A \end{cases}}$ Indicator Function

$$\langle k^2 \rangle = \sum_k P(k) k^2 = \sum_{k=1}^{+\infty} \frac{k^2}{Z(\alpha) |k|^\alpha} = \frac{1}{Z(\alpha)} \sum_{k=1}^{\infty} \frac{1}{|k|^{\alpha - 2}}$$

So: $\langle k^2 \rangle < +\infty$ if $\alpha - 2 > 1 \rightsquigarrow \alpha > 3$

$\langle k^2 \rangle = +\infty$ if $\alpha - 2 < 1 \overset{⊛}{\rightsquigarrow} 1 < \alpha < 3$

Harmonic series $\sum_{k=1}^{\infty} \frac{1}{k} = +\infty$

PS Generalization in 3D: The particle is moving on a 3D lattice and $\vec{k}$ now is a vector of integers

If we assume: $P(\vec{k}) \equiv P(|\vec{k}|)$ and $\langle k^2 \rangle_p < +\infty$ $\Rightarrow$ We can derive all like we do in 1D

Scale invariance of the Diffusion Equation

In the previous lecture from the Master Equation ME in the continuum limit we have obtained:

$$\frac{\partial}{\partial t} W(x,t) = D \frac{\partial^2}{\partial x^2} W(x,t) \quad (*)$$

Let's introduce a new function $\hat{W}(x,t)$: $W(x,t) = \hat{W}(\lambda x, \lambda^2 t)$ with $\lambda \in \mathbb{R}$

$$\Rightarrow \hat{W}(x,t) = W\left(\frac{x}{\lambda}, \frac{t}{\lambda^2}\right)$$

$$(*) \quad \frac{\partial}{\partial t} \hat{W}(\lambda x, \lambda^2 t) = \frac{\partial \hat{W}}{\partial \tau} \frac{\partial \tau}{\partial t}\Big|_{\tau=\lambda^2 t} = \frac{\partial}{\partial \tau} \hat{W}(\lambda x, \tau)\Big|_{\tau = \lambda^2 t} \cdot \lambda^2$$

$$= D \frac{\partial^2}{\partial x^2} \hat{W}(\lambda x, \lambda^2 t) = D \frac{\partial^2 \hat{W}}{\partial y^2} \left(\frac{dy}{dx}\right)^2 = D \frac{\partial^2}{\partial y^2} \hat{W}(y, \lambda^2 t)\Big|_{y=\lambda x} \cdot \lambda^2$$

$$\Rightarrow \frac{\partial}{\partial \tau} \hat{W}(y,\tau) = D \frac{\partial^2}{\partial y^2} \hat{W}(y,\tau)$$

$$\Rightarrow \frac{\partial}{\partial t} \hat{W}(x,t) = D \frac{\partial^2}{\partial y^2} \hat{W}(x,t)$$

So also $\hat{W}(x,t)$ it's a solution of the diffusion equation!

What changes with respect to $W(x,t)$ solution? Let's see, starting from the choice of the initial condition:

$W(x,t) \underset{\text{i.c.}}{\rightsquigarrow} W(x, t=0) = \delta(x - x_0)$, so then $\hat{W}(x,t)$:

$$\hat{W}(x,t) = W\left(\frac{x}{\lambda}, \frac{t}{\lambda^2}\right) \xrightarrow{\text{i.c.}} \hat{W}(x,0) = W\left(\frac{x}{\lambda}, 0\right) = \delta\left(\frac{x}{\lambda} - x_0\right)$$

$$\overset{!}{=} |\lambda|\, \delta(x - \lambda x_0)$$

The initial condition has changed!

$(\delta(\lambda t) = \delta(t)/|\lambda|)$

In particular, from the conservation of probability in the whole lattice (remember that the particle cannot disappear):

$$\int \hat{W}(x,t)\,dx = \int \hat{W}(x,0)\,dx = |\lambda| \int \delta(x - \lambda x_0)\,dx = |\lambda|$$

If we want $\hat{W}(x,t)$ to be normalized to 1 as usual, we can define finally:

$$\boxed{\hat{\hat{W}}(x,t|x_0\lambda,0) = \frac{1}{|\lambda|}\hat{W}(x,t) = \frac{1}{|\lambda|} W\left(\frac{x}{\lambda}, \frac{t}{\lambda^2}\middle| x_0, 0\right)}$$

→ SCALE INVARIANCE: involves both space and times!

Ex $x_0 = 0$: $\hat{\hat{W}}(x,t|0,0) = \frac{1}{|\lambda|} W\left(\frac{x}{\lambda}, \frac{t}{\lambda^2}\middle| 0,0\right)$ with $\lambda \in \mathbb{R}$

So we can arbitrarily choose $\lambda = \sqrt{t}$, so we have:

$$\hat{\hat{W}}(x,t|0,0) = \frac{1}{\sqrt{t}} W\left(\frac{x}{\sqrt{t}}, \frac{t}{t}\middle| 0,0\right) = \frac{1}{\sqrt{t}} W\left(\frac{x}{\sqrt{t}}, 1 \middle| 0,0\right)$$

$$\overset{!}{=} \frac{1}{\sqrt{t}} f\left(\frac{x}{\sqrt{t}}\right)$$

- This gave us the form of the generic solution of the starting ⊛, the most general possible!
- Also here we have that $x \sim \sqrt{t}$ (stochastic fundamental relation)

Notice that the old solution have this form:

$$W(x,t|0,0) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$

$$\overset{!}{=} \frac{1}{\sqrt{t}} \frac{1}{\sqrt{4\pi D}} \exp\left(-\frac{1}{4D}\left(\frac{x}{\sqrt{t}}\right)^2\right) \implies f(z) = \frac{1}{\sqrt{4\pi D}} \exp\left(-\frac{z^2}{4D}\right)$$

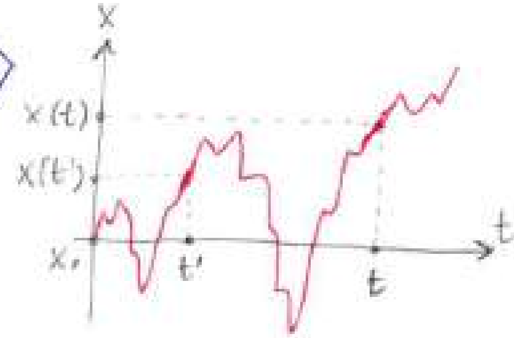
1.4 Propagators

See Manzali-Nicolai's Notes for the ESCK property - pag.28 ch1.5.1 Propagators

We have seen that we can compute the average of the observable f at time t over all possible trajectories $x(t)$ like:

$$\langle f(x(t)) \rangle = \int_{\mathbb{R}} W(x,t) f(x)\, dx$$

But how to compute the average $\langle f(x(t), x(t')) \rangle$ at times t and t' over all possible trajectories?
The joint probability density to be at x at time t and at x' at time t' is:



$$W(x,t;x',t') = \int_{\mathbb{R}} W(x,t|x',t') W(x',t'|x_0,t_0) W(x_0,t_0)\, dx_0$$

$$\Rightarrow \langle f(x(t), x(t')) \rangle = \int_{\mathbb{R}^2} dx\, dx'\, f(x,x') W(x,t;x',t') \quad \text{usual definition}$$

$$= \int_{\mathbb{R}^2} dx\, dx'\, f(x,x') \int_{\mathbb{R}} dx_0\, W(x,t|x',t') W(x',t'|x_0,t_0) W(x_0,t_0)$$

$$= \int_{\mathbb{R}} dx_0 \int_{\mathbb{R}^2} d\mathbb{P}_{t,t'}(x,x'|x_0,t_0) \cdot W(x_0,t_0) \cdot f(x,x')$$

where $d\mathbb{P}_{t,t'}(x,x'|x_0,t_0) = dx\, dx'\, W(x,t|x',t') W(x',t'|x_0,t_0)$

and $t_0 < t' < t$ fixed times

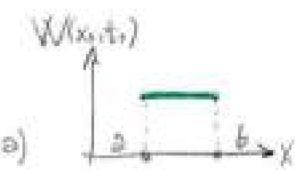
In General:

$$\langle f(x(t_0), x(t_1) \cdots x(t_n)) \rangle = \int_{\mathbb{R}} dx_0 \int_{\mathbb{R}^n} d\mathbb{P}_{t_1 \cdots t_n}(x_1 \cdots x_n|x_0,t_0) \cdot W(x_0,t_0)\, f(x_0 \cdots x_n)$$

where $d\mathbb{P}_{t_1 \cdots t_n}(x_1, x_2 \cdots x_n|x_0,t_0) = W(x_n,t_n|x_{n-1},t_{n-1}) \cdots W(x_1,t_1|x_0,t_0)\, dx_1 \cdots dx_n$

and $t_0 < t_1 < \cdots < t_n$

For example: $W(x_0,t_0) = \delta(x_0 - x_K)$
$W(x_0,t_0) = e^{-(x_0-x_K)^2/2\sigma^2} / \sigma\sqrt{2\pi}$
$W(x_0,t_0) = \mathbb{1}_{[a,b]}(x_0) / (b-a)$



$\boxed{\text{Ex}}$ Calculate $\langle x(t)x(t')\rangle$ where $t, t' > 0$

Initial condition

and $W(x, t_0) = \delta(x - \tilde{x}_{1c})$

$$\Rightarrow \langle x(t)x(t')\rangle = \int_{\mathbb{R}} dx_0 \int_{\mathbb{R}^2} d\mathbb{P}_{t,t'}(x, x' | x_0, t_0) \cdot W(x_0, t_0) \cdot x x'$$

$$\stackrel{!}{=} \int_{\mathbb{R}} dx_0 \int_{\mathbb{R}^2} dx\, dx'\, W(x, t | x', t')\, W(x', t' | x_0, t_0) \cdot W(x_0, t_0) \cdot x x'$$

where: $t_0 < t' < t$

$$\stackrel{!}{=} \int_{\mathbb{R}^3} dx_0\, dx'\, dx\, W(x, t | x', t')\, W(x', t' | x_0, t_0)\, \delta(x_0 - x_{1c}) \cdot x x'$$

where $W(x_0, t_0) = \delta(x_0 - x_{1c})$ and remember that: $W(x, t | x_0, t_0) = \dfrac{e^{-\frac{(x - x_0)^2}{4D(t - t_0)}}}{\sqrt{4\pi D(t - t_0)}}$

$$\Rightarrow \langle x(t)x(t')\rangle = \int_{\mathbb{R}^2} dx'\, dx\, W(x, t | x', t')\, W(x', t' | x_{1c}, t_0) \cdot x x'$$

$$\stackrel{!}{=} \int_{\mathbb{R}^2} dx'\, dx\, \frac{e^{-\frac{(x - x')^2}{4D(t - t')}}}{\sqrt{4\pi D(t - t')}}\, \frac{e^{-\frac{(x' - x_{1c})^2}{4D(t' - t_0)}}}{\sqrt{4\pi D(t' - t_0)}} \cdot x x'$$

Let's change the variables:

$x - x' = z \qquad x' - x_{1c} = y$

$\rightsquigarrow x' = y + x_{1c}$

$x = z + x' = z + y + x_{1c}$

$$\Rightarrow \begin{cases} x = z + y + x_{1c} \\ x' = y + x_{1c} \end{cases} = T(z, y)$$

$$\Rightarrow J_T(z, y) = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

Recall that, when we change variables:

$$\iint_D f(x, x')\, dx\, dx' = \iint_{D^*} dy\, dz\, f(T(z, y))\, |\det J_T(z, y)|$$

$$\Rightarrow = \frac{1}{4\pi D\sqrt{(t - t')(t' - t_0)}} \iint_{\mathbb{R}^2} dy\, dz\, e^{-\frac{z^2}{4D(t - t')} - \frac{y^2}{4D(t' - t_0)}} \cdot (z + y + x_{1c})(y + x_{1c})$$

$$(z + y + x_{1c})(y + x_{1c}) \stackrel{!}{=} \cancel{z x_{1c}} + \cancel{y x_{1c}} + x_{1c}^2 + \cancel{z y} + y^2 + \cancel{y x_{1c}}$$

Odd terms multiplied by an even function $f(y, z)$ to be integrals over a symmetric domain are zero!

$$\stackrel{!}{=} \frac{1}{4\pi D\sqrt{(t - t')(t' - t_0)}} \int_{\mathbb{R}} dy\, e^{-\frac{y^2}{4D(t' - t_0)}} \int_{\mathbb{R}} dz\, e^{-\frac{z^2}{4D(t - t')}} \cdot (x_{1c}^2 + y^2)$$

$$\langle x(t)x(t')\rangle = \frac{1}{4\pi D\sqrt{(t-t')(t'-t_0)}}\Big\{ x_{ic}^2\sqrt{4\pi D(t-t')}\sqrt{4\pi D(t'-t_0)} + $$
$$+\sqrt{4\pi D(t-t')}\,4D(t'-t_0)\sqrt{\pi D(t'-t_0)}\Big\}$$

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$$= x_{ic}^2 + \sqrt{4D^2}\,(t'-t_0) = x_{ic}^2 + 2D(t'-t_0)$$

where $\int_{\mathbb{R}} e^{-\frac{1}{2}ax^2}dx = \sqrt{\frac{2\pi}{a}}$ In our case: $a = \frac{1}{2D\Delta t} \rightsquigarrow \sqrt{\frac{2\pi}{1/2D\Delta t}} = \sqrt{4\pi D\Delta t}$

and $\int_{\mathbb{R}} dx\, x^2 e^{-\frac{1}{2}ax^2} = -2\frac{d}{da}\int dx\, e^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a^3}} \rightsquigarrow \sqrt{\frac{2\pi}{1/8D^3\Delta t^3}} = 4\sqrt{\pi D^3\Delta t^3}$

$$= 4D\Delta t\sqrt{\pi D\Delta t}$$

$\Rightarrow \langle x(t)x(t')\rangle = x_{ic}^2 + 2D(t'-t_0)$ where $t_0 < t' < t$

In the case where $t_0 < t < t'$ we have $x' \leftrightarrow x$, $t' \leftrightarrow t$ and the integration it's the same: $\langle x(t)x'(t)\rangle = x_{ic}^2 + 2D(t-t_0)$

$\Rightarrow$ So then in general we have: $\underline{\langle x(t)x(t')\rangle} = x_{ic}^2 + 2D\min(t-t_0, t'-t_0)$

While: $\langle x^2(t)\rangle = \int dx_0 \int dx\, W(x,t|x_0,t_0)\, W(x_0,t_0)\, x^2$ ... a lot of passages are like before...

$$= \int dx\, W(x,t|x_{ic},t_0)\,x^2 = \int dx\, \frac{e^{-(x-x_{ic})^2/4D(t-t_0)}}{\sqrt{4D\pi(t-t_0)}}\cdot x^2$$

$$= \int dz\, \frac{e^{-z^2/4D(t-t_0)}}{\sqrt{4\pi D(t-t_0)}}\underbrace{(z+x_{ic})^2}_{= z^2 + \cancel{2z x_{ic}} + x_{ic}^2} \quad \text{where } z = x - x_{ic}$$

$$= \frac{1}{\sqrt{4D\pi(t-t_0)}}\int dz\,(z^2+x_{ic}^2)\,e^{-\frac{z^2}{4D(t-t_0)}} = \frac{4D(t-t_0)\sqrt{\pi D(t-t_0)} + x_{ic}^2\sqrt{4\pi D(t-t_0)}}{\sqrt{4D\pi(t-t_0)}}$$

$$\Rightarrow \underline{\underline{\langle x^2(t)\rangle}} = x_{1c}^2 + 2D(t-t_0)$$

Furthermore: $\langle x(t)\rangle = \int dx_0 \int dx\, W(x,t\,|\,x_0,t_0)\, W(x_0,t_0)\, x$

$$\overset{!}{=} \int dx\, W(x,t\,|\,x_{1c},t_0)\, x = \int dx \frac{e^{-(x-x_{1c})^2/4D(t-t_0)}}{\sqrt{4D\pi(t-t_0)}}\cdot x$$

where $z = x - x_{1c}$, $dz = dx$

$$\overset{!}{=} \int dz \frac{e^{-\frac{z^2}{4D(t-t_0)}}}{\sqrt{4D\pi(t-t_0)}}(\cancel{z} + x_{1c}) = x_{1c}$$

$$\Rightarrow \underline{\underline{\langle x(t)\rangle}} = x_{1c}$$

So then the variance: $\underline{\underline{Var(x(t))}} = \langle x^2(t)\rangle - \langle x(t)\rangle^2 = 2D(t-t_0)$

↳ we find again $\sqrt{Var} = \sigma \propto \sqrt{t}$ a characteristic lenght of the diffusion stocastic motion!

2 The Wiener Path Integral

2.1 Remark

⋆ New material ⋆

Remark on the Wiener Measure:

$$dP_{t_1 \cdots t_n}(x_1 \cdots x_n | x_0, t_0)$$

$$= \prod_{i=1}^{n} \frac{dx_i}{\sqrt{4\pi D \Delta t}}\, e^{-\sum_{i=1}^{n} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i}}$$

$$= \frac{1}{4D} \sum_{i=1}^{n} \Delta t_i \left(\frac{\Delta x_i}{\Delta t_i}\right)^2$$

$$\xrightarrow[n \to \infty]{} dX_W = \prod_{\tau = t_0^+}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}}\, e^{-\frac{1}{4D}\int_{t_0}^{t} \dot{x}^2(\tau)\, d\tau}$$

Formal limit!

The above expression ($dX_W = \cdots$) is meaningless unless we has in mind its discretized version. However we will see it's a very useful formula to do calculations without using explicitly the discretized form. If we don't have in mind the discretized form the dX_W expression may seem very strange: one can show that $x(\tau)$ is continuous but not differentiable. Thus, strictly speaking $\dot{x}(\tau)$ doesn't exists!

2.2 Examples of Path Integrals

See Manzali-Nicolai's Notes - pag.36 ch2.2 Examples of path integrals

Wiener Measure: $dX_w(\tau) = \text{"}\lim_{n\to\infty}\text{"}\, d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0,t_0)$

⇝ Definition à la Physicist (not mathematically accurate) that permit us to introduce the notion of path integral

While the expected value of a functional f that depend on the trajector $x(\tau)$ with $\tau = 0\dots t$ is defined as:

$$\langle f(\{x(\tau)\}_{\tau=0}^{t})\rangle_W = \text{"}\lim_{n\to\infty}\text{"} \int_{\mathbb{R}^n} d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0 t_0)\cdot f_{\text{discretized}}(x_0 x_1\cdots x_n)$$

for fixed initial conditions $x(t_0) = x_0$

Notice that: $\langle 1\rangle_W = \text{"}\lim_{n\to\infty}\text{"} \int_{\mathbb{R}^n} d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0 t_0) = \int_{\mathbb{R}^n} dX_w(\tau) = 1$

Calculating Path Integrals

Ex (Transition Probabilities)

We want to calculate the wiener integral of the functional:

$f(\{x(\tau)\}_{\tau=0}^{t}) = \delta(x - x(t))$ } Probability density: when integrated takes a function of the position x and evaluates it in $x(t)$ the final trajectory point $(\tau = t)$

⇝ Fixes the final point!

If we average this functional over all possible path $x(\tau)|_{\tau=0}^{t}$ we already know the result:

$\langle \delta(x - x(t))\rangle_W = W(x,t|x_0,0)$ giving the i.c. $x(0)=x_0,\ t_0=0$

Why $\langle \delta(x-x(t))\rangle_W$ is the propagator? Because the average of the delta is the prob. density that the final point of the trajectory is at $x(t)$; in fact suppose we want to average $f(x(t))$:

$$\langle f(x(t))\rangle_{x_0} = \int dx\, \underline{W(x,t|x_0,0)}\, f(x)$$

Take out the average and inserting the delta

$$= \left\langle \int dx\, \delta(x-x(t))\, f(x)\right\rangle_{x_0}$$

$$= \int dx\, \underline{\langle \delta(x-x(t))\rangle}_{x_0}\, f(x)$$

$x(t)$ is the only random variable: the rest is constant for $\langle\cdot\rangle$!

Different from the previous definition of discrete traj. average:

$$\int dx_0 dx\, W(x,t|x_0,t_0)\, W(x_0,t_0) f(x) \overset{!}{=} \int dx\, W(x,t) f(x) = \langle f(x(t))\rangle$$

In fact below we are calculating the average giving the fact that the initial point is fixed! $\begin{cases} x(t=0)=x_0 \\ t_0=0\end{cases}$

$$\Rightarrow W(x,t|x_0,t_0) = \langle \delta(x-x(t))\rangle_{x_0}$$

We want to show that we get the same result using the Wiener measure

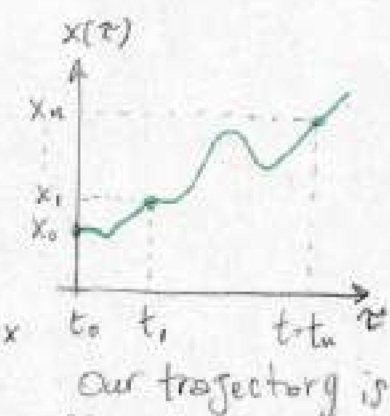
Let's calculate it using the Wiener measure. Initially we discretize time and space for finite n: $\underline{x(t)=x(t_n)=x_n \text{ and } t=t_n}$

$$\langle \delta(x-x(t))\rangle_{\text{discr}} = \int \prod_{i=1}^{n} \frac{dx_i}{\sqrt{4\pi D\Delta t_i}}\, e^{-\sum_{i=1}^{n}\frac{(x_i-x_{i-1})^2}{4D\Delta t_i}} \cdot \delta(x-x_n)$$

$$= \left[\int \prod_{i=1}^{n-1} \frac{dx_i}{\sqrt{4\pi D\Delta t_i}}\, e^{-\sum_{i=1}^{n-1}\frac{(x_i-x_{i-1})^2}{4D\Delta t_i}}\right]\left[\int \frac{dx_n}{\sqrt{4\pi D\Delta t_n}}\, e^{-\frac{(x_n-x_{n-1})^2}{4D\Delta t_n}}\delta(x-x_n)\right]$$

$$= \left[\cdots\right]\left[\frac{e^{-\frac{(x-x_{n-1})^2}{4D\Delta t_n}}}{\sqrt{4\pi D\Delta t_n}}\right] = \underline{\frac{1}{\sqrt{4\pi D\Delta t_n}}\int \prod_{i=1}^{n-1}\frac{dx_i}{\sqrt{4\pi D\Delta t_i}}\, e^{-\sum_{i=1}^{n}\frac{(x_i-x_{i-1})^2}{4D\Delta t_i}}\Big|_{x_n=x}}$$

☆



Our trajectory is given by discretized points

So then x_0, x_n fixed initial and final point, but we are integrating over the intermediate points: it's a convolution of $n-1$ gaussians (propagators)!

$$\langle \delta(x-x(t))\rangle_{discr.} = \frac{e^{-\frac{(x-x_{n-1})^2}{4D\Delta t_n}}}{\sqrt{4\pi D\Delta t_n}} \int W(x_{n-1}t_{n-1}|x_{n-2}t_{n-2})\cdots W(x_1t_1|x_0t_0)\,dx_{n-1}\dots dx_1$$

$$= \int W(x_nt_n|x_{n-1}t_{n-1})\Big|_{x_n=x} W(x_{n-1}t_{n-1}|x_{n-2}t_{n-2})\cdots W(x_1t_1|x_0t_0)\,dx_{n-1}\dots dx_2dx_1$$

$$= W(x_nt_n|x_0t_0)\Big|_{x_n=x} = \frac{e^{-\frac{(x-x_0)^2}{4Dt}}}{\sqrt{4\pi Dt}} \quad \forall n$$

Result indipendent on n so there's no need to take n to infinity: $n \to +\infty$

(Recall that: $t=\sum_{i=1}^{n}\Delta t_i$ and $\Delta x_i = x_i - x_{i-1}$ indip. random variables)

This is not the way we want to use to solve this integral: we want to use PATH INTEGRALS a more complicated but general method.

$$\langle \delta(x-x(t))\rangle_{discr.} \overset{\star}{=} \frac{1}{\sqrt{4\pi D\Delta t_n}}\int \prod_{i=1}^{n-1}\frac{dx_i}{\sqrt{4\pi D\Delta t_i}}\, e^{-\sum_{i=1}^{n}\frac{(x_i-x_{i-1})^2}{4D\Delta t_i}}\Big|_{x_n=x}$$

Let's define $n=N+1$
$\to N=n-1$

$\Delta t_i = \varepsilon$
$t_n - t_0 = t - t_0$
$\overset{!}{=} n\varepsilon = (N+1)\varepsilon$

$$= \frac{1}{\sqrt{4\pi D\Delta t_{N+1}}}\int \prod_{i=1}^{N}\frac{dx_i}{\sqrt{4\pi D\Delta t_i}}\, e^{-\sum_{i=1}^{N+1}\frac{(x_i-x_{i-1})^2}{4D\Delta t_i}}\Big|_{x_n=x}$$

$$= \frac{1}{\sqrt{4\pi D\varepsilon}}\int \prod_{i=1}^{N}\frac{dx_i}{\sqrt{4\pi D\varepsilon}}\, e^{-\frac{\vec{x}^TA\vec{x}}{4D\varepsilon}}$$

when $\sum_i (x_i-x_{i-1})^2$ is a polynomial of order 2 $\to$ quadratic form!

In particular we choose $x = x_n = x_{N+1} = 0 = x_0$, so then:

$$\sum_{i=1}^{N+1}(x_i-x_{i-1})^2 = (\cancel{x_{N+1}^2} - \cancel{2x_{N+1}x_N} + x_N^2) + \dots + (x_2^2 - 2x_1x_2 + x_1^2) + (x_1^2 - \cancel{2x_1x_0} + \cancel{x_0^2})$$

$$\overset{!}{=} 2(x_1^2+x_2^2+\dots+x_N^2) - 2(x_1x_2+\dots+x_Nx_{N-1}) = \sum_{i,j=1}^{N} x_ix_jA_{ij} = \vec{x}^TA\vec{x}$$

So we have $\vec{x}^T = (x_1, x_2, \dots x_N)$ and we are calculating the probability to be back at the origin ($x = 0 = x_0$) at time t:

$$W(0,t|0,t_0) = \langle \delta(x(t)) \rangle_{discr.} = \frac{1}{\sqrt{4\pi D\varepsilon}} \int \prod_{i=1}^{N} \frac{dx_i}{\sqrt{4\pi D\varepsilon}}\, e^{-\frac{\vec{x}^T A \vec{x}}{4D\varepsilon}}$$

So the A_N matrix is an $N \times N$ matrix, but how to represent it?

$$\vec{x}^T A_N \vec{x} = \sum_{i,j=1}^{N} x_i A_{ij} x_j = 2\left(\sum_{i=1}^{N} x_i^2\right) - 2\left(\sum_{i=1}^{N-1} x_i x_{i+1}\right)$$

Direct method: $\frac{\partial^2}{\partial x_m \partial x_n}(\vec{x}^T A \vec{x}) = \frac{\partial^2}{\partial x_m \partial x_n}\left(\sum_{i,j=1}^{N} x_i A_{ij} x_j\right)$

$$\overset{!}{=} \frac{\partial}{\partial x_m}\left[\sum_{j=1}^{N} A_{nj} x_j + \sum_{i=1}^{N} x_i A_{in}\right] = A_{nm} + A_{nm} = 2A_{nm}$$

$$\frac{\partial^2}{\partial x_m \partial x_n}\left[2\sum_i^N x_i^2 - 2\sum_i^{N-1} x_i x_{i+1}\right] = \frac{\partial}{\partial x_m}\left[\sum_i 2\left(2x_n \frac{\partial x_i}{\partial x_n}\right) - 2\left(\sum_i \underbrace{\frac{\partial x_i}{\partial x_n}}_{\neq 0 \text{ if } i=n} x_{i+1} + x_i \underbrace{\frac{\partial x_{i+1}}{\partial x_n}}_{\neq 0 \text{ if } i+1=}\right.\right.$$

$$\overset{!}{=} \frac{\partial}{\partial x_m}\left[4x_n - 2(x_{n+1} + x_{n-1})\right] = 4\delta_{nm} - 2(\delta_{n+1,m} + \delta_{n-1,m})$$

$\Rightarrow A_{nm} = 2\delta_{nm} - (\delta_{n+1,m} + \delta_{n-1,m})$

$\Rightarrow A_{n,n\pm1} = -1$

$A_{nn} = 2$

$$B_{n,m} = \begin{cases} 1 & \text{if } n+1=m \\ 0 & \text{otherwise} \end{cases} \overset{!}{=} \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ & 0 & 1 & & \vdots \\ & & 0 & & \\ \vdots & & & \ddots & 1 \\ 0 & \cdots & & & 0 \end{pmatrix}$$

$$\Rightarrow A_N = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ & & & & -1 \\ 0 & & \cdots & & 2 \end{pmatrix}$$

(Professor: $AN[i,j] = 2 \quad AN[i,j] = -\delta_{i,j-1} - \delta_{i,j+1}$)

Substituting back in ☆ we have:

$$W(0,t|0,t_0) = \langle \delta(x(t)) \rangle_{discr.}$$

$$= \frac{1}{(\sqrt{4\pi D\varepsilon})^{N+1}} \int_{\mathbb{R}^N} dx_1 \dots dx_N \, e^{-\frac{\vec{x}^T A \vec{x}}{4D\varepsilon}}$$

where $Z(A) = \int_{\mathbb{R}^N} d\vec{x} \, e^{-\frac{1}{2}\vec{x}^T A \vec{x}} = \frac{(2\pi)^{N/2}}{\sqrt{\det A}}$

and $\det A = \prod_{i=1}^{N} a_i$ a_i = eigenvalues of A

$$= \frac{1}{(\sqrt{4\pi D\varepsilon})^{N+1}} \frac{(2\pi)^{N/2}}{\left(\prod_{i=1}^{N} \frac{a_i}{2D\varepsilon}\right)^{1/2}}$$

$$= \frac{1}{(4\pi\varepsilon D)^{\frac{N+1}{2}}} \frac{(4\pi D\varepsilon)^{N/2}}{\sqrt{\det A_N}} = \frac{1}{\sqrt{4\pi\varepsilon D}\,\sqrt{\det A_N}}$$

$$\Rightarrow W(0,t|0,t_0) = \frac{1}{\sqrt{4\pi D\varepsilon}} (\det A_N)^{-1/2}$$

So all is left is to calculate the determinant of A_N

(... See Marzoli notes pag. 39)

$$\Rightarrow \underline{\underline{W(0,t|0,t_0)}} = \frac{1}{\sqrt{4\pi D\varepsilon}} \frac{1}{\sqrt{N+1}}$$

$$= \frac{1}{\sqrt{4\pi D(t-t_0)}}$$ where $(N+1)\varepsilon = t - t_0$

Ex **Integral functional ~ Maiton method**

We want to compute $\left\langle F\left(\int_0^t a(\tau) x(\tau) d\tau \right) \right\rangle_W$ and to do this we use a special trick, to make easier the computation.

Let's introduce $A(\tau)$ such that:

$a(\tau) = -\dot{A}(\tau)$ $\Rightarrow$ We put $A(\tau) = \int_\tau^t a(\tau') d\tau'$ because we want that $A(t) = 0$ holds!

Separation of variables:

$a(\tau) = -\frac{dA}{d\tau}$ $\quad \int a(\tau) d\tau = -\int dA \quad \Rightarrow A(\tau) = -\int a(\tau') d\tau' + const$

The reason we want $A(t) = 0$ is because we have also $x(t_0) = 0$ which is convenient when we calculate:

$$\int_0^t a(\tau) x(\tau) d\tau = -\int_0^t \dot{A}(\tau) x(\tau) d\tau = -\cancel{\left[A(\tau) x(\tau) \right]_{\tau=0}^{\tau=t}} + \int_0^t A(\tau) \dot{x}(\tau) d\tau$$

$$= \int_0^t A(\tau) \dot{x}(\tau) d\tau$$

$$\Rightarrow F\left(\int_0^t A(\tau) \dot{x}(\tau) d\tau \right) \rightsquigarrow F_{discr.}\left(\sum_{i=1}^N \frac{x_i - x_{i-1}}{\Delta t_i} \Delta t_i A_i \right)$$

(Discretization) where $A_i = A(t_i)$ and $\Delta x_i = x_i - x_{i-1}$

$$\Rightarrow \langle F_{discr.} \rangle_N = \int \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} e^{-\sum_{i=1}^N \frac{\Delta x_i^2}{4D\Delta t_i}} F_{discr.}\left(\sum_{i=1}^N \Delta x_i A_i \right)$$

$\overset{!}{=}$ Manzali pag. 43/45 $= \cdots$

2.3 Integral Functional (Special cases) and Functional Derivative

$\star$ **New material** $\star$ done after ch2.2.2 of Manzali-Nicolai's Notes (see pag.46 - **Example 3** (Generating function))

$\boxed{\text{Ex}}$ Integral functional ~ special cases

$\boxed{1A}$

- If $F(z) = e^{hz}$, then we have:

$$\left\langle e^{h \int_0^t a(\tau) x(\tau) d\tau} \right\rangle_W = \frac{1}{\sqrt{4\pi R(t) D}} \int dz \, e^{hz - \frac{z^2}{4DR(t)}}$$

Gauss integral: $\int_{\mathbb{R}} dx \, e^{-\frac{a}{2}x^2 + bx} = \sqrt{\frac{2\pi}{a}} \, e^{\frac{b^2}{2a}}$ | In our case: $a \to \frac{1}{2DR(t)}$ $b \to h$

$$\Rightarrow \int dz \, e^{hz - \frac{z^2}{4DR(t)}} = \sqrt{4\pi D R(t)} \, e^{h^2 D R(t)}$$

$$\Rightarrow \left\langle e^{h \int_0^t a(\tau) x(\tau) d\tau} \right\rangle_W = e^{h^2 D R(t)} \equiv G(h)$$

Notice that $G(h)$ is the moment generating function of the integral $I = \int_0^t a(\tau) x(\tau) d\tau$, so then we can compute the n-th moment of I calculating the n-th derivative of $G(h)$:

$$\frac{d^n}{dh^n} G(h) \Big|_{h=0} = \langle I^n \rangle_W$$

$$\langle I \rangle_W = \left\langle \int_0^t a(\tau) x(\tau) d\tau \right\rangle_W = \frac{d}{dh} G(h) \Big|_{h=0}$$

$$= 2hDR(t) \, e^{h^2 R(t) D} \Big|_{h=0} = 0$$

For a random variable X, the mom. generating function is:

$$M_X(h) = \mathbb{E}(e^{hX})$$

with $h \in \mathbb{R}$

In particular:

$$\mu_n = \frac{d^n}{dh^n} M_X(h) \Big|_{h=0}$$

where

$$\mu_n = \mathbb{E}(X^n)$$

$$\langle I^2\rangle_W = \left\langle\left(\int_0^t a(\tau)x(\tau)d\tau\right)^2\right\rangle_W = \frac{d^2}{dh^2}G(h)\Big|_{h=0}$$

$$= \frac{d}{dh}\left(2hDRe^{h^2DR}\right)\Big|_{h=0} = 2DRe^{h^2DR} + (2hDR)^2e^{h^2DR}\Big|_{h=0}$$

$$= 2DR(t)$$

Considering a generic odd moment we have:

$$\left\langle\left(\int_0^t a(\tau)x(\tau)d\tau\right)^{2k+1}\right\rangle_W = \frac{d^{2k+1}}{dh^{2k+1}}G(h)\Big|_{h=0} = 0$$

In fact if we expand $G(h) = e^{h^2DR(t)}$ we get:

$$G(h) = \sum_{n=0}^{\infty}\frac{h^{2n}}{n!}(DR)^n = 1 + DRh^2 + \frac{(DR)^2}{2}h^4 + \dots$$

So differentiating respect to h an odd number of times and imposing $h=0$ we will always get zero because there will be all terms containing power of h (at least of order one)!

