From the CLT to Stirling ... and back !

1°) a) the sum of two $\mathcal{P}(\lambda)$ is a $\mathcal{P}(2\lambda)$, if the variables summed are independent.

b) $S_n = \sum_{i=1}^{n} x_i$ where $x_i$ IID $\to \mathcal{P}(1)$

then $S_n$ follows a $\mathcal{P}(n1) = \mathcal{P}(n)$ ie

$$\Pr[S_n = k] = e^{-n} \frac{n^k}{k!}$$

, and the CLT, which applies here (all moments finite) tells us that $S_n$ tends to a gaussian of mean $\langle S_n \rangle = n$ and variance $V(S_n) = n V(x_1) = n$

c) $$\Pr\left[n - \tfrac{1}{2} \leqslant S_n \leqslant n + \tfrac{1}{2}\right] = \Pr[S_n = n] = e^{-n} \frac{n^n}{n!}$$ using the definition of Poisson var

$$= \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{1}{\sqrt{2\pi n}} \exp\left[-\frac{s^2}{2n}\right] ds$$ (from CLT $s = S_n - n$)

$$\simeq \frac{1}{\sqrt{2\pi n}}$$

$$n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \Rightarrow \text{Stirling formula}$$

2°) R.W: $x_0 = 0$

$x_{k+1} = x_k + \eta_k$ ; $\eta_k \begin{cases} \to 1, & \text{proba } 1/2 \\ \to -1, & \text{proba } 1/2 \end{cases}$ ; $n$ steps made, $n$ even

a) $$\Pr[x_n = 0] = \frac{1}{2^n}\binom{n}{n/2}$$ since we have to make $\frac{n}{2}$ steps to the right, and $\frac{n}{2}$ to the left

b) $$\Pr[x_n = 0] = \frac{1}{2^n}\frac{n!}{\left[\left(\frac{n}{2}\right)!\right]^2} \sim \frac{1}{2^n}\frac{\sqrt{2\pi n}\, n^n e^{-n}}{\left[\sqrt{\pi n}\left(\frac{n}{2}\right)^{n/2} e^{-n/2}\right]^2} \sim \frac{\sqrt{2}}{\sqrt{\pi}}\frac{\cancel{n^n}\, \cancel{e^{-n}}\sqrt{n}}{n\, \cancel{n^n}\, \cancel{e^{-n}}} = \sqrt{\frac{2}{\pi n}}$$

c) the walker makes $n_+$ steps to the right, $n_-$ to the left:

$$\begin{cases} n_+ + n_- = n \\ n_+ - n_- = m \end{cases} \Rightarrow \begin{cases} n_+ = \frac{n+m}{2} \\ n_- = \frac{n-m}{2} \end{cases}$$

$m = 2n_+ - n$

if $n$ even, $m$ is even
($n$ odd, $m$ is odd)

$$\Pr[x_n = m] = \frac{1}{2^n}\binom{n}{n_+} \sim \frac{1}{\cancel{2^n}} \frac{\sqrt{2\pi n}\, n^n \cancel{e^{-n}}}{\sqrt{2\pi\frac{n+m}{2}}\left(\frac{n+m}{\cancel{2}}\right)^{\frac{n+m}{2}}} \frac{1}{\sqrt{2\pi\frac{n-m}{2}}\left(\frac{n-m}{\cancel{2}}\right)^{\frac{n-m}{2}} \cancel{e^{-\frac{n+m}{2}}}\, \cancel{e^{-\frac{n-m}{2}}}}$$

$$\sim \sqrt{\frac{2}{\pi}}\sqrt{\frac{n}{n^2-m^2}}\frac{n^n}{(n+m)^{\frac{n+m}{2}}(n-m)^{\frac{n-m}{2}}}$$

$$\sim \sqrt{\frac{2}{\pi}}\sqrt{\frac{n}{n^2-m^2}}\underbrace{\left(1+\frac{m}{n}\right)^{-\frac{n+m}{2}}}_{\exp\left[-\left(\frac{n+m}{2}\right)\log\left(1+\frac{m}{n}\right)\right]}\left(1-\frac{m}{n}\right)^{-\frac{n-m}{2}} \to e^{-\left(\frac{n-m}{2}\right)\log\left(1-\frac{m}{n}\right)}$$