While for the even moments we have:

$$\left\langle\left(\int_0^t a(\tau)x(\tau)d\tau\right)^{2k}\right\rangle = \frac{d^{2k}}{dh^{2k}}G(h)\Big|_{h=0} = \left(\frac{DR(t)}{2}\right)^k\frac{(2k)!}{2^k\cdot k!}$$

Using the previous expansion we get:

$$\frac{d^2}{dh^2}G(h) = 2DR \quad \frac{d^4}{dh^4}G(h) = \frac{(DR)^2}{2}4! \quad \frac{d^6}{dh^6}G(h) = \frac{(DR)^3}{3!}6! \quad \frac{d^8}{dh^8}G(h) = \frac{(DR)^4}{4!}8!$$

$$\Rightarrow \frac{d^{2k}}{dh^{2k}}G(h)\Big|_{h=0} = \frac{(DR)^k}{k!}(2k)! \quad (?)$$

- If $a(\tau) = \delta(\tau - t^-)$, where $t^- < t$, so we have:

$$\int_0^t x(\tau) a(\tau)\, d\tau = \int_0^t x(\tau)\, \delta(\tau - t^-)\, d\tau = x(t) \qquad \boxed{1B}$$

and if $F(z) = \delta(z - x)$

$$\Rightarrow F\left(\int_0^t a(\tau) x(\tau)\, d\tau\right) = F(x(t)) = \delta(x(t) - x)$$

$\Rightarrow$ With this choice of $a(\tau)$ and $F(z)$ we get the previous transition probability:

$$\left\langle F\left(\int_0^t a(\tau) x(\tau) d\tau\right)\right\rangle_W = \left\langle F(x(t))\right\rangle_W = \left\langle \delta(x(t) - x)\right\rangle_W = W(x,t|0,0)$$

So then:

$$A(\tau) = \int_\tau^t a(\tau')\, d\tau' = \int_\tau^t \delta(\tau' - t^-)\, d\tau' = 1 \quad \text{for } \forall \tau: 0 < \tau < t$$

$$R(t) = \int_0^t d\tau \left(\int_\tau^t a(s)\, ds\right)^2 = \int_0^t A^2(\tau)\, d\tau = t$$

$$\Rightarrow W(x,t|0,0) = \frac{1}{\sqrt{4\pi R(t)D}} \int dz\, F(z)\, e^{-\frac{z^2}{4DR(t)}}$$

$$= \frac{1}{\sqrt{4\pi Dt}} \int dz\, \delta(z - x)\, e^{-\frac{z^2}{4Dt}} = \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}$$

which is result we expected!

• If $F(z)=e^z$ and $a(\tau)=h_1\delta(\tau-t_1)+h_2\delta(\tau-t_2)$ $\left(\begin{array}{c}\text{Case 1A}\\ \text{with } h=1\end{array}\right)$

where $0<t_1, t_2<t$

$\boxed{1C}$

$$\int_0^t a(\tau)x(\tau)\,d\tau = \int_0^t \big(h_1x(\tau)\delta(\tau-t_1)+h_2x(\tau)\delta(\tau-t_2)\big)d\tau$$

$$= h_1x(t_1)+h_2x(t_2)$$

$$A(\tau)=\int_\tau^t a(\tau')\,d\tau' = \int_\tau^t \big(h_1\delta(t_1-\tau')+h_2\delta(t_2-\tau')\big)d\tau'$$

$$= \int_\tau^t \left[h_1\dot{\theta}(t_1-\tau')+h_2\dot{\theta}(t_2-\tau')\right]d\tau' \quad \text{where } \delta(x)=\frac{d}{dx}\theta(x)$$

$$= h_1\theta(t_1-\tau')\Big|_\tau^t + h_2\theta(t_2-\tau')\Big|_\tau^t \quad \text{and } \theta(x-a)=\begin{cases}1 & \text{if } x>a\\ 1/2 & \text{if } x=a\\ 0 & \text{if } x<a\end{cases}$$

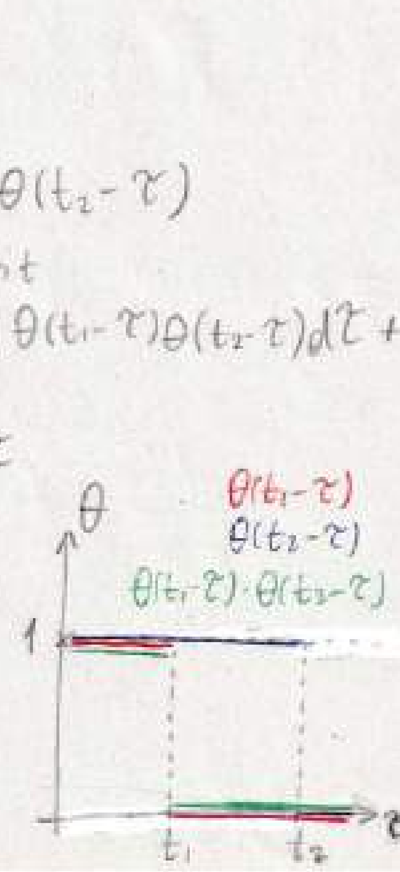
$$= h_1\Big[\cancel{\underbrace{\theta(t_1-t)}_{<0}}-\theta(t_1-\tau)\Big]+h_2\Big[\cancel{\underbrace{\theta(t_2-t)}_{<0}}-\theta(t_2-\tau)\Big]$$

$$= -\big(h_1\theta(t_1-\tau)+h_2\theta(t_2-\tau)\big)$$

$$A^2(\tau)=h_1^2\theta(t_1-\tau)+2h_1h_2\theta(t_1-\tau)\theta(t_2-\tau)+h_2^2\theta(t_2-\tau)$$

$$R(t)=\int_0^t A^2(\tau)\,d\tau = h_1^2\int_0^t\theta(t_1-\tau)\,d\tau+2h_1h_2\int_0^t\theta(t_1-\tau)\theta(t_2-\tau)\,d\tau+$$

$$+h_2^2\int_0^t\theta(t_2-\tau)\,d\tau$$



$$= h_1^2\int_0^{t_1}d\tau + h_2^2\int_0^{t_2}d\tau + 2h_1h_2\int_0^{\min(t_1,t_2)}d\tau$$

$$= h_1^2t_1+h_2^2t_2+2h_1h_2\min(t_1,t_2)$$

$$\Rightarrow \left\langle e^{k_1 x(t_1) + k_2 x(t_2)} \right\rangle_W = \left\langle F\left(\int_0^t a(\tau) x(\tau) d\tau \right) \right\rangle_W$$

$$= \frac{1}{\sqrt{4\pi R(t) D}} \int dz F(z) e^{-\frac{z^2}{4DR(t)}} = e^{k^2 DR(t)} \Big|_{k=1}$$

$$= e^{D(k_1^2 t_1 + k_2^2 t_2 + 2k_1 k_2 \min(t_1, t_2))} \equiv G(k_1, k_2)$$

Notice that differenciating the two sides of the equation above:

$$\frac{\partial^2}{\partial k_1 \partial k_2} G(k_1, k_2) \Big|_{k_1 = k_2 = 0} = \langle x(t_1) x(t_2) \rangle_W = 2D \min(t_1, t_2)$$

$\rightsquigarrow$ That is the result we have obtain at the end of the last chapter when we calculate $\langle x(t_1) x(t_2) \rangle$ with $x_{10} = 0$ and $W(x_0, t_0 = 0) = \delta(x_0 - x_{10})$

So the particle starts from $x_0 = 0$ at $t_0 = 0$: recall that if the particle starts at $x_0 \neq 0$ then:

$$\langle x(t_1) x(t_2) \rangle = 2D \min(t_1, t_2) + x_0^2$$

$$\langle x(t_i) \rangle = \frac{\partial}{\partial k_i} G(k_1, k_2) \Big|_{k_1 = k_2 = 0} = 0 \,!$$

Recalling also that

- The same result of 1C can be obtained as follow. $\boxed{1D}$

$$\left\langle e^{\int_0^t a(\tau) x(\tau) d\tau} \right\rangle_W = \mathcal{G}\left(\{a(\tau)\}_{\tau=0}^t\right)$$

we introduce $\mathcal{G}$ a functional depending on the generic function $a(\tau)$

$\Rightarrow$ Functional derivative of the integral at the exponent:

$$\frac{\delta}{\delta a(\tau')} \int_0^t a(\tau) x(\tau) d\tau = x(\tau')$$

Def: Functional Derivative of $\mathcal{G}(\{a(\tau)\}_{\tau=0}^{t})$

If we take the difference: $\Delta \mathcal{G} = \mathcal{G}(\{a(\tau)+\delta a(\tau)\}_{\tau=0}^{t}) - \mathcal{G}(\{a(\tau)\}_{\tau=0}^{t})$

$$\overset{!}{=} \int d\tau \, \hat{\mathcal{G}}(\{a(\tau)\}_{\tau=0}^{t}) \, \delta a(\tau)$$

$$\Rightarrow \hat{\mathcal{G}} \equiv \frac{\delta}{\delta a(\tau)} \mathcal{G}(\{a(\tau)\}_{\tau=0}^{t})$$

Functional Derivative of $\mathcal{G}(\{a(\tau)\}_0^t)$

Examples

① Functional: $\mathcal{G}_1 = \int_0^t a(\tau') x(\tau') d\tau'$

$a \to a + \delta a$

$$\Rightarrow \Delta \mathcal{G}_1 = \int_0^t [a(\tau') + \delta a(\tau')] \cdot x(\tau') d(\tau') - \int_0^t a(\tau') x(\tau') d\tau'$$

$$\overset{!}{=} \int_0^t \delta a(\tau') x(\tau') d\tau'$$

$$\Rightarrow \hat{\mathcal{G}}_1 \equiv \frac{\delta \mathcal{G}}{\delta a(\tau)} = x(\tau)$$

(That is similar to: $\partial/\partial a_i \sum_i x_i a_i = x_i$!)

② Functional: $\mathcal{G}_2 = e^{\int_0^t a(\tau') x(\tau') d\tau'} = e^{\mathcal{G}_1}$

$a \to a + \delta a$

$$\Rightarrow \Delta \mathcal{G}_2 = e^{\int_0^t (a+\delta a) x \, d\tau'} - e^{\int_0^t a x \, d\tau'} = e^{\int_0^t a x \, d\tau'} \left(e^{\int_0^t \delta a x \, d\tau'} - 1 \right)$$

$$\overset{!}{=} e^{\mathcal{G}_1} (\Delta \mathcal{G}_1 - 1)$$

$$\Rightarrow \hat{\mathcal{G}}_2 \equiv \delta \mathcal{G}_2 / \delta a(\tau) = e^{\mathcal{G}_1} \frac{\delta \mathcal{G}_1}{\delta a(\tau)} = x(\tau) \, \mathcal{G}_2$$

or we can do it directly using a sort of (functional) chain rule:

$$\frac{\delta G_2}{\delta a(\tau)} = \frac{\delta}{\delta a(\tau)} e^{\int_0^t a(\tau')x(\tau')d\tau'}$$

Chain rule!

$$= e^{\int_0^t a(\tau')x(\tau')d\tau'} \frac{\delta}{\delta a(\tau)}\Big[\underbrace{\int_0^t a(\tau')x(\tau')d\tau'}_{\overset{!}{=} G_1}\Big]$$

$$= e^{G_1}\frac{\delta G_1}{\delta a(\tau)} = G_2 x(\tau)$$

3 More in General – Functions of a functional

Functional: $G_3 = F\left(\int_0^t a(\tau')x(\tau')d\tau'\right) = F(G_1)$

where $F: \mathbb{R} \to \mathbb{R}$

$$\Delta G_3 = \Delta F(G_1) = F(G_1 + \Delta G_1) - F(G_1)$$

$$\overset{!}{=} F'(G_1)(\Delta G_1 + \mathcal{O}(\Delta G_1^2))$$

$$\Rightarrow \frac{\delta G_3}{\delta a(\tau)} = F'(G_1)\frac{\delta G_1}{\delta a(\tau)} = F'(G_1)\,x(\tau)$$

4 Euler-Lagrange equations with the action:

$$S = \int_0^t d\tau\, \underbrace{\mathcal{L}(x(\tau), \dot{x}(\tau))}_{\text{Lagrangian (Functional)}}$$

$x(\tau) \to x(\tau)+\delta x(\tau)$, $\dot{x}(\tau) \to \dot{x}(\tau)+\delta\dot{x}(\tau)$ and neglecting $\mathcal{O}(\delta x^2, \delta\dot{x}^2)$.

$$\Rightarrow \Delta S = \int_0^t d\tau \left[\mathcal{L}(x(\tau)+\delta x(\tau), \dot{x}(\tau)+\delta\dot{x}(\tau)) - \mathcal{L}(x(\tau),\dot{x}(\tau))\right]$$

$$= \int_0^t d\tau \left[\delta x(\tau)\frac{\partial \mathcal{L}}{\partial x}(x,\dot{x}) + \underline{\delta\dot{x}(\tau)\frac{\partial \mathcal{L}}{\partial \dot{x}}(x,\dot{x})}\right]_{\substack{x=x(\tau)\\ \dot{x}=\dot{x}(\tau)}}$$

Integration by parts

$$= \int_0^t d\tau\, \delta x(\tau)\left[\frac{\partial \mathcal{L}}{\partial x}(x,\dot{x}) - \underline{\frac{d}{dt}}\frac{\partial \mathcal{L}}{\partial \dot{x}}(x,\dot{x})\right]_{\substack{x=x(\tau)\\ \dot{x}=\dot{x}(\tau)}} + \underline{\delta x(\tau)\frac{\partial \mathcal{L}}{\partial \dot{x}}(x(\tau),\dot{x}(\tau))\Big|_0^t}$$

Thus if $\tau \in (0,t)$

$$\Rightarrow \frac{\delta S}{\delta x(\tau)} = \left[\frac{\partial \mathcal{L}}{\partial x}(x,\dot{x}) - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}}(x,\dot{x})\right]_{\substack{x=x(\tau)\\ \dot{x}=\dot{x}(\tau)}}$$

Euler Lagrange equation

$\to$ The equation of motion (classic ones) are such that the action is stationary respect to $x(\tau)$!

So returning to the exercise 1D we have:

$$\left\langle e^{\int_0^t a(\tau)x(\tau)d\tau}\right\rangle_W = \mathcal{G}\left(\{a(\tau)\}_{\tau=0}^t\right)$$

$$\frac{\delta}{\delta a(\tau)}\mathcal{G} = \langle x(\tau)\,\mathcal{G}\rangle_W = \left\langle e^{\int_0^t a(\tau')x(\tau')d\tau'}\, x(\tau)\right\rangle_W$$

$$\frac{\delta}{\delta a(\tau_1)\delta a(\tau_2)}\mathcal{G}\Big|_{a=0} = \frac{\delta}{\delta a(\tau_1)}\left\langle e^{\int_0^t a(\tau')x(\tau')d\tau'}\, x(\tau_2)\right\rangle_W\Big|_{a=0}$$

$$= \left\langle e^{\int_0^t a(\tau')x(\tau')d\tau'} x(\tau_1)x(\tau_2) \right\rangle_W \Big|_{a=0} = \langle x(\tau_1)x(\tau_2)\rangle_W$$

So if we use: $\left\langle e^{k\int_0^t a(\tau)x(\tau)d\tau} \right\rangle_W = e^{k^2 D R(t)} = G(k)$ with $k=1$

and: $R(t) = \int_0^t A^2(\tau)d\tau = \int_0^t \left(\int_\tau^t a(\tau')d\tau' \right)^2 d\tau$

we get the previous result: $\frac{\delta}{\delta a(\tau_1)\delta a(\tau_2)} G \Big|_{a=0} = \langle x(\tau_1)x(\tau_2)\rangle_W = 2D\min(\tau_1,\tau_2)$

3 Diffusion with Forces

3.1 Fokker-Planck equation

See Manzali-Nicolai's Notes - pag.56 ch3.1 Fokker-Planck equation

FOKKER-PLANK EQUATION

Let's start considering a particle that moves inside a continuum lattice (so we drop the discretization of space, moving from $\mathbb{Z}$~lattice to $\mathbb{R}$) of dimension d and that can jump to another position after a time step ε (jump of size $\vec{z}$ (= z later on) of any size)

So then considering jumps $\in \mathbb{R}$ the ME becomes:

$$\underbrace{\omega(x,t_{n+1})}_{\substack{\text{Prob. to be at} \\ \text{position } x \text{ at} \\ \text{time } t_{n+1}}} = \int_{\mathbb{R}^d} d^d z \, \underbrace{W(z|x-z)}_{\substack{\text{jump of} \\ \text{of size } z \text{ giving} \\ \text{the fact we were at position } x-z}} \underbrace{\omega(x-z,t_n)}_{\substack{\text{Prob. to be at position} \\ x-z \text{ at time } t_n}}$$

In particular: $W(z|x-z)d^d z$ ~ prob. to do a jump of size $z \in \mathbb{R}^d$ given that at the previous time the particle was at position $x-z$

Moreover: $\int_{\mathbb{R}^d} d^d z \, W(z|x) = 1 \quad (*) \quad \Leftrightarrow \sum_i W_{ij} = 1$

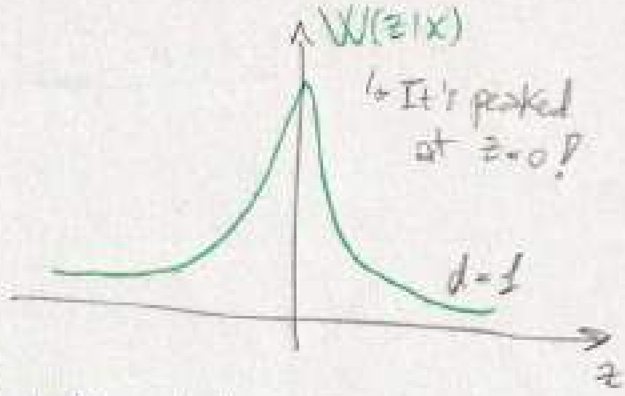
⇝ If we are at a generic position x, the probability to do a jump of any size must be equal to certainty!

So we start from $(*)$ and multiply both sides of it by $\omega(x,t_n)$:

$\int_{\mathbb{R}^d} \omega(x,t_n) W(z|x) d^d z = \omega(x,t_n)$ ⇝ We subtract each side by $\omega(x,t_{n+1})$ and use the ME

$$\omega(x,t_{n+1}) - \omega(x,t_n) = \int_{\mathbb{R}^d} d^d z \left[W(z|x-z)\omega(x-z,t_n) - W(z|x)\omega(x,t_n) \right]$$

Hyp: let's assume that small jumps $z \ll 1$ are more likely than bigger ones, so $W(z|x)$ will have the shape in the figure (something like that)



- Notice that $W(z|x)$ depends only on the jump z (is a function of z): it's indipendent on the position x where the particle is!

Then starting from the last equation, we define the function $f(x)$:

$$\omega(x,t_{n+1}) - \omega(x,t_n) = \int_{\mathbb{R}^d} d^d z \Big[\underbrace{W(z|x-z)\,\omega(x-z,t_n)}_{\stackrel{!}{=} f(x-z)} - \underbrace{W(z|x)\,\omega(x,t_n)}_{\stackrel{!}{=} f(x)} \Big]$$

Notice that the main contribution to $f(x-z)$ are given by the part of W that is peaked ($z \sim 0$), so we can expand it in series:

$$f(x-z) - f(x) = \Big[\cancel{f(x)} - z \frac{d}{dx} f(x) + \frac{z^2}{2} \frac{d^2}{dx^2} f(x) + \cdots \Big] - \cancel{f(x)}$$

↳ Expansion at $z \sim 0 \Rightarrow x - z = x$

Rearranging the starting equation with the expansion, substituting $t_n \to t$ and expanding $\omega(x,t_{n+1}) = \omega(x,t_n+\varepsilon)$ for $\varepsilon \sim 0$ we have:

$$\underbrace{\Big[\cancel{\omega(x,t)} + \varepsilon\, \dot{\omega}(x,t) + \mathcal{O}(\varepsilon^2) \Big]}_{\text{Expansion at } \varepsilon \sim 0:\ t_n + \varepsilon = t_n} - \cancel{\omega(x,t)} = \int d^d z \Big[-z \frac{d}{dx} f(x) + \frac{z^2}{2} \frac{d^2}{dx^2} f(x) + \cdots \Big]$$

$$\varepsilon\, \dot{\omega}(x,t) + \mathcal{O}(\varepsilon^2) = \int d^d z \Big[-z \frac{d}{dx} W(z|x)\,\omega(x,t) + \frac{z^2}{2} \frac{d^2}{dx^2} W(z|x)\,\omega(x,t) + \cdots \Big]$$

Generic k order

$$\stackrel{!}{=} -\frac{d}{dx} \Big[\omega(x,t) \int_{\mathbb{R}^d} d^d z\, W(z|x)\, z \Big] + \frac{1}{2} \frac{d^2}{dx^2} \Big[\omega(x,t) \int_{\mathbb{R}^d} d^d z\, W(z|x)\, z^2 \Big] + \cdots + \frac{(-1)^k}{k!} \frac{d^k}{dx^k} \Big[\omega(x,t) \int_{\mathbb{R}^d} d^d z\, W(z|x)\, z^k \Big]$$

We have just obtained the Kramer-Moyal expansion, in order to give a meaning to this expansion (we don't know what is the expansion parameter, and furthermore if it converges!) we divide by ε and take $\varepsilon \to 0$:

$$\dot{\omega}(x,t) = -\frac{\partial}{\partial x}\left[\omega(x,t)\lim_{\varepsilon\to 0}\underbrace{\int_{R^d} d^d z\, W(z|x)\frac{z}{\varepsilon}}_{\langle z\rangle_J \propto \varepsilon}\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[\omega(x,t)\lim_{\varepsilon\to 0}\underbrace{\int_{R^d} d^d z\, W(z|x)\frac{z^2}{\varepsilon}}_{\langle z^2\rangle_J \propto \varepsilon}\right]$$

$$+ \frac{(-1)^k}{k!}\frac{\partial^k}{\partial x^k}\left[\omega(x,t)\lim_{\varepsilon\to 0}\overbrace{\int_{R^d} d^d z\, W(z|x)\frac{z^k}{\varepsilon}}^{\langle z^k\rangle}\right] + \dots$$

PS. RW with no bias ($P_+ = P_- = 1/2$), in this case we have:

$\langle z\rangle_{jump} = 0$

$\langle z^2\rangle_{jump} \propto \varepsilon$

If we assume there's an external force $F_{ext} \neq 0$ that is affecting the particle, we expect it to have a preferred jump direction: $\langle z\rangle_J \propto \varepsilon F_{ext}$

(See pag 59 Manzoli)

$$\underbrace{\langle z^2\rangle_J}_{\propto \varepsilon \text{ a part from higher orders}} - \underbrace{\langle z\rangle_J^2}_{\propto \varepsilon} \propto \varepsilon$$

(... Manzoli pag. 59-60 ...) $\Rightarrow$ $\lim_{\varepsilon\to 0}\frac{\langle z^3\rangle_J}{\varepsilon} = \varepsilon^{\frac{3}{2}-1} \xrightarrow[\varepsilon\to 0]{} 0$

$\lim_{\varepsilon\to 0}\frac{\langle z^k\rangle_J}{\varepsilon} = \varepsilon^{\frac{k}{2}-1} \xrightarrow[\varepsilon\to 0]{} 0$ for $k \geq 3$

So taking $\varepsilon \to 0$ in the $k \geq 3$ orders cancels out and we get the F-P Equation:

$$\dot{\omega}(x,t) = -\frac{\partial}{\partial x}\omega(x,t)\left[\frac{\varepsilon f(x)}{\varepsilon}\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\omega(x,t)\left[\frac{2\varepsilon D(x) + \varepsilon^2 f^2}{\varepsilon}\right] + 0 \text{ when } \varepsilon \to 0$$

$$\boxed{= \frac{\partial}{\partial x}\left[-f(x)\omega(x,t) + \frac{\partial}{\partial x}\left(D(x)\,\omega(x,t)\right)\right]}$$

$\boxed{\text{P.S.}}$ f and $\hat{D}$ (or D) might depend on time t!

FOKKER-PLANK EQUATION:

If we define $J(x,t) = f(x)\omega(x,t) - \frac{d}{dx}(D(x)\omega(x,t))$ like a probab. current, then we retrieve the usual diffusion equation:

$$\mathring{\omega}(x,t) = -\frac{d}{dx} J(x,t) \quad \text{in 1-DIM}$$

While in d-DIM: $\mathring{\omega}(x,t) = -\vec{\nabla}\cdot\vec{J}(x,t)$ where $x \in \mathbb{R}^d$ and the prob. current in components is:

$$J_\mu(x,t) = f_\mu(x)\,\omega(x,t) - \sum_{\nu=1}^{d} \frac{d}{dx_\nu}\left(D_{\mu\nu}\,\omega(x,t)\right)$$ where $D_{\mu\nu} = D_{\nu\mu}$ symmetric and positive definite

While: $$W(z|x) = \frac{1}{\varepsilon^{d/2}|\hat{D}|^{1/2}} F\left(\sum_{\mu\nu}(x_\mu - f_\mu(x)\varepsilon)\frac{\hat{D}^{-1}_{\mu\nu}(x)}{\varepsilon}(x_\nu - f_\nu(x)\varepsilon)\right)$$

Notice that if $f=0$ and $D(x)=D$ is indipendent of x and t then we have:

$$\mathring{\omega}(x,t) = D\nabla^2\omega(x,t)$$

$$\int dy\, F(y) = 1$$

$$W(z|x) = \frac{1}{\sqrt{\varepsilon\hat{D}}} F\left(\frac{z}{\sqrt{\varepsilon\hat{D}}}\right)$$

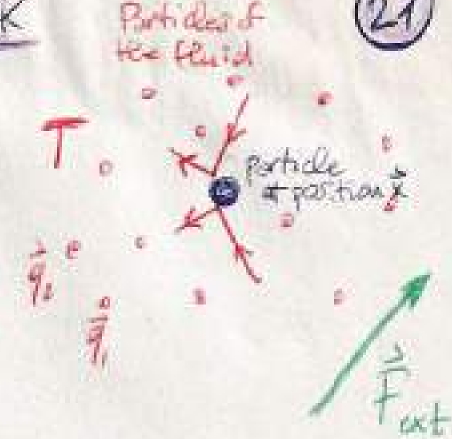
$$\int dy\, y\, F(y) = 0$$

3.2 New Final Chapters

⋆ **New material** ⋆ **-** Final chapters treated differently respect the previous years

From NEWTON to FOKKER - PLANK

In order to understand what is f and $\hat{D}$ in the F-P equation from a physical point of view we have to start from the Newton equation trying to understand what is going on in a diffusion process with an external force:



$$\text{①}\quad m\ddot{\vec{x}} = \underbrace{\vec{F}_{ext}(x)}_{\text{All external interaction with the particle = EM, gravitational ...}} + \underbrace{\vec{F}_{int}(\vec{x}, \{\vec{q}\})}_{\text{Interaction between the particle and the particles of the fluid}}$$

If $\vec{F}_{int}$ derives from a potential (conservative force) then we can write it like:

$\rightarrow$ Fluid system = typical form

$$\vec{F}_{int} = -\vec{\nabla}_{x} U(\vec{x}, \{\vec{q}\}) \quad \text{where} \quad U(\vec{x}, \{\vec{q}\}) = \underbrace{\sum_i u(\vec{x} - \vec{q}_i)}_{\text{Interaction between } \vec{x} \text{ particle and the fluid's one}} + \underbrace{\sum_{i<j} v(\vec{q}_i - \vec{q}_j)}_{\text{Mutual interactions of fluid's particles}}$$

(x) we are interested in the blue ($\vec{x}$) particle!

Or more in general: $\vec{F}_{int}(\vec{x}(t), \{\vec{q}(t)\}) = \sum_{i=1}^{N} \vec{F}(\vec{x}(t) - \vec{q}_i(t))$

In order to understand the behaviour of the system we should solve a number of $\sim 10^{23}$ equation for the fluid particles $m_i \ddot{\vec{q}}_i = -\vec{\nabla}_{q_i} U$ besides the ① for our $\vec{x}$ particle.

$\rightarrow$ Statistical mechanics come to the assistance of us and permit us to avoid solving the eq.s of newton, calculating averages of the observables in an equilibrium situation (Boltzmann weight: canonical ens.).

$\rightarrow$ If $\vec{F}_{ext}$ can be derived from a potential $V_{ext}(x)$, then if we are at equilibrium and we know this potential, then we everything we need!

$$\vec{F}_{ext} = -\vec{\nabla}_x V_{ext}(x)$$

So at equilibrium:

$$w_{eq} = \frac{e^{-\beta V_{ext}(x)}}{Z} \quad \text{where } Z = \int d^d x\, e^{-\beta V_{ex}(x)} = \text{Partition function}$$

$$\Rightarrow \int w_{eq}(x)\, \mathcal{O}(x)\, d^d x = \langle \mathcal{O} \rangle_{eq} \qquad \beta = 1/k_B T$$

But the reality is we are concerned to dynamics: in particular how we arrive to equilibrium? Instead of solving the full ~10^{23} newton equation, we would like to rewrite $\vec{F}_{int}$ such as an effective force acting upon the single particle $\vec{x}$ generated by all the $\vec{q}_i$ particles collectively:

$$m\ddot{x}(t) = F_{ext}(x(t)) \overbrace{- \underbrace{\gamma \cdot \dot{x}(t)}_{\text{Viscous force}} + \vec{F}_{noise}(t)}^{= \vec{F}_{int}(\vec{x}(t), \{\vec{q}(t)\})}$$

Viscous force where γ = friction coefficient

$$-\gamma \dot{x} = \langle \vec{F}_{int}(\vec{x}, \{\vec{q}\}) \rangle$$

the viscous force must come from the interaction with the fluid!

P.S. We expect that at large times the dynamics of the system will lead/will relax to a Boltzmann distribution where the fluid is a temperature T and all is at equilibrium
→ Equilibrium distribution!

Notice that if we have $\vec{F}_{ext} = 0$, then on average the particle is not moving $\langle \vec{x} \rangle = 0$, then only when the is motion, and so $\vec{F}_{ext} \neq 0$ and $\dot{x} \neq 0$, there will be a viscous force acting on the blu $\vec{x}$ particle!

$\Rightarrow$ Viscous force : Average force that the fluid acts upon the particle $\vec{x}$

So then: $\vec{F}_{int} = \underbrace{\langle \vec{F}_{int} \rangle_{\{\vec{q}\}}}_{\text{Average over the } \{\vec{q}_i\}} + \vec{F}_{Noise}$ Then we want to model the $\vec{F}_{Noise}$ in such a way the system relax at equilibrium at large times

(22)

So then if $\vec{F}_{ext} = 0$ then on average the particle is at rest $\langle \vec{x} \rangle = 0$ and the motion is due only to the random collision with the particles in the fluid (Brownian motion). This means that on average no force is acting on our particle ('cause it's at rest), so then:

$$\underbrace{\langle \vec{F}_{int} \rangle_{env}}\quad \begin{cases} = 0 \text{ if } \dot{\vec{x}}(t) = \vec{v}(t) = 0 \\ \vec{F}_{ave}(\vec{v}) \neq 0 \text{ if } \underbrace{\dot{\vec{x}}(t) = \vec{v}(t) \neq 0} \end{cases}$$

Viscous force is acting on $\vec{x}$ particle: the ext. force $\vec{F}_{ext}$ is non zero!

If we suppose the $\vec{x}$ particle velocity is less than a characteristic velocity of the system (that we will find later) then we can expand $\vec{F}_{ave}(\vec{v})$ in series:

$$\underbrace{\vec{F}_{ave}(\vec{v})} = \sum_{\mu=1}^{d} v_\mu \frac{\partial}{\partial v_\mu} \vec{F}_{ave}(\vec{v})\Big|_{\vec{v}=0} + \mathcal{O}(v^2)$$

where v_μ velocity's component (of $\vec{x}$ particle)

McLaurin expansion around $\vec{v} \sim 0$

$$= -\gamma \cdot \vec{v} + \mathcal{O}(v^2)$$

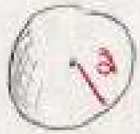
$\boxed{\text{P.S.}}$ We write $\gamma \cdot \vec{v}$ just for semplicity (it doesn't hold every time!) Notice that typically γ has to be a matrix ($= \partial_{v_\mu} \vec{F}_{ave}(\vec{v})$): if computed for $\vec{v} = 0$ it's just a constant matrix.
For the moment we can consider it just a constant multiplicated by the identity matrix ($\gamma \cdot \mathbb{1}$)

γ = Friction coefficient $\qquad 1/\gamma$ = Mobility

If $\gamma = 0 \rightsquigarrow \frac{1}{\gamma} = \infty$ so there's no viscous force!

Stokes Formula: holds if the particle is spherical with radius a $\qquad \eta_{H_2O} \simeq 10^{-3}\ kg/m \cdot s$

$\Rightarrow \gamma = 6\pi a \eta$ where η = viscosity coefficient



Dimensionality:
$[\gamma \cdot v] = kg\ m/s^2 \quad [\gamma] = kg/s$
$\rightsquigarrow [\eta] = kg/m \cdot s$

Returning to our Newton eq. for the $\vec{x}$ particle:

$$m\ddot{\vec{x}}(t) = \vec{F}_{ext}(\vec{x}(t)) - \gamma\cdot\dot{\vec{x}}(t) + \vec{F}_{noise}(t)$$

Notice that: $\langle \vec{F}_{noise} \rangle = 0$

$$\rightsquigarrow \underbrace{\frac{m}{\gamma}\ddot{\vec{x}}(t)}_{} = \underbrace{\frac{\vec{F}_{ext}(\vec{x}(t))}{\gamma} - \dot{\vec{x}}(t) + \frac{\vec{F}_{noise}(t)}{\gamma}}_{} \circledast$$

$\left[\frac{m}{\gamma}\right]\left[\ddot{\vec{x}}\right] = \left[\frac{m}{\gamma}\right]\frac{m}{s^2}$

Have all the dimension of a velocity: $\left[\frac{F}{\gamma}\right] = \frac{kg\ m/s^2}{kg/s} = \frac{m}{s}$

$\Rightarrow [m/\gamma] = s = [\text{Time}]$

$\Rightarrow \frac{m}{\gamma}$ is a time: it's a characteristic timescale of our system

$\boxed{\text{Ex}}$ $\vec{x}$ Spherical particle of radius a in H_2O

$m = \rho V$
$= \rho \frac{4}{3}\pi a^3$
$\sim 4\cdot 10^{-24}$ kg

$a \simeq 10^{-9}$ m

Radius of a H_2O molecule $\simeq 2{,}75\,\text{Å} = 2{,}75\cdot 10^{-10}$ m

$\vec{x}$ particle density $= \rho \simeq \rho_{H_2O} \sim 10^{-3}$ kg/m^3

$\Rightarrow \gamma = 6\pi a \eta \sim 2\cdot 10^{-12}$ kg/s

$\Rightarrow m/\gamma \equiv$ Characteristic time $\sim 10^{-13}$ s

So if we are observing our $\vec{x}$ particle at timescale much greater than $m/\gamma \sim 10^{-13}$s then the left side of $\circledast$ is negligible

$\rightsquigarrow$ m/γ is so small respect to the remaining term that we can neglect the $m/\gamma\, \ddot{\vec{x}}(t)$ term!

(= Overdamped equation)

Overdamped Equation: it's like the particle is moving in a very dense fluid (light particle in water, than water it's like honey for it!):

$$0 = \vec{F}_{ext} - \gamma\cdot\dot{\vec{x}} + \vec{F}_{noise}$$

Let's study the Overdamped case (Time scale $\gg m/\gamma$):

$$\dot{\vec{x}}(t) = \underbrace{\frac{\vec{F}_{ext}(\vec{x}(t))}{\gamma}} + \underbrace{\frac{\vec{F}_{noise}(t)}{\gamma}} = \underbrace{f(\vec{x}(t))}_{\text{Deterministic part}} + \underbrace{\sqrt{2D}\,\vec{\xi}(t)}_{\text{Stocastic part}}$$

We introduce the 2 new terms!!

→ Fokker-Plank equation: Deterministic equation for the probability distribution of a diffusing particle

Langevin equation: It's a stocastic quasi-equation that describe the motion of a diffusing particle in presence of an external field

OVERDAMPED LANGEVIN EQUATION

$$\boxed{\dot{\vec{x}}(t) = f(\vec{x}(t)) + \sqrt{2D}\,\vec{\xi}(t)}$$

→ $\vec{\xi}(t)$? Firstly we have seen it must have zero average, because derives from a noise that derives from the environment, but also γ derives from the environment. So then D and $\vec{\xi}(t)$ not only must depend on the enviroment through γ but also through the $\vec{F}_{noise}$, and we have seen that this force must guarantees that if the $\vec{x}$ particle is in a system with fixed temperature T and the external force can be derived by a potential, then at large times the system must be described by the canonical distribution → Equilibrium!

So $\vec{\xi}(t)$ term has to led to the thermalization of the $\vec{x}$ particle in such a way to have the Boltzmann distribution at large times! Idea for D!

① $\vec{F}_{ext} = 0$ Case

In this case our particle behaves like a brownian particle: $\vec{x}(t)$ is a Brownian trajectory. So we have:

$$\dot{x}(t) = \sqrt{2D}\,\xi(t)$$

Integration between $[t, t+\Delta t]$ $= \int_t^{t+\Delta t} \dot{x}(t')\,dt' = \sqrt{2D}\int_t^{t+\Delta t} \xi(t')\,dt'$ where $\Delta B(t) = \int_t^{t+\Delta t} \xi(t')\,dt'$

$$\Rightarrow \Delta x(t) \equiv x(t+\Delta t) - x(t) = \sqrt{2D}\,\Delta B(t) \quad ☆$$

Recall from the $d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0,t_0)$ expression that the increment $x(t_i)-x(t_{i-1})=\Delta x_i$, the jumps at successive discrete times, are independent random variables: $d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0,t_0)$ is the product of their prob. gaussian distributions.

So then from $d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0,t_0)$ we know that:

$$P(\Delta x) = \frac{e^{-\frac{(\Delta x)^2}{4D\Delta t}}}{\sqrt{4\pi D\Delta t}} \quad \text{where} \quad x(t_i)-x(t_{i-1})\sim\mathcal{N}(0,\underbrace{2D\Delta t_i}_{\text{Variance}=\sigma^2})$$

$$\vec{x}(t_i)-\vec{x}(t_{i-1})\sim\mathcal{N}_d(0,2D\Delta t_i)$$

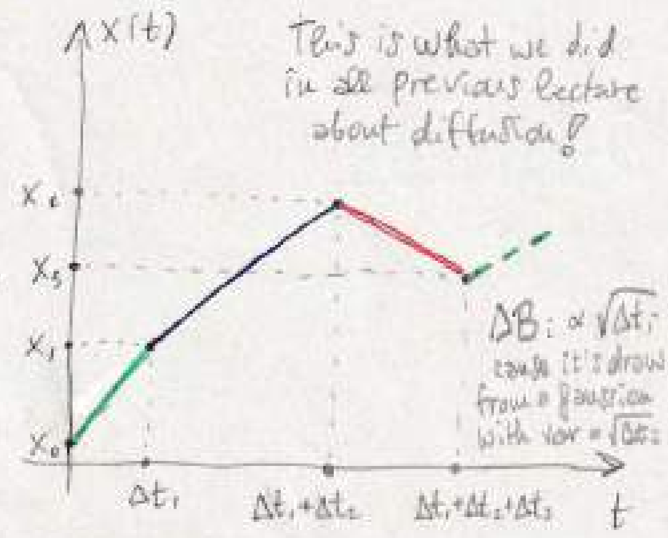
So then from ☆ we can change variables: $P(\Delta B)\,d\Delta B = P(\Delta x)\,d\Delta x$

$$\Rightarrow \frac{d(\Delta x)}{d(\Delta B)} = \sqrt{2D}\,.$$

$$\Rightarrow P(\Delta B) = \frac{1}{\sqrt{2\pi\Delta t}}\,e^{-\frac{(\Delta B)^2}{2\Delta t}} = \mathcal{N}(0,\Delta t)$$

$$\boxed{\underline{\text{Gaussian}} \quad \mathcal{N}(0,\sigma^2) = \frac{e^{-x^2/2\sigma^2}}{\sqrt{2\pi}\,\sigma}}$$

So then ☆: $\boxed{x(t+\Delta t) = x(t) + \sqrt{2D}\,\Delta B(t)}$ will describe us the trajectory of a brownian particle where $\Delta B\sim\mathcal{N}(0,\Delta t)$ is a random variable distributed as a gaussian with mean zero and variance Δt: his role is to update the particle position at each timestep!



x_0 at time $t_0=0$

$x_1 = x_0 + \Delta x_1 = x_0 + \sqrt{2D}\,\Delta B_1$ at time Δt_1

$x_2 = x_1 + \Delta x_2 = x_1 + \sqrt{2D}\,\Delta B_2$ at time $\Delta t_1+\Delta t_2$

$\vdots$

$x_n = x_{n-1} + \Delta x_n = x_{n-1} + \sqrt{2D}\,\Delta B_n$ at $\sum_{i=1}^{n}\Delta t_i$

where $\Delta B_1, \Delta B_2 \cdots \Delta B_n \sim \mathcal{N}(0,\Delta t)$

<u>N.B.</u> In order to construct a trajectory with fine details we have to make the Δt_i smaller and smaller

2) $\vec{F}_{ext} \neq 0$ Case

We have (in 1Dim): $\dot{x}(t) = f(x(t)) + \sqrt{2D}\,\xi(t)$

Like before: $\int_t^{t+\Delta t} \dot{x}(t')dt' = \int_t^{t+\Delta t} f(x(t'))dt' + \sqrt{2D}\int_t^{t+\Delta t} \xi(t')dt'$

$\Rightarrow \Delta x(t) = x(t+\Delta t) - x(t) = \Delta t\, f(x(t)) + \sqrt{2D}\,\Delta B(t)$

↳ Given that the time is small: $\Delta t \ll 1$

where $\Delta B(t) = \int_t^{t+\Delta t} \xi(t')dt' \sim \mathcal{N}(0,\Delta t)$

and where we assumed that the external force to be a smooth function (also $x(t)$ is smooth, is $\dot{x}(t)$ that is not!)

So then $\boxed{x(t+\Delta t) = x(t) + \Delta t\, f(x(t)) + \sqrt{2D}\,\Delta B(t)}$ will descibe the trajectory of the brownian particle in presence of an external force: each timestep the position is updated by the random gaussian distributed variable $\Delta B \sim \mathcal{N}(0,\Delta t)$ and also by the external $x(t)$ dependent force $f(x(t))$

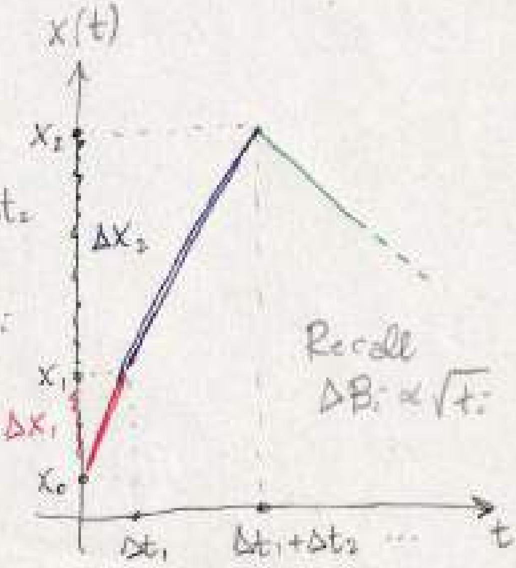
x_0 at time $t_0 = 0$

$x_1 = x_0 + \Delta x_1 = x_0 + \Delta t_1 f(x_0) + \sqrt{2D}\,\Delta B_1$ at time Δt_1

$x_2 = x_1 + \Delta x_2 = x_1 + \Delta t_2 f(x_1) + \sqrt{2D}\,\Delta B_2$ at time $\Delta t_1 + \Delta t_2$

$\vdots$

$x_n = x_{n-1} + \Delta x_n = x_{n-1} + \Delta t_n f(x_{n-1}) + \sqrt{2D}\,\Delta B_n$ at $\sum_{i=1}^{n} \Delta t_i$



We can also write the equation ⑱ in a more mathematically rigorous way:

$$\boxed{dx(t) = f(x(t))\,dt + \sqrt{2D}\,dB(t)}$$

DIFFERENTIAL FORM of the LANGEVIN EQUATION (OVERDAMPED)

or like the physicists: $\underbrace{\dot{x}(t) = \overbrace{f(x(t))}^{\text{Deterministic}} + \overbrace{\sqrt{2D}\,\xi(t)}^{\text{Stocastic term}}}_{\text{QUASI-DIFFERENTIAL EQUATION}}$ where $\xi(t) = \frac{dB(t)}{dt}$

QUASI-DIFFERENTIAL EQUATION (definition introduced by Van-Kampen)

Recall that the Brownian trajectories are not differentiable $\dot{x}(t)$: so then $\nexists\ \xi(t)$ in a mathematical rigorous way

Nevertheless it's interesting for us studying the properties of this $\xi(t)$, thing that we'll do starting from $\Delta B(t)$ features.

Recall $\Delta B \sim \mathcal{N}(0, \Delta t)$ and in particular at each timestep Δt_i the trajectory is update (also) by ΔB_i: the $\{\Delta B_i\}_{i=1,2\ldots}$ are indipendent random variables gaussian distributed!

Δt_1, Δt_2 ... t

ΔB_1 ΔB_2 ...

Indipendent random variables

In particular:

$$\langle \Delta B_i \rangle = 0 \qquad \overbrace{\langle \Delta B_i \Delta B_J \rangle}^{\text{Covariance matrix}} = \begin{cases} 0 & \text{when } i \neq J \\ \langle \Delta B_i^2 \rangle = \Delta t_i & \text{when } i = J \end{cases}$$

If $i \neq J$: $\langle \Delta B_i \Delta B_J \rangle \overset{\{\Delta B\}\text{ are indipendent}}{=} \langle \Delta B_i \rangle \langle \Delta B_J \rangle = 0$

If $i = J$: $\langle \Delta B_i \Delta B_i \rangle = \langle \Delta B_i^2 \rangle = \langle \Delta B_i^2 \rangle - \cancel{\langle \Delta B_i \rangle^2} = \mathrm{Var}(\Delta B_i) = \Delta t_i$

If we divide by Δt: $\left\langle \frac{\Delta B_i}{\Delta t_i} \frac{\Delta B_J}{\Delta t_J} \right\rangle = \frac{\delta_{iJ}}{\Delta t_i} \qquad \left\langle \frac{\Delta B_i}{\Delta t_i} \right\rangle = 0$

When $\Delta t_{i,J} \to 0$ and $t = t_i$, $t' = t_J$: $\boxed{\langle \xi(t)\xi(t') \rangle \overset{⑲}{=} \delta(t - t')} \quad \boxed{\langle \xi(t) \rangle = 0}$

$\xi(t)$ is a gaussian distributed var. derived by ΔB!

6 Let's consider: $\sum_j \frac{\delta_{ij}}{\Delta t_i} h(t_j)\Delta t_j = h(t_i)$ for a generic h

Continuous limit: $\Delta t_k \to 0$ $\forall k$ $\quad \sum_j h(t_j)\Delta t_j \rightsquigarrow \int h(t')dt' \Rightarrow \int h(t')\delta(t'-t)dt' = h(t)$

$(t = t_i, t' = t_j)$

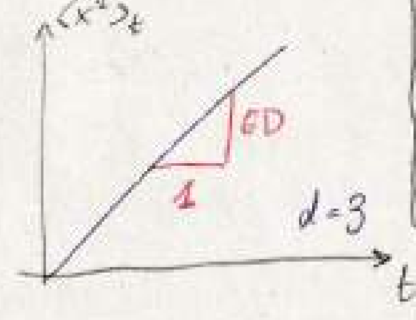
$$\Rightarrow \frac{\delta_{ij}}{\Delta t_i} \xrightarrow{\Delta t_i \to 0} \delta(t-t')$$

Heuristic Argument

Remark: Experiments on Brownian Motion

In order to measure D we take usually $\vec{F}_{ext} = 0$, and we exploit the relation:

$$\langle x^2\rangle_t = 2Dt \text{ in } d=1 \quad \text{where } x_0 = 0$$
$$\overset{!}{=} 6Dt \text{ in } d=3$$



Then we'll find that there's a relation between D, γ and T temperature

$\rightsquigarrow$ Einstein Relation

$\rightsquigarrow$ The relation guarantees that at large times the system reach equilibrium

In order to measure γ we exploit ($\vec{F}_{ext} = 0$):

$$m\ddot{x} = \cancel{F_{ext}} - \gamma\dot{x} + F_{noise} \underset{\text{average}}{\rightsquigarrow} m\langle\ddot{x}\rangle = -\gamma\langle\dot{x}\rangle \quad \text{where } \langle F_{noise}\rangle = 0$$

$\Rightarrow$ Solution: $\langle\dot{x}\rangle = e^{-\gamma/m\, t}\langle\dot{x}\rangle_0$ The exponential decay allow us to compute γ

If we stop pushing bicycle pedal's when riding a bike, our velocity starts decreasing exponentially?

Going on in 1Dim for simplicity we can generalize the differential form of the Langevin equation like:

$$\boxed{dx(t) = \underbrace{A(x(t),t)\,dt}_{\text{Deterministic part: drift } (\mathcal{O}(dt))} + \underbrace{C(x(t),t)\,dB(t)}_{\text{Stocastic part: noise } (\mathcal{O}(\sqrt{t}))}}$$

where before we have $A = f$ and $C = \sqrt{2D}$ indipendent of x and t

→ Interpretation Problem: we always to have in mind the discretization

$$\Delta x(t) = x(t+\Delta t) - x(t) \overset{!}{=} A(x(t),t)\Delta t + C(\underbrace{\,?\,}_{\text{What to write here?}})\Delta B(t) \quad \text{where } \Delta B(t) \sim \mathcal{N}(0,\Delta t)$$

We could compute C at $C(x(t),t)$ like A, but suppose we calculate A in the average position between $[t, t+\Delta t]$ like $A\Big(\underbrace{\frac{x(t)+x(t+\Delta t)}{2}, \frac{t+(t+\Delta t)}{2}}_{\text{Intermediate position and intermediate time } t+\Delta t/2}\Big)$.

At this point recall that:

- $\Delta B \propto \sqrt{\Delta t}$ the lenght of each step of a BM is drawn by a gaussian distribution with variance $= \sqrt{\Delta t}$
- Taylor expansion at $\Delta t \sim 0$:

> $$A\left(t+\frac{\Delta t}{2}\right)\Delta t = \left[A(t) + \dot{A}(t)\frac{\Delta t}{2} + \mathcal{O}(\Delta t^2)\right]\Delta t \overset{!}{\simeq} A(t)\Delta t + \dot{A}(t)\frac{\Delta t^2}{2} \simeq A(t)\Delta t + \mathcal{O}(\Delta t^2)$$

> $$A\Big(\frac{x(t)}{2} + \underbrace{\frac{x(t+\Delta t)}{2}}\Big)\Delta t = \left[A\left(\frac{x(t)}{2} + \frac{x(t)+\mathcal{O}(\sqrt{\Delta t})}{2}\right)\right]\Delta t = \dots$$

where $x(t+\Delta t) = x(t) + \overbrace{\Delta t\, f(x(t))}^{\text{order} \propto \Delta t} + \overbrace{\sqrt{2D}\,\Delta B(t)}^{\text{order} \propto \sqrt{\Delta t}} = x(t) + \mathcal{O}(\sqrt{\Delta t})$

$$\dots = \left[A\left(x(t)+\mathcal{O}(\sqrt{\Delta t})\right)\right]\Delta t = \left[A(x(t)) + \dot{A}(x(t))\,\mathcal{O}(\sqrt{\Delta t}) + \mathcal{O}\left[(\mathcal{O}(\sqrt{\Delta t}))^2\right]\right]\Delta t$$ (26)

$$= A(x(t))\Delta t + \dot{A}(x(t))\,\mathcal{O}(\Delta t^{3/2}) + \underbrace{\mathcal{O}\left[\mathcal{O}(\Delta t)\right]\Delta t}_{} \quad = \mathcal{O}(\Delta t)\cdot\Delta t = \mathcal{O}(\Delta t^2)$$

$$= A(x(t))\Delta t + \dot{A}(x(t))\,\mathcal{O}(\Delta t^{3/2}) + \mathcal{O}(\Delta t^2)$$

$$= A(x(t))\Delta t + \mathcal{O}(\Delta t^{3/2})$$

We have:

- $A(t+\frac{\Delta t}{2})\Delta t = A(t)\Delta t + \mathcal{O}(\Delta t^2)$
- $A\left(\frac{x(t)}{2}+\frac{x(t+\Delta t)}{2}\right) = A(x(t))\Delta t + \mathcal{O}(\Delta t^{3/2})$

$\Rightarrow A\left(\frac{x(t)}{2}+\frac{x(t+\Delta t)}{2}, t+\frac{\Delta t}{2}\right)\Delta t = A(x(t),t)\Delta t + \mathcal{O}(\Delta t^{3/2})$

If $\Delta t \ll 1$ then all the higher order goes to zero faster than Δt

$\Rightarrow$ So calculating A in the average point we are doing an error of order $\Delta t^{3/2}$ which we can neglect when $\Delta t \ll 1$

$\Rightarrow$ So the function A can be computed at <u>any point we like</u> as far as is between $[t, t+\Delta t]$: we always get the $A(x(t),t)\Delta t$ term and high orders that go to zero!

$\sim$ Langevin equation: $x(t+\Delta t) = x(t) + A(\dots)\Delta t + C(\dots)\Delta B(t)$

So then to compute the trajectory x at time $t+\Delta t$ we need only the previous positions for what concernes A! It's not important what previous point because $\mathcal{O}(\Delta t^{3/2})$ goes to zero when $\Delta t \ll 1$: the previous point is arbitrary when computing the amplitude A!

$\Rightarrow$ Concerning the <u>amplitude C</u> we have to make a <u>choice</u>: now it's not like the A situation's where one thing is worth the other in the $\Delta t \ll 1$ limit (all points led to the same result), now the amplitude of the noise C will depend on the point in which is computed!

=> Two famous choices are:

ITO PRESCRIPTION

We compute C on the previous timestep $C(x(t),t)$ leading to:

$$\Delta x(t) = A(x(t),t)\Delta t + \underbrace{C(x(t),t)\Delta B}$$

I'm calculating, C, the amplitude of the noise part, before the noise takes place

~> It's physically what we expect: the noise acts at time t in order to calculate the position at time $t+\Delta t$

~> The Ito-prescription applied to this stocastic differential equation lead to stocastic calculus: is different from the ordinary one and its rules depend on this prescription

~> Langevin equation makes more sense (it's more physical) in Ito framework

STRATONOVICH PRESCRIPTION

We compute C on a middle point, for example if we choose the middle one $C\left(\frac{x(t)}{2}+\frac{x(t+\Delta t)}{2}, t+\frac{\Delta t}{2}\right)$ we are led to:

$$\Delta x = A(x(t),t)\Delta t + \underbrace{C\left(\frac{x(t)}{2}+\frac{x(t+\Delta t)}{2}, t+\frac{\Delta t}{2}\right)\Delta B}$$

Less physical than the Ito prescription: it seems that we are missing causality with the Stratonovich prescription

~> It's calculating the amplitude C at an intermediate position between the old and the new so in some way (not precise) it's like is "predicting the future" (it's not so, but it seems)

~> The rules of calculus for the Stratonovic prescription are different from the rules of the Ito's one: the Straton. rules are the same of ordinary calculus (~ easier)

~> Stocastic integrals makes more sense in Stratonovic framework

Let's go on using the Ito prescription studing the generalized overdamped Langevin equation:

$$x(t+\Delta t)-x(t)=\underbrace{A(x(t),t)\Delta t}_{\text{Deterministic part}}+\underbrace{C(x(t),t)\Delta B(t)}_{\text{Stocastic part}}$$

Amplitude of noise term — Noise term

⤳ Notice that the trajectory at time t, that is $x(t)$, depends only on $\Delta B(s)$ for $s<t$ in the Ito-interpretation (so then $x(t)$ doesn't depend on $\Delta B(s)$ with $s \geq t$). In this case $x(t)$ is said to be non-anticipating! That's due to causality!

In fact: $\Delta B(t)=\int_t^{t+\Delta t}\xi(s)ds$ ⇒ The trajectory at times $x(t+\Delta t)$ depends on $\Delta B(t)$, while $\Delta B(t)$ depends on $\xi(s)$ only for times $s\in(t,t+\Delta t)$

⇒ $x(t+\Delta t)$ depends on $\xi(s)$ with $s<t+\Delta t$

⇒ $x(t)$ depends on $\xi(s)$ with $s<t$ ⤳ so depends only on previous time!

This fact tell us that $C(x(t),t)$ is indipendent of $\xi(s)$ with $s\in(t,t+\Delta t)$

⤳ Ito: $C(x(t),t)$ depends only on previous time t

$\Delta B(t)$ depends on $\xi(s)$ at times $s\in(t,\Delta t+t)$

So then: $\langle C(x(t),t)\Delta B(t)\rangle=\langle C(x(t),t)\rangle\underbrace{\langle\Delta B(t)\rangle}_{=0}=0$

⤳ Stratonovic: $C\left(\frac{x(t)}{2}+\frac{x(t+\Delta t)}{2},t+\frac{\Delta t}{2}\right)$ depends on $t+\frac{\Delta t}{2}$

$\Delta B(t)$ depends on $s\in(t,t+\Delta t)$

In this case are dependent! $\langle C\Delta B\rangle\neq 0$!

So let's continue our discussion using Ito prescription:

$$\langle \Delta x(t) \rangle = \langle A(x(t),t)\Delta t \rangle + \cancel{\langle C(x(t),t)\Delta B(t) \rangle}$$

$$\overset{!}{=} \langle A(x(t),t) \rangle \Delta t \neq A(\langle x(t) \rangle, t)\Delta t$$

We can't do that because averaging $\langle x(t) \rangle$ we are neglecting the fluctation of the $x(t)$ position!

→ Can be true (=) only if fluctations ~ 0:

$$\langle x^2(t) \rangle - \langle x(t) \rangle^2 \overset{!}{=} Var(x(t)) \approx 0$$

Then the evolution of the position it's deterministic!

So we can't get a deterministic evolution even for the averages!

- A is linear: $A(x) = -kx$

$\Rightarrow \langle A(x) \rangle = -k\langle x \rangle = A(\langle x \rangle)$

$\Rightarrow$ In this case it's true

- A is non linear: $A(x) = -kx^3$

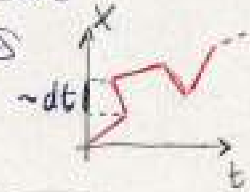
$\Rightarrow \langle A(x) \rangle = -k\langle x^3 \rangle \neq -k\langle x \rangle^3 = A(\langle x \rangle)$

$\Rightarrow$ False

Deterministic World

$dx = A\,dt$ where the stocastic term $C = 0$

Ex Hamilton equations of N particles



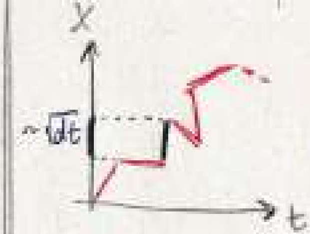
$\{\vec{p}_i, \vec{q}_i\}_{i=1 \dots N}$ ($\vec{p}_i$: momenta, $\vec{q}_i$: positions)

$$X = \begin{pmatrix} \vec{q}_1 \\ \vdots \\ \vec{q}_N \\ \vec{p}_1 \\ \vdots \\ \vec{p}_N \end{pmatrix} \xrightarrow[\text{evolution}]{\text{time}} dX = \underbrace{\begin{pmatrix} \vec{\nabla}_{q_1} \\ \vdots \\ \vec{\nabla}_{q_N} \\ -\vec{\nabla}_{p_1} \\ \vdots \\ -\vec{\nabla}_{p_N} \end{pmatrix} H(q,p)}_{=A(x)} dt$$

Stocastic World

$$dx(t) = \underbrace{A(x(t),t)dt}_{\sim\mathcal{O}(dt)} + \underbrace{C(x(t),t)dB(t)}_{\sim\mathcal{O}(\sqrt{dt})}$$

$\sim\mathcal{O}(dt)$ Deterministic part — $\sim\mathcal{O}(\sqrt{dt})$ Stocastic part



If $C \neq 0$ then the stocastic part is the dominant when $\Delta t \ll 1$!

In this case $x(t)$ it's no more deterministic: in order to have deterministic equations we have to consider $W(x,t)$, the probab. distribution of x

If we make a statistics of $x(t)$ over the numbers of trials $\to \infty$, we get the prob. distribution of the position of the particle at time t

So we are intrested in getting a deterministic evolution equation for $W(x,t)$, where:

$$\int_D W(x,t)\,dx = \text{Prob. that our system at time } t \text{ is found in the position domain } D$$

What we already know is: $\frac{\partial}{\partial t} W(x,t) = D\nabla^2 W(x,t)$ in the case where $A = 0$, $C = \underbrace{\sqrt{2D}}_{\text{Indipendent of } x}$

$\to$ "Pure" brownian motion: let's generalize!

In order to generalize the case on both A and C dependent on x and t we use the following trick.

Let's introduce the compact support function h and for simplicity let's work in 1D:

$h(x) \in C_c(\mathbb{R})$ where $x \in \mathbb{R}$

(Generalization in d-Dim: $x \in \mathbb{R}^d$ $d\vec{B} = \begin{pmatrix} dB_1 \\ \vdots \\ dB_d \end{pmatrix}$ where dB_μ are indip. and ident. dist.)

We want to compute: $\langle h(x(t)) \rangle = \int \omega(x,t) h(x) dx \quad \langle h(x(t+\Delta t)) \rangle = ?$

$$x(t+\Delta t) - x(t) = \Delta x(t) = A(x(t),t)\Delta t + C(x(t),t)\Delta B(t) \sim \mathcal{O}(\sqrt{dt})$$

where $\Delta B(t) \sim \mathcal{N}(0, \Delta t)$ stocastic part is dominant

$\rightsquigarrow h(x(t+\Delta t)) = h(x(t) + \Delta x(t))$ Taylor expansion

$$= h(x(t)) + \Delta x(t) h'(x(t)) + \frac{1}{2}(\Delta x(t))^2 h''(x(t)) + \mathcal{O}(\Delta x(t)^3)$$

$\mathcal{O}(\Delta t^{3/2})$

Stocastic calculus: we can't be satisfied with the first order, we must go to the second one!

If we want to compute the derivative and so divide by Δt we have different approaches for the two different frameworks:

- Deterministic: as far as $\Delta x(t) \sim \mathcal{O}(\Delta t)$ all the terms of the expansion $\geq 2^{nd}$ order goes to zero when $\Delta t \ll 1$, so we are satisfied with the first order
- Stocastic: $\Delta x(t) \sim \mathcal{O}(\sqrt{\Delta t})$ all terms $> 2^{nd}$ order ..., so we need the second order!

$$= h(x(t)) + h'(x(t))\left[A(x(t),t)\Delta t + C(x(t),t)\Delta B(t)\right] + \frac{1}{2} h''(x(t))\left[\cdots\right]^2 + \mathcal{O}([\cdots]^3)$$

$$\Rightarrow \langle h(x(t+\Delta t))\rangle = \langle h(x(t))\rangle + \langle h'(x(t))[A(x(t),t)\Delta t +$$
$$+ C(x(t),t)\Delta B(t)\rangle + \frac{1}{2}\langle h''(x(t))[\cdots]^2\rangle + \cdots$$

- Recall that $\Delta B(t) = \int_t^{t+\Delta t} B(s)\,ds$ and $x(t)$ depend only on $B(s)$ with $s<t$
  $\rightsquigarrow$ $\Delta B(t)$ is in the future of $x(t)$: $x(t)$ is indip. on $\Delta B(t)$
  $\rightsquigarrow$ We can factorize the average

$$\langle h'(x(t))A(x(t),t)\rangle\Delta t + \langle h'(x(t))C(x(t),t)\Delta B(t)\rangle$$
$$\stackrel{!}{=} \langle \cdots\rangle\Delta t + \langle h'(x(t))\cdot C(x(t),t)\rangle\underbrace{\langle\Delta B(t)\rangle}_{=0} = \langle h'A\rangle\Delta t$$

- $$\frac{1}{2}\langle h''(x(t))[\underbrace{A(x(t),t)^2\Delta t^2}_{\sim\mathcal{O}(\Delta t^2)} + \underbrace{2A(x(t),t)C(x(t),t)\Delta t\Delta B(t)}_{\sim\mathcal{O}(\Delta t^{3/2})} +$$
$$+ \underbrace{C(x(t),t)^2\Delta B^2(t)}_{\sim\mathcal{O}(\Delta t)}]\rangle$$

Double product $= 0$ 'cause we can factorize ΔB
$\langle 2AC\rangle\langle\Delta B\rangle\Delta t = 0$

$$= \frac{1}{2}\langle h''(x(t))C(x(t),t)^2\Delta B^2(t)\rangle + \mathcal{O}(\Delta t^2)$$
$$\stackrel{!}{=} \frac{1}{2}\langle h''(x(t))C(x(t),t)^2\rangle\underbrace{\langle\Delta B^2(t)\rangle}_{\stackrel{!}{=}\Delta t \rightsquigarrow \text{Variance}} + \mathcal{O}(\Delta t^2)$$

Putting together • and • we get:

$$\langle h(x(t+\Delta t)) - h(x(t))\rangle = \langle h'(x(t))A(x(t),t)\rangle\Delta t + \frac{\Delta t}{2}\langle h''(x(t))C^2(x(t),t)\rangle$$
$$+ \mathcal{O}(\Delta t^2)$$

Now if we divide by Δt and take $\Delta t \to 0$ we get:

$$\Rightarrow \frac{d}{dt}\langle h(x(t))\rangle = \left\langle h'(x(t))A(x(t),t) + \frac{h''(x(t))}{2}C^2(x(t),t)\right\rangle$$

Now we can finally exploit: $\langle h(x(t))\rangle = \int w(x,t)\,h(x)\,dx$

$$\Rightarrow \frac{d}{dt}\int w(x,t)h(x)dx = \int \frac{dw(x,t)}{dt}h(x)\,dx = \text{Right}_{\text{side}}$$

$$\text{Left side} = \int dx\, w(x,t)\left[h'(x)A(x,t) + \frac{h''(x)}{2}C^2(x,t)\right]$$

$$\overset{*!}{=} \int dx\, h(x)\frac{d}{dx}\left[-A(x,t)w(x,t) + \frac{1}{2}\frac{d}{dx}\left(C^2(x,t)w(x,t)\right)\right]$$

* Integrations by part

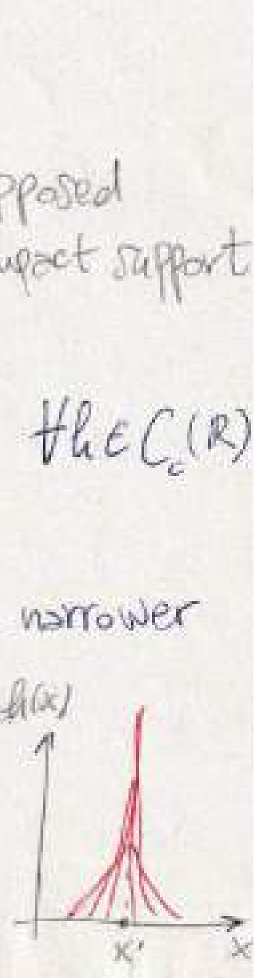
$$\int_{\mathbb{R}} dx\, w h' A = \cancel{w \underset{=0}{\underset{\sim}{h}} A}\Big|_{-\infty}^{+\infty} - \int dx\, h\frac{d}{dx}(wA)$$ if $h(x)$ has a compact support

$$\int_{\mathbb{R}} dx\, w\frac{h''}{2}C^2 = \cancel{w\frac{h'}{2}C^2}\Big|_{\mathbb{R}} - \int dx\,\frac{h'}{2}\frac{d}{dx}(wC^2)$$

$$\overset{!}{=} -\cancel{\frac{h}{2}\frac{d}{dx}(wC^2)}\Big|_{\mathbb{R}} + \int dx\,\frac{h}{2}\frac{d^2}{dx^2}(wC^2)$$ if $h(x)$ is supposed to have a compact support

$$\Rightarrow \int \frac{dw}{dt}h\,dx = \int dx\, h\frac{d}{dx}\left[-Aw + \frac{1}{2}\frac{d}{dx}(wC^2)\right] \quad \forall h\in C_c(\mathbb{R})$$

$\Rightarrow$ If we take $h(x)$'s compact support narrower and narrower we get a delta function: $h(x) = \delta(x-x')$



$$\boxed{\frac{d}{dt}w(x,t) = -\frac{d}{dx}J(x,t) \quad \text{with } J(x,t) = A(x,t)w(x,t) - \frac{1}{2}\frac{d}{dx}\left[C^2(x,t)w(x,t)\right]}$$

FOKKER-PLANK EQUATION

This is the FP equation that correspond to the Langevin equation:

$$dx = A(x,t)\,dt + C(x,t)\,dB(t) \quad \text{(where } x(t)=x\text{)}$$

Notice that if $A = f(x)$ and $C = \sqrt{2D(x)}$ ($C^2/2 = D$) than we recover the previous resul (Manzoli pag. 61 and before)!

FOKKER-PLANK EQUATION (with $h(x) = \delta(x-x')$ starting from the Langevin eq.)

$$\frac{\partial}{\partial t} w(x,t) = -\frac{\partial}{\partial x} J(x,t) \quad \text{where}$$

$$J(x,t) = A(x,t)\,w(x,t) - \frac{1}{2}\frac{\partial}{\partial x}\left[C^2(x,t)\,w(x,t)\right]$$

~ Particle moving in an environment with an external force $\vec{F}_{ext}$ and diffusion constant D: we retrieve what we get in Manzoli notes at pag. 61 in 3-dim.

$$f(x) = \frac{\vec{F}_{ext}}{\gamma} \qquad D(x) = \text{constant} = D$$

$$\Rightarrow \boxed{\frac{\partial}{\partial t} w(\vec{x},t) = \vec{\nabla}\left[-\frac{\vec{F}_{ext}(\vec{x})}{\gamma} w(\vec{x},t) + D\vec{\nabla} w(\vec{x},t)\right]}$$

~ In general:

$$\frac{\partial}{\partial t} w(x,t) = \frac{\partial}{\partial x}\left[-A(x,t)\,w(x,t) + \frac{1}{2}\frac{\partial}{\partial x}\left(w(x,t)\,C^2(x,t)\right)\right]$$

and if we introduce $C(x,t) = \sqrt{2D(x,t)}$ we get:

$$\boxed{\dot{w}(x,t) = \frac{\partial}{\partial x}\left[-A(x,t)\,w(x,t) + \frac{\partial}{\partial x}\left(w(x,t)\,D(x,t)\right)\right]}$$

Generalized FOKKER-PLANK EQUATION

EINSTEIN RELATION and CONVERGENCE to EQUILIBRIUM

Problem: how do we choose D in equation ⊛ ? (See previous page)

⇝ D must encode the effects of collision between our particle and the particle of the fluid so it's strictly related to the noise part. Moreover D must be related to γ, which encodes the average force generated by the collisions

$\Rightarrow$ D and γ have a common origin! The origin is the collisions of fluid particles with our target particle!

⇝ If we also assume that the prob. distribution $\omega(x,t)$ tends to the Boltzmann distribution at the infinite time limit, then D has also to be related to the temperature!

$\Rightarrow$ We have $D = \underline{D(\gamma, T)}$

If our particle $\vec{x}$ lives in an environment at fixed temperature T with an external potential $U(x)$ and so an external force $\vec{F}_{ext} = -\vec{\nabla}U(x)$, then we expect that:

$$\omega(\vec{x},t) \xrightarrow[t\to\infty]{} e^{-\beta U(\vec{x})}/Z_U \equiv W_{eq}(\vec{x}) \;\Big\}\; \text{marginalized version}$$

where $Z_U = \int d^3x \, e^{-\beta U(\vec{x})}$ = Partition function

while the complete version is:

$$W_{eq}(\vec{x},\vec{p}) = \frac{e^{-\beta(p^2/2m + U(\vec{x}))}}{Z} \qquad \text{where } Z = \int d^3x \, e^{-\beta\left(\frac{p^2}{2m} + U(\vec{x})\right)}$$

and where: $\underbrace{W_{eq}(\vec{x})}_{} = \int d^3p \, W_{eq}(\vec{x},\vec{p}) = \dfrac{e^{-\beta U(\vec{x})}}{Z_U}$

We get this for $t \to +\infty$ cause we are dealing only with positions $\vec{x}$!