$$\frac{m}{n} \ll 1$$

$$\Pr[x_n = m] \sim \sqrt{\frac{2}{\pi}} \sqrt{\frac{n}{n^2-m^2}}\, e^{-\frac{n+m}{2}\left(\frac{m}{n} - \frac{m^2}{2n^2}\right)}\; e^{-\frac{n-m}{2}\left(-\frac{m}{n} - \frac{m^2}{2n^2}\right)}$$

$$\log(1+\varepsilon) \underset{0}{\simeq} \varepsilon - \frac{\varepsilon^2}{2}$$

$$\sim \sqrt{\frac{2}{\pi}} \underbrace{\sqrt{\frac{n}{n^2-m^2}}}_{\simeq 1/\sqrt{n}} \exp\left[ -\cancel{\frac{nm}{2n}} - \frac{m^2}{2n} + \frac{m^2}{4n} + \cancel{\frac{nm}{2n}} - \frac{m^2}{2n} + \frac{m^2}{2n} + O(m^3) \dots \right]$$

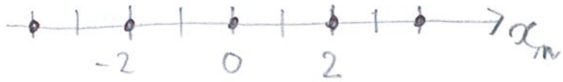
$$\sim \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{n}}\, e^{-m^2/2n}$$

d) With our random walk, $\langle x_n \rangle = 0$ ; $\langle x_n^2 \rangle = V(x_n) = n$

and the CLT tells us that $x_n$ becomes $\mathcal{G}(0, \sqrt{n})$, hence with pdf

$$p(x) = \frac{1}{\sqrt{2\pi n}}\, e^{-x^2/2n} \quad \dots \text{ almost as above, but for a factor } 2.$$

The reason is that $x_n$ takes even values, or more precisely, that it changes by 2 from a value to the next




Hence the relation between the discrete $\Pr[x_n = m]$ and the pdf $p(m)$

$$\Pr[x_n = m] = \int_{m-1}^{m+1} p(x)\,dx \simeq 2\,p(m)$$

and thus, the CLT agrees with our combinatorial calculation

## Consistency of Itō-Doblin and Stratonovich calculus

$$\dot{x} = \mu F + \sqrt{2D}\,\eta(t)$$

→ <u>Stratonovich calculus</u>: $\frac{d}{dt}\langle \varphi(x(t))\rangle = \left\langle \frac{d\varphi(x(t))}{dt}\right\rangle = \langle \varphi'(x(t))\,\dot{x}\rangle = \mu\langle F(x)\varphi'(x)\rangle + \underbrace{\sqrt{2D}\,\langle \varphi'(x)\,\eta(t)\rangle}_{= D\langle \varphi''(x)\rangle}$

$$\Rightarrow \frac{d}{dt}\langle \varphi(x(t))\rangle = \mu\langle F(x)\varphi'(x)\rangle + D\langle \varphi''(x)\rangle$$

→ <u>Itô calculus</u>: $\frac{d}{dt}\langle \varphi(x(t))\rangle = \underbrace{\langle \varphi'(x)\,\dot{x}\rangle}_{\langle \varphi'(x)\mu F\rangle + \underbrace{\langle \varphi'(x)\sqrt{2D}\,\eta(t)\rangle}_{0}} + D\langle \varphi''(x)\rangle$

$$= \mu\langle F(x)\varphi'(x)\rangle + D\langle \varphi''(x)\rangle$$

consistent!

---

## Itō-Doblin, Stratonovich and Wick

$\dot{x} = \sqrt{2D}\,\eta(t)$ defines Wiener process, which is gaussian: $\langle x\rangle = 0$; $\langle x^2(t)\rangle = 2Dt$.

Thus, from the vanishing of cumulants / Wick theorem, we get

$$\langle x^4\rangle = 3\langle x^2\rangle^2 \quad\Rightarrow\quad \langle x^4\rangle = 3(2Dt)^2 = 12D^2t^2$$

$$\langle x^6\rangle = 15\langle x^2\rangle^3 \qquad\quad \langle x^6\rangle = 15(2Dt)^3 = 120D^3t^3$$

→ <u>Stratonovich calculus</u>: $\frac{d}{dt}\langle x^4\rangle = \langle 4x^3\dot{x}\rangle = \sqrt{2D}\,4\langle x^3\eta(t)\rangle = 4\times 3\langle x^2\rangle D$

$$= 12D\cdot 2Dt = 24D^2t$$

$\Rightarrow \langle x^4\rangle = 12D^2t^2$ ✓ since $\langle x^4\rangle = 0$ at $t=0$.