N.B. $w(\vec{x},\vec{p}) \equiv$ Prob. distribution of observing a particle with momentum $\vec{p}$ and position $\vec{x}$ in an external potential $U(\vec{x})$ and at equilibrium at temp. T

$$= \frac{1}{Z} e^{-\beta\left(\frac{p^2}{2m}+U(\vec{x})\right)}$$ where m = particle mass

$$Z = \int d^3p \int d^3x \, e^{-\beta\left(\frac{p^2}{2m}+U(\vec{x})\right)} = (2\pi m k_B T)^{3/2} Z_U$$

we have two things to verify:

① $w_{eq}(\vec{x})$ must satisfy the stationary F-P equation, that is:

$$\partial/\partial t \, w(\vec{x},t) = \vec{\nabla}\left[-\frac{\vec{F}_{ext}(\vec{x})}{\gamma} w(\vec{x},t) + D\vec{\nabla} w(\vec{x},t)\right]$$

Since $\frac{\partial}{\partial t} w_{eq}(\vec{x}) = 0$ cause $w_{eq}(\vec{x})$ is indipendent of time t

we must get: $\vec{\nabla}\left[-\frac{\vec{F}_{ext}}{\gamma} w_{eq}(\vec{x}) + D\vec{\nabla}(w_{eq}(\vec{x}))\right] = 0$

This is true in two cases:

- $\vec{\nabla}[\dots] = 0 \overset{⊙}{\Longleftrightarrow} [\dots] = 0$
- $\vec{\nabla}[\dots] = 0 \Longleftrightarrow [\dots] = \vec{\nabla}\times\vec{V}$ with $\vec{V} \in \mathbb{R}$

(Recall that the divergence of a curl is always zero)

⊙ $[\dots] = 0$ $\quad \frac{\vec{\nabla} w_{eq}(\vec{x})}{w_{eq}(\vec{x})} = + \frac{\vec{F}_{ext}}{\gamma D} \quad \vec{\nabla}(\ln w_{eq}(\vec{x})) = + \frac{\vec{F}_{ext}}{\gamma D} = -\frac{\vec{\nabla}U(\vec{x})}{\gamma D}$

$$\vec{\nabla}\left(\ln w_{eq}(\vec{x}) - \frac{U(\vec{x})}{\gamma D}\right) = 0 \Longleftrightarrow \ln w_{eq}(\vec{x}) - \frac{U(\vec{x})}{\gamma D} = \text{constant}$$

$$\Longleftrightarrow w_{eq}(\vec{x}) \propto e^{-U(\vec{x})/\gamma D}$$

$\Longleftrightarrow$ $[\dots] = 0$ Holds only if we retrieve the expression of $w_{eq}(\vec{x})$!

$$\Rightarrow D\gamma = 1/\beta = k_B T$$

EINSTEIN RELATION
(Dissipation fluctuation Relation)

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

→ Fluctuation - Dissipation Relation:
- D is related to the fluctuation of the average force acting on the particle by the environment: recall that in this case D is the amplitude $C(x(t),t)$ in front of $\Delta B(t)$!
- γ is related to the friction and so to the dissipation of energy

→ This relation has been found by Einstein on 1905: an epoch where great part of scientific community believed that matter was continuous and not made by atoms.
Through this relation experiments had made possible the measurement of the avogadro number and so proven indirectly the discontinuity of matter:

$PV = Nk_BT$ then for one mole: $N = (\text{mole's } \#) \cdot N_A \overset{!}{=} N_A$

$\overset{!}{=} N_A k_B T$

$\overset{!}{=} RT$ where R is the gas constant (at that times was known)

$[R] = \text{energy}/\text{Temperature}$

If we measure: $\langle \vec{x}^2(t)\rangle - \langle \vec{x}(t)\rangle^2 = 6Dt$ so we can get D just looking on how the cloud of our diffusing particles evolves in time from a central source.
We can also measure the friction coefficient $\gamma = 6\pi a\eta$ knowing the viscosity η and also the size of the particles a.

$\Rightarrow k_B = \frac{D\gamma}{T}$ we get k_B $\Rightarrow N_A = \frac{R}{k_B}$ we get the avogadro number!

$\sim 6 \cdot 10^{23}$ first estimate of the avogadro number! Einstein!

What we get is that the Boltzmann distribution satisfy the stationary F-P equation if the Einstein relation holds, but what guarantees that $w(x,t)$ converges to the equilibrium one $w_{eq}(\vec{x})$ at large times?

2. In order to solve the F-P equation we need an initial condition, that is $w_0(\vec{x}) \equiv w(\vec{x}, t=0)$, and we want to prove that:

$$w(\vec{x},t) \xrightarrow[t\to\infty]{} w_{eq}(\vec{x})$$

3D-stationary FP equation: $\partial_t w = \vec{\nabla}\left(\frac{\vec{\nabla}U}{\gamma} w + D\vec{\nabla} w\right) = D\vec{\nabla}\left(\frac{\vec{\nabla}U}{\gamma D} w + \vec{\nabla} w\right)$

① $= D\vec{\nabla}\left(\beta\vec{\nabla}U w + \vec{\nabla} w\right)$ where $1/\gamma D = 1/k_B T = \beta$

Einstein relation

Recall that: $\vec{\nabla}_x\left(e^{\varphi(x)} f(x)\right) = \left(\vec{\nabla}_x e^{\varphi(x)}\right) f(x) + e^{\varphi(x)}\vec{\nabla}_x f(x)$

$$\stackrel{!}{=} \left(e^{\varphi(x)}\vec{\nabla}_x\varphi(x)\right) f(x) + e^{\varphi(x)}\vec{\nabla}_x f(x)$$

$$\stackrel{!}{=} e^{\varphi(x)}\left[\vec{\nabla}_x\varphi(x) + \vec{\nabla}_x\right] f(x)$$

$$\rightsquigarrow \vec{\nabla}(e^{\varphi} f) = e^{\varphi}(\vec{\nabla} + \vec{\nabla}\varphi) f \quad \circledast$$

Trick, let's define: $w(\vec{x},t) = e^{-\beta\frac{U(\vec{x})}{2}}\Psi(\vec{x},t)$

① $\Rightarrow \frac{\partial}{\partial t}\left(e^{-\beta\frac{U(\vec{x})}{2}}\Psi(\vec{x},t)\right) = D\vec{\nabla}_x\left[\beta w\vec{\nabla}_x U(\vec{x}) + \underbrace{\vec{\nabla}_x\left(e^{-\beta\frac{U(\vec{x})}{2}}\Psi(\vec{x},t)\right)}_{\circledast}\right]$

$$\frac{\partial}{\partial t} w(\vec{x},t) = D\vec{\nabla}_x\left[\beta e^{-\beta\frac{U(\vec{x})}{2}}\Psi(\vec{x},t)\vec{\nabla}_x U(\vec{x}) + e^{-\beta\frac{U(\vec{x})}{2}}\left(\vec{\nabla}_x + \vec{\nabla}_x\left(-\frac{\beta}{2}U(\vec{x})\right)\right)\Psi(\vec{x},t)\right]$$

Let's continue neglecting the x and t dependencies:

$$e^{-\beta\frac{U}{2}}\frac{\partial}{\partial t}\Psi = D\vec{\nabla}\left[\beta e^{-\beta\frac{U}{2}}\Psi\vec{\nabla}U + e^{-\beta\frac{U}{2}}\left(\vec{\nabla}-\frac{\beta}{2}\vec{\nabla}U\right)\Psi\right]$$

$$\stackrel{!}{=} D\vec{\nabla}\left[\beta e^{-\beta\frac{U}{2}}\Psi\vec{\nabla}U + e^{-\beta\frac{U}{2}}\vec{\nabla}\Psi - \frac{\beta}{2}e^{-\beta\frac{U}{2}}\vec{\nabla}U\Psi\right]$$

$$\stackrel{!}{=} D\vec{\nabla}\left[\frac{\beta}{2}e^{-\beta\frac{U}{2}}\Psi\vec{\nabla}U + e^{-\beta\frac{U}{2}}\vec{\nabla}\Psi\right]$$

$$\stackrel{!}{=} D\left[\frac{\beta}{2}\vec{\nabla}\left(e^{-\beta\frac{U}{2}}\right)\Psi\vec{\nabla}U + \frac{\beta}{2}e^{-\beta\frac{U}{2}}\vec{\nabla}\Psi\vec{\nabla}U + \frac{\beta}{2}e^{-\beta\frac{U}{2}}\Psi\vec{\nabla}^2U + \vec{\nabla}\left(e^{-\beta\frac{U}{2}}\right)\vec{\nabla}\Psi + e^{-\beta\frac{U}{2}}\vec{\nabla}^2\Psi\right]$$

$$= De^{-\beta\frac{U}{2}}\left[-\frac{\beta^2}{4}\Psi(\vec{\nabla}U)^2 + \cancel{\frac{\beta}{2}\vec{\nabla}\Psi\vec{\nabla}U} + \frac{\beta}{2}\Psi\vec{\nabla}^2U - \cancel{\frac{\beta}{2}\vec{\nabla}U\vec{\nabla}\Psi} + \vec{\nabla}^2\Psi\right]$$

$$\Rightarrow \frac{\partial}{\partial t}\Psi = D\left[-\frac{\beta^2}{4}(\vec{\nabla}U)^2 + \frac{\beta}{2}\vec{\nabla}^2U + \vec{\nabla}^2\right]\Psi$$

$$\text{©}\qquad \stackrel{!}{=} D\left[\vec{\nabla}-\frac{\beta}{2}\vec{\nabla}U\right]\left[\vec{\nabla}+\frac{\beta}{2}\vec{\nabla}U\right]\Psi$$

Notice that if we define the momentum operator $\hat{p} = -i\vec{\nabla}$ and we let it acts only on function that goes to zero at infinity, then we have $\hat{p}^\dagger = \hat{p}$. Let's define an operator: $\hat{A} = \hat{p} - i\frac{\beta}{2}\vec{\nabla}U$ then we have: $\hat{A}^\dagger = \hat{p}^\dagger + i\frac{\beta}{2}(\vec{\nabla}U)^\dagger = \hat{p} + i\frac{\beta}{2}\vec{\nabla}U$ and substituting in ©:

$$\frac{\partial}{\partial t}\Psi = -D\hat{A}^\dagger\hat{A}\Psi \longleftrightarrow$$

Quantum Harmonic Oscillator

$\hat{A}, \hat{A}^\dagger$ annihilation/creation operators

Harmonic potential $U(x) = x^2$

N.B. Quantum Mechanics & Stocastic Processes

The two are completely different worlds, but the mathematical tools used are interchangeable and identical!

$$\frac{d}{dt}\Psi = -D\hat{A}^{+}\hat{A}\Psi = -D\hat{H}\Psi \quad \text{where } \hat{H} = \hat{A}^{+}\hat{A}$$

and $\hat{H} = \hat{H}^{+}$ self-adjoint operator $\rightsquigarrow$ its eigenvalue are real!

$\underline{\hat{H} \text{ operator}}$: $\hat{H}\Psi_i = \lambda_i \Psi_i$ where $\lambda_i \in \mathbb{R}$

$\rightsquigarrow$ We want to show that $\lambda_0 = 0$ and $\lambda_i > 0 \ \forall i > 0$

$\rightsquigarrow$ $\hat{H}$ has a discrete spectrum but we aren't gonna prove it

$\underline{\lambda_0 = 0}$: $\hat{A}^{+}\hat{A}\Psi_0 = 0 \iff \hat{A}\Psi_0 = 0$

$$\iff \left(\vec{\nabla} + \frac{\vec{\nabla}U}{2}\beta\right)\Psi_0 = 0 \quad \text{...like before...}$$

$$\iff \Psi_0(\vec{x}) \propto e^{-\frac{U(\vec{x})\beta}{2}}$$

If then we impose the normalization $\int_{\mathbb{R}^3} dx \, \|\Psi_0(\vec{x})\|^2 = 1$ we then find: $\Psi_0(\vec{x}) = e^{-\frac{U(\vec{x})\beta}{2}} / \sqrt{Z_U}$ (this is because $\Psi_0(\vec{x}) \propto W_{eq}(\vec{x})$)

$$\underline{\lambda_i > 0}: \quad \lambda_i \int \Psi_i^2(x)\, dx = \int \Psi_i \underbrace{\hat{H}\Psi_i}_{=\lambda_i\Psi_i} dx = \int dx\, \Psi_i \hat{A}^{+}\hat{A}\Psi_i$$

$$\overset{!}{=} \int dx\, (\hat{A}\Psi_i)(\hat{A}\Psi_i) = \int dx\, (\hat{A}\Psi_i)^2 > 0 \implies \lambda_i > 0$$

The spectrum is non-degenerate so then:

$A\Psi_0 = 0$ has only one solution

$A\Psi_i \neq 0$ if $\lambda_i \neq 0$!

Given that the spectrum of $\hat{H}$ is non degenerate, then ψ_i eigenvectors form an orthonormal basis of the Hilbert space. Then we can expand:

$$\Psi(x,t) = \sum_i c_i(t)\psi_i(x) = \sum_i |\psi_i\rangle\langle\psi_i|\Psi\rangle \quad \boxtimes$$

$$\Rightarrow \partial_t \Psi = -D\hat{H}\Psi \qquad \sum_i \dot{c}_i(t)\psi_i(x) \overset{!}{=} -D\hat{H}\left(\sum_i c_i(t)\psi_i(x)\right)$$
$$= -D\sum_i c_i(t)\lambda_i\psi_i(x)$$

$\Rightarrow \dot{c}_i(t) = -D\lambda_i c_i(t)$ which led to $c_i(t) = c_i(0)e^{-D\lambda_i t}$

$\Rightarrow c_i(0)$ is computed using the i.c. $\omega(x,t=0) = \omega_0(x)$:

$$\boxtimes\ c_i(t) = \langle\psi_i|\Psi\rangle = \int dx\,\psi_i(x)\,\Psi(x,t) = \int dx\,\psi_i(x)e^{\beta\frac{U(x)}{2}}\omega(\vec{x},t)$$
$$c_i(0) = \int dx\,\psi_i(x)\,\Psi(x,0) = \int dx\,\psi_i(x)e^{\beta\frac{U(x)}{2}}\omega(\vec{x},0)$$
$$\overset{!}{=} \int dx\,\psi_i(x)e^{\beta\frac{U(x)}{2}}\omega_0(\vec{x})$$

$$\Rightarrow \omega(x,t) = e^{-\frac{\beta}{2}U(x)}\Psi(\vec{x},t) = e^{-\frac{\beta}{2}U(x)}\sum_i c_i(t)\psi_i(x)$$
$$\overset{!}{=} e^{-\frac{\beta}{2}U(x)}\sum_i c_i(0)e^{-D\lambda_i t}\psi_i(x) \quad \text{where } \lambda_i = \begin{cases} 0 & \text{if } i=0 \\ >0 & \text{otherwise}\end{cases}$$
$$\xrightarrow{t\to\infty} e^{-\frac{\beta}{2}U(x)}c_0(0)\psi_0(x) = \frac{e^{-\beta U(x)}}{\sqrt{Z_U}}c_0(0) \quad \text{where } \psi_0(x) = \frac{e^{-\frac{\beta}{2}U(x)}}{\sqrt{Z_U}}$$

We are left to compute $c_0(0) = \int dx\,\psi_0(x)e^{\beta\frac{U(x)}{2}}\omega_0(x) = \int dx\,\frac{\omega_0(x)}{\sqrt{Z_U}} = \frac{1}{\sqrt{Z_U}}$ (Normalization)

$$\Rightarrow \underline{\omega(x,t) \xrightarrow{t\to\infty} \frac{e^{-\beta U(x)}}{Z_U}}$$

So indipendently on the initial condition it tends to the equilibrium distribution!

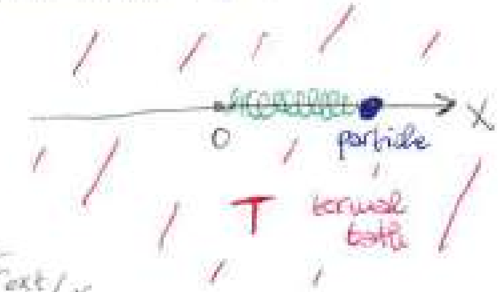
Recap:

- From the overdamped Langevin equation we get the F-P equation
  ⇝ They are equivalent!
- The F-P equation, with this choice of D and of the conservative $\vec{F}_{ext}$, guarantees that the solution $w(\vec{x},t)$ tents to the equilibrium distribution $w_{eq}(\vec{x})$ indipendentely on the choice of $w_0(\vec{x})$
- So we can describe the dinamics of the particle which we're interested in neglecting the surrounding environment fluid's particle: the environment it's all encoded/collapses on the constants D, γ and the temperature T!
  ⇝ In this way we can studing a very reduced dynamics on the particle of interest (avoiding to solve the hamilton dynamics for $\sim 10^{23}$ particle) while all the environment is treated in a stocastic way

THE ORNSTEIN-UHLENBECK PROCESS

The Ornstein-Uhlenbeck process is an application of the overdamped Langevin equation in 1D and describes the motion of a particle subjected to an harmonic force $F_{ext}(x)$ at temperature T:

$$F_{ext}(x) = -m\omega^2 x \quad \leftrightsquigarrow \quad U(x) = m\frac{\omega^2 x^2}{2}$$



$$\Rightarrow dx(t) = f(x(t))\,dt + \sqrt{2D}\,dB(t) \quad \text{where } f = F_{ext}/\gamma$$

$$= -m\frac{\omega^2}{\gamma}x(t)\,dt + \sqrt{2D}\,dB(t)$$

$$= -kx(t)\,dt + \sqrt{2D}\,dB(t) \quad \text{where } k \equiv \frac{m\omega^2}{\gamma}$$

LANGEVIN EQUATION

While the corresponding FP EQUATION will be:

$$\dot{\omega}(x,t) = \frac{\partial}{\partial x}\left[kx\,\omega(x,t) + D\frac{\partial}{\partial x}\omega(x,t)\right]$$

where $A(x,t) = -kx$

$C(x,t) = \sqrt{2D}$

We would like to find the solution to this FP equation given the initial condition $\omega(x,t_0) = \delta(x-x_0)$, this solution is the usual propagator $W(x,t|x_0,t_0)$ which obeys to the same FP equation!

Two ways to proceed:

- Fourier transform in x and then use the method of characteristics
- Discretize the Langevin equation $\rightsquigarrow$ We will follow only this approach in the following

Discretized Langevin equation with time discretization $\frac{t-t_0}{N} = \varepsilon$ where N is any large integer:

$$x(t+\varepsilon) - x(t) = -Kx(t)\varepsilon + \sqrt{2D}\,\Delta B(t)$$

$$x(t+\varepsilon) = x(t)(1-K\varepsilon) + \sqrt{2D}\,\Delta B(t)$$

Let's iterate using the previous timestep of the Lan. eq.

$$= \left[x(t-\varepsilon)(1-K\varepsilon) + \sqrt{2D}\,\Delta B(t-\varepsilon)\right](1-K\varepsilon) + \sqrt{2D}\,\Delta B(t)$$

1st iter.

$$= \left[x(t-2\varepsilon)(1-K\varepsilon) + \sqrt{2D}\,\Delta B(t-2\varepsilon)(1-K\varepsilon)\right](1-K\varepsilon) + \sqrt{2D}\left[\Delta B(t) + (1-K\varepsilon)\Delta B(t-\varepsilon)\right]$$

2nd iter.

$$= x(t-2\varepsilon)(1-K\varepsilon)^2 + \sqrt{2D}\left[\Delta B(t) + (1-K\varepsilon)\Delta B(t-\varepsilon) + (1-K\varepsilon)^2\Delta B(t-2\varepsilon)\right]$$

$= \dots$ iterating N times $\rightsquigarrow N\varepsilon = t - t_0$

$\rightsquigarrow t - N\varepsilon = t_0$

Nth iteration

$$= x(t-N\varepsilon)(1-K\varepsilon)^N + \sqrt{2D}\sum_{i=0}^{N}(1-K\varepsilon)^i\,\Delta B(t-i\varepsilon) \qquad i = N-J$$

$$= x(t_0)(1-K\varepsilon)^N + \sqrt{2D}\sum_{J=N}^{0}(1-K\varepsilon)^{N-J}\,\Delta B(t-N\varepsilon+J\varepsilon)$$

$$= x(t_0)(1-K\varepsilon)^N + \sqrt{2D}\sum_{J=0}^{N}(1-K\varepsilon)^{N-J}\,\Delta B(t_0+J\varepsilon)$$

$$\Rightarrow x(t+\varepsilon) = x(t_0)(1-K\varepsilon)^N + \sqrt{2D}\sum_{i=0}^{N}(1-K\varepsilon)^{N-i}\,\Delta B_i$$

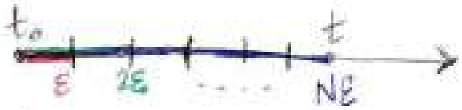
where $\Delta B_i \equiv \Delta B(t_0+i\varepsilon)$, $\Delta B_N = \Delta B(t)$

$$\sim \mathcal{N}(0,\varepsilon) = \frac{1}{\sqrt{2\pi}\,\varepsilon}\, e^{-\Delta B_i^2/2\varepsilon^2}$$

Holds the same argument that we've found see in the next page!

While for a generic $n \in [1, N]$ we have:

$$x_n = (1-k\varepsilon)x_{n-1} + \sqrt{2D}\,\Delta B_{n-1} \quad \underline{0\ \text{iter.}}$$



$t_n - t_0 = n\varepsilon$
$x_n = x(t_0 + n\varepsilon)$
where $n \in \mathbb{N}$
$1 \le n \le N$

$$= (1-k\varepsilon)\left[(1-k\varepsilon)x_{n-2} + \sqrt{2D}\,\Delta B_{n-2}\right] + \sqrt{2D}\,\Delta B_{n-1}$$

$$= (1-k\varepsilon)^2 x_{n-2} + \sqrt{2D}\left[\Delta B_{n-1} + (1-k\varepsilon)\Delta B_{n-2}\right] \quad \underline{1^{st}\ \text{iter.}}$$

$$= (1-k\varepsilon)^2\left[(1-k\varepsilon)x_{n-3} + \sqrt{2D}\,\Delta B_{n-3}\right] + \sqrt{2D}\left[\cdots\right]$$

$$= (1-k\varepsilon)^3 x_{n-3} + \sqrt{2D}\left[\Delta B_{n-1} + (1-k\varepsilon)\Delta B_{n-2} + (1-k\varepsilon)^2\Delta B_{n-3}\right] \quad \underline{2^{nd}\ \text{iter.}}$$

$$= (1-k\varepsilon)^3\left[(1-k\varepsilon)x_{n-4} + \sqrt{2D}\,\Delta B_{n-4}\right] + \sqrt{2D}\left[\cdots\right] \quad \underline{3^{rd}\ \text{iter.}}$$

$$= (1-k\varepsilon)^4 x_{n-4} + \sqrt{2D}\left[\Delta B_{n-1} + (1-k\varepsilon)\Delta B_{n-2} + (1-k\varepsilon)^2\Delta B_{n-3} + (1-k\varepsilon)^3\Delta B_{n-4}\right]$$

$\underline{(n-1)^{th}\ \text{iter.}}$

$$= (1-k\varepsilon)^n x_0 + \sqrt{2D}\left[\Delta B_{n-1} + (1-k\varepsilon)\Delta B_{n-2} + \dots + (1-k\varepsilon)^{n-1}\Delta B_0\right]$$

$$= (1-k\varepsilon)^n x_0 + \sqrt{2D}\sum_{i=0}^{n-1}(1-k\varepsilon)^{n-1-i}\Delta B_i$$

$$\Rightarrow\ x_n = \underbrace{(1-k\varepsilon)^n x_0}_{\text{Constant term}} + \underbrace{\sqrt{2D}\sum_{i=0}^{n-1}(1-k\varepsilon)^{n-1-i}\Delta B_i}_{\text{Sum of indipendent random gaussian distributed variables } \Delta B_i \text{ with different coefficients}} \quad \text{with } n \in \mathbb{N},\ 1 \le n \le N$$

and $\underbrace{\Delta B_i}_{} \sim \mathcal{N}(0, \varepsilon)$

They are all indipendent between each other and identically distributed

$\Rightarrow$ We know that a sum of normally distributed random variables which are indipendent between each other is still a gaussian distribution, so then we expect $x_n = x(t_0 + n\varepsilon)$ to be distributed as a gaussian!

P.S. X, Y indip. random variables
$X \sim \mathcal{N}(\mu_X, \sigma_X^2)$ $\quad Y \sim \mathcal{N}(\mu_Y, \sigma_Y^2)$ $\Rightarrow Z = X + Y \sim \mathcal{N}(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2)$

=> **ANSATZ**: we suppose that our solution has gaussian form

$$W(x,t|x_0,t_0) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} e^{-\frac{(x-\bar{x}(t))^2}{2\sigma^2(t)}}$$ } Most general gaussian form

where $\bar{x}(t)$, $\sigma^2(t)$ are two functions of t such that the initial condition is satisfied and that $W(x,t|x_0,t_0)$ is the solution of the previous Fokker-Plank equation

How to calculate this two functions $\bar{x}(t)$ and $\sigma^2(t)$? There are at least two methods:

1. Is based on simple observation of the properties of the first two moments of $x(t)$ random variable.

2. Substitute the ansatz for $W(x,t|x_0,t_0)$ in the FP equation together with the initial condition.

1. $$\langle x\rangle_t = \int_{\mathbb{R}} W(x,t|x_0,t_0)\, x\, dx \overset{\text{Ansatz}}{=} \bar{x}(t)$$

$$\langle x^2\rangle_t - \langle x\rangle_t^2 = Var(x)_t = \int_{\mathbb{R}} W(x,t|x_0,t_0)\, x^2 dx - \langle x\rangle_t^2 \overset{\text{Ansatz}}{=} \sigma^2(t)$$

$$\Rightarrow \partial_t \langle x\rangle_t = \int_{\mathbb{R}} \dot{W}(x,t|x_0,t_0)\, x\, dx$$ FP equation

$$\overset{!}{=} \int_{\mathbb{R}} x\, dx\, \partial_x \left[kxW(x,t|x_0,t_0) + D\partial_x W(x,t|x_0,t_0)\right]$$ Integration by parts

$$\overset{!}{=} x\underbrace{\left[kxW + D\partial_x W\right]}_{\substack{=0 \text{ cause } W(x,t|x_0,t_0) \\ \text{and its derivatives goes} \\ \text{to zero at infinity for the} \\ \text{probability conservation}}}\Big|_{-\infty}^{+\infty} - \int_{\mathbb{R}} kxW + \widetilde{D\partial_x W}\, dx$$

$$D\int_{\mathbb{R}} \partial_x W dx = DW\Big|_{-\infty}^{+\infty} = 0$$

$$= -k\int_{\mathbb{R}} xW(x,t|x_0,t_0)dx = -k\langle x\rangle_t$$

$\Rightarrow \partial_t \langle x\rangle_t = -k\langle x\rangle_t$ and so we have $\langle x\rangle_t = e^{-kt}\cdot \text{const.}$

Initial condition t_0 : $\langle x \rangle_{t=t_0} = e^{-kt_0} \cdot \text{const.}$

$$= \int_{\mathbb{R}} W(x,t_0|x_0,t_0)\, x\, dx = \int_{\mathbb{R}} \delta(x-x_0)\, x\, dx \overset{*}{=} x_0$$

$$\rightsquigarrow \text{const.} = x_0 e^{kt_0}$$

$$\Rightarrow \underline{\langle x \rangle_t = x_0 e^{-k(t-t_0)} = \bar{x}(t)}$$

While we have : $\partial_t \langle x^2 \rangle_t = \int_{\mathbb{R}} \dot{W}(x,t|x_0,t_0)\, x^2 dx$ FP equation.

$$= \int_{\mathbb{R}} x^2 dx\, \partial_x [kxW + D\partial_x W]$$ Integration by parts

$$= x^2 [\underbrace{kxW + D\partial_x W}_{=0}]\Big|_{-\infty}^{\infty} - 2\int_{\mathbb{R}} x\, dx\, [kxW + D\partial_x W]$$

$$= -2k\int_{\mathbb{R}} x^2 W dx - 2D \underbrace{\int_{\mathbb{R}} x \partial_x W\, dx}_{\text{Integrate by parts}} \quad \cancel{xW\Big|_{-\infty}^{+\infty}} - \overbrace{\int_{\mathbb{R}} W\, dx}^{\text{Normalization}} = -1$$

$$= -2k \langle x^2 \rangle_t + 2D$$

Initial condition t_0 : $\langle x^2 \rangle_{t=t_0} - \langle x \rangle^2_{t=t_0} = \sigma^2(t_0) = 0$

It's zero because the i.c. is $\delta(x-x_0)$ so the variance of this initial distribution (at time t_0) will be zero!

$$\Rightarrow \langle x^2 \rangle_{t=t_0} = \langle x \rangle^2_{t=t_0} \overset{*}{=} x_0^2$$

Let's solve $\partial_t \langle x^2 \rangle_t = -2k \langle x^2 \rangle_t + 2D$

$\Rightarrow$ Homogeneous solution : $\partial_t \langle x^2 \rangle_t = -2k \langle x^2 \rangle_t \iff \langle x^2 \rangle_t^H = A e^{-2kt}$

$\Rightarrow$ Particular solution : $\partial_t \langle x^2 \rangle_t = 0 = -2k \langle x^2 \rangle_t + 2D \iff \langle x^2 \rangle^P_t = \frac{2D}{2k} = \frac{D}{k}$

$\Rightarrow \langle x^2 \rangle_t = \langle x^2 \rangle_t^H + \langle x^2 \rangle_t^P = A e^{-2kt} + \frac{D}{k}$ $\oplus$ Initial condition $\langle x^2 \rangle_{t_0} = x_0^2$

$$\Rightarrow \langle x^2\rangle_{t=t_0} = Ae^{-2kt_0} + \frac{D}{k} = x_0^2 \qquad A = e^{2kt_0}\left(x_0^2 - \frac{D}{k}\right)$$

$$\Rightarrow \langle x^2\rangle_t = \frac{D}{k} + \left(x_0^2 - \frac{D}{k}\right)e^{-2k(t-t_0)}$$

and so we have : $$\underline{\sigma^2(t)} = \langle x^2\rangle_t - \langle x\rangle_t^2 = \left[\frac{D}{k} + \left(x_0^2 - \frac{D}{k}\right)e^{-2k(t-t_0)}\right] - \left[x_0 e^{-k(t-t_0)}\right]^2$$

$$\stackrel{!}{=} \underline{\frac{D}{k}\left(1 - e^{-2k(t-t_0)}\right)}$$

Finally we can compute $W(x,t|x_0,t_0)$:

$$\boxed{W(x,t|x_0,t_0) = \left[\frac{2\pi D}{k}\left(1 - e^{-2k(t-t_0)}\right)\right]^{-\frac{1}{2}} e^{-\frac{\left[x - x_0 e^{-k(t-t_0)}\right]^2}{\frac{2D}{k}\left(1 - e^{-2k(t-t_0)}\right)}}}$$

~> Does $W(x,t|x_0,t_0)$ satisfy the initial condition?

If $t \to t_0^+$: $$W(x,t|x_0,t_0) = \underbrace{\left[\frac{2\pi D}{k}\left(1-e^{-2k(t-t_0)}\right)\right]^{-1/2}}_{\to (0)^{-1/2} = +\infty} e^{-\frac{\left[x-x_0e^{-k(t-t_0)}\right]^2 \;\to (x-x_0)^2}{\frac{2D}{k}\left(1-e^{-2k(t-t_0)}\right) \;\to 0}}$$

$e^{-\frac{(x-x_0)^2}{0}}$ scales like an exponential

Goes to infinity like a power law - Taylor

$$= \begin{cases} \infty \cdot e^{-\infty} \to 0 & \text{when } t \to t_0^+ \text{ and } x \neq x_0 \\ \infty \cdot e^{0} \to \infty & \text{when } t \to t_0^+ \text{ and } x = x_0 \end{cases}$$

The numerator goes to zero faster than the denominator *

$$= \delta(x - x_0)$$

* $$\frac{(x - x_0 e^{-\tau})^2}{\frac{2D}{k}(1 - e^{-2\tau})} \quad \text{with } \tau = k(t-t_0) \xrightarrow[t\to t_0]{} 0^+$$

$$\stackrel{!}{=} \frac{\left[x - x_0\left(1 - \tau + \frac{\tau^2}{2}\right)\right]^2}{\frac{2D}{k}\left[1 - \left(1 - 2\tau + \frac{(2\tau)^2}{2}\right)\right]}$$

$$= \begin{cases} (x-x_0)^2/0 \to +\infty & \text{if } x \neq x_0 \\ \dfrac{(\tau - \tau^2/2)^2 x_0^2}{\frac{2D}{k}(2\tau - 2\tau^2)} = \dfrac{\left(\tau - \tau^2 - \frac{\tau^3}{4}\right)x_0^2}{\frac{4D}{k}(1-\tau)} \to 0 & \text{if } x = x_0 \end{cases}$$

~> Does $W(x,t|x_0,t_0)$ tend to the Maxwell-Boltzmann distribution of the harmonic oscillator when $t \to +\infty$?

$$Z_U = \int_{\mathbb{R}} dx\, e^{-\beta U(x)} = \int_{\mathbb{R}} dx\, e^{-\frac{m}{2}\omega^2 x^2 \beta} = \sqrt{\frac{2}{m\beta\omega^2}} \int_{\mathbb{R}} dy\, e^{-y^2} = \sqrt{\frac{2\pi}{m\beta\omega^2}} \quad \text{with } \frac{m}{2}\omega^2 x^2 \beta = y^2,\ \sqrt{\frac{m}{2}\beta}\,\omega x = y,\ \sqrt{\frac{m}{2}\beta}\,\omega\, dx = dy$$

$$\lim_{t\to\infty} W(x,t|x_0,t_0) = \left(\frac{2\pi D}{k}\right)^{-\frac{1}{2}} e^{-\frac{x^2}{2D/k}} = \left(\frac{2\pi D\gamma}{m\omega^2}\right)^{-\frac{1}{2}} e^{-\frac{1}{2D}\frac{m\omega^2}{\gamma}x^2} = \left(\frac{2\pi}{\beta\omega^2 m}\right)^{-\frac{1}{2}} e^{-\frac{m}{2}\omega^2 x^2 \beta} \quad \text{with } D\gamma = \frac{1}{\beta}$$

$$\stackrel{!}{=} e^{-\beta U(x)} / Z_U$$

More in general for an arbitrary i.c. $\omega(x, t=t_0)$ we can write the solution of the FP equation like:

$$\omega(x,t) = \int dx' \, W(x,t|x',t_0)\, \omega(x', t=t_0)$$

$\rightsquigarrow$ Indeed $\dot{\omega}(x,t) \equiv \partial_t \omega(x,t) = \int dx' \, \dot{W}(x,t|x',t_0)\, \omega(x',t=t_0)$

$$\stackrel{!}{=} \int dx' \, \partial_x \left[Kx\, W(x,t|x',t_0) + D\partial_x W(x,t|x',t_0) \right] \omega(x',t=t_0)$$

$$\stackrel{!}{=} \partial_x \left[Kx \int dx' \, W(x,t|x',t_0)\,\omega(x',t=t_0) + D\partial_x \int dx' \, W(x,t|x',t_0)\,\omega(x',t_0) \right]$$

$$\stackrel{!}{=} \partial_x \left[Kx\, \omega(x,t) + D\partial_x \omega(x,t) \right]$$

we obtain again the FP equation!

As in quantum mechanics (Schrodinger equation) in stocastic processes (FP equation) we are dealing with linear differential equations so the tricks are always the same: we calculate the particular solution of the differential equation (Green function ~ Propagator) and we get automatically the general solution!