$$\frac{d}{dt}\langle x^6\rangle = 6\langle x^5\dot{x}\rangle = 6\times 5\cdot D\langle x^4\rangle = 30D\cdot 12D^2t^2$$

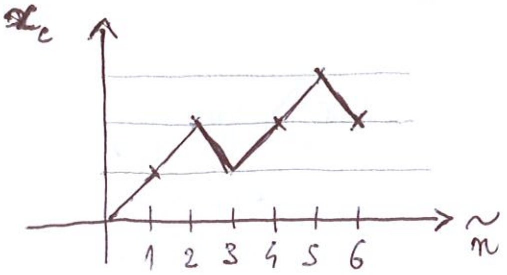
$\Rightarrow \langle x^6\rangle = \frac{1}{3}\cdot D^3\,30\cdot 12\cdot t^3 = 120D^3t^3$ ✓

→ <u>Itô calculus</u>: $\frac{d}{dt}\langle x^4\rangle = \langle 4x^3\dot{x}\rangle + 4\cdot 3D\langle x^2\rangle = 12\langle x^2\rangle D = 24D^2t$

$$\frac{d}{dt}\langle x^6\rangle = \langle 6x^5\dot{x}\rangle + 6\cdot 5\langle x^4\rangle D = 30D\langle x^4\rangle$$

all is consistent

## The Wiener process from the scaling limit of a random walk




From this signal $x_c(\tilde{n})$, we define
$$x_\varepsilon(t) = \varepsilon\, x_c\left(\frac{t}{\Delta t}\right)$$
which is the same as defining $\Delta t$ as the time step between 2 jumps, and $\varepsilon$ as the amplitude of the left/right jumps.

For $t \gg \Delta t$, the process $x_\varepsilon(t)$ becomes gaussian : the variable itself $x_\varepsilon(t)$ is gaussian distributed, but also, the joint pdf of $x_\varepsilon(t)$ and $x_\varepsilon(t')$ is gaussian, for $|t-t'| \gg \Delta t$, and both $t, t' \gg \Delta t \Rightarrow$ same result for the $n$-point pdf, hence the whole process is gaussian

$$\langle x_\varepsilon(t)\rangle = 0$$

$$\langle x_\varepsilon(t)\, x_\varepsilon(t')\rangle = \varepsilon^2 \left\langle x_c\left(\frac{t}{\Delta t}\right) x_c\left(\frac{t'}{\Delta t}\right)\right\rangle \simeq \varepsilon^2 \underbrace{\langle x_n\, x_{n'}\rangle}_{\min(n,n')} \qquad n = \left\lfloor \frac{t}{\Delta t} \right\rfloor$$

$$\simeq \varepsilon^2 \min\left(\frac{t}{\Delta t}, \frac{t'}{\Delta t}\right) \qquad n' = \left\lfloor \frac{t'}{\Delta t} \right\rfloor$$

For the Wiener process, we have $\langle W(t)\, W(t')\rangle = 2D \min(t, t')$ and we thus have to take
$$\left[\begin{array}{l} \varepsilon \to 0 \\ \Delta t \to 0 \end{array}\right. , \quad \frac{\varepsilon^2}{\Delta t} = 2D, \text{ fixed} \quad (\text{diffusive scaling})$$

## Markovian, or non Markovian ?

$x_n$ is a non Markovian process since the jump proba depends on the position the step before, $x_{n-1}$. Yet, the "augmented" process $\left|\begin{array}{l} x_n \\ x_{n-1} \end{array}\right.$, which is now vectorial, is Markovian : from $\left|\begin{array}{l} x_n \\ x_{n-1} \end{array}\right.$, the jump proba is known, from which $x_{n+1}$ follows, so that the jump proba to $\left|\begin{array}{l} x_{n+1} \\ x_n \end{array}\right.$ is fully specified.

Position and velocity process in the Langevin equation

$$m\ddot{x} = -\gamma m \dot{x} + R(t)$$
$$\langle R(t) R(t')\rangle = 2m^2\Gamma\,\delta(t-t')$$

1°) Velocity

a) $$v(t) = v_0\, e^{-\gamma t} + \frac{1}{m}\int_0^t e^{-\gamma(t-t')} R(t')\,dt'$$

b) $v(t) \to$ gaussian, as a sum of gaussian variables

$\to$ Markovian, since obeys a first order diff equation : $\dot{v} = -\gamma v + \frac{1}{m} R$

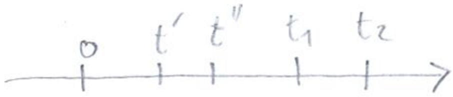
We will denote $v(t)$ the process where $v_0$ is fixed

$\tilde{v}(t)$ " " $v_0$ is distributed according to equilibrium Maxwellian

Since $v(t)$ is gaussian, the process is entirely characterized by $\langle v(t)\rangle$ and $\langle v(t_1) v(t_2)\rangle$.

Same thing for $\tilde{v}$, obtained from $v$ by an extra averaging over $v_0$.

$$\langle v(t)\rangle = v_0 e^{-\gamma t} \; ; \quad \langle \tilde{v}(t)\rangle = 0$$




Calculation $\langle v(t_1) v(t_2)\rangle$.

brute force $\rightarrow$ $$\langle v(t_1) v(t_2)\rangle = v_0^2 e^{-\gamma(t_1+t_2)} + 0 + 0 + \frac{1}{m^2}\int_0^{t_1} dt' \int_0^{t_2} dt''\, e^{-\gamma(t_1-t')}\, e^{-\gamma(t_2-t'')} \underbrace{\langle R(t') R(t'')\rangle}_{2m^2\Gamma\delta(t'-t'')}$$

$$= v_0^2 e^{-\gamma(t_1+t_2)} + 2\Gamma e^{-\gamma(t_1+t_2)} \underbrace{\int_0^{t_1} e^{+\gamma(t'+t')}\,dt'}_{\frac{1}{2\gamma}\left(e^{2\gamma t_1}-1\right)}$$

take $t_1 < t_2$, the integral vanishes for $t'' > t_1 = \min(t_1,t_2)$

$$= v_0^2 e^{-\gamma(t_1+t_2)} + \frac{\Gamma}{\gamma}\left[e^{-\gamma\underbrace{(t_1+t_2-2t_1)}_{t_2-t_1}} - e^{-\gamma(t_1+t_2)}\right]$$

($\hookrightarrow$ means $t_2 - \min(t_1,t_2)) = |t_2 - t_1|$ in all generality

$$\boxed{\langle v(t_1) v(t_2)\rangle = v_0^2 e^{-\gamma(t_1+t_2)} + \frac{\Gamma}{\gamma}\left[e^{-\gamma|t_1-t_2|} - e^{-\gamma(t_1+t_2)}\right]}$$

which is symmetric $t_1 \leftrightarrow t_2$, as it should

variant $\rightarrow$ $$\left\langle v(t')\frac{dv}{dt}\right\rangle = -\gamma\langle v(t') v(t)\rangle + \frac{1}{m}\underbrace{\langle v(t') R(t)\rangle}_{0 \text{ for } t>t'}$$

$$\Rightarrow \langle v(t') v(t)\rangle = A(t') e^{-\gamma t}, \quad \text{for } t > t'$$

$$\Rightarrow A(t) = e^{-\gamma t}\langle v^2(t)\rangle \; ; \quad \langle v^2(t)\rangle - \langle v(t)\rangle^2 = \frac{\Gamma}{\gamma}\left(1-e^{-2\gamma t}\right)$$ seen in class

here $\langle v\rangle = v_0$

Hence we get $\langle v(t') v(t)\rangle$ for $t > t'$ ; we complete by symmetry for $t < t'$ and get same as above.

Besides, the fluctuation-dissipation relation reads $\frac{\Gamma}{\gamma} = \frac{kT}{m}$. Finally, averaging over the equilibrium Maxwellian for $v_0$ yields: $\langle v_0^2 \rangle = \frac{kT}{m}$

$$\Rightarrow \langle \tilde{v}(t_1)\tilde{v}(t_2)\rangle = \frac{kT}{m} e^{-\gamma|t_1-t_2|} \quad \text{and} \quad \langle \tilde{v}(t)\rangle = 0$$