General Langevin & Fokker-Plank equations and Kramer's Equation

We want to generalize the Langevin equation for a particle that lives in a d-dimensional space:

- $\vec{x}(t) \in \mathbb{R}^d$ with components $x^\alpha(t)$ and $\alpha = 1, 2, \dots d$
- For each component we introduce a gaussian noise $B^\alpha(t)$ such that they are indipendent between each others (what happens in each dimension α is indipendent of all the others!). In other words:

$$dP_{t_1 \dots t_N}(\vec{B}_1, \dots, \vec{B}_N | \vec{B}_0, t_0) = \prod_{\alpha=1}^{d} \prod_{i=1}^{N} \frac{dB_i^\alpha}{\sqrt{2\pi \Delta t_i}} \, e^{-\frac{(\Delta B_i^\alpha)^2}{2\Delta t_i}}$$

Discretized Wiener Measure: for each timestep Δt_i of a fixed α component ΔB_i^α is normally distributed $N(0, \Delta t_i)$

where $\Delta B_i^\alpha = B^\alpha(t_i) - B^\alpha(t_{i-1})$

$\Rightarrow$ Not only ΔB_i^α are indipendent at each timestep i, but indip. at each dimension α

In this case we can proceed in the same way we have seen in the 1-dim. case:

$\langle \Delta B^\alpha(t) \rangle = 0$; Each $\Delta B^\alpha(t)$ is gaussian distributed with zero average

$\langle \Delta B^\alpha(t) \Delta B^\beta(t) \rangle = \Delta t \, \delta^{\alpha\beta}$

$\langle \Delta B^\alpha(t) \Delta B^\beta(t) \Delta B^\gamma(t) \rangle = 0$

$\langle \Delta B^\alpha(t) \Delta B^\beta(t) \Delta B^\gamma(t) \Delta B^\delta(t) \rangle = \Delta t^2 (\delta^{\alpha\beta}\delta^{\gamma\delta} + \delta^{\alpha\gamma}\delta^{\beta\delta} + \delta^{\alpha\delta}\delta^{\beta\gamma})$

$\vdots$

Recall that: $$P_{t_1 \dots t_N}(\vec{B}_1 \dots \vec{B}_N | \vec{B}_0, t_0) = \prod_{\alpha=1}^{d} \prod_{i=1}^{N} \frac{e^{-\frac{(\Delta B_i^\alpha)^2}{2\Delta t_i}}}{\sqrt{2\pi \Delta t_i}} = \mathcal{N}_{dN}(0, \Sigma) \sim \Delta \vec{B}$$

$$P^\alpha_{t_1 \dots t_N}(B_1^\alpha \dots B_N^\alpha | B_0^\alpha, t_0) = \prod_{i=1}^{N} \frac{e^{-\frac{(\Delta B_i^\alpha)^2}{2\Delta t_i}}}{\sqrt{2\pi \Delta t_i}} = \mathcal{N}_N(0, \tilde{\Sigma}) \sim \Delta B^\alpha$$

$\boxed{\text{P.S.}}$ Multivariate Gaussian Distribution of a $\vec{x}$ random variable

$$\vec{x} \sim \mathcal{N}_d(\vec{\mu}, \Sigma) \equiv \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} e^{-\frac{1}{2}(\vec{x}-\vec{\mu})^T \Sigma^{-1} (\vec{x}-\vec{\mu})}$$

where $\vec{x} = (x_1, x_2 \dots x_d)$

$\vec{\mu} = \mathbb{E}[\vec{x}] = (\mathbb{E}(x_1), \dots, \mathbb{E}(x_d))$ Mean vector

$\Sigma_{ij} = \mathbb{E}[(x_i - \mu_i)(x_j - \mu_j)] = Cov(x_i, x_j)$ Covariance Matrix

and where $\Sigma = \mathbb{E}[(\vec{x}-\vec{\mu})(\vec{x}'-\vec{\mu}')]$ is positive definite

- $\langle \Delta B^\alpha(t) \rangle = 0$
- $\langle \Delta B^\alpha(t) \Delta B^\beta(t) \rangle = \begin{cases} \langle (\Delta B^\alpha(t))^2 \rangle = \langle (\Delta B^\alpha(t))^2 \rangle - \langle \Delta B^\alpha(t) \rangle^2 = \tilde{\Sigma} & \text{if } \alpha = \beta \\ \langle \Delta B^\alpha(t) \rangle \langle \Delta B^\beta(t) \rangle = 0 & \text{if } \alpha \neq \beta \end{cases}$

where $\tilde{\Sigma} = \begin{pmatrix} \Delta t_1 & & 0 \\ & \ddots & \\ 0 & & \Delta t_N \end{pmatrix}$ $\Rightarrow \langle \Delta B^\alpha(t) \Delta B^\beta(t) \rangle = \tilde{\Sigma} \, \delta_{\alpha\beta}$

$\Rightarrow \langle \Delta B^\alpha(t) \Delta B^\beta(t) \rangle = \Delta t \, \delta_{ij} \delta_{\alpha\beta}$ with $\Delta t_i = \Delta t \;\; \forall i$

- $\langle \Delta B^{\alpha}(t)\Delta B^{\beta}(t)\Delta B^{\gamma}(t)\rangle = \langle \Delta B^{\alpha}(t)\Delta B^{\beta}(t)\rangle\langle \Delta B^{\gamma}(t)\rangle = 0$ Derives from the previous results
- $\langle \Delta B^{\alpha}(t)\Delta B^{\beta}(t)\Delta B^{\gamma}(t)\Delta B^{\delta}(t)\rangle$ Wick's theorem

$$= \langle \Delta B^{\alpha}(t)\Delta B^{\beta}(t)\rangle\langle \Delta B^{\gamma}(t)\Delta B^{\delta}(t)\rangle + \langle \Delta B^{\alpha}(t)\Delta B^{\gamma}(t)\rangle\langle \Delta B^{\beta}(t)\Delta B^{\delta}(t)\rangle + \langle \Delta B^{\alpha}(t)\Delta B^{\delta}(t)\rangle\langle \Delta B^{\beta}(t)\Delta B^{\gamma}(t)\rangle$$

$$= (\tilde{\Sigma})^2\left[\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}\right]$$

and we get $= \left(\sum_{k=1}^{N}\Delta t^2\delta_{ik}\delta_{kj}\right)[\cdots] = (\Delta t^2\delta_{ij})\left[\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}\right]$
if and only if we have $\Delta t_i = \Delta t\ \forall i$.

Moreover if $\Delta t_i = \Delta t\ \forall i$ the distribution of $\Delta\vec{B}$ for a single timestep follow the normal distribution:

$$P(\Delta\vec{B}) = \frac{1}{(2\pi\Delta t)^{d/2}}e^{-\frac{(\Delta\vec{B})^2}{2\Delta t}} \quad \text{where } (\Delta\vec{B})^2 = \sum_{\alpha=1}^{d}(\Delta B^{\alpha})^2$$

$$= \mathcal{N}_d(0,\bar{\Sigma})$$

$$\Delta\vec{B}^T\bar{\Sigma}^{-1}\Delta\vec{B} = \begin{pmatrix}\Delta B_1\\ \vdots\\ \Delta B_d\end{pmatrix}\begin{pmatrix}\frac{1}{\Delta t} & & 0\\ & \ddots & \\ 0 & & \frac{1}{\Delta t}\end{pmatrix}(\Delta B_1 \cdots \Delta B_d) = \frac{1}{\Delta t}\Delta\vec{B}^T\mathbb{1}\Delta\vec{B} = \frac{(\Delta\vec{B})^2}{\Delta t}$$

$$\Rightarrow \boxed{dx^{\alpha}(t) = f^{\alpha}(x(t),t)\,dt + \sqrt{2D^{\alpha}(x(t),t)}\,dB^{\alpha}(t)}$$

d-DIM. LANGEVIN EQUATION

Ito prescription: so $\vec{x}(t)$ is indipendent of $\vec{B}(s)$ $\forall s > t \rightsquigarrow$ Causality!

It's derived following the same steps of the 1-D case

$$\boxed{\dot{\omega}(\vec{x},t) = \sum_{\alpha=1}^{d}\partial_{\alpha}\left[-f^{\alpha}(\vec{x},t)\,\omega(\vec{x},t) + \partial_{\alpha}\left(D^{\alpha}(\vec{x},t)\,\omega(\vec{x},t)\right)\right]} = -\vec{\nabla}\cdot\vec{J}(\vec{x},t)$$

d-DIM. FOKKER PLANK EQUATION

We are now ready to take into account the inertial force (that we have neglect in the case of the overdamped Langevin equation) in our equation of motion (we are in 3D):

$$m\ddot{\vec{r}}(t) = \vec{F}_{ext}(\vec{r}(t)) - \gamma \cdot \dot{\vec{r}}(t) + \gamma\sqrt{2D}\,\vec{\xi}(t) \qquad \underline{\text{Quasi-equation}}$$

where $\vec{\xi}(t) = \dfrac{d\vec{B}(t)}{dt}$ and $\vec{F}_{noise}(t) = \gamma\sqrt{2D}\,\vec{\xi}(t)$ (see pag. 23)

The trick to write this equation such as a Langevin equation of the previous form is to define the 6-dimensional vector:

$$\vec{x} = \begin{pmatrix}\vec{r}\\ \vec{v}\end{pmatrix} \Rightarrow \begin{cases}\dot{\vec{r}}(t) = \vec{v}(t)\\ \dot{\vec{v}}(t) = \dfrac{\vec{F}_{ext}(\vec{r}(t))}{m\gamma} - \dfrac{\gamma}{m}\vec{v}(t) + \gamma\dfrac{\sqrt{2D}}{m}\vec{\xi}(t)\end{cases}$$

$$\Rightarrow \begin{cases} dr^{\alpha}(t) = v^{\alpha}(t)\,dt\\ dv^{\alpha}(t) = \dfrac{F^{\alpha}_{ext}(\vec{r}(t)) - \gamma v^{\alpha}(t)}{m}\,dt + \gamma\dfrac{\sqrt{2D}}{m}\,dB^{\alpha}(t)\end{cases}$$

Or without components:

$$\boxed{\begin{aligned} d\vec{r}(t) &= \vec{v}(t)\,dt\\ d\vec{v}(t) &= \left[\frac{\vec{F}_{ext}(\vec{r}(t)) - \gamma\vec{v}(t)}{m}\right]dt + \frac{\gamma}{m}\sqrt{2D}\,d\vec{B}(t)\end{aligned}}$$

This is a Langevin equation that has the form of the previous d-Dim. one ⊛ with ($\hat{u} = (1,1,1)$):

$$\vec{x}(t) = \begin{pmatrix}\vec{r}(t)\\ \vec{v}(t)\end{pmatrix} \qquad \vec{f}(\vec{x}(t),t) = \begin{pmatrix}\vec{v}(t)\\ \frac{1}{m}\left[\vec{F}_{ext}(\vec{r}(t)) - \gamma\vec{v}(t)\right]\end{pmatrix} \qquad \vec{D} = \begin{pmatrix}0\\ \frac{\gamma^2}{m^2}D\hat{u}\end{pmatrix}$$

→ So it corresponds to ⊛ with $d = 6$, $D^1 = D^2 = D^3 = 0$ and $D^4 = D^5 = D^6 \equiv D > 0$!

So then the equation ⊛ becomes:

$$\boxed{\dot{\omega}(\vec{r},\vec{v},t) = -\vec{\nabla}_r\cdot(\vec{v}\,\omega(\vec{r},\vec{v},t)) + \vec{\nabla}_v\cdot\left[\frac{\gamma\vec{v}-\vec{F}_{ext}(\vec{r})}{m}\,\omega(\vec{r},\vec{v},t) + \frac{\gamma^2 D}{m^2}\vec{\nabla}_v\,\omega(\vec{r},\vec{v},t)\right]}$$

KRAMER'S EQUATION

$$\dot{\omega}(\vec{x},t) = \sum_{\alpha=1}^{d}\partial_\alpha\left[-f^\alpha(\vec{x},t)\,\omega + \partial_\alpha\left(D^\alpha(\vec{x},t)\,\omega\right)\right]$$

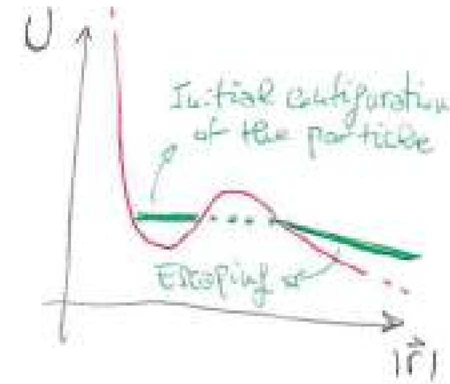
$$= \partial_{r_1}\left[-v_1\,\omega + \cancel{\partial_{r_1}(0\cdot\omega)}\right] + \partial_{r_2}\left[\dots 2\right] + \partial_{r_3}\left[\dots 3\right] +$$

$$+ \partial_{v_1}\left[-\frac{F_{ext,1}(\vec{r})-\gamma v_1}{m}\,\omega + \partial_{v_1}\frac{\gamma^2}{m^2}D\,\omega\right] + \partial_{v_2}\left[\dots 2\right] + \partial_{v_3}\left[\dots 3\right]$$

$$= \vec{\nabla}_r\cdot\left(-\vec{v}\cdot\omega(\vec{x},t)\right) + \vec{\nabla}_v\cdot\left[\frac{\gamma\vec{v}-\vec{F}_{ext}(\vec{r})}{m}\,\omega(\vec{x},t) + \vec{\nabla}_v\frac{\gamma^2}{m^2}D\,\omega(\vec{x},t)\right]$$

$$= -\vec{\nabla}_r\cdot\left(\vec{v}\,\omega(\vec{x},t)\right) + \vec{\nabla}_v\cdot\left[\frac{\gamma\vec{v}-\vec{F}_{ext}(\vec{r})}{m}\,\omega(\vec{x},t) + \frac{\gamma^2}{m^2}D\,\vec{\nabla}_v\,\omega(\vec{x},t)\right]$$

⇝ It allows to compute the analogous of the tunnel effect in quantum mechanics: if we have a particle that lives in a potential well initially (like in the figure) sooner or later it can cross the potential barrier thanks to the stocastic noise with a certain probability! Once it cross the barrier the particle escapes to infinity! This effect is related to the probability that two molecules get binded or unbinded due to stocasticity (thermal effects in this case ≠ quantum mechanical effects).



⇝ The Kramer's equation is also related to a lot of process in chemistry, ecology and so on...

If our external force $\vec{F}_{ext}$ can be derived from a potential (3D: this is not always guaranteed, the domain must be simply connected and the curl of the force must be zero. 1D: this is always guaranteed if the force is integrable and have a definite primitive) then:

$$\vec{F}_{ext}(\vec{r}) = -\vec{\nabla}_r\,U(\vec{r})$$

And by direct substitution in the Kramer's equation one can verify that the stationary state $\omega_{st}(\vec{r},\vec{v})$:

$$-\vec{\nabla}_r\cdot(\vec{v}\,\omega_{st}(\vec{r},\vec{v})) + \vec{\nabla}_v\cdot\left[\frac{\gamma\vec{v}+\vec{\nabla}_r U(\vec{r})}{m}\,\omega_{st}(\vec{r},\vec{v}) + \frac{\gamma^2}{m^2} D\,\vec{\nabla}_v\,\omega_{st}(\vec{r},\vec{v})\right] = 0$$

is given by the Boltzmann distribution of $\vec{r}$ and $\vec{v}$ for large times:

$$\omega(\vec{r},\vec{v},t) \xrightarrow{t\to\infty} \frac{1}{Z}\, e^{-\beta\left(\frac{m}{2}\vec{v}^2 + U(\vec{r})\right)} = \omega_{st}(\vec{r},\vec{v}) = \mathbb{P}_{eq}(\vec{r},\vec{v})$$

where $Z = \left(\frac{2\pi k_B T}{m}\right)^{3/2} Z_U$, $Z_U = \int d^3r\, e^{-\beta U(\vec{r})}$

and D is given by the Einstein relation $\gamma D = k_B T$

Checking $\omega_{eq}(\vec{r},\vec{v})$ satisfy the Kramer's equation of stationarity:

$$\underbrace{-\vec{\nabla}_r\cdot(\vec{v}\,\omega_{eq})}_{1} + \vec{\nabla}_v\cdot\left[\underbrace{\frac{\gamma\vec{v}+\vec{\nabla}_r U}{m}\,\omega_{eq}}_{2} + \underbrace{\frac{\gamma^2}{m^2} D\,\vec{\nabla}_v\,\omega_{eq}}_{3}\right]$$

A little of Stochastic Calculus

What we already know about integrals is about the Riemann definition of integrals:

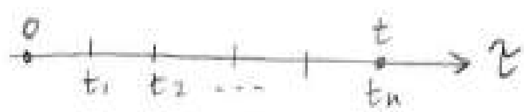
$$\int_0^t f(\tau)\,d\tau = \lim_{\max \Delta t_i \to 0} \sum_i \Delta t_i\, f(\tau_i) \quad \text{where} \quad \begin{array}{l} t_{i-1} \le \tau_i \le t_i \text{ arbitrary} \\ \Delta t_i = t_i - t_{i-1} \end{array}$$

What are STOCASTIC INTEGRALS? They occours when for examples we integrate both sides of the Langevin equation: we have ordinary integrals (Riemann type) when we integrate the deterministic part but also stocastic integrals when we integrate the stocastic part with the noise term!
This new type of integrals will have the form:

$\int_0^t G(\tau)\,dB(\tau)$ with $G(\tau)$ arbitrary function of τ and where $\{\underbrace{B(\tau)}_{\text{Random variable}}, 0 \le \tau \le t\}$ is a brownian trajectory with its associated measure in the trajectory space:

$$\boxed{\times}\ d\mathbb{P}(\{B\}) = \text{"} \prod_{0 \le \tau \le t} \frac{dB(\tau)}{\sqrt{2\pi\, d\tau}}\, e^{-\frac{1}{2}\int_0^t \dot{B}^2(\tau)\,d\tau} \text{"}$$

Since $B(\tau)$ is a random variable we define $S = \int_0^t G(\tau)\,dB(\tau)$ as follow.
We discretize our time line with a generic mesh (all time-point are not necessarily equally spaced) and define a discretized version of S, that is:



$$S_n = \sum_{i=1}^{n} G(\tau_i)\underbrace{\left(B(t_i) - B(t_{i-1})\right)}_{=\Delta B_i}$$

where $t_i < \tau_i < t_{i-1}$, for example we can choose

$\tau_i = \lambda t_i + (1-\lambda)\, t_{i-1}$ with $0 \le \lambda \le 1$

- $\lambda = 0$ => Ito Integral
- $\lambda = 1/2$ -> Stratonovic Integral

$\Rightarrow$ S is such that : $\boxed{\lim_{n\to\infty} \langle (S-S_n)^2 \rangle = 0}$ ①

where the limit has to be such that $\max_{i=1\dots n} \Delta t_i \to 0$ and where the average $\langle \cdot \rangle$ has to be done with the discretized version of the measure ⊠ (Wiener measure for $B(\tau)$)

$\boxed{\text{Ex}}$ Calculate the stocastic integral:

$S = \int_0^t B(\tau)\, dB(\tau)$ where $B(\tau)$ is such that the discretized probab. is: $d\mathbb{P}_{t_1 \dots t_n}(B_1 \dots B_n | B_0, 0) = \prod_{i=1}^{n} \frac{dB_i}{\sqrt{2\pi \Delta t_i}}\, e^{-\sum_{i=1}^{n} \frac{(\Delta B_i)^2}{2\Delta t_i}}$

with $\Delta B_i = B_i - B_{i-1}$

Firstly we discretize S using $\lambda = 0$ (Ito integral).

$$S_n = \sum_{i=1}^{n} B(t_{i-1}) \left[B(t_i) - B(t_{i-1}) \right]$$

or in general we can compute S_n using whatever λ:

$$S_n = \sum_{i=1}^{n} B(\tau_i) \left[B(t_i) - B(t_{i-1}) \right]$$

$$\langle S_n \rangle = \sum_{i=1}^{n} \left[\langle B(\tau_i) B(t_i) \rangle - \langle B(\tau_i) B(t_{i-1}) \rangle \right] \circledast$$

$$= \sum_{i=1}^{n} (\tau_i - t_{i-1}) = \sum_{i=1}^{n} \left(\lambda t_i + (\cancel{1} - \lambda) t_{i-1} - \cancel{t_{i-1}} \right) = \sum_{i=1}^{n} \lambda (t_i - t_{i-1})$$

$$= \lambda \sum_{i=1}^{n} \Delta t_i = \lambda (t - t_0) = \lambda t \quad \text{where } \begin{matrix} t_0 = 0 \\ t_n = t \end{matrix} \text{ and } \Delta t_i = t_i - t_{i-1}$$

⊛ Recall that (see previous lectures) : $\langle B(t_1) B(t_2) \rangle = \min(t_1, t_2)$ with $B_0 = 0$ and $t_0 = 0$

$\rightsquigarrow$ It's computed using the Wiener measure for B (discretized and then taken the discretization to the "continuous limit")

Notice that $\langle S_n \rangle = 0$ if $\lambda = 0$: we get this because $\langle S_n \rangle = \sum_{i=1}^{n} \langle B(t_{i-1}) \Delta B_i \rangle$ and $B(t_{i-1}) = \sum_{j=1}^{i-1} \Delta B_j$ so $B(t_{i-1})$ is independent of ΔB_i ❢ Successive jumps ΔB_k are independent between each others ❢ $\langle \Delta B_k \rangle = 0$

So when $\lambda = 0$:

$$S_n = \sum_{i=1}^{n} \sum_{j=1}^{i-1} \Delta B_j \Delta B_i \qquad \langle S_n \rangle = \sum_{i=1}^{n} \sum_{j<i} \langle \Delta B_j \rangle \langle \Delta B_i \rangle = 0$$

$$\Rightarrow S_n = \sum_{i=1}^{n} \sum_{j<i} \Delta B_j \Delta B_i = \sum_{i=1}^{n} B(t_{i-1}) \Delta B_i = \sum_{i=1}^{n} B_{i-1} \Delta B_i$$

$$= \frac{1}{2} \sum_{i=1}^{n} \left[(B_{i-1} + \Delta B_i)^2 - B_{i-1}^2 - (\Delta B_i)^2 \right] \quad \text{where } \Delta B_i = B_i - B_{i-1}$$

$$= \frac{1}{2} \sum_{i=1}^{n} \left[B_i^2 - B_{i-1}^2 \right] - \frac{1}{2} \sum_{i=1}^{n} (\Delta B_i)^2 = \frac{1}{2} \left(B_n^2 - B_0^2 \right) - \frac{1}{2} \sum_{i=1}^{n} (\Delta B_i)^2$$

$$= \underbrace{\frac{1}{2} \left[B^2(t) - B^2(0) \right]} - \underbrace{\frac{1}{2} \sum_{i=1}^{n} (\Delta B_i)^2}$$

That's what we expect in ordinary calculus: all it's fine!

$$\int_{t=0}^{t} x\, dx = \frac{x^2(t) - x^2(0)}{2}$$

New unexpected term: it's what makes the difference between ordinary calculus and stocastic calculus!!

How to compute it? ... continues ...

From Hölder inequality we have:

$$|\langle S \rangle - \langle S_n \rangle| = |\langle S - S_n \rangle| \leq \langle (S - S_n)^2 \rangle^{1/2}$$

We know from ⓪ (pag. 41-b) that:

$$\lim_{n \to \infty} \langle (S - S_n)^2 \rangle = 0$$

$$\Rightarrow \langle (S - S_n)^2 \rangle^{1/2} = 0 \quad \text{when } n \to \infty$$

$$\Rightarrow \lim_{n \to \infty} |\langle S \rangle - \langle S_n \rangle| = 0$$

$$\Rightarrow \boxed{\lim_{n \to \infty} \langle S_n \rangle = \langle S \rangle}$$

or equivalently:

$$\boxed{\text{ms-}\lim_{n \to \infty} S_n = S}$$

where ms = mean square

Theorem (Hölder's inequality)

Let (S, Σ, μ) be a measure space and let $p, q \in [1, \infty]$ where:

$$1/p + 1/q = 1$$

$$\Rightarrow \|f g\|_1 \leq \|f\|_p \|g\|_q$$

$\forall f, g$ measurable functions on S

When we consider averages with respect to the discretized version of ⊠ (see pag. 41), that is:

$$d\mathbb{P}_{t_1 \cdots t_n}(B_1, B_2 \cdots B_n | B_0, t_0) = \prod_{i=1}^{n} \left[\frac{dB_i}{\sqrt{2\pi \Delta t_i}} e^{-\frac{(\Delta B_i)^2}{2\Delta t_i}} \right]$$

with $t_0 = 0$, $B_0 = 0$, $t_n = t$

of $(\Delta B_i)^2 F(\{B\})$, where F is a function of the whole B trajectory, and we are interested in the leading order in Δt_i then we can substitute $(\Delta B_i)^2$ with Δt_i.

Proof.

Since $\{B\}$ is determined by ΔB_J with $i = 1 \cdots n$, in fact:

$$B_J = \sum_{k=1}^{J} \Delta B_k \quad \text{where } B_0 = 0 \quad \left(B_J = \sum_{k=1}^{J} \Delta B_k + B_0 \text{ if } B_0 \text{ is fixed} \right)$$

Then $F(\{B\})$ is a function of all ΔB_J's $\rightsquigarrow F\{\Delta B\}$.

Now we can expand this function F in McLaurin series in ΔB_i with i fixed (so we are expanding in a single fixed variable, recall that F is a function of all $\{\Delta B\}$)

$$F\{B\} = F(\Delta B_J : J \neq i, \Delta B_i = 0) + \Delta B_i \left(\frac{\partial}{\partial(\Delta B_i)} F \right)_{|\Delta B_i = 0} + $$

$$+ \frac{\Delta B_i^2}{2} \left(\frac{\partial^2}{\partial^2(\Delta B_i)} F \right)_{|\Delta B_i = 0} + \cdots$$

$$= \sum_{k \geq 0} (\Delta B_i)^k F^{(k)} (\Delta B_J : J \neq i, \Delta B_i = 0)$$

$$(\Delta B_i)^2 F(\{B\}) = (\Delta B_i)^2 F(\Delta B_J : J \neq i, \Delta B_i = 0) + (\Delta B_i)^3 \left(\frac{\partial}{\partial(\Delta B_i)} F \right)_{|\Delta B_i = 0} + $$

$$+ \frac{(\Delta B_i)^4}{2} \left(\frac{\partial^2}{\partial^2(\Delta B_i)} F \right)_{|\Delta B_i = 0} + \cdots$$

$$= \sum_{k \geq 0} (\Delta B_i)^{k+2} F^{(k)} (\Delta B_J : J \neq i, \Delta B_i = 0)$$

$\langle (\Delta B_i)^2 F(\Delta B_j) \rangle$

$= \langle \Delta B_i^2 \rangle \langle F(\Delta B_j : j \neq i, \Delta B_i = 0) \rangle + \cancel{\langle (\Delta B_i)^3 \rangle \langle \frac{\partial}{\partial (\Delta B_i)} F|_{\Delta B_i = 0} \rangle} +$

= 0 in fact we know that $\langle \Delta B_i \rangle = 0$ from the previous lessons

$+ \frac{1}{2} \langle (\Delta B_i)^4 \rangle \langle \frac{\partial^2}{\partial^2 (\Delta B_i)} F|_{\Delta B_i = 0} \rangle + \dots$

All the averages factorizes because $\Delta B_j : j \neq i$ is indipendent of ΔB_i

$$= \sum_{k \geq 0} \langle (\Delta B_i)^{k+2} \rangle \langle F^{(k)}(\Delta B_j : i \neq j, \Delta B_i = 0) \rangle$$

Moreover:

$$\langle (\Delta B_i)^{k+2} \rangle = \int \frac{dB_i}{\sqrt{2\pi \Delta t_i}} (\Delta B_i)^{k+2} e^{-\frac{(\Delta B_i)^2}{2\Delta t_i}}$$

substitution: $x^2 = \frac{(\Delta B_i)^2}{\Delta t_i}$

$dx = \frac{dB_i}{\sqrt{\Delta t_i}}$

$$= \frac{1}{\sqrt{2\pi}} \int dx \, (\sqrt{\Delta t_i}\, x)^{k+2} e^{-\frac{x^2}{2}}$$

$$= \frac{(\Delta t_i)^{k+2/2}}{\sqrt{2\pi}} \int dx \, x^{k+2} e^{-\frac{x^2}{2}} = \begin{cases} 0 \text{ if } k \text{ is odd} \\ \Delta t_i \text{ if } k = 0 \\ \mathcal{O}\left((\Delta t_i)^{\frac{k+2}{2}}\right) \text{ if } k = 2, 4, \dots \end{cases}$$

In fact: $\int dx \, x^{k+2} e^{-a x^2}$ with $a = \frac{1}{2}$ and notice that: $(-1)^i \frac{\partial^i}{\partial^i a}(e^{-ax^2}) = x^{2i} e^{-ax^2}$

- Let $\underline{k}$ be <u>odd</u> such that $k+2 = 2i+1$:

$$\int dx \, x^{k+2} e^{-ax^2} = \int dx \, x^{2i+1} e^{-ax^2} = (-1)^i \frac{\partial^i}{\partial^i a} \int dx \, e^{-ax^2} \cdot x = 0$$

- Let $\underline{k}$ be <u>even</u> such that $k+2 = 2i$:

$$\int dx \, x^{k+2} e^{-ax^2} = \int dx \, x^{2i} e^{-ax^2} = (-1)^i \frac{\partial^i}{\partial^i a} \int dx \, e^{-ax^2} = (-1)^i \frac{\partial^i}{\partial^i a} \left(\sqrt{\frac{\pi}{a}} \right)$$

$\underline{k=0}$ $(i=1)$: $-\frac{\partial}{\partial a}\left(\sqrt{\frac{\pi}{a}}\right) = -\frac{1}{2}\left(\frac{\pi}{a}\right)^{-\frac{1}{2}}\left(-\frac{\pi}{a^2}\right) = \frac{1}{2}\sqrt{\frac{a}{\pi}}\left(\frac{\pi}{a^2}\right) = \frac{1}{2}\frac{\sqrt{\pi}}{a\sqrt{a}}$

$\int dx \, x^2 e^{-\frac{x^2}{2}} = \sqrt{2\pi}$

$\underline{k=1}$ $(i=2)$: $(-1)^2 \frac{\partial^2}{\partial^2 a}\left(\sqrt{\frac{\pi}{a}}\right) = \frac{3\sqrt{\pi}}{4}(a)^{\frac{5}{2}} \rightsquigarrow 3\sqrt{2\pi} \dots$

$$\Rightarrow \langle (\Delta B_i)^2 F(\{B\}) \rangle = \Delta t_i \langle F(\Delta B_j : j \neq i, \Delta B_i = 0) \rangle + \mathcal{O}((\Delta t_i)^2)$$

Moreover notice that taking $\Delta t_i F(\{B\})$ on the other hand we have:

$$\langle \Delta t_i F(\{B\}) \rangle = \Delta t_i \langle F(\{B\}) \rangle = \Delta t_i \sum_{k \geq 0} \langle (\Delta B_i)^k F^{(k)}(\Delta B_j : i \neq j, \Delta B_i = 0) \rangle$$

$$= \Delta t_i \sum_{k \geq 0} \langle (\Delta B_i)^k \rangle \langle F^{(k)}(\Delta B_j : i \neq j, \Delta B_i = 0) \rangle$$

$$= \Delta t_i \langle F(\Delta B_j : i \neq j, \Delta B_i = 0) \rangle + \mathcal{O}((\Delta t_i)^2)$$

End of the proof. $\square$

ITO-RULE $\Delta t_i F(\{B\})$ and $(\Delta B_i)^2 F(\{B\})$ behave in the same way at the leading order in Δt_i as far as we are interested in their averages.

⇝ They are the same if we are dealing with their averages! The error in doing so it's of higher order in Δt_i, instead if at the end we take all the $\Delta t_i \to 0$ then this result is exact!

⇝ Exact in the continuum limit $\Delta t \to 0$

Ex Let's continue the computation of $S = \int_0^t B(\tau) dB(\tau)$

We were at $(\lambda = 0)$: $S_n = \frac{1}{2}\left[B^2(t) - B^2(0)\right] - \frac{1}{2}\sum_{i=1}^{n} \underbrace{(\Delta B_i)^2}_{\text{Ito rule}}$

$$S = \frac{1}{2}\left[B^2(t) - B^2(0)\right] - \frac{1}{2}\sum_{i=1}^{n} \Delta t_i = \frac{B^2(t) - B^2(0)}{2} - \frac{t}{2} \quad \text{with } t_0 = 0$$

So one can easily check that:

$$\lim_{n \to \infty} \langle (S - S_n)^2 \rangle = \lim_{n \to \infty} \left\langle \sum_{i=1}^{n} \left[(\Delta B_i)^2 - \Delta t_i\right] \right\rangle = 0$$

In general with a generic λ: $S = \int_{t_0}^{t} B_\lambda(\tau) dB(\tau) = \frac{B^2(t) - B^2(t_0)}{2} + \left(\lambda - \frac{1}{2}\right)(t - t_0)$

with $t_0 = 0$

On the other hand if we use $\lambda = 1/2$ (Stratonovic integral):

$$S_n = \sum_{i=1}^{n} \underline{B\left(\frac{t_i + t_{i-1}}{2}\right)} \left[B(t_i) - B(t_{i-1})\right]$$

$$= \sum_{i=1}^{n} \underline{\frac{B(t_i) + B(t_{i-1})}{2}} \left[B(t_i) - B(t_{i-1})\right] = \sum_{i=1}^{n} \frac{B^2(t_i) - B^2(t_{i-1})}{2}$$

$$= \frac{B^2(t) - B^2(0)}{2} \quad \text{with } t_0 = 0$$

$$B\left(\frac{t_i + t_{i-1}}{2}\right) = B\left(\frac{\tau}{2} + \frac{\tau - \Delta\tau}{2}\right) = B\left(\tau - \frac{\Delta\tau}{2}\right) \overset{\Delta\tau \to 0}{=} B(\tau) - \frac{\Delta\tau}{2}\dot{B}(\tau) + \frac{\Delta\tau^2}{4}\ddot{B}(\tau) + O(\Delta\tau^3)$$

while: $B(t_{i-1}) = B(\tau - \Delta\tau) = B(t) - \Delta\tau \dot{B}(\tau) + \frac{\Delta\tau^2}{2}\ddot{B}(\tau) + O(\Delta\tau^3)$

$$\frac{B(t_i) + B(t_{i-1})}{2} = B(\tau) - \frac{\Delta\tau}{2}\dot{B}(\tau) + \frac{\Delta\tau^2}{4}\ddot{B}(\tau) + O(\Delta\tau^3)$$

=> Thus if we take $\lambda = 1/2$ then $S = \frac{B^2(t) - B^2(0)}{2}$ and we trivially have $\langle (S_n - S)^2 \rangle = 0 \ \forall n$

Finally:
$$\int_{t_0}^{t} B(\tau)\, dB(\tau) = \begin{cases} \frac{B^2(t) - B^2(t_0)}{2} - \frac{t - t_0}{2} & \text{\underline{Ito} integ\underline{ral} } (\lambda = 0) \\ \frac{B^2(t) - B^2(t_0)}{2} & \text{\underline{Stratonovich} integ\underline{ral} } (\lambda = \frac{1}{2}) \end{cases}$$

where $t_0 = 0$

Recap (valid in general!):

- At variance what happens in ordinary calculus/integrals, stocastic integrals depends on the choice of λ
  - ⇝ Ito and Stratonovic integrals have different values for the same integrand! The choice is done according to what you have to compute!
- Notice that the Stratonovic integrals coincide with the result of ordinary integrals (ordinary calculus!)

Differentiation Rules

In general stocastic integrals are hard to compute but sometimes they can be reduced to ordinary integrals ($dB(\tau)$ is mapped to $d\tau$!). In order to do this we must introduce some differentiation rules.

As a result of the ito rule we can derive the following differentiation rule. Suppose that we have a generic function h of $B(t)$ and of the time t, that is $h(B(t),t)$. Let's introduce:

$$\Delta h(B(t),t) = h(\underline{B(t+\Delta t)}, t+\Delta t) - h(B(t),t)$$

$$\stackrel{!}{=} h(\underline{B(t)+\Delta B(t)}, t+\Delta t) - h(B(t),t) \quad \text{where } \Delta B(t) = B(t+\Delta t) - B(t)$$

$$\stackrel{!}{=} \Big[\cancel{h(B,t)} + \partial_B h(B,t)\Delta B(t) + \partial_t h(B,t)\Delta t + \tfrac{1}{2}\partial_B h(B,t)(\Delta B^2(t)) + $$

$$+ \mathcal{O}(\Delta t^2, \Delta B^3(t))\Big]\Big|_{B=B(t)} - \cancel{h(B(t),t)}$$

Taylor expansion where $\Delta t \sim 0$, $\Delta B(t) \sim 0$

Ito Rule

$$= \left\{\Delta t\left[\partial_t h(B,t) + \tfrac{1}{2}\partial_B^2 h(B,t)\right] + \partial_B h(B,t)\Delta B(t)\right\}\Big|_{B=B(t)} + \mathcal{O}(\Delta t^2, \Delta B^3(t))$$

$\Rightarrow$ Differential Form:

$$\boxed{\begin{aligned} dh(B(t),t) &= \left(\partial_t h + \tfrac{1}{2}\partial_B^2 h\right)dt + (\partial_B h)\,dB \\ &\stackrel{!}{=} \Big[\underline{\partial_t h(B,t)} + \underline{\tfrac{1}{2}\partial_B^2 h(B,t)}\Big]\Big|_{B=B(t)} dt + \underline{\partial_B h(B,t)}\Big|_{B=B(t)} \cdot \underline{dB(t)} \end{aligned}}$$

Δ

Terms that we expect: are the same of ordinary calculus!

New term due to stocasticity: stocastic calculus!

If $h(B(t))$ doesn't depend explicity on time (t is a continuous variable: we don't have problems dealing with it!):

$$\boxed{dh(B(t)) = \underline{\partial_B^2 h(B)}\Big|_{B=B(t)} \cdot \frac{dt}{2} + \underline{\partial_B h(B)}\Big|_{B=B(t)} \cdot \underline{dB(t)}}$$

If we integrate Δ from t_0 to t we can derive a method to transform stocastic integrals to ordinary one.
Recall that $dh(B(t))$ is an exact differential so then we have.

$$\int_{t_0}^{t} dh(B(\tau))d\tau = h(B(t)) - h(B(t_0))$$ Left side of Δ

Exact differential so it can be approximated as : $\sum_i \Delta h_i = h_n - h_0 = h(t) - h(t_0)$

$$\underbrace{\int_{t_0}^{t} \frac{\partial h(B)}{\partial B}\bigg|_{B=B(\tau)} dB(\tau)}_{\text{Stocastic integral !}} + \underbrace{\frac{1}{2}\int_{t_0}^{t} \frac{\partial^2 h(B)}{\partial B^2}\bigg|_{B=B(\tau)} d\tau}$$ Right side of Δ

ordinary integral: notice that $B(\tau)$ is continuous (never differentiable) and also that h is defined to be differentiable!

$$\Rightarrow \boxed{\int_{t_0}^{t} \frac{\partial h(B)}{\partial B}\bigg|_{B=B(\tau)} dB(\tau) = h(t) - h(t_0) - \frac{1}{2}\int_{t_0}^{t} \frac{\partial^2 h(B)}{\partial B^2}\bigg|_{B=B(\tau)} d\tau}$$

Δ From Stocastic to Ordinary Integral

Ex Suppose that $h(B) = \frac{B^2}{2}$

We have: $\frac{\partial h}{\partial B} = B \qquad \frac{\partial^2 h}{\partial B^2} = 1$ so from Δ we get.

$$\int_{t_0}^{t} B(\tau)dB(\tau) = \frac{B^2(t)}{2} - \frac{B^2(t_0)}{2} - \frac{1}{2}\int_{t_0}^{t} d\tau$$

$$= \frac{B^2(t) - B^2(t_0)}{2} - \frac{t - t_0}{2}$$

We recover the previous exercise!

$\boxed{Ex}$ Suppose that $h(B) = \frac{B^{m+1}}{m+1}$

We have: $\frac{dh}{dB} = B^m$ and $\frac{d^2h}{dB^2} = mB^{m-1}$, so then from Δ we get:

$$\int_{t_0}^{t} B^m(\tau)\, dB(\tau) = \frac{B^{m+1}(t) - B^{m+1}(t_0)}{m+1} + \frac{m}{2}\int_{t_0}^{t} \underbrace{B^{m-1}(\tau)\, d\tau}$$

Ordinary integral: recall that B is continuous!

Path Integrals for the general FP equation & Feynmann-Kac Formula

Our next goal is to repeat the discussion of path integrals for the diffusion process in the more general case, so when we have also an external force acting on our system $\rightsquigarrow$ Path integrals for the general Langevin equation

We've already seen that if we're dealing with the overdamped Langevin equation in absence of external force we have:

$dx(t) = \sqrt{2D}\, dB(t)$ where the wiener measure for this process is:

$$dX_w = \text{"}\prod_{t_0 < \tau \le t} \frac{dx(\tau)}{\sqrt{4\pi D\, d\tau}}\, e^{-\frac{1}{4D}\int_{t_0}^{t} \left(\frac{dx(\tau)}{d\tau}\right)^2 d\tau}\text{"} \xleftarrow{n\to\infty} \prod_{i=1}^{n} \frac{dx_i}{\sqrt{4D\pi\, \Delta t_i}}\, e^{-\frac{1}{4D}\sum_{i=1}^{n} \frac{(\Delta x_i)^2}{\Delta t_i}}$$

What happens in the case of the general overdamped Langevin equation? Let's see keeping the 1D case:

$$dx(t) = f(x(t), t)\, dt + \sqrt{2D(x(t), t)}\, dB(t)$$

Now we discretize the time line and we apply the Ito prescription:

$$\Delta x_i = x_i - x_{i-1} = f_{i-1}\Delta t_i + \sqrt{2D_{i-1}}\, \Delta B_i$$

where $x_i = x(t_i)$ $\quad \Delta t_i = t_i - t_{i-1}$ $\quad f_i = f(x(t_i), t_i)$

$B_i = B(t_i)$ $\quad \Delta B_i = B_i - B_{i-1}$ $\quad D_i = D(x(t_i), t_i)$

$\Delta B_i = B_i - B_{i-1}$

Now let's do a change of variable from B to x that depend on each other.

$$d\mathbb{P}_{t_1 \cdots t_n}(B_1 \cdots B_n | B_0, t_0) = \prod_{i=1}^{n} \frac{dB_i}{\sqrt{2\pi \Delta t_i}} e^{-\sum_{i=1}^{n} \frac{(\Delta B_i)^2}{2\Delta t_i}}$$

$$= d\mathbb{P}_{t_1 \cdots t_n}(x_1 \cdots x_n | x_0, t_0) \left| \underbrace{\det \left[\frac{\partial(x_1 \cdots x_n)}{\partial(B_1 \cdots B_n)} \right]}_{\text{Jacobian}} \right|$$

Let's compute the Jacobian: $x_i = f_{i-1} \Delta t_i + \sqrt{2D_{i-1}} (B_i - B_{i-1}) + x_{i-1}$

$$\Rightarrow \frac{\partial x_i}{\partial B_j} = \begin{cases} 0 & \text{if } j > i \\ \sqrt{2D_{i-1}} & \text{if } i = j \\ \frac{\partial x_i}{\partial B_j} & \text{if } j < i \end{cases}$$

with $i, j = 1 \dots n$

It's some complicate expression: we don't know

$\Rightarrow$ We obtain a triangular matrix! So then its determinant J is simply the product of the diagonal:

$$J = \prod_{i=1}^{n} \sqrt{2D_{i-1}}$$

and

$$\Delta B_i = \frac{(\Delta x_i - f_{i-1} \Delta t_i)}{\sqrt{2D_{i-1}}}$$

This result derives directly from the Ito prescription otherwise, using the Stratonovic prescription, the result would be more complicated (a mess in generic dimension: D becomes a positive definite matrix that play the role of a metric in the manifold of the trajectories, so then the path integrals are done in a curved space)

$$d\mathbb{P}_{t_1 \cdots t_n}(x_1 \cdots x_n | x_0, t_0) = \prod_{i=1}^{n} \frac{dx_i}{\sqrt{4\pi D_{i-1} \Delta t_i}} e^{-\sum_{i=1}^{n} \frac{(\Delta x_i - \Delta t_i f_{i-1})^2}{4D_{i-1} \Delta t_i}}$$

$$\xrightarrow{n \to \infty} \text{“} \prod_{t_0^+ < \tau \le t} \frac{dx(\tau)}{\sqrt{4\pi D(\tau)\, d\tau}} e^{-\int_{t_0}^{t} \frac{(\dot{x}(\tau) - f(x(\tau), \tau))^2}{4D(x(\tau), \tau)} d\tau} \text{”}$$

So when $f = 0$ and D is constant we get back the Wiener measure!

Now comes the interesting part that explain why, when we introduced the path integrals, we have done certain obscure calculation: we're gonna map this problem to something we already know how to compute.

Ex Let's exploit ✡ and take $D = \text{const}$.

$$d\mathbb{P}_{t_1 \cdots t_n}(x_1 \dots x_n | x_0, t_0) = \underbrace{\prod_{i=1}^{n} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}}\, e^{-\frac{1}{4D}\sum_{i=1}^{n} \frac{(\Delta x_i)^2}{\Delta t_i}}}_{dX_W \text{ in the continuum limit}} .$$

$$\cdot\, e^{\underbrace{\frac{1}{2D}\sum_{i=1}^{n} \Delta x_i f_{i-1}}_{\text{Stocastic integral}} - \underbrace{\frac{1}{4D}\sum_{i=1}^{n} \Delta t_i f_{i-1}^2}_{\text{ordinary integral}}}$$

Stocastic integral: ① $\int dx(\tau) f(x(\tau),\tau)$

ordinary integral: $\int_{t_0}^{t} d\tau\, f^2(x(\tau),\tau)$ ②

Notice that the ratio between the x measure $d\mathbb{P}$ and the wiener discretized measure (we should go to the continuum limit to be formally correct) is given by the last line and represent the random Malliavin (?) derivative of the x measure with respect to the wiener measure!

Now we'll consider external forces with no explicit dependence of t time, so then it can be written exploiting a potential because we are in 1D:

$$f(x(t)) = -\frac{\partial}{\partial x} \frac{U(x)}{\gamma}\Big|_{x=x(t)}$$

① $$\int_{t_0}^{t} dx(\tau)\, f(x(\tau)) = -\int_{t_0}^{t} \frac{dx(\tau)}{\gamma} \frac{\partial U(x)}{\partial x}\Big|_{x=x(\tau)}$$

$$= -\frac{1}{\gamma}\left[U(t) - U(t_0) - D\int_{t_0}^{t} \frac{\partial^2 U(x)}{\partial x^2}\Big|_{x=x(\tau)} d\tau \right]$$

Let's use ⚠ remembering to change variable from B to x and recalling that:

$\langle \Delta B^2 \rangle = \Delta t \quad (dB)^2 = d\tau$

$\langle \Delta x^2 \rangle = 2D\Delta t \quad (dx)^2 = 2D d\tau$

So we get:

$$d\mathbb{P}_{t_1\cdots t_n}(x_1\cdots x_n|x_0,t_0) \xrightarrow{n\to\infty} d\mathbb{P}(\{x(\tau): t_0<\tau\le t\}) \quad \oplus$$

$$= \underbrace{\prod_{t_0<\tau\le t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}}\, e^{-\frac{1}{4D}\int_{t_0}^{t} d\tau\, \dot{x}^2(\tau)}}_{dX_W} \; \underbrace{e^{-\frac{1}{2D\gamma}(U(t)-U(t_0))}}_{2} {}^{+\int_{t_0}^{t}\left[\frac{1}{2\gamma}\frac{\partial^2 U(x)}{\partial x^2} - \underbrace{\frac{1}{4D\gamma^2}\left(\frac{\partial U(x)}{\partial x}\right)^2}_{1}\right]_{x=x(\tau)} d\tau}$$

$$= dX_W(\tau)\, e^{-\frac{\beta}{2}[U(x(t))-U(x(t_0))]}\, e^{-\int_{t_0}^{t} d\tau\, V(x(\tau))} \quad \text{with } V = -\frac{U''}{2\gamma} + \frac{U'^2}{4D\gamma^2}$$

$\boxed{\text{Ex}}$ We want to compute the propagator $W(x,t|x_0,t_0)$: average of the path integral with the dirac delta that fixes the final point x

$$W(x,t|x_0,t_0) = \int d\mathbb{P}(\{x(\tau): 0<\tau\le t\})\, \delta(x(t)-x)$$

where $x(\tau)$ is such that $x(0)=x_0$

Let's use $\oplus$: $d\mathbb{P}(\{x(\tau): 0<\tau\le t\})$

$$= e^{-\frac{1}{2D\gamma}[U(x(t))-U(x(0))]}\, e^{-\int_{t_0}^{t} d\tau\, V(x(\tau))}\, dX_W \quad \text{and } \frac{1}{D\gamma} = \beta$$

$$\Rightarrow W(x,t|x_0,t_0) = e^{-\frac{\beta}{2}[U(x)-U(x_0)]} \underbrace{\left\langle e^{-\int_{t_0}^{t} V(x(\tau))d\tau}\, \delta(x(t)-x)\right\rangle_W}_{\text{we have computed it in the previous lessons!}}$$

Ex Harmonic oscillator: Ornstein-Uhlenbeck process

In this case: $U(x) = \frac{m\omega^2}{2}x^2 \qquad U'(x) = \omega^2 m x \qquad U''(x) = m\omega^2$

$$\Rightarrow V(x) = -\frac{k}{2} + \frac{k^2}{4D}x^2 \quad \text{where } k = \frac{m}{\gamma}\omega^2$$

We have:

$$\int_{t_0}^{t} V(x(\tau))\,d\tau = -\frac{k}{2}(t-t_0) + \frac{k^2}{4D}\int_{t_0}^{t} x^2(\tau)\,d\tau$$

$\Rightarrow W(x,t\,|\,0,0) \equiv$ Propagator for the Ornstein-Uhlenbeck process with $t_0=0$, $x_0=0$ and $D=1/4$

$$= e^{-\frac{\beta}{4}\frac{m\omega^2}{2}x^2}\left\langle e^{-\int_0^t d\tau\left(-\frac{k}{2}+\frac{k^2}{4D}x^2(\tau)\right)}\delta(x(t)-x)\right\rangle_W$$

$\frac{\beta m\omega^2}{4} = \frac{m\omega^2}{4D\gamma} \stackrel{!}{=} \frac{k}{4D} = k,\ D=\frac{1}{4}$

$$= e^{-kx^2}\left\{e^{\frac{k}{2}t}\sqrt{\frac{k}{\pi\sinh(kt)}}\,e^{-kx^2\coth(kt)}\right\}$$

$$= \sqrt{\frac{2k}{\pi(1-e^{-2kt})}}\,e^{-2k\frac{x^2}{1-e^{-2kt}}}$$

$$\text{where } \left\langle e^{-\frac{k^2}{4D}\int_0^t x^2(\tau)\,d\tau}\delta(x(t)-x)\right\rangle_W = \sqrt{\frac{k}{\pi\sinh(kt)}}\,e^{-kx^2\coth(kt)}$$

[See Wiener integral's section with $P(\tau)=k^2$ and $D=1/4$!]

In all this cases we have chosen V such that it's not explicitly dependent on time, but this is not the general case! In general could depend on time: so we get $V(x(\tau),\tau)$.

We can introduce the **BLOCH FUNCTION**:

$$W_B(x,t\,|\,x_0,t_0) = \left\langle e^{-\int_{t_0}^{t} V(x(\tau),\tau)\,d\tau}\,\delta(x(t)-x)\right\rangle_W$$

where $\langle \cdot \rangle = \int \cdot \, dX_W$ and $x(t_0) = 0$

→ The Bloch function it's <u>not</u> a propagator because it's integral over x it's not necessarily one (W_B it's not normalized !).
In fact:

$$\int dx \, W_B(x,t|x_0,t_0) = \left\langle e^{-\int_{t_0}^{t} V(x(\tau),\tau)\, d\tau} \right\rangle_W \neq 1 \,!$$

Moreover it satisfy the <u>BLOCH EQUATION</u>:

$$\boxed{\frac{\partial}{\partial t} W_B(x,t|x_0,t_0) = D\,\partial_x^2 W_B(x,t|x_0,t_0) - V(x,t)\, W_B(x,t|x_0,t_0)}$$

→ It looks like a Schrodinger equation of a free particle on a potential $V(x,t)$ where in quantum mecanics we have:

$$D_{QM} = -\frac{i\hbar}{2m} \quad \text{and} \quad V_{QM} = \frac{i}{\hbar} V$$

→ Perfect analogy between the Schrodinger equation and the Langevin equation with a force derived from a potential: the solution of the Sch. eq. can be mapped to the solutions of the FP equation !

$\psi \to W_B \quad i\hbar\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} \quad -\frac{\hbar^2}{2m} \to D$

$i\hbar \frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2 \partial_x^2}{2m} + V\right)\psi$

From Schrodinger to Bloch equation

Path Integrals for the general d-DIM FP equation

Now we would like to extend what we have seen on the previous lecture, extending it in the more general d-dimensional case: in particular we want to derive the concept of measure in the space of the d-DIM stochastic trajectories subjected to an external force (See pag. 39 ~ d-DIM Langevin eq. and pag. 46 and so on for the derivation).

From pag. 49 we know that the d-Dim Langevin equation (Trajectory in dimension d):

$$dx^\alpha(t) = f^\alpha(x(t),t)\,dt + \sqrt{2D^\alpha(x(t),t)}\;dB^\alpha(t) \quad \text{where } \alpha = 1,2,\dots,d \text{ and } D^\alpha \geq 0$$

Ito prescription!

The discretized version of this expression is (time discretization $i = 1 \cdots N$):

$$\Delta x^\alpha_i = f^\alpha_{i-1}\,\Delta t_i + \sqrt{2D^\alpha_{i-1}}\,\Delta B^\alpha_i .$$

where:

$$\Delta x^\alpha_i = x^\alpha_i - x^\alpha_{i-1} \equiv x^\alpha(t_i) - x^\alpha(t_{i-1}) = \Delta x^\alpha(t_i)$$

$$f^\alpha_{i-1} \equiv f^\alpha(x(t_{i-1}), t_{i-1}) \qquad D^\alpha_{i-1} \equiv D^\alpha(x(t_{i-1}), t_{i-1})$$

$$\Delta B^\alpha_i = B^\alpha_i - B^\alpha_{i-1} \equiv B^\alpha(t_i) - B^\alpha(t_{i-1}) = \Delta B^\alpha(t_i)$$

Now we change variable from $\vec{B}$ to $\vec{x}$, $x^\alpha_i = f^\alpha_{i-1}\Delta t_i + \sqrt{2D^\alpha_{i-1}}\,(B^\alpha_i - B^\alpha_{i-1}) + x^\alpha_{i-1}$

Let's compute the Jacobian of the change of variable:

$$J^{\alpha\beta}_{ij} = \frac{\partial x^\alpha_i}{\partial B^\beta_j} = \begin{cases} 0 & \text{if } j > i \\ \sqrt{2D^\alpha_{i-1}}\,\delta^\alpha_\beta & \text{if } j = i \\ \dfrac{\partial x^\alpha_i}{\partial B^\beta_j} & \text{if } j < i \end{cases}$$

$\Rightarrow J = Nd \times Nd$ matrix is triangular

$$\Rightarrow |J| = \det J \stackrel{!}{=} \prod_{i=1}^{N} \prod_{\alpha=1}^{d} \sqrt{2D^\alpha_{i-1}}$$

Finally we can exploit the multidimensional change of random variable:

$$d\mathbb{P}_{t_1\cdots t_N}(\vec{B}_1\cdots\vec{B}_N|\vec{B}_0,t_0) = \left|\det\left[\frac{\partial(\vec{x}_1\cdots\vec{x}_N)}{\partial(\vec{B}_1\cdots\vec{B}_N)}\right]\right| d\mathbb{P}_{t_1\cdots t_N}(\vec{x}_1\cdots\vec{x}_N|\vec{x}_0,t_0)$$

$$\Rightarrow d\mathbb{P}_{t_1\cdots t_N}(\vec{x}_1\cdots\vec{x}_N|\vec{x}_0,t_0) = \frac{d\mathbb{P}_{t_1\cdots t_N}(\vec{B}_1\cdots\vec{B}_N|\vec{B}_0,t_0)}{|J|}$$

$$\boxed{\Rightarrow d\mathbb{P}_{t_1\cdots t_N}(\vec{x}_1\cdots\vec{x}_N|\vec{x}_0,t_0) = \left[\prod_{i=1}^{N}\prod_{\alpha=1}^{d}\frac{dx_i^\alpha}{\sqrt{4\pi\Delta t_i D_{i-1}^\alpha}}\right] e^{-\sum_{i=1}^{N}\sum_{\alpha=1}^{d}\frac{(\Delta x_i^\alpha - f_{i-1}^\alpha\Delta t_i)^2}{4D_{i-1}^\alpha\Delta t_i}}}$$

(In pag. 38 you can find $d\mathbb{P}_{t_1\cdots t_N}(\vec{B}_1\cdots\vec{B}_N|B_0,t_0)$ expression and furthermore recall that: $\prod_{i=1}^{n}\prod_{j=1}^{m} A_i^j e^{C_i^j} = \prod_{i=1}^{n}\prod_{j=1}^{m} A_i^j e^{\sum_{i=1}^{n}\sum_{j=1}^{m} C_i^j}$)

While in the <u>continuum limit</u>:

$$\boxed{d\mathbb{P}(\{\vec{x}(\tau):0<\tau\leq t\}) = \prod_{\tau=0^+}^{t}\prod_{\alpha=1}^{d}\frac{dx^\alpha(\tau)}{\sqrt{4\pi d\tau D^\alpha(x(\tau),\tau)}}\, e^{-\sum_{\alpha=1}^{d}\int_0^t d\tau\frac{(\dot{x}^\alpha(\tau)-f^\alpha(x(\tau),\tau))^2}{4D^\alpha(x(\tau),\tau)}}}$$

→ The trajectories are constrained at the origin $x(t_0)=x_0$ ($x(0)=x_0$): that's why time starts immediately after t_0 (0) at t_0^+ (0^+)!

Bloch equation & Feynmann-Kac formula

Using the expressions in pag. 49-b and taking the D^{α}'s as constants D and if $\vec{f}(\vec{x}) = -\vec{\nabla}_x U(\vec{x})/\gamma$ we can proceed as in pag. 47-a/47-b and get an expression for the propagator:

$$\underline{W(\vec{x},t|\vec{x}_0,t_0)} = e^{-\frac{\beta}{2}[U(\vec{x})-U(\vec{x}_0)]} \left\langle e^{-\int_{t_0}^{t} V(\vec{x}(\tau))d\tau} \delta^d(\vec{x}(t)-x) \right\rangle_W$$

Thus we are faced with the evaluation of averages with the d-DIM Wiener measure:

$$d^d X_W(\tau) \propto e^{-\int_{t_0}^{t} \dot{\vec{x}}^2(\tau)d\tau} \quad \text{with} \quad \begin{array}{l} \vec{x}(0)=\vec{x}_0 \\ \vec{x}(t)=\vec{x} \end{array}$$

Fixed initial and final point ! (See pag. 49b)

Let's introduce the Bloch function $W_B(\vec{x},t|\vec{x}_0,t_0)$ whose expression is called Feynmann-Kac formula:

$$\boxed{W_B(\vec{x},t|\vec{x}_0,t_0) = \left\langle e^{-\int_{t_0}^{t} V(\vec{x}(\tau))d\tau} \delta^d(\vec{x}(t)-x) \right\rangle_W}$$

$$\Rightarrow W(\vec{x},t|\vec{x}_0,t_0) = e^{-\frac{\beta}{2}[U(\vec{x})-U(\vec{x}_0)]} W_B(\vec{x},t|\vec{x}_0,t_0) \quad \circledast$$

where $V(\vec{x}) = -\frac{1}{2\gamma}\nabla^2 U(\vec{x}) + \frac{1}{4D\gamma^2}\left(\vec{\nabla}U(\vec{x})\right)^2$

We know that $W(\vec{x},t|\vec{x}_0,t_0)$ follow the d-dim FP equation (pag. 39).
In particular $\vec{f} = -\vec{\nabla}U/\gamma$ and $\vec{D} = D\hat{u}_d$ in our d-DIM overdamped Langevin equation case ($\hat{u}_d = (1,1,\cdots,1)$):

$$\dot{W}(\vec{x},t|\vec{x}_0,t_0) = \sum_{\alpha=1}^{d} \partial_\alpha \left[\partial_\alpha U(\vec{x}) \frac{W}{\gamma} + D \partial_\alpha W \right]$$

$$\stackrel{!}{=} \sum_{\alpha=1}^{d} \left[\partial_\alpha^2 U(\vec{x}) \frac{W}{\gamma} + \frac{1}{\gamma} \partial_\alpha U(\vec{x}) \partial_\alpha W + D \partial_\alpha^2 W \right]$$

$$\stackrel{!}{=} \vec{\nabla}_x^2 U(\vec{x}) \frac{W}{\gamma} + \frac{1}{\gamma} \vec{\nabla}_x U(\vec{x}) \cdot \vec{\nabla}_x W + D \vec{\nabla}_x^2 W$$

$$\stackrel{!}{=} \vec{\nabla}_x \cdot \left[\frac{\vec{\nabla}_x U}{\gamma} W + D \vec{\nabla}_x W \right]$$

$$\Rightarrow \dot{W}(\vec{x},t|\vec{x}_0,t) = \vec{\nabla}_x \cdot \left[\frac{\vec{\nabla}_x U(\vec{x})}{\gamma} W(\vec{x},t|\vec{x}_0,t_0) + D \vec{\nabla}_x W(\vec{x},t|\vec{x}_0,t_0) \right]$$

We would like to find an analogous equation for W_B starting from this FP's one and from ⊛ in the previous page : the Bloch equation!

$$\dot{W} = \partial_t \left\{ e^{-\frac{\beta}{2}[U(\vec{x}) - U(\vec{x}_0)]} W_B \right\} = e^{-\frac{\beta}{2}\Delta U} \dot{W}_B$$

LEFT SIDE

where $U(\vec{x}) - U(\vec{x}_0) = \Delta U(\vec{x}) = \Delta U$

RIGHT SIDE

$$\vec{\nabla} \cdot \left[\frac{\vec{\nabla} U}{\gamma} W + D \vec{\nabla} W \right] = \nabla^2 U \frac{W}{\gamma} + \frac{1}{\gamma} \vec{\nabla} U \cdot \vec{\nabla} W + D \nabla^2 W$$

$$\stackrel{!}{=} D \left[\beta \nabla^2 U W + \beta \vec{\nabla} U \cdot \vec{\nabla} W + \nabla^2 W \right] = ⊛$$

$$W = e^{-\frac{\beta}{2}\Delta U} W_B \qquad \vec{\nabla} W = e^{-\frac{\beta}{2}\Delta U} \left[\vec{\nabla} - \frac{\beta}{2} \vec{\nabla} U \right] W_B \qquad \frac{1}{D\gamma} = \beta$$

$$\nabla^2 W = \vec{\nabla}\cdot\vec{\nabla}W = \vec{\nabla}\cdot\left[e^{-\frac{\beta}{2}\Delta U}\vec{\nabla}W_B - \frac{\beta}{2}e^{-\frac{\beta}{2}\Delta U}W_B\vec{\nabla}U\right]$$

$$= \vec{\nabla}\left(e^{-\frac{\beta}{2}\Delta U}\right)\cdot\vec{\nabla}W_B + e^{-\frac{\beta}{2}\Delta U}\nabla^2 W_B - \vec{\nabla}\left(\frac{\beta}{2}e^{-\frac{\beta}{2}\Delta U}W_B\right)\cdot\vec{\nabla}U +$$

$$-\frac{\beta}{2}e^{-\frac{\beta}{2}\Delta U}W_B\nabla^2 U$$

Recall that: $\vec{\nabla}\cdot(\varphi\vec{F}) \overset{!}{=} \vec{\nabla}\varphi\cdot\vec{F} + \varphi(\vec{\nabla}\cdot\vec{F})$

$$= e^{-\frac{\beta}{2}\Delta U}\left[\cancel{-\frac{\beta}{2}\vec{\nabla}U\cdot\vec{\nabla}} + \nabla^2 + \frac{\beta^2}{4}(\vec{\nabla}U)^2 \cancel{-\frac{\beta}{2}\vec{\nabla}U\cdot\vec{\nabla}} - \frac{\beta}{2}\nabla^2 U\right]W_B$$

$$\circledast = D\left[\beta\nabla^2 U\left(e^{-\frac{\beta}{2}\nabla U}W_B\right) + \beta\vec{\nabla}U\cdot\left[e^{-\frac{\beta}{2}\Delta U}\left(\vec{\nabla}-\frac{\beta}{2}\vec{\nabla}U\right)W_B\right] + \dots\right]$$

$$= De^{-\frac{\beta}{2}\nabla U}\left[\beta\nabla^2 U + \cancel{\beta\vec{\nabla}U\cdot\vec{\nabla}} - \frac{\beta^2}{2}(\vec{\nabla}U)^2 + \dots\right]W_B$$

$$= De^{-\frac{\beta}{2}\nabla U}\left[\nabla^2 - \frac{\beta^2}{4}(\vec{\nabla}U)^2 + \frac{\beta}{2}\nabla^2 U\right]W_B \qquad \left(D\beta : \frac{(D\beta)^2}{D} = \frac{1}{D\gamma^2}\right)$$

$$\Rightarrow \cancel{e^{-\frac{\beta}{2}\Delta U}}\dot{W}_B = \cancel{e^{-\frac{\beta}{2}\Delta U}}\left[D\nabla^2 - \frac{(\vec{\nabla}U)^2}{4D\gamma^2} + \frac{1}{2\gamma}\nabla^2 U\right]W_B$$

$\Rightarrow$ Bloch equation

$$\boxed{\dot{W}_B(\vec{x},t|x_0,t_0) = D\nabla_x^2 W_B(\vec{x},t|\vec{x}_0,t_0) - V(\vec{x})W_B(\vec{x},t|\vec{x}_0,t_0)}$$

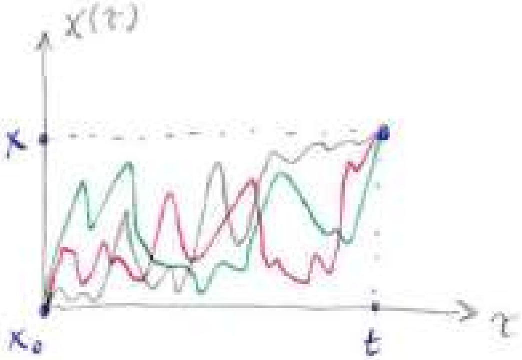
where $V(\vec{x}) = \dfrac{(\vec{\nabla}U(\vec{x}))^2}{4D\gamma^2} - \dfrac{1}{2\gamma}\nabla^2 U(\vec{x})$

Since $W(\vec{x},t_0|\vec{x}_0,t_0) = \delta^d(\vec{x}-\vec{x}_0)$ it implies that the i.c. for W_B is also $W_B(\vec{x},t_0|\vec{x}_0,t_0) = \delta^d(\vec{x}-\vec{x}_0)$: this derives from $\circledast$ and the FK formula when $\begin{matrix} t = t_0 \\ x(t) = x_0 \end{matrix}$!

⇝ The Bloch function W_B is the solution of the Bloch equation but can also be expressed using the Feynman-Kac formula!

⇝ More in general V potential could depend also explicitly on time: $V(\vec{x},t)$!

What is the meaning of the Bloch eq. and of the Feynman Kac formula?
Notice that in the Bloch equation $\vec{x}$ and time τ are independent variables, while in the FK formula we are averaging over trajectories according to the Wiener measure.



Let's see what's going on: we generate (sample) N trajectories according to the Wiener measure ($d=1$ in our figure) or equivalently using:

$$dx(\tau) = \sqrt{2D}\, dB(\tau) \text{ with } dB(\tau) = \mathcal{N}(0, d\tau)$$

So then we have that:

$$\left\langle e^{-\int_{t_0}^{t} d\tau\, V(x(\tau))} \delta(x(t)-x) \right\rangle_W = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} e^{-\int_{t_0}^{t} d\tau\, V(x_i(\tau))}$$

where $\{x_i(\tau)\}_{i=1..N}$ are the sampled trajectories

Using the path integral formulation one can show a similar Bloch equation with all the derivative respect to the initial condition: the **Backward Bloch equation**:

$$\boxed{\partial_{t_0} W_B(\vec{x},t|\vec{x}_0,t_0) = -\left[D\nabla^2_{\vec{x}_0} - V(\vec{x}_0,t_0)\right] W_B(\vec{x},t|\vec{x}_0,t_0)}$$

$\rightsquigarrow$ The usual Bloch eq. it's the Forward Bloch equation: it concerns times that are successive to t_0!
whereas the Backward one regards the previous time!

If V is indipendent of time t explicitly, then due to time translational invariance we have:

$$W_B(\vec{x},t|\vec{x}_0,t_0) = W_B(\vec{x},t-t_0|\vec{x}_0,0)$$

If we derive both sides by t_0 we get:

$$\partial_{t_0} W_B(\vec{x},t|\vec{x}_0,t_0) = \partial_{t_0} W_B(\vec{x},t-t_0|\vec{x}_0,0) = \frac{\partial(t-t_0)}{\partial t_0}\frac{\partial W_B(\vec{x},t-t_0|\vec{x}_0,0)}{\partial(t-t_0)}$$

$$= -\frac{\partial W_B(\vec{x},t-t_0|\vec{x}_0,0)}{\partial(t-t_0)} \stackrel{\bullet}{=} -\frac{\partial W_B(\vec{x},t|\vec{x}_0,t_0)}{\partial t} \quad \text{where } \begin{array}{l} t-t_0 \to t \\ 0 \to 0+t_0 \\ t \to t+t_0 \end{array} \bullet$$

or in the same way: $\partial_t W_B(\vec{x},t|\vec{x}_0,t_0) = \dots = -\partial_{t-t_0} W_B(\vec{x},t-t_0|\vec{x}_0,0) = -\partial_{t-t_0} W_B(\vec{x},t|\vec{x}_0,t_0)$

$$\stackrel{\bullet}{=} -\partial_t W_B(\vec{x},t+t_0|\vec{x}_0,2t_0) = -\partial_t W_B(\vec{x},t-t_0|\vec{x}_0,0)$$

$$\Rightarrow \partial_{t_0} W_B(\vec{x},t|\vec{x}_0,t_0) = -\partial_t W_B(\vec{x},t-t_0|\vec{x}_0,0) = -\partial_t W_B(\vec{x},t|\vec{x}_0,t_0)$$

$\Rightarrow$ The Backward Bloch equation can be rewritten as:

$$\partial_t W_B(\vec{x},t|\vec{x}_0,t_0) = \left[D\nabla^2_{x_0} - \underbrace{V(\vec{x}_0)}_{\text{Time independence!}} \right] W_B(\vec{x},t|\vec{x}_0,t_0)$$

Path Integrals & Quantum Mechanics

We've already seen that the Bloch eq., up to some adjustment, resembles the Schrodinger equation. Furthermore the Bloch equation is related to the FP's one ($W_B \leftrightarrow W$ propagator), so at this point we will indeed apply some techniques to formulate QM in terms of path integrals. This will led us to Feynman path integrals!

In quantum mechanics we deal with wave functions $\psi(\vec{x},t)$ such that:

$|\psi(\vec{x},t)|^2 d^dx =$ Probability to find the particle in d^dx around $\vec{x}$

$\int_D |\psi(\vec{x},t)|^2 d^dx =$ Probability to find the particle in the domain D

$\rightsquigarrow$ In QM we deal with probability amplitudes ψ (probability $|\psi|^2$) while in stochastic processes the propagator W it's already a probability!

In non relativistic QM the wave function obey to the Schrodinger equation:

$$i\hbar\, \partial_t \psi(\vec{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\,\psi(\vec{x},t)$$

$\rightsquigarrow$ $V(\vec{x})$ is the potential where the quantum particle lives, while for the Bloch eq. (or FP equa.) the particle lives in the $U(\vec{x})$ potential that is connected through $V(\vec{x})$ using the expression at pag. 51!

Divide by $i\hbar$: $\partial_t \psi(\vec{x},t) = -\frac{\hbar}{2mi}\nabla^2\psi(\vec{x},t) + \frac{V(\vec{x})}{i\hbar}\psi(\vec{x},t)$

We get: $\partial_t \Psi(\vec{x},t) = \left[\frac{i\hbar}{2m}\nabla^2 + \frac{V(\vec{x})}{i\hbar} \right] \Psi(\vec{x},t)$

$$= \left[D_{QM}\nabla^2 - V_{QM}(\vec{x}) \right] \Psi(\vec{x},t)$$

$\Rightarrow$ We can retrieve the Bloch equation from this Schrodinger's one the right substitutions:

$$W_B(\vec{x},t|\vec{x}_0,t_0) \leftrightarrow \Psi(\vec{x},t) \qquad D \leftrightarrow \frac{i\hbar}{2m} = D_{QM} \qquad V \leftrightarrow \frac{iV}{\hbar} = V_{QM}$$

$\boxed{\text{Free particle}}$

$V(\vec{x}) = 0 = V_{QM}(\vec{x})$ so the Schrodinger equation becomes:

Θ $\partial_t \Psi(\vec{x},t) = \frac{i\hbar}{2m}\nabla^2\Psi(\vec{x},t)$ with i.c. $\Psi(\vec{x},t_0) = \Psi_0(\vec{x})$, for example we can take $\Psi_0(\vec{x}) = \langle \vec{x}|\vec{x}_0\rangle = \delta^d(\vec{x}-\vec{x}_0)$

This equation resembles the diffusion equation with $\Psi \to W_B$, $D_{QM} \to D$:

$\partial_t W(\vec{x},t|\vec{x}_0,t_0) = D\nabla^2 W(\vec{x},t|\vec{x}_0,t_0)$?

which has the solution in d-DIM:

$$W(\vec{x},t|\vec{x}_0,t_0) = \frac{e^{-\frac{(\vec{x}-\vec{x}_0)^2}{4D(t-t_0)}}}{\left(4\pi D(t-t_0)\right)^{d/2}}$$

In this case the FP eq. it's a particular case of Bloch equation: the two coincides for the free diffusion! In facts from $*$ at pag. 50 we know that $U=0$ and so then $W = W_B$!

Let's introduce the propagator $K(\vec{x},t|\vec{x}_0,t_0)$ for the free particle in QM: in particular $\Psi(\vec{x},t) = \int K(\vec{x},t|\vec{x}_0,t_0)\Psi_0(\vec{x}_0)\,d^d x_0$ satisfies the previous Schrodin. equation with the previous initial condition $\Psi_0(\vec{x}) = \delta^d(\vec{x}-\vec{x}_0)$ Θ if the propagator K satisfies the same Schrodinger equation with the initial condition $K(\vec{x},t_0|\vec{x}_0,t_0) = \delta^d(\vec{x}-\vec{x}_0)$!