Thus the autocorrelations:

$$\boxed{\begin{aligned} \langle v(t_1)v(t_2)\rangle - \langle v(t_1)\rangle\langle v(t_2)\rangle &= \frac{kT}{m}\left[e^{-\gamma|t_1-t_2|} - e^{\gamma(t_1+t_2)}\right] \\ \langle \tilde{v}(t_1)\tilde{v}(t_2)\rangle - \langle \tilde{v}(t_1)\rangle\langle \tilde{v}(t_2)\rangle &= \frac{kT}{m} e^{-\gamma|t_1-t_2|} \end{aligned}}$$

$\tilde{v}$ is stationnary, but not $v$

2°) a) $x(t) = \int_0^t v(t')\,dt'$ | $x(t) = \frac{v_0}{\gamma}(1-e^{-\gamma t}) + \frac{1}{m}\int_0^t dt' \int_0^{t'} dt''\, R(t')\, e^{-\gamma(t'-t'')}$

$\tilde{x}(t) = 0 \quad + \quad$ ″

b) $x(t)$ obeys a 2nd order differential equation $\Rightarrow$ not Markovian; $\tilde{x}(t)$ is Markovian

But: $\{x(t), v(t)\}$ is Markovian, obeys a first order (vectorial) equation.

Besides, since $v(t)$ is gaussian, $x(t)$ is also Gaussian. Same thing for $\tilde{x}$.

To characterize the processes $x(t)$, and $\tilde{x}(t)$, we need the first moment and the autocorrelation function: $\langle x(t)\rangle = \int_0^t \langle v(t')\rangle dt' = \frac{v_0}{\gamma}\left(1-e^{-\gamma t}\right)$ ; $\langle \tilde{x}(t)\rangle = 0$

$$\langle x(t_1)x(t_2)\rangle = \int_0^{t_1} dt' \int_0^{t_2} dt'' \langle v(t')v(t'')\rangle$$

$$= \left(v_0^2 - \frac{kT}{m}\right)\underbrace{\int_0^{t_1} dt' \int_0^{t_2} dt''\, e^{-\gamma(t'+t'')}}_{\frac{1}{\gamma^2}(1-e^{-\gamma t_1})(1-e^{-\gamma t_2})} + \underbrace{\frac{kT}{m}\int_0^{t_1} dt' \int_0^{t_2} dt''\, e^{-\gamma|t'-t''|}}_{\text{take } t_1 < t_2 \text{ and symmetrize in the end}} \quad \mathrm{I}$$

$$\mathrm{I} = \int_0^{t_1} dt' \left[\int_0^{t'} e^{-\gamma(t'-t'')} dt'' + \int_{t'}^{t_2} e^{-\gamma(t''-t')} dt''\right]$$

$$= \int_0^{t_1} dt' \left[\frac{1}{\gamma}(1-e^{-\gamma t'}) + \frac{1}{\gamma}\left(1-e^{-\gamma(t_2-t')}\right)\right]$$

$$= \frac{1}{\gamma}\left[2t_1 + \frac{1}{\gamma}\left(e^{-\gamma t_1}-1\right) - \frac{1}{\gamma}\left(e^{-\gamma(t_2-t_1)} - e^{-\gamma t_2}\right)\right]$$

$$= \frac{1}{\gamma^2}\left[2\gamma t_1 + e^{-\gamma t_1} + e^{-\gamma t_2} - e^{-\gamma(t_2-t_1)} - 1\right]$$

$t_1 = \min(t_1, t_2)$

$t_2 - t_1 \Rightarrow |t_2 - t_1|$

$$\boxed{\begin{aligned} \langle x(t_1)x(t_2)\rangle &= \left(v_0^2 - \frac{kT}{m}\right)\frac{1}{\gamma^2}\left(1-e^{-\gamma t_1}\right)\left(1-e^{-\gamma t_2}\right) + \frac{kT}{m\gamma^2}\left\{2\gamma \min(t_1,t_2) + e^{-\gamma t_1} + e^{-\gamma t_2} - e^{-\gamma|t_2-t_1|} - 1\right\} \\ \langle \tilde{x}(t_1)\tilde{x}(t_2)\rangle &= \frac{kT}{m\gamma^2}\left\{2\gamma \min(t_1,t_2) + e^{-\gamma t_1} + e^{-\gamma t_2} - e^{-\gamma|t_2-t_1|} - 1\right\} \end{aligned}}$$