In fact: $\psi(xt) = \int k(xt|x_0t_0)\psi(x_0t_0)dx_0$

Let's derive respect to t: $\partial_t\psi(xt) = \partial_t \int k(xt|x_0t_0)\psi(x_0t_0)dx_0$

$$\frac{i\hbar}{2m}\nabla^2\psi(xt) = \frac{i\hbar}{2m}\nabla^2\int k(xt|x_0t_0)\psi(x_0t_0)dx_0$$

$$\Rightarrow \int \partial_t k(xt|x_0t_0)\psi(x_0t_0)dx_0 = \int \frac{i\hbar}{2m}\nabla^2 k(xt|x_0t_0)\psi(x_0t_0)dx_0$$

$$\Rightarrow \partial_t k(xt|x_0t_0) = \frac{i\hbar}{2m}\nabla^2 k(xt|x_0t_0)$$

while for the initial condition $k(xt_0|x_0t_0)$:

$$\psi(xt_0) = \int k(xt_0|x_0t_0)\psi(x_0t_0)dx_0$$

$$= \psi(xt_0) \quad \Leftrightarrow \quad k(xt_0|x_0t_0) = \delta(x-x_0)$$

□

The solution of the Schrodinger eq. for the free propagator $K(\vec{x}t|\vec{x}_0t_0)$ it's the same for the diffusion equation $W(\vec{x}t|\vec{x}_0t_0)$ with the right substitutions:

$$K(\vec{x}t|\vec{x}_0t_0) = W(\vec{x}t|\vec{x}_0t_0)|_{D=D_{QM}}$$

$$= \frac{e^{-\frac{(\vec{x}-\vec{x}_0)^2}{4D_{QM}(t-t_0)}}}{(4\pi D_{QM}(t-t_0))^{d/2}} = \left[\frac{m}{i\hbar(t-t_0)}\right]^{\frac{d}{2}} e^{im\frac{(\vec{x}-\vec{x}_0)^2}{2\hbar(t-t_0)}} \;!$$

Notice that:

$$\int W(\vec{x}t|\vec{x}_0t_0)\,d^d\vec{x} = 1$$

$$\underbrace{\int |K(\vec{x}t|\vec{x}_0t_0)|^2 d^d\vec{x}}_{\text{Prob. density}} = \left[\frac{m}{\hbar(t-t_0)}\right]^{d}\int_{\mathbb{R}^d} d^dx = +\infty$$

So we get that the probability diverges and so that $K(\vec{x}t|\vec{x}_0t_0)$ is not normalizable! We expect this because the prob. is conserved and the I.C. it's a Dirac delta $\delta^d(\vec{x}-\vec{x}_0)$ so then:

$$\int |K(\vec{x}t_0|\vec{x}_0t_0)|^2 dx \overset{!}{=} \int \delta^d(\vec{x}-\vec{x}_0)\delta^d(\vec{x}-\vec{x}_0)dx \overset{!}{=} \delta^d(\vec{x}_0-\vec{x}_0) = +\infty \;!$$

Path integral for the free particle

We know that the propagator for the pure diffusion process can be written also exploiting the Wiener measure (recall that the trajectories starts at $\vec{x}(t_0)=\vec{x}_0$):

$$W(\vec{x}t|\vec{x}_0t_0)=\int\prod_{\tau=t_0^+}^{t}\frac{d^d\vec{x}(\tau)}{(4\pi D d\tau)^{d/2}}\,e^{-\frac{1}{4D}\int_{t_0}^{t}\dot{\vec{x}}^2(\tau)d\tau}\,\delta^d(\vec{x}-\vec{x}(t))$$

$$=\int d^dX_W(\tau)\,\delta^d(\vec{x}-\vec{x}_0)="\lim_{N\to\infty}"\int\prod_{j=1}^{N}\prod_{\alpha=1}^{d}\frac{dx_j^\alpha}{\sqrt{4\pi D\Delta t_j}}\,e^{-\frac{1}{4D}\sum_{j=1}^{N}\sum_{\alpha=1}^{d}\frac{(x_j^\alpha-x_{j-1}^\alpha)^2}{\Delta t_j}}\,\delta^d(\vec{x}-\vec{x}_N)$$

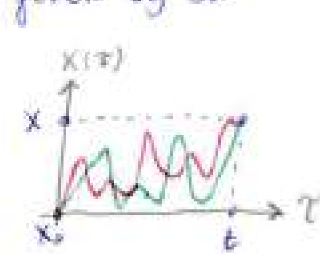
We can get the same result for $K(\vec{x}t|\vec{x}_0t_0)$ with the right substitutions $D\to D_{QM}$:

$$K(\vec{x}t|\vec{x}_0t_0)=\int\prod_{\tau=t_0^+}^{t}\left(\frac{m}{i\hbar d\tau}\right)^{\frac{d}{2}}d^d\vec{x}(\tau)\,e^{\underbrace{\frac{i}{\hbar}\int_{t_0}^{t}\frac{m}{2}\dot{\vec{x}}^2(\tau)d\tau}_{\boxtimes}}\,\delta^d(\vec{x}-\vec{x}(t))$$

$$=\int\underbrace{d^dX_F(\tau)}_{\text{Feynmann "measure"!}}\,\delta^d(\vec{x}-\vec{x}_0)="\lim_{N\to\infty}"\int\prod_{j=1}^{N}\prod_{\alpha=1}^{d}\left(\frac{m}{i\hbar\Delta t_j}\right)^{\frac{d}{2}}dx_j^\alpha\,e^{\frac{i}{\hbar}\sum_{j=1}^{N}\sum_{\alpha=1}^{d}\frac{m}{2}\frac{(x_j^\alpha-x_{j-1}^\alpha)^2}{\Delta t_j}}\,\delta^d(\vec{x}-\vec{x}_N)$$

- Notice that in $\boxtimes$ we have the Lagrangian $\mathcal{L}(x,\dot{x})=\frac{m}{2}\dot{\vec{x}}(\tau)=T(x,\dot{x})$, that in this case coincide with the kinetic energy! In particular $S(t|x_0t_0)=S(\{x(\tau)\})=\int\mathcal{L}(x,\dot{x})d\tau$ is the action!

- So in QM the propagator $K(\vec{x}t|\vec{x}_0t_0)$, that can be used to find a solution of the Schrodinger equation given an initial condition, is given by an average over $x(\tau)$ trajectories with a complex weight that is $e^{\frac{i}{\hbar}S(\{x(\tau)\}_{\tau=t_0^+}^{t})}$ with a fixed $\vec{x}(t_0)=\vec{x}_0$ i.c.!



- That's what Feynmann has done: reformulating QM in terms of this new path integral! Nevertheless this is not a proper measure, well defined like the Wiener's one, and Feynmann path integrals are not a well defined objects: they can also depend on the assumed discretization!

→ Wiener measure: the argument of the path integral has a well defined meaning and that's the probability of a given trajectory

Feynman measure: the argument of the path integral has not a well defined meaning and we can't talk about probability because we are dealing with prob. amplitudes

---

$\boxed{\text{General case } V \neq 0}$

In this case the Schrodinger equation is:

$$\partial_t \Psi(\vec{x}t) = \left[\frac{i\hbar}{2m} \nabla^2 + \frac{V(\vec{x})}{i\hbar} \right] \Psi(\vec{x}t) \quad \text{where } D_{QM} = \frac{i\hbar}{2m}, \; V_{QM} = \frac{V(\vec{x})}{\hbar} i$$

Recall that is equivalent to the Bloch eq. with the right substitutions so we can easily follow the same steps of the free particle case (indeed the i.c. for $k(\vec{x}t|\vec{x}_0t_0)$ is a Dirac delta):

$$W_B(\vec{x}t|\vec{x}_0t_0) = \left\langle e^{-\int_{t_0}^t V(\vec{x}(\tau))d\tau} \delta^d(\vec{x} - \vec{x}(t)) \right\rangle_W$$

$$= \int \prod_{\tau=t_0^+}^{t} \frac{d^d\vec{x}(\tau)}{(4\pi D d\tau)^{d/2}} e^{-\frac{1}{4D}\int_{t_0}^t \dot{\vec{x}}^2(\tau)d\tau - \int_{t_0}^t V(\vec{x}(\tau))d\tau}$$

$$K(\vec{x}t|\vec{x}_0t_0) = W_B(\vec{x}t|\vec{x}_0t_0)\Big|_{V=V_{QM},\, D=D_{QM}}$$

$$= \int \prod_{\tau=t_0^+}^{t} \left(\frac{m}{i h d\tau}\right)^{\frac{d}{2}} d^d\vec{x}(\tau)\, e^{\frac{i}{\hbar}\int_{t_0}^t \frac{m}{2}\dot{\vec{x}}(\tau)d\tau - \frac{i}{\hbar}\int_{t_0}^t V(\vec{x}(\tau))d\tau}$$

$$= \int \prod_{\tau=t_0^+}^{t} \left(\frac{m}{i h d\tau}\right)^{\frac{d}{2}} d^d\vec{x}(\tau)\, e^{\frac{i}{\hbar}\int_{t_0}^t \left[\frac{m}{2}\dot{\vec{x}}(\tau) - V(\vec{x}(\tau))\right]d\tau}$$

where the lagrangian: $\mathcal{L}(x,\dot{x}) = \frac{m}{2}\dot{\vec{x}}(\tau) - V(\vec{x}(\tau))$

and the action: $S(\{\vec{x}(\tau)\}) = \int_{t_0}^t \mathcal{L}(x,\dot{x})d\tau$

→ What Feynman has done is to avoid the use of operators and map the QM problem in the classical problem, that enters in the calculation of the wave function through the complex weight of the exponential of the classical action $S(\{x(\tau)\})$!

→ That's counter-intuitive: it's not like the classical deterministic mechanics where we minimize the action and we get the Newton dynamics of $x(\tau)$, in this case all $x(\tau)$ contribute to the wave function acting as a weight in the integral through the corresponding action $S(\{x(\tau)\})$! Also the classical trajectory contributes, but that's not the only!

$\boxed{\text{Harmonic Oscillator: special case}}$

Let's apply what we've just seen in the case of the harmonic oscillator. The QM harmonic potential is (1DIM):

$$V(x) = \frac{m}{2}\omega^2 x^2 \rightsquigarrow V_{QM}(x) = \frac{i}{\hbar}\frac{m}{2}\omega^2 x^2 = k_{QM}^2 x^2 \quad \text{with } k_{QM}^2 = \frac{i}{\hbar}\frac{m\omega^2}{2}$$

We can compute the Bloch function using the Feynman-Kac formula:

$$W_B(x\,t|0,0) = \left\langle e^{-\int_0^t k^2 x^2(\tau)\,d\tau}\,\delta(x(t)-x)\right\rangle_W \quad \text{with } \begin{matrix} x_0 = x(t_0) = 0 \\ t_0 = 0 \end{matrix}$$

$$k^2 = \frac{m}{2}\omega^2$$

$$= \left[\frac{k^2}{2\pi\sqrt{Dk^2}\,\mathrm{sh}(2\sqrt{Dk^2}\,t)}\right]^{\frac{1}{2}} e^{-\frac{k^2x^2}{2\sqrt{k^2D}}\coth(2\sqrt{Dk^2}\,t)} \qquad (?)$$

We want to compute the propagator $K(x,t|0,0)$ using the suitable substitutions $D\to D_{QM}$, $V\to V_{QM}$, $k\to k_{QM}$:

$$2\sqrt{k^2D} \to 2\sqrt{k_{QM}^2 D_{QM}} = 2\sqrt{\frac{im\omega^2}{2\hbar}\frac{\hbar i}{2m}} = \sqrt{-\omega^2} = \pm i\omega$$

$$2\sqrt{k^2D}\,\mathrm{sh}(2\sqrt{Dk^2}\,t) \to \pm i\omega\,\mathrm{sh}(\pm i\omega t) = i\omega\,\mathrm{sh}(i\omega t) \quad \mathrm{sh} \text{ is odd!}$$

$$= -\omega\,\mathrm{sen}(\omega t)$$

$$\mathrm{ch}(2\sqrt{k^2 D}\, t) \to \mathrm{ch}(\pm i\omega t) = \mathrm{ch}(i\omega t) \quad \text{ch is even!}$$
$$= \cos(\omega t)$$

$$\mathrm{coth}(2\sqrt{k^2 D}\, t) = \frac{\mathrm{ch}(\cdots)}{\mathrm{sh}(\cdots)} \to -\frac{1}{\omega}\frac{\cos(\omega t)}{\sin(\omega t)} = -\frac{1}{\omega}\cot g(\omega t)$$

$$\Rightarrow K(\vec{x},t|0,0) = W_B(\vec{x},t|0,0)\Big|_{D=D_{an},\, K=K_{an}}$$

$$= \sqrt{\frac{m\omega}{i\hbar \sin(\omega t)}}\; e^{i\frac{m\omega}{2\hbar}\cot g(\omega t)\, x^2}$$

For $t_0 \neq 0$ we just exploit the time translational invariance of the propagator:

$$K(x,t|x_0,t_0) = K(x,t-t_0|x_0,0)$$

$\rightsquigarrow$ We just have to substitute $t \to t-t_0$ in the $K(\vec{x}t|0,0)$ expression to get a solution $K(\vec{x}t|0,t_0)$ for $t_0 \neq 0$!

Instead if we want to get the propagator for $x_0 \neq 0$, that is $K(\vec{x}t|x_0t_0)$, we have to change strategy exploiting the following trick.

From the Ornstein-Uhlenbeck process section (pag. 35) we found that the solution of the FP equation for this process has the form (see pag. 37b for the complete expression):

$$W(x,t|x_0,t_0) = \frac{1}{\sqrt{2\pi}\,\sigma(t)}\, e^{-\frac{(x-\bar{x}(t))^2}{2\sigma^2(t)}}$$

and indeed from ⊛ at pag. 50 we have:

$$= e^{-\frac{\beta}{2}[U(x)-U(x_0)]}\, W_B(x,t|x_0,t_0) \quad \text{with } U(x) = \frac{m\omega^2}{2}x^2$$

Furthermore: $V = -\frac{1}{2\gamma}\partial_x^2 U + \frac{1}{4D\gamma^2}(\partial_x U)^2$ $\qquad \partial_x^2 U = m\omega^2$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \partial_x U = m\omega^2 x$

$$= -\frac{m\omega^2}{2\gamma} + \frac{1}{4D\gamma^2}(m\omega^2 x)^2$$

$$= -\frac{m\omega^2}{2\gamma} + \frac{m^2\omega^2}{4D\gamma^2}x^2$$

$$\Rightarrow W_B(xt|x_0t_0) = \left\langle e^{-\int_{t_0}^{t} V(x(\tau))d\tau}\,\delta(x(t)-x)\right\rangle_W \quad ✡$$

$$= e^{\frac{m\omega^2}{2\gamma}(t-t_0)}\left\langle e^{-\frac{m^2\omega^2}{4D\gamma^2}\int_{t_0}^{t} x^2(\tau)d\tau}\,\delta(x(t)-x)\right\rangle_W$$

So for the QM case, where we want $K(xt|x_0t_0)$, we can find it through the solution of the FP eq. at pag. 55b exploiting also the previous ✡ expression for the Black function $W_B(xt|x_0t_0)$ using the right usual substitutions $V \to V_{QM}$, $D \to D_{QM}$ and so on.

In this way we find the solution of the quantum armonic oscillator, either $K(xt|x_0t_0)$ and also $\psi(xt)$ if we have the propagator's i.c., in a much easier way than the traditional one, exploiting or the creation/annihilation operators or the Hermite polinomials and their orthonormality proprierties

$\rightsquigarrow$ Some problems are easier in QM formalism, others are easier in stochastic process formalism: it depends! Thanks to this mapping we can work out everything!

Part II
Baiesi's Lectures

4 Anomalous Diffusion

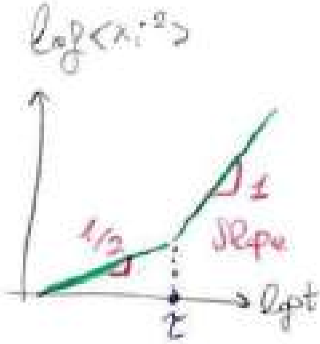
See Manzali-Nicolai's Notes - pag.150 ch7.3 Subdiffusion and superdiffusion

Subdiffusion & Superdiffusion

Subdiffusion: Position of a monomer in a polymer

$$\langle x_i^2(t)\rangle = \begin{cases} \sim t^{1/2} & \text{subdiffusion for short times} \\ \sim t & \text{usual diffusion for long times} \end{cases}$$

In this case the diffusion of the monomer involves memory and the interactions between far away monomers. For short times that's different from the usual fluid behaviour: the monomer has difficulty to diffuse. At longer times, above a certain characteristic time τ given by the length of the polymer chain, we have the usual diffusion and the all configuration (polymer) is diffusing as the single monomer.



Levy flights

$\langle x^2(t)\rangle$ is not even defined and in particular it's not finite. Furthermore the prob. distribution $W(x)$ has no finite variance!

$\boxed{\text{Ex}}$ Cauchy distribution

$$W(x) = \frac{1}{\pi}\,\frac{1}{1+x^2} \qquad \langle x\rangle = \int x\, W(x)\, dx = 0$$

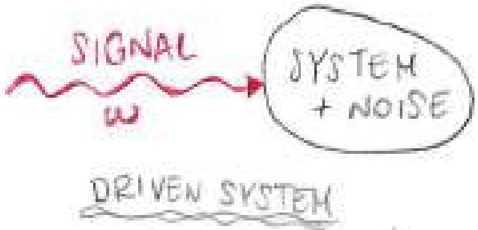
$$\langle x^2\rangle = \sigma^2 = +\infty \rightsquigarrow \text{Not defined}$$

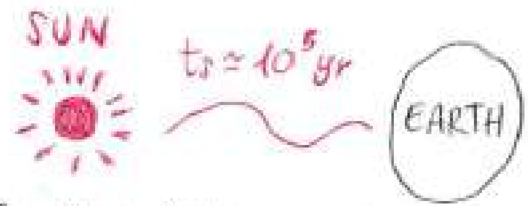
5 Stochastic Resonance

See Manzali-Nicolai's Notes - pag.154 ch8 Stochastic Resonance

Stochastic Resonance

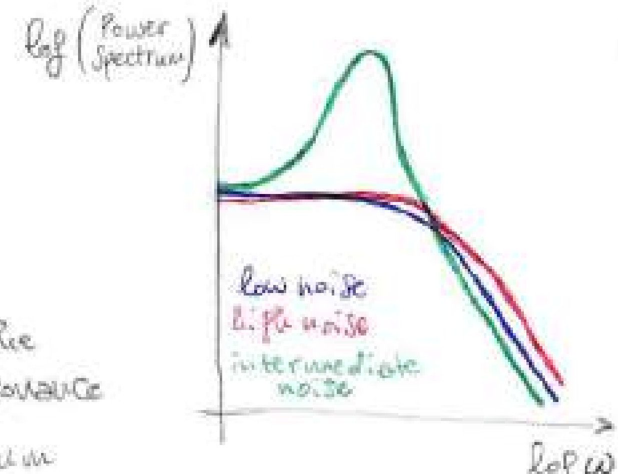
We have a system upon which is acting some noise and so introducing stochasticity. Moreover we have have a signal characterized by a given (angular) frequency ω that is driving the system and comes from the outside.





Sun "drives" the climate of the earth with a signal of period t_S: ice ages on earth have the same periodicity of the sun signal (even if very weak)

Introduced by Benzi, Sutera and Vulpiani in 1981 (also by Parisi in 1982) this process can be also applied to lasers, biology, quantum, climate, magnetic resonance ...



low noise: almost a deterministic system → No resonance in the low noise power spectrum

high noise: Similar to the low noise case

intermediate noise: Right amount of noise in the system that generates the resonance
→ peak in the power spectrum
→ even if the "driving signal" is weak the system can react significantly and generate an output / power spectrum peaked

Power Spectrum: Concept introduced in the space of frequencies ω that measures the amount of signal at every angular frequency

PERTURBED SYSTEM with MODULATION

Modulation $\leftrightarrow$ so we introduce the signal with ω_s frequency that modulates the energy potential

stochastic equation of motion : $\dot{x}(t) = V'(x,t) + \xi(t)$

$\boxed{\text{Hyp.}}$ $\frac{1}{\omega_s} \gg$ Equilibration time within minima } The time of the modulation is much longer than the typical timescale of the system within the minima!

Best moment to jump? When the system sees a barrier which is the at minimum so then:

$$e^{-\frac{2}{k}(\Delta V - V_1)} \iff \sin(\omega_s t) = \mp 1 \quad \text{for } W_{12}, W_{21}$$

$$\iff W_{12}) \;\; \omega_s t = \frac{3}{2}\pi \qquad t = \frac{3}{4} t_s$$

$$W_{21}) \;\; \omega_s t = \frac{\pi}{2} \qquad t = \frac{t_s}{4}$$

In this case the system is barely able to overtake the minimum barrier so then:

$K \sim \Delta V - V_1$ same order

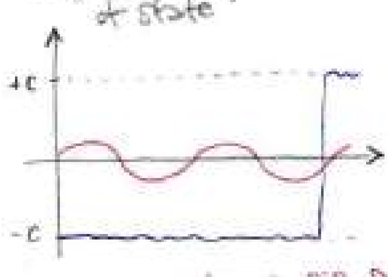
with the assumption $V_1 \ll \Delta V$, but still even a small change could be very effective for a change of state of the system given that we have an exponential dependence!

Moreover we don't want K to be a number close to zero or one but of the right amount which generates the wanted behaviour.

Qualitatively what we expect?

SMALL K NOISE : stuck

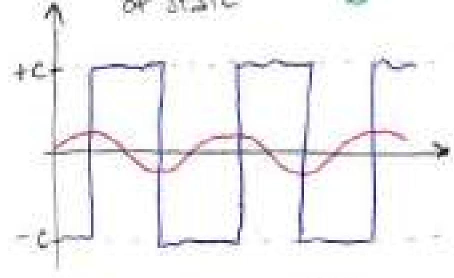
very rare change of state



external signal

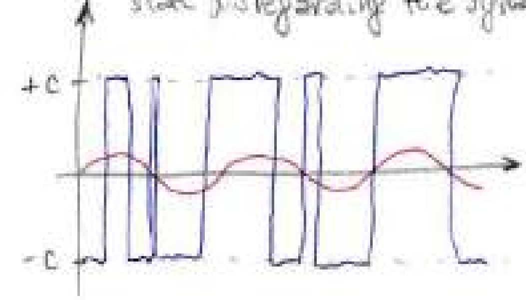
INTERMEDIATE K : in phase

periodic change of state



LARGE K NOISE : random

stochastic change of state disregarding the signal



POWER SPECTRUM $P(\omega) = \lim_{t_{max} \to 0} \frac{1}{2\pi t_{max}} \left| \underbrace{\int_0^{t_{max}} dt\, x(t) e^{-i\omega t}}_{\text{Sort of finite time Fourier transform}} \right|^2$

⇝ $P(\omega)$ will converge to a constant since this is a stochastic system, if it was a deterministic system $P(\omega)$ could diverge

SYSTEM with MODULATION ($\varepsilon \neq 0$) .....

In practise we consider a given sampling which takes place in a given Δt (shorter possible time that we consider) which in turn generates the highest possible frequency ω_{max}. Moreover for our pratical purpose we will consider also a given $\Delta\omega$.

Is there the deterministic ω_s within or not $\Delta\omega$ intervals? We introduce:

$$\underline{\underline{SNR}} = \frac{S_1 + \Delta\omega P^0(\omega_s)}{\Delta\omega P^0(\omega_s)} \simeq \frac{S_1}{\Delta\omega P^0(\omega_s)}$$

⇝ It compares how high it's the peak in ω_s compared to the previous signal $P_0(\omega)$

⇝ The fact we have a t_{max} bring us to a protocol in which we have $\Delta\omega = 2\pi / t_{max}$

Part III
Gradenigo's Lectures

6 Hopfield Model

See Manzali-Nicolai's Notes - pag.176 ch9.4 Hopfield Model (from the deterministic to the "probabilistic" model)

Now we want to add the temperature (possibility of fluctuations and noisy dynamics) to our model: recall that up to now the dynamics of the neurons is deterministic and evolves according to

$$\circledast \quad S_i(t+1) = \mathrm{sgn}\left(\sum_{j=1}^{N} J_{ij} S_j(t)\right) = \mathrm{sgn}(h_i(t))$$

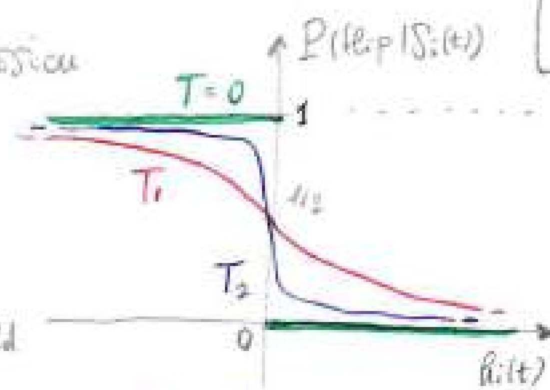
We introduce a noisy dynamics assuming that our previous expression has a probabilistic meaning: given the value of the field $h_i(t)$ on a given neuron i at time t we have a finite probability that the system will follow the previous deterministic behaviour.
The probability to flip the neuron i, given it's value $S_i(t)$ at time t, at a later time is:

$$P(\text{FLIP} \mid S_i(t)) = \frac{1}{1 + e^{2\beta S_i(t) h_i(t)}}$$

$\boxed{\text{Ex}}$

$$P(\text{FLIP} \mid S_i(t) = 1) = \frac{1}{1 + e^{2\beta h_i(t)}} \quad \text{where } \beta = \frac{1}{k_B T}$$

- When $T \to 0$ ($\beta \to \infty$) we recover the $\circledast$ expression and so the deterministic dynamics
- So if at t we have an acting neuron ($=1$) then for later times at temperature T:
  - Active neuron if $h_i(t)$ is positive and $|h_i(t)| \to \infty$ } +1 neuron with positive field
  - Inactive neuron if $h_i(t)$ is negative and $|h_i(t)| \to \infty$ } −1 neuron with negative field



$T_1 > T_2 > T = 0$

If we the probabilities to flip for all the neurons $\forall i = 1 \ldots N$ we can then construct a transition matrix $W(\vec{S}' \mid \vec{S})$ that is the probability to switch from $\vec{S}$ at time t to $\vec{S}'$ at later times ($\vec{S} = \{S_1 \ldots S_N\}$ neurons' configuration)

Thanks to this transition matrix we can write the master equation for the probability $P_t(\vec{S})$ to have a given $\vec{S}$ neurons' configuration at time t:

$$\frac{\partial}{\partial t} P_t(\vec{S}) = \sum_{\{\vec{S}'\}} W(\vec{S}|\vec{S}')\, P_t(\vec{S}')$$

⤳ This ME led to a stationary solution at a given temperature $P^{\beta}_{EQ}(\vec{S})$ which has the form of a Boltzmann distribution:

$$\dot{P}_t(\vec{S}) = 0 \Rightarrow P_t(\vec{S}) \equiv P^{\beta}_{EQ}(\vec{S}) = \frac{e^{-\beta E(\vec{S})}}{Z}$$

$$\text{where } Z = \sum_{\vec{S}} e^{-\beta E[\vec{S}]}$$

$$\text{and } E[\vec{S}] = -\sum_{i<j} J_{ij} S_i S_j$$

(...Energy landscape at low temperature - Pag. 180) Let us compute the partition function:

$$E[\vec{S}] \equiv E = -\sum_{i<j} J_{ij} S_i S_j = -\frac{1}{2}\sum_{i\neq j} J_{ij} S_i S_j$$

Recall that we can shift the energy wrt a constant value: thermodinamic and statistical mechanics properties don't change!

$$E \to E_{NEW} + \text{Const.}$$

$$E_{NEW} = -\frac{1}{2}\sum_{i\neq j} J_{ij} S_i S_j - \frac{N}{2}$$

$$= -\frac{1}{2}\sum_{i\neq j} J_{ij} S_i S_j - \frac{1}{2}\sum_{i=1}^{N} S_i S_i$$

$$= -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij} S_i S_j \quad \text{where } J_{ii} = \frac{1}{N}\sum_{\mu=1}^{p} \xi_i^{\mu}\xi_i^{\mu} = 1 \ (?)$$

$$\Rightarrow Z = \sum_{\vec{S}} e^{-\beta E} = \sum_{\vec{S}} e^{\frac{\beta}{2}\sum_{i,j} J_{ij} S_i S_j} = \mathrm{Tr}\, e^{\frac{\beta}{2}\sum_{ij}\left(\frac{1}{N}\sum_{\mu=1}^{p}\xi_i^{\mu}\xi_j^{\mu}\right) S_i S_j}$$

$$\Rightarrow Z = \mathrm{Tr}\, e^{\frac{\beta}{2N}\sum_\mu \left(\sum_{i=1}^N S_i \xi_i^\mu\right)\left(\sum_{j=1}^N S_j \xi_j^\mu\right)} \stackrel{!}{=} \mathrm{Tr}\, e^{\frac{\beta}{2N}\sum_{\mu=1}^p \left(\sum_{i=1}^N S_i \xi_i^\mu\right)^2}$$

$\left(\sum_{\vec{S}} \equiv \mathrm{Tr}\right.$ Sum over all configurations$\left.\right)$

$$e^{\frac{1}{2N}\left(\sum_{i=1}^N \xi_i^\mu S_i\right)^2} = \int_{\mathbb{R}} dq_\mu\, e^{-\frac{N}{2} q_\mu^2 + q_\mu \sum_{i=1}^N \xi_i^\mu S_i}$$

Hubbard-Stratonovic transformation with $b = \frac{1}{N}$ (pag. 169)

$$e^{\frac{\beta}{2N}\left(\sum_i \xi_i^\mu S_i\right)^2} = \int_{\mathbb{R}} dq_\mu\, e^{-\frac{\beta N}{2} q_\mu^2 + \beta q_\mu \sum_i \xi_i^\mu S_i}$$

$$\boxed{\text{SH transformation (more general)}: \quad e^{\frac{\beta}{2N}x^2} = \int_{\mathbb{R}} e^{-q^2\frac{N\beta}{2} + \beta q x}\, dq}$$

$$Z = \mathrm{Tr} \prod_{\mu=1}^p e^{\frac{\beta}{2N}\left(\sum_i S_i \xi_i^\mu\right)^2} \underset{HS}{=} \mathrm{Tr} \int_{\mathbb{R}} \prod_\mu dq_\mu\, e^{-\frac{\beta N}{2}\sum_{\mu=1}^p q_\mu^2 + \beta \sum_{\mu=1}^p q_\mu \sum_i \xi_i^\mu S_i} \;\square$$

$$\square\; \mathrm{Tr}\, e^{\beta \sum_{\mu=1}^p q_\mu \sum_i \xi_i^\mu S_i} = \sum_{S_1} \cdots \sum_{S_N} e^{\beta \sum_\mu q_\mu (\xi_1^\mu S_1 + \cdots + \xi_N^\mu S_N)}$$

$$= \left[\sum_{S_1} e^{\beta \sum_\mu q_\mu \xi_1^\mu S_1}\right]\left[\cdots\right]\left[\sum_{S_N} e^{\beta \sum_\mu q_\mu \xi_N^\mu S_N}\right] = \prod_{i=1}^N \left[\sum_{S_i} e^{\beta \sum_\mu q_\mu \xi_i^\mu S_i}\right]$$

$$= \prod_{i=1}^N \left[\sum_{S_i = \pm 1} e^{\beta \vec{q}\cdot\vec{\xi}_i S_i}\right] = \prod_{i=1}^N \left(e^{\beta \vec{q}\cdot\vec{\xi}_i} + e^{-\beta \vec{q}\cdot\vec{\xi}_i}\right) \quad \text{where } \sum_{\mu=1}^p q_\mu \xi_i^\mu = \vec{q}\cdot\vec{\xi}_i$$

$$= \prod_{i=1}^N \left[2\cosh(\beta \vec{q}\cdot\vec{\xi}_i)\right] = e^{\ln \prod_i (2\cosh \beta \vec{q}\cdot\vec{\xi}_i)} = e^{\sum_i \ln\left[2\cosh(\beta \vec{q}\cdot\vec{\xi}_i)\right]}$$

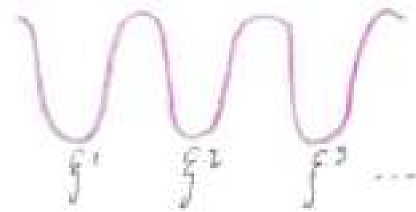
$$\Rightarrow Z = \int_{\mathbb{R}} \prod_\mu dq_\mu\, e^{-\frac{N\beta}{2}\sum_\mu q_\mu^2 + \sum_i \ln\left[2\cosh(\beta \vec{q}\cdot\vec{\xi}_i)\right]}$$

$$\stackrel{!}{=} \int_{\mathbb{R}} \prod_\mu dq_\mu\, e^{-N\beta u(\vec{q})}$$

- So we have removed the spins/neurons dependence from Z: we have replaced the trace over N variables/spins ($N \to \infty$ in the therm. limit) with an integration over P variables q_μ (P stays finite when $N \to \infty$)
- q_μ are more meaningful from a physical point of view: they are the similarities/overlaps between a given configuration of the spins ξ and one of the patterns ξ^μ

$$q_\mu = \frac{1}{N} \sum_{i=1}^{N} \xi_i \xi_i^\mu \quad \text{where } \mu = 1 \dots P$$

- In this way we "forget" about the small details of the spins configuration and we understand better if we are close to one or another of the P patterns ξ^μ / Minima of the free energy stored in memory



- $q_1 \dots q_P$ are the degree of similarity over the P possible patterns $\xi^1 \dots \xi^P$

$$u(\vec{q}) = \frac{1}{2} \sum_{\mu=1}^{P} q_\mu^2 - \frac{1}{\beta N} \sum_{i=1}^{N} \log\left[2\cosh(\beta \vec{q} \cdot \vec{\xi}_i)\right]$$

$$\frac{\partial u(\vec{q})}{\partial q_\nu} = q_\nu - \frac{1}{\beta N} \sum_i \frac{2\sinh(\beta \vec{q} \cdot \vec{\xi}_i)}{2\cosh(\beta \vec{q} \cdot \vec{\xi}_i)} \beta \xi_i^\nu = q_\nu - \frac{1}{N} \sum_{i=1}^{N} \xi_i^\nu \tanh(\beta \vec{q} \cdot \vec{\xi}_i)$$

Stationarity: $\frac{\partial u(\vec{q})}{\partial q_\nu} = 0 \iff q_\nu = \frac{1}{N} \sum_{i=1}^{N} \xi_i^\nu \tanh(\beta \vec{q} \cdot \vec{\xi}_i)$ P equations $\nu = 1 \dots P$

If (assumption) $\vec{q}^* = (0, 0 \dots q_\mu \dots 0)$ then we have: $q_\nu = \frac{1}{N} \sum_{i=1}^{N} \xi_i^\nu \, \text{th}(\beta q_\mu \xi_i^\mu)$

$\Rightarrow q_\nu = \mathbb{E}\left[\text{th}(\beta q_\mu \xi_i^\mu) \xi_i^\nu\right]$ P equations $\nu = 1 \dots P$

empirical average respect to ξ_i^ν

$\Rightarrow$ $\mu \neq \nu$: $q_\nu = 0$ agrees with our assumption

$\mu = \nu$: $q_\nu = \text{th}(\beta q_\nu)$ where $\nu = 1 \dots P$

OVERLAP IN HOPFIELD MODEL ($N \to \infty$)

Along our calculations of the partition function we got, after the HS transformation, that:

$$\mathcal{Z} = \sum_{\vec{S}} \int_{\mathbb{R}} \prod_{\mu=1}^{P} dq_\mu \, e^{-N\beta f(\vec{q}, \xi^1 \cdots \xi^P, \vec{S})} \quad \text{with } f(\vec{q}, \xi^1 \cdots \xi^P, \vec{S}) = \frac{1}{2}\sum_{\mu=1}^{P} q_\mu^2 - \frac{1}{N}\sum_{\mu=1}^{P} q_\mu \sum_{i=1}^{N} \xi_i^\mu S_i$$

⇝ The overlaps q_μ come out as an auxiliary variable in the HS transf.: in disordered systems' calculation this happens all the time, we introduce an auxiliary variable that turns out to have some physical meaning

⇝ We can understand the q_μ meaning at $N \to \infty$ so when we perform a saddle point approx. in $\mathcal{Z}$ above. We want the q_μ that stationarize the function f:

$$\frac{\partial f}{\partial q_\mu} = 0 \quad \Longleftrightarrow \quad q_\mu = \frac{1}{N}\sum_{i=1}^{N} \xi_i^\mu S_i$$ Definition of overlap

---

The overlaps q_μ:

- They're the rate of similarity between a neuron's configuration and a pattern
- They're macroscopic variables which denotes a macroscopic state: for a given pattern ξ^μ there are a lot of microscopic configurations (of the neurons) $\vec{S} = \{S_1 \cdots S_N\}$ that gives the same overlap value q_μ

Statistical mechanics: Which is the probability of a microscopic configuration $\vec{S}$ in the canonical ensemble? Boltzmann factor normalized

$$\frac{e^{-\beta H_J[\vec{S}]}}{\mathcal{Z}_J} \underset{\text{High temperature}}{\sim} \frac{1}{\#\text{ of all possible spins configurations}} = \frac{1}{2^N} \xrightarrow{N \to \infty} 0$$

we're not interested in a specific microscopic configuration but in the macroscopic one (energy, pressure ... overlap q_μ in our case)

That's the reason why we translated our problems to the spins/neurons $\vec{S}$ to the overlaps q_μ: they're more meaningful from the physical purpose we're interested in!

So after our calculations we get that:

$$\mathcal{Z} = \int_{\mathbb{R}} \prod_{\mu=1}^{p} dq_\mu \, e^{-\beta N u(\vec{q})}$$

Saddle point approximation $(N \to \infty)$: The only relevant contribution to $\mathcal{Z}$ comes from the stationary points of $u(\vec{q})$ which have the form

$$= \sum_{s=1}^{p} e^{-\beta N u(\vec{q}_s^*)}$$

Sum over all stationary points

$\vec{q}_1^* = (q^*, 0 \cdots 0)$

$\vdots$

$\vec{q}_\mu^* = (0 \cdots q^* \cdots 0)$

$\vdots$

$\vec{q}_p^* = (0 \cdots 0, q^*)$

p stationary points (minima) for a given fixed temperat.