Neither $x(t)$ nor $\tilde{x}(t)$ are stationnary

Doob's theorem

1°) a) $p(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$

b) Both $p(x)$ and $p(x,0;y,\tau)$ are gaussian. Hence $p(y,\tau|x,0) = \frac{p(x,0;y,\tau)}{p(x)}$ also is

$$\boxed{p(y,\tau|x;0) = d\, \exp(-ax^2 - 2bxy - cy^2)} \quad , a>0 \ ; c>0$$

c) $$\int dy\, p(y,\tau|x,0) = 1 = d \int dy\, \exp\left\{-c\left(y+\frac{bx}{c}\right)^2 + \frac{b^2x^2}{c}\right\} e^{-ax^2}$$

$$= d\sqrt{\frac{\pi}{c}}\, e^{x^2(b^2/c - a)} \qquad \forall x$$

$$\Rightarrow \boxed{a = \frac{b^2}{c}} \ ; \ \boxed{d = \sqrt{\frac{c}{\pi}}}$$

d) $$p(y) = \int dx\, p(y,\tau|x;0)\, p(x)$$

$$\Rightarrow \cancel{\frac{1}{\sqrt{2\pi}}} e^{-y^2/2} = \int dx\, d\, e^{-ax^2-2bxy-cy^2} \cancel{\frac{1}{\sqrt{2\pi}}} e^{-x^2/2}$$

$$= d\, e^{-cy^2} \underbrace{\int dx\, e^{-(a+\frac{1}{2})x^2 - 2bxy}}_{\sqrt{\frac{\pi}{a+1/2}} \langle e^{-2byx} \rangle}$$

$\to$ gauss weight $e^{-(a+\frac{1}{2})x^2}$

$\to$ moment generating function

$$= \sqrt{\frac{\pi}{a+\frac{1}{2}}}\, e^{-\frac{1}{2}(2by)^2\frac{1}{1+2a}}$$

$\frac{\sigma^2}{2} = \frac{1}{a+1/2}$

$\sigma^2 = \frac{1}{1+2a}$

$$e^{-y^2/2} = \sqrt{\frac{c}{\cancel{\pi}}}\, e^{-cy^2} \sqrt{\frac{2\cancel{\pi}}{1+2a}}\, e^{+\frac{2b^2y^2}{1+2a}}$$

$$c = \frac{1+2a}{2} \quad \text{and} \quad \frac{1}{2} = c - \frac{2b^2}{1+2a} \ ; \ \boxed{c = \frac{1}{2} + \frac{2b^2}{1+2a}}$$

$$\boxed{a = c - \frac{1}{2}}$$

e) We note above that $c > \frac{1}{2}$, Hence, we choose to write $c = \frac{1}{2}\frac{1}{1-\gamma^2}$ ; $0<\gamma<1$

$$a = c - \frac{1}{2} = \frac{\gamma^2}{2(1-\gamma^2)} \quad > 0$$

Note that we have 3 relations $a, b, c$ but only 2 are independent. Indeed,

$$a = \frac{b^2}{c} \quad \text{and} \quad \left(c-\frac{1}{2}\right) = \frac{2b^2}{1+2a} \quad \text{are redundant}$$

$$\hookrightarrow b^2 = ac = a\left(a+\frac{1}{2}\right) \qquad \hookrightarrow b^2 = \left(c-\frac{1}{2}\right)(1+2a)\frac{1}{2} = a\left(a+\frac{1}{2}\right)$$

$$b^2 = ac = \frac{\gamma^2}{2(1-\gamma^2)} \frac{1}{2} \frac{1}{(1-\gamma^2)} \; ; \; b = \frac{\gamma}{2(1-\gamma^2)}$$

and the sign of $\gamma$ is not known (depends on which root we pick... not important at this point). Take $b = -\sqrt{ac}$ for later convenience

$$\Rightarrow a x^2 + 2bxy + by^2 = \frac{1}{2(1-\gamma^2)} \left[ \gamma^2 x^2 + -2\gamma x y + y^2 \right]$$

$$= \frac{1}{2(1-\gamma^2)} \left[ y - \gamma x \right]^2 \qquad \square$$

f) $$p(y; \tau | x, 0) = \frac{1}{\sqrt{2\pi(1-\gamma^2)}} e^{-\frac{(y-\gamma x)^2}{2(1-\gamma^2)}}$$

which means that

$$\langle x(\tau) | x, 0 \rangle = \gamma x$$

and we can compute $\langle x(\tau) x(0) \rangle$ in 2 steps: for fixed $x(0)$, we average over $x(\tau)$ (which gives $\gamma x(0)$) and then we average over $x(0)$. In other words

$$\langle x(0) x(\tau) \rangle = \int dx dy \; x \cdot y \underbrace{p(x, 0; y; \tau)}_{p(y; \tau | x, 0) \, p(x, 0)}$$