⇝ If we low temperature the # of minima grows

⇝ We assume also q^* fixed for all

Which is the probability to have a configuration of the neurons which has a given overlap $\vec{q}_\mu^*$ (overlap q^* with one of the pattern ξ^μ)?

$$P = \frac{\text{\# of configuration } \vec{S} \text{ that gives a certain value of the overlap}}{\text{\# of all possible configurations } \vec{S}}$$

$$\frac{e^{-\beta N u(\vec{q}_s^*)}}{\sum_{\mu=1}^{p} e^{-\beta N u(\vec{q}_\mu^*)}} = \frac{1}{p} = P(\vec{q}_s^*)$$

The prob. to have a given overlap with one of the patterns / macroscopic state is finite $1/p$!

$\boxed{\text{N.B.}}$ We have plenty of stationary points / minima of $u(\vec{q})$, which are increasing in number as the temperature decreases.

In particular:

- $T > T_c$: the only minima has the form $\vec{q} = (0 \dots q \dots 0)$ ⇝ Higher tempert. phase
- $T < T_c$: the minima can has the form $\vec{q} = (\underbrace{q, \dots, q, q}_{m \text{ times}}, 0 \dots 0)$

⇝ Low temperature phase

⇝ We start having a finite probability of non-zero overlap with several patterns (not only one!)

7 Sherrington-Kirkpatrick Model

Professors' notes - pag.86 ch7.4 Sherrington-Kirkpatrick (SK) model (check the reference of the formulas)

The Sherrington-Kirkpatrick model can be viewed as a generalization of the Hopfield model (infinite number of patterns):

<u>Hopfield model</u>

$$J_{ij} = \frac{1}{N}\sum_{\mu=1}^{p} \xi_i^\mu \xi_j^\mu \longrightarrow$$

<u>SK model</u>

$$J_{ij} = \frac{1}{N}\sum_{\mu=1}^{N} \xi_i^\mu \xi_j^\mu = \frac{1}{N}\sum_{\mu=1}^{N} \underset{\sim}{C_{ij}^\mu}$$

with $N \to \infty$

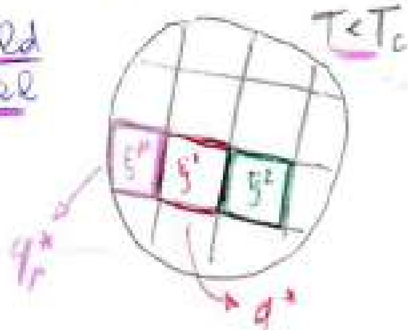
↳ Random variable with a symmetric probability distr. with finite mean and variance

So then the prob. distribution of J_{ij} coincide with a gaussian when $N \to \infty$ due to the central limit theorem!

QUALITATIVE DIFFERECE BETWEEN SK and HOPFIELD MODELS

Instead concerning the phase space of all configurations:

- **Hopfield model**



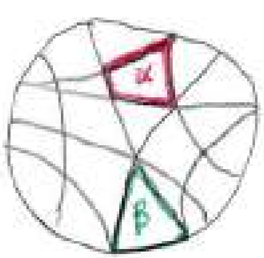
The phase space is composed by a finite number of disjoint components, each one grouping a pool of microscopic configurations of the spins which have a finite overlap q_μ^* with a given pattern ξ^μ

→ We can still organize/distinguish the pool of configurations in groups, each caracterized by a finite overlap with one of the patterns

Recall that the overlaps are embedded in the coupling coefficients through the expression:

$$q_\mu = \frac{1}{N}\sum_{i=1}^{N} \xi_i^\mu S_i$$

- **SP model**



$q_{\alpha\beta}$ ~ matrix order parameter

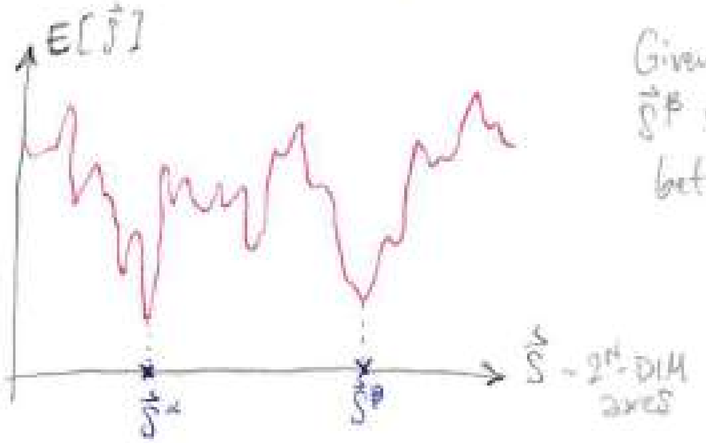
We have so many patterns that we can't keep track of any of them: we loose the capability to retrieve any information to the J_{ij} and so in each piece of the phase space we don't have anymore a reference pattern ξ that tells us that all the configurations inside this piece have a finite overlap with ξ (we loose the possibility to detect the similarity with a given pattern)

The only thingh we can retrieve is the similarity degree between two different configurations: no more patterns with which we can compare our configurations, we can only compare configurations among themselves.

$T > T_c$: $q_{\alpha\beta} = 0$ So every config. is different from the others!

$T < T_c$: $q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^\alpha S_i^\beta \in [0,1]$ Spin glass transition!

Pictorial representation of the energy landscape of our system $E[\vec{S}]$ in terms of a given spin configuration $\vec{S}$.



Given two different spins configurations $\vec{S}^\alpha$ and $\vec{S}^\beta$ we want to know the grade of similarity between the two:

$$q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^\alpha S_i^\beta \equiv \text{Order parameter (it's a matrix)}$$

How to compute the order parameter $q_{\alpha\beta}$? We have to compute the free-energy:

$$F_J = \langle E_J[\vec{S}]\rangle - TS \overset{!}{=} \langle \mathcal{H}_J[\vec{S}]\rangle - TS \implies \text{Minimization of the free-energy}$$

⇝ Notice that as always we can change the temperature (noisyness of the system), but what is the role of the quenched disorder represented by the J_{ij} couplings? If we fix the level of noise / temperature, then how much the behaviour of the system depends on the choice of the random coefficients J_{ij}? Self averaging tell us that the system's behaviour and so its associated macroscopic properties do not depend on the choice of this J_{ij} values in the $N \to \infty$ limit!

The free energy F_J is itself a random variable that depends on the values of the J_{ij} random variable. It's probability distribution can be derived starting from the J_{ij} one:

$$P(F) = \int \prod_{i<j} P(J_{ij})\,\delta(F - F_J)\,dJ_{ij}$$

$$\boxed{\begin{aligned}\mathcal{H}_J[\vec{S}] &= -\sum_{i<j} J_{ij} S_i S_j \\ F_J &= -\frac{1}{\beta}\log Z_J\end{aligned}}$$

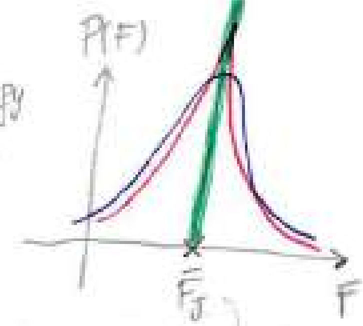
Self averaging can be defined exploiting:

$$\sigma_F = \sqrt{\overline{F_J^2} - (\overline{F_J})^2} \quad \text{with } \overline{F_J} = \int dF\, P(F)\,F \quad \overline{F_J^2} = \int dF\, P(F)\,F^2$$

SELF AVERAGING: $\frac{\sigma_F}{\overline{F}_J} \underset{N\to\infty}{\sim} \frac{1}{\sqrt{N}}$

$N < N \ll N \to \infty$

This tell us that the free energy prob. distr. $P(F)$ becomes more and more piked around a given value, until it becomes a Dirac delta when $N \to \infty$



The most likely value coincide with the mean value of the free energy: that's not true for all the prob. distributions!

$$\Rightarrow \boxed{\lim_{N\to\infty} F_J = \overline{F}_J}$$

where

F_J = free energy for a given realization of the disorder

$\overline{F}_J$ = average value of the free energy over all instances of disorder

Thanks to this considerations we can calculate the minima of the free energy exploiting the free energy averaged over the disorder:

$$\textcircled{} = \lim_{N\to\infty} -\frac{1}{N\beta} \log Z_J = \lim_{N\to\infty} -\frac{1}{N\beta} \overline{\log Z_J} \quad \text{where } F_J = -\frac{1}{\beta}\log Z_J$$

$$\textcircled{} = \int_{\mathbb{R}} \prod_{i<j} dJ_{ij}\, P(J_{ij}) \log\left(\sum_{\{S\}} e^{\beta \sum_{i<j} J_{ij} S_i S_j}\right) \quad \text{and } Z_J = \sum_{\{S\}} e^{-\beta H_J[S]}$$

Impossible to be computed: exploit the replica trick! $\log x = \lim_{n\to 0} \frac{x^n - 1}{n}$

$$\lim_{n\to 0} \frac{x^n-1}{n} = \lim_{n\to 0} \frac{e^{n\ln x} - 1}{n} = \lim_{n\to 0} \frac{\cancel{1} + n\log x + O(n^2) - \cancel{1}}{n}$$

$$= \lim_{n\to 0} \log x + O(n) = \log x$$

$$\textcircled{} = \int_{\mathbb{R}} \prod_{i<j} dJ_{ij}\, P(J_{ij}) \log Z_J = \int_{\mathbb{R}} \prod_{i<j} dJ_{ij}\, P(J_{ij}) \lim_{n\to 0} \frac{Z_J^n - 1}{n}$$

$$= \lim_{n\to 0} \frac{\overline{Z_J^n} - 1}{n}$$

$$\Rightarrow \quad ⓪ = \lim_{N\to\infty}\lim_{n\to 0} -\frac{1}{nN\beta}\left(\overline{Z_J^n}-1\right) \equiv f$$

where
$$\overline{Z_J^n} = \int_{\mathbb{R}} \prod_{i<j} dJ_{ij}\, P(J_{ij})\, Z_J^n = \int_{\mathbb{R}} \prod_{i<j} dJ_{ij}\, P(J_{ij}) \left[\sum_{\{S\}} e^{\beta \sum_{i<j} J_{ij} S_i S_j}\right]^n$$
$$= \int_{\mathbb{R}} \prod_{i<j} dJ_{ij}\, P(J_{ij}) \left[\sum_{\{S^1 \dots S^n\}} e^{\beta \sum_{\alpha=1}^{n} \sum_{i<j} J_{ij} S_i^\alpha S_j^\alpha}\right]$$

and where $P(J_{ij}) = \sqrt{\dfrac{N}{2\pi \delta^2}}\, e^{-\frac{N}{2\delta^2} J_{ij}^2}$

Following the book's missing calculation starting from pag. 88 and so on...

(7.102) $$\int_{\mathbb{R}} dJ_{ij}\, e^{-\frac{N}{2\delta^2} J_{ij}^2 + \beta J_{ij} \sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha}$$
$$\propto e^{\frac{\delta^2}{2N}\beta^2 \left(\sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha\right)^2}$$
$$\propto e^{\frac{\delta^2\beta^2}{2N}\left(\sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha\right)\left(\sum_{\beta=1}^{n} S_i^\beta S_j^\beta\right)}$$

$$\int_{\mathbb{R}} e^{-ax^2+bx}\, dx = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}}$$
where $a = \dfrac{N}{2\delta^2}$ and $b = \beta \sum_\alpha S_i^\alpha S_j^\alpha$

(7.104) $$\sum_{i<j} S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta = \frac{1}{2}\sum_{i\neq j} S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta = \frac{1}{2}\sum_{i\neq j} S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta + \frac{N}{2}$$
$$= \frac{1}{2}\sum_{i\neq j} S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta + \frac{1}{2}\sum_{i=1}^{N} S_i^\alpha S_i^\beta S_i^\alpha S_i^\beta = \frac{1}{2}\sum_{i,j=1}^{N} S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta$$
$$= \frac{1}{2}\left(\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right)\left(\sum_{j=1}^{N} S_j^\alpha S_j^\beta\right) = \frac{1}{2}\left(\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right)^2$$

Recall that a constant shift of the energy doesn't change the system properties

(7.101) + (7.103) + (7.105) + (7.102)
$$\overline{Z_J^n} = \prod_{i<j} \sum_{\{S^1 \dots S^n\}} e^{\frac{\delta^2\beta^2}{2N}\sum_{\alpha,\beta} S_i^\alpha S_j^\alpha S_i^\beta S_j^\beta} = \sum_{\{S^1 \dots S^n\}} e^{\frac{\delta^2\beta^2}{2N}\sum_{\alpha,\beta}\sum_{i<j} S_i^\alpha S_j^\alpha S_i^\beta S_j^\beta}$$
$$= \sum_{\{S^1 \dots S^n\}} e^{\frac{\delta^2\beta^2}{4N}\sum_{\alpha,\beta=1}^{n}\left(\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right)^2} = \sum_{\{S^1 \dots S^n\}} e^{\frac{\delta^2\beta^2}{2N}\left(\frac{nN^2}{2} + \sum_{\alpha<\beta}\left(\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right)^2\right)}$$

$$\overline{Z^n_J} = e^{\frac{nN\beta^2 J^2}{4}} \mathrm{Tr}\left[e^{\frac{\beta^2 J^2}{2N}\sum_{\alpha<\beta}^{n}\left(\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right)^2}\right]$$

Hubbard-Stratonovich transformation
⇝ We introduce the auxiliary variables $q_{\alpha\beta} \equiv$ overlaps

HS considering a single term:

$$e^{\frac{\beta^2 J^2}{2N}\left(\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right)^2} = \int_{\mathbb{R}} dq_{\alpha\beta}\, e^{-\frac{N\beta^2 J^2}{2} q_{\alpha\beta}^2 + \beta^2 J^2 q_{\alpha\beta}\sum_{i=1}^{N} S_i^\alpha S_i^\beta}$$

where we neglected the prefactors which do not matter?

Recall that: $e^{\frac{b}{2}z^2} = \int_{\mathbb{R}} dx\, e^{-\frac{x^2}{2b}+xz}$ where $b = 1/N$, $x = q_{\alpha\beta}$, $z = \sum_i S_i^\alpha S_i^\beta$

$$\Rightarrow \overline{Z^n_J} = e^{\frac{nN\beta^2 J^2}{4}} \sum_{\{S^1 \dots S^n\}} \int_{\mathbb{R}} \prod_{\alpha<\beta} dq_{\alpha\beta}\, e^{-\frac{N\beta^2 J^2}{2}\sum_{\alpha<\beta} q_{\alpha\beta}^2 + \beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta}\sum_{i=1}^{N} S_i^\alpha S_i^\beta} \quad (7.109)$$

⊛

We can write the integrand exponential as: $e^{-\frac{N}{2}u(q_{\alpha\beta}, \vec{S}^1 \dots \vec{S}^n)}$ where $u(\dots) = \beta^2 J^2\left[q_{\alpha\beta}^2 - \frac{2}{N} q_{\alpha\beta}\sum_{i=1}^{N} S_i^\alpha S_i^\beta\right]$

⇝ In order to understand the physical meaning of $q_{\alpha\beta}$ we can exploit the saddle point approx. when $N\to\infty$ and see that the only $q_{\alpha\beta}$s that make sense are the ones for which:

$$\frac{\partial u}{\partial q_{\alpha\beta}} = 0 \quad \forall q_{\alpha\beta} \quad \Rightarrow q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^\alpha S_i^\beta$$

⇒ $q_{\alpha\beta}$ are the overlaps / grade of similarity between two different replica configurations when $N\to\infty$

First sum = $\{S_1^1 = \pm 1, S_2^1 = \pm 1 \dots S_N^n = \pm 1\}$

Second sum = $\{S^1 = \pm 1 \dots S^n = \pm 1\}$

(7.109) and (7.110) ... ⊛

$$\sum_{\{S^1 \dots S^n\}} e^{\beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} \underbrace{\sum_i S_i^\alpha S_i^\beta}_{\text{Diagonal term in spin index } i}} = \sum_{\{S^1 \dots S^n\}} \prod_{i=1}^{N} e^{\beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} S_i^\alpha S_i^\beta} = \prod_{i=1}^{N} \overbrace{\sum_{\{S^1 \dots S^n\}} e^{\beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} S_i^\alpha S_i^\beta}}^{\text{All identical terms}}$$

$$= \left(\sum_{\{S^1 \dots S^n\}} e^{\beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} S^\alpha S^\beta}\right)^N$$

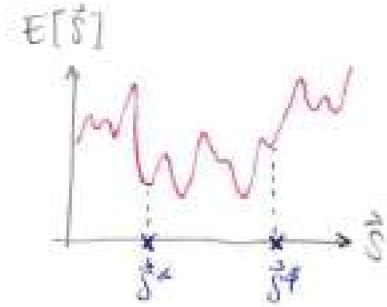
$$\left(\sum_{\{S^1 \dots S^n\}} e^{\beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} S^\alpha S^\beta}\right)^N = \left(\mathrm{Tr}\, e^{L(q_{\alpha\beta})}\right)^N \text{ where } L(q_{\alpha\beta}) = \beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} S^\alpha S^\beta$$

$\Rightarrow \overline{Z^n_J} = (7.111)$ and $A[q_{\alpha\beta}] = (7.112)$

... until free energy calculation (9.115)

REPLICA SYMMETRIC ANSATZ : $q_{\alpha\beta} = \begin{pmatrix} 0 & \ddots & q \\ q & \ddots & 0 \end{pmatrix}$ All the elements outside the diagonal are the same with value q

→ This means that, taking two different configurations of the spins (replicas) $\vec{S}^\alpha$ and $\vec{S}^\beta$, they're different always in the same way!



We want to compute the stationary points of $A[q_{\alpha\beta}]$ in order to apply the saddle point approx. :

$$\frac{\delta A}{\delta q_{\alpha\beta}} = 0 \xrightarrow[\text{Ansatz (RSA)}]{\text{Replica Sym.}} \frac{\delta A}{\delta q} = 0$$

So then : $A[q_{\alpha\beta}] \overset{!}{=} -\frac{\beta^2 J^2}{4} + \frac{\beta^2 J^2}{2n} \sum_{\alpha<\beta} q^2_{\alpha\beta} - \frac{1}{n} \log\left[\mathrm{Tr}\, e^{L(q_{\alpha\beta})}\right]$

$$\overset{RSA}{\underset{!}{=}} -\frac{\beta^2 J^2}{4} + \underbrace{\frac{\beta^2 J^2}{2n} \frac{n(n-1)}{2} q^2}_{\text{energetic term}} + \text{entropic term}$$

$$\text{entropic term} = -\frac{1}{n} \log\left(\mathrm{Tr}\, e^{L(q_{\alpha\beta})}\right) = -\frac{1}{n} \log\left(\mathrm{Tr}\, e^{\beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} S^\alpha S^\beta}\right)$$

$$\overset{!}{=} -\frac{1}{n} \log\left(\mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2} \sum_{\alpha\neq\beta} q_{\alpha\beta} S^\alpha S^\beta}\right) \overset{RSA}{=} -\frac{1}{n} \log\left(\mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2} q \sum_{\alpha\neq\beta} S^\alpha S^\beta}\right)$$

$$\overset{!}{=} -\frac{1}{n} \log\left[\mathrm{Tr}\left(e^{\frac{\beta^2 J^2}{2} q \sum_{\alpha\neq\beta} S^\alpha S^\beta + \frac{\beta^2 J^2}{2} q n - \frac{\beta^2 J^2}{2} q n}\right)\right] = -\frac{1}{n} \log\left(\mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2} q \sum_{\alpha,\beta=1}^{n} S^\alpha S^\beta - \frac{\beta^2 J^2}{2} q n}\right)$$

entropic term $= -\frac{1}{n}\log\left[\left(\mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2} q \sum_{\alpha,\beta} S^\alpha S^\beta}\right) e^{-\frac{\beta^2 J^2}{2} q n}\right] = -\frac{1}{n}\log\left(\mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2} q \sum_{\alpha\beta} S^\alpha S^\beta}\right) + \frac{\beta^2 J^2}{2} q$

$$= -\frac{1}{n}\log\left(\sum_{\{S^1\dots S^n\}} e^{\frac{\beta^2 J^2}{2} q \sum_\alpha S^\alpha \sum_\beta S^\beta}\right) + \frac{\beta^2 J^2}{2} q$$

$$= -\frac{1}{n}\log\left(\sum_{\{S^1\dots S^n\}} \underbrace{e^{\frac{\beta^2 J^2}{2} q \left(\sum_{\alpha=1}^n S^\alpha\right)^2}}_{\bullet\ \text{single replica term}}\right) + \frac{\beta^2 J^2}{2} q$$

$$\bullet \overset{HS}{=} \int_{\mathbb{R}} \sqrt{\frac{\beta^2 J^2 q}{2\pi}}\, dz\, e^{-\frac{\beta^2 J^2 q}{2} z^2 + \beta^2 J^2 q z \sum_{\alpha=1}^n S^\alpha}$$

$$= \int_{\mathbb{R}} d\mu(z)\, e^{\beta^2 J^2 q z \sum_\alpha S^\alpha}$$

Substituting: $\sigma_z^2 = \frac{1}{\beta^2 J^2 q}$

$d\mu(z) = \frac{1}{\sqrt{2\pi\sigma_z^2}} e^{-\frac{z^2}{2\sigma_z^2}} dz$

$$\sum_{\{S^1\dots S^n\}} \bullet = \int_{\mathbb{R}} d\mu(z)\left(\sum_{S=\pm 1} e^{\beta^2 J^2 q z S}\right)^n = \int_{\mathbb{R}} d\mu(z)\left(2\cosh(\beta^2 J^2 q z)\right)^n$$

$$= \int_{\mathbb{R}} d\mu(z)\, e^{n\log[2\cosh(\beta^2 J^2 q z)]} \underset{\substack{\text{expon. expansion}\\ n\to 0}}{=} \int_{\mathbb{R}} \underbrace{d\mu(z)}_{\text{Gaussian integral normalized}} \left[1 + n\log(\dots) + \mathcal{O}(n^2)\right]$$

$$= 1 + n\int_{\mathbb{R}} d\mu(z) \log\left[2\cosh(\beta^2 J^2 q z)\right] + \mathcal{O}(n^2)$$

entropic term $= -\frac{1}{n}\log\left\{1 + n\int_{\mathbb{R}} d\mu(z)\dots + \mathcal{O}(n^2)\right\} + \frac{\beta^2 J^2}{2} q$

$$\underset{\substack{\text{logarithm expansion}\\ n\to 0}}{=} -\int_{\mathbb{R}} d\mu(z) \log\left(2\cosh(\beta^2 J^2 q z)\right) - \frac{\mathcal{O}(n^2)}{n} + \frac{\beta^2 J^2}{2} q$$

We can do all the expansions at $n\to 0$ because in the end we will take the $n \to 0$ limit!

$$\Rightarrow A[q_{\alpha\beta}] = -\frac{\beta^2 J^2}{4} + \frac{\beta^2 J^2}{4}(n-1) q^2 - \int_{\mathbb{R}} d\mu(z)\log\left(2\cosh(\beta^2 J^2 q z)\right) + \frac{\beta^2 J^2}{2} q$$

$$= -\frac{\beta^2 J^2}{4}(1-q)^2 - \int_{\mathbb{R}} d\mu(z)\log\left(2\cosh(\beta^2 J^2 q z)\right) \quad \text{when } n \to 0$$

$$\Rightarrow f_J = \frac{1}{\beta} A[q_{\alpha\beta}] = -\frac{\beta J^2}{4}(1-q^2) - \frac{1}{\beta}\int_{\mathbb{R}} d\mu(z) \log\left[2\cosh(\beta^2 J^2 q z)\right]$$

We can finally compute the <u>Saddle point equation</u>:

$$\frac{df}{dq} = 0 \iff \boxed{q = \int_{\mathbb{R}} d\mu(z) \tanh^2(\beta^2 J^2 q z)}$$

NB We get f_J, the free energy of the SK model, in the replica symmetric ansatz for the overlap matrix $q_{\alpha\beta}$

→ Notice that now we have only one variational parameter that is q!
(The temperature β is fixed and also the variance J of the disorder couplings is fixed)

Recall that the saddle point equation for the Random Field Ising Model (RFIM) is:

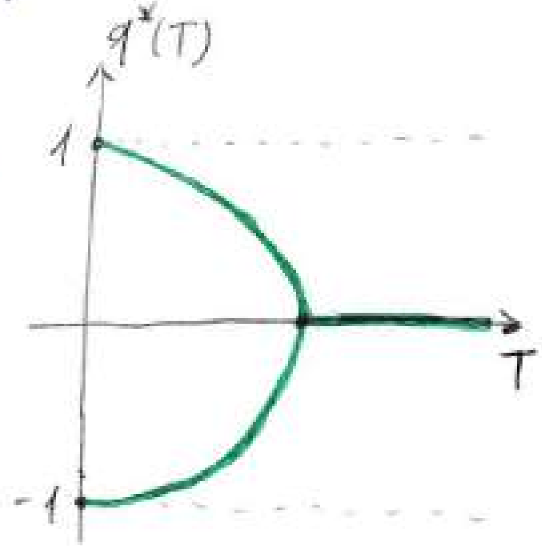
$$m = \int_{\mathbb{R}} d\mu(h) \tanh(2\beta J m + \beta h)$$

→ The order parameter was m, the magnetization

→ In either cases we get a gaussian integral: for the RFIM over the local field (disorder)

If we solve the saddle point equation for the SK model in the replica symmetric ansatz we get a <u>Bifurcation</u> of the solution $q^*(T)$:

- $T < T_c$: $q^*(T)$ bifurcates
- $T \geq T_c$: $q^*(T) = 0$



! What turns out is that this result and in particular the replica symmetry (replica symm. ansatz) are <u>WRONG</u>: the ansatz led to a negative entropy that is not possible for a discrete system (spin system in our case)! In particular:

$$f_J[q^*(T)] \xrightarrow{T\to 0} -\sqrt{\frac{2}{\pi}}J + \frac{T}{2\pi} \iff \underset{\text{Free energy}}{F} = \langle E \rangle - TS \Rightarrow S = -\frac{1}{2\pi} < 0$$

We can have a negative entropy only for continuous variables: recall that from the Boltzmann definition:

$$S = k_B \log W \quad \text{where } W = \text{volume in the phase space}$$

⇝ If the continuous variable occupies a phase space volume that is less then one, then we can have a negative entropy

⇝ If we have discrete variables W becomes the number of possible configurations of these discrete variables (spin on a lattice) and so $W = N$ is an integer and $S = k_B \log N$ cannot be negative

Parisi discovered that the replica symmetry assumption was wrong and that we are in presence of a REPLICA SYMMERY BREAKING (RSB)

If we pick up randomly two different replica configurations $\vec{S}^\alpha$ and $\vec{S}^\beta$ we can notice that they can have different degrees of similarity, which is encoded in the overlap matrix $q_{\alpha\beta}$ (that we are plugging into $A[q_{\alpha\beta}]$ for our calculation)
Beside the replica symmetry assumption, we can study a replica symmetry breaking situation with different "breaking" degrees:

- ONE STEP RSB

In this case we assume that the overlap matrix $q_{\alpha\beta}$ is a block diagonal matrix of the form:

$m_1 \times m_1$ Block

$$m_1 \text{ size} \left\{ \underbrace{\boxed{\begin{matrix} 0 & q_1 & \cdots & q_1 & q_1 \\ q_1 & 0 & q_1 & \cdots & q_1 \\ \vdots & q_1 & \ddots & & \vdots \\ \vdots & & & \ddots & q_1 \\ q_1 & q_1 & \cdots & q_1 & 0 \end{matrix}}}_{m_1 \text{ size}} \right. \equiv \boxed{\begin{matrix} 0 & q_1 \\ q_1 & 0 \end{matrix}}$$

$m_1 \times m_1$ Block

$$m_1 \text{ size} \left\{ \underbrace{\boxed{\begin{matrix} q_0 & \cdots & q_0 \\ \vdots & \ddots & \vdots \\ q_0 & \cdots & q_0 \end{matrix}}}_{m_1 \text{ size}} \right. \equiv \boxed{q_0}$$

$$q_{\alpha\beta} = \underbrace{\begin{pmatrix} \boxed{\begin{matrix} 0 & q_1 \\ q_1 & 0 \end{matrix}} & \boxed{q_0} & & \boxed{q_0} \\ \boxed{q_0} & \boxed{\begin{matrix} 0 & q_1 \\ q_1 & 0 \end{matrix}} & & \vdots \\ \vdots & & \ddots & \boxed{q_0} \\ \boxed{q_0} & \cdots & & \boxed{\begin{matrix} 0 & q_1 \\ q_1 & 0 \end{matrix}} \end{pmatrix}}_{n \text{ size}} \left. \right\} n \text{ size}$$

with this assumption the calculation of $A[q_{\alpha\beta}]$ can be repeated and so get the free energy f_J, that now will depends on m_1, q_0 and q_1 = the three new variational parameters! Moreover it turns out that $q_1 > q_0$ and so we can have two possible outcomes for the overlap matrix:

$$q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^\alpha S_i^\beta <\begin{matrix} q_0 \\ q_1 \end{matrix}$$

=> In particular the probability distr. of the overlaps of two different replicas is:

$$P(q) = m_1 \delta(q-q_0) + (1-m_1)\delta(q-q_1)$$

= Prob. distr. to find q_0 or q_1 as overlap for 2 different replicas

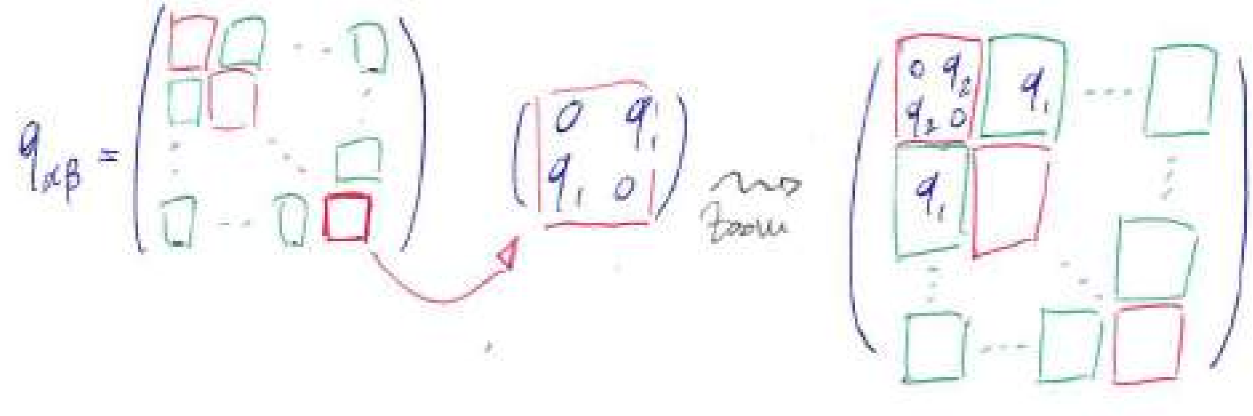
=> Consistently with this result we find that $\frac{\partial f}{\partial m_1} = 0$ led to $m_1 \in [0,1]$
~~so that the prob. distr. is normalized~~

(? Strange result: m_1 should be an integer and $< n$ but it works. Recall that before calculating $\partial f / \partial m_1$ we have send $n \to 0$!)

=> Even with this assumption we find a negative entropy, unless it is less negative (greater) than the replica symmetry case !

• <u>FULL RSB</u> (Parisi)

In this case we have to consider the same structure of $q_{\alpha\beta}$ in the one step RSB case but now the diagonal blocks have each the same structure of the original matrix ... and so on iteratively:



$\begin{pmatrix} 0 & q_2 \\ q_2 & 0 \end{pmatrix} \rightsquigarrow$ zoom And so on ....

where $\{q_1, q_2 \cdots q_k\}$ are K overlap parameters

If we iterate this procedure up to infinity we get an infinite number of variational parameters where $K \to +\infty$, so then $\{q_1 \cdots q_k\}$ in this limit becomes a prob. distribution:

$\{q_1 \cdots q_k\} \xrightarrow[K\to\infty]{} q(X) = [0,1] \to [0,1]$ which can be computed solving the saddle point equation and has inverse $X(q)$

$X(q)$: prob. distr. of the overlaps

Part IV

Additional Material

8 Fractional Calculus

See Manzali-Nicolai's Notes - pag.150 ch7.4 Levy Flights (Deepening on the structure of the generalized diffusion equation)

Deepening: FRACTIONAL CALCULUS & FRACTIONAL DERIVATIVE

Fractional calculus is a branch of mathematical analysis that studies the several different possibility of defining real and complex number powers of the differentiation operator D^α and of the integration operator J^α in such a way that, when $\alpha \in \mathbb{N}$ the two operators coincide with the usual derivative and integration operation.

⇝ Fractional differential equations also called extraordinary differential equations are a generalization of differential equations through the application of fractional calculus

Fractional Derivative of a power function

Let's take $f(x) = x^k$, then in ordinary calculus we have:

$$f'(x) = \frac{d}{dx} f(x) = k x^{k-1} \qquad f^\alpha(x) = \frac{d^\alpha}{dx^\alpha} f(x) = \frac{k!}{(k-\alpha)!} x^{k-\alpha} \qquad \alpha \in \mathbb{N}$$

$$f^\alpha(x) = \frac{d^{\alpha-1}}{dx^{\alpha-1}} \left(k x^{k-1} \right) = \frac{d^{\alpha-2}}{dx^{\alpha-2}} \left(k \cdot k-1 \right) x^{k-2} = \left(k \cdot k-1 \cdot \dots \cdot k-\alpha+1 \right) x^{k-\alpha}$$

⇒ We can define the fractional derivative exploiting the gamma function, the continuous generalization of the factorial $\Gamma(n+1) = n!$

Positive integer power: $$\frac{d^\alpha}{dx^\alpha} x^k = \frac{\Gamma(k+1)}{\Gamma(k-\alpha+1)} x^{k-\alpha} \quad \text{where } k > 0$$

Negative integer power: $$\frac{d^\alpha}{dx^\alpha} x^{-k} = (-1)^\alpha \frac{\Gamma(k+\alpha)}{\Gamma(k)} x^{-(k+\alpha)} \quad \text{where } k \geq 0$$

$\boxed{\text{Ex}}$ $$\frac{d^{1/2}}{dx^{1/2}} x = \frac{\Gamma(1+1)}{\Gamma(1-\frac{1}{2}+1)} x^{1-\frac{1}{2}} = \frac{1}{\frac{\sqrt{\pi}}{2}} x^{\frac{1}{2}} = \frac{2}{\sqrt{\pi}} \sqrt{x}$$

Notice that: $$\frac{d^{1/2}}{dx^{1/2}} \left[\frac{d^{1/2}}{dx^{1/2}} x \right] = \frac{2}{\sqrt{\pi}} \frac{\Gamma(1+\frac{1}{2})}{\Gamma(\frac{1}{2}-\frac{1}{2}+1)} x^{\frac{1}{2}-\frac{1}{2}} = \frac{2}{\sqrt{\pi}} \frac{\frac{\sqrt{\pi}}{2}}{1} = 1 = \frac{d}{dx} x$$

⇝ We retrieve the usual derivative result!

For a general function $f(x)$ and for $0<\alpha<1$ the fractional derivative is defined as:

$$\boxed{\mathcal{D}^{\alpha} f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x \frac{f(t)}{(x-t)^{\alpha}} dt} \quad \text{where } 0<\alpha<1$$

→ For a generic α it's necessary to see α as a sum of an integer number and a fractional part!

Recall that the set $\{\mathcal{D}^{\alpha} \mid \alpha \in \mathbb{R}\}$ with the composition operation form a continuous semigroup with parameter α:

$$(\mathcal{D}^{\alpha} \mathcal{D}^{\beta}) \mathcal{D}^{\gamma} = \mathcal{D}^{\alpha} (\mathcal{D}^{\beta} \mathcal{D}^{\gamma}) \quad \forall \alpha, \beta, \gamma \in \mathbb{R}$$

$\boxed{\text{Ex}}$ $\mathcal{D}^{3/2} f(x) = \mathcal{D}^{1/2} \mathcal{D}^{1} f(x) = \mathcal{D}^{1/2} \frac{d}{dx} f(x)$

Riesz Derivative

That's a particular fractional derivative defined exploiting the Fourier transform $\mathcal{F}$:

$$\mathcal{F}\left\{ \frac{d^{\alpha} u}{d|x|^{\alpha}} \right\}(k) = -|k^{\alpha}| \, \mathcal{F}\{u\}(k)$$