Shortcut: $\langle x(0) x(\tau) \rangle = \langle \langle x(\tau) | x(0) \rangle x(0) \rangle_{x(0)} = \langle \gamma x(0) x(0) \rangle_{x(0)} = \gamma$

Hence the meaning of $\gamma$, which depends on $\tau$: $\boxed{\gamma(\tau) = \langle x(\tau) x(0) \rangle}$

g) Chapman-Kolmogorov: $$p(z, \tau_1 + \tau_2 | x, 0) = \int dy \underbrace{p(z, \tau_2 | y, 0)}_{= p(z, \tau_1 + \tau_2 | y, \tau_1)} p(y, \tau_1 | x, 0)$$

We multiply by $x z \, P(x, 0)$ and $\int dx dz$

$$\int dx dz \; x z \; p(z, \tau_1 + \tau_2 | x, 0) p(x, 0) = \int dx dy dz \; x z \; p(z, \tau_2 | y, 0) \; p(y, \tau_1 | x, 0) \; p(x, 0)$$

$$= \underbrace{\langle x(\tau_1 + \tau_2) x(0) \rangle}_{\gamma(\tau_1 + \tau_2)} = \int dx dy \; x \underbrace{\int dz \; z \; p(z, \tau_2 | y, 0)}_{y \gamma(\tau_2)} \; p(y, \tau_1 | x, 0) \; p(x, 0)$$

$$= \int dx \, x \underbrace{dy \; y \; p(y, \tau_1 | x, 0)}_{x \gamma(\tau_1)} p(x, 0) \; \gamma(\tau_2)$$

$$= \gamma(\tau_1) \gamma(\tau_2) \int dx \; x^2 \; p(x, 0)$$

$$\gamma(\tau_1 + \tau_2) = \gamma(\tau_1) \gamma(\tau_2) \Rightarrow \text{exponential.}$$

2) Reciprocal: the process that is gaussian, stationary, with exponential correlation function is the same as Ornstein-Uhlenbeck (up to scale), which is markovian.

## Fokker-Planck from Itō-Doblin calculus

The Fokker-Planck eq associated to $\dot{x} = \mu F(x) + \sqrt{2D}\, \eta(t)$ is

$$\partial_t P(x,t) = -\partial_x \left[ \mu F(x) P \right] + D\, \partial_x^2 P$$

We can retrieve this from Itō-Doblin calculus: we take an arbitrary $\varphi(x)$, that does not depend on time.

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

$$\frac{d}{dt} \langle \varphi(x(t)) \rangle = \langle \varphi'(x)\, \dot{x} \rangle + D \langle \varphi''(x) \rangle \qquad \text{(Itō-Doblin rule)}$$

$$= \cancel{\sqrt{2D} \langle \varphi'(x)\, \eta(t) \rangle} + \langle \varphi'(x) \mu F(x) \rangle + D \langle \varphi''(x) \rangle$$

Besides: $\frac{d}{dt} \langle \varphi(x(t)) \rangle = \int \varphi(x)\, \partial_t P(x,t)$

Thus $\int \varphi(x)\, \partial_t P(x,t)\, dx = \mu \int \varphi'(x) F(x) P(x,t) + D \int \varphi''(x)\, P(x,t)\, dx$

$$= -\mu \int \varphi(x)\, \partial_x [F P]\, dx + D \int \varphi(x)\, \partial_x^2 P\, dx$$

from integration by parts, assuming fast enough decay of $P$ at infinity.

The above equation is true $\forall\, \varphi(x)$

$$\Rightarrow \partial_t P = -\mu\, \partial_x [F P] + D\, \partial_x^2 P$$

---

## Several solutions to the diffusion equation

The conditional density obeys $\partial_t P = D\, \partial_x^2 P$, where $P(x,t|x_0,t_0)$
the problem is both time and space translation invariant. It is thus innocuous to choose $t_0 = 0$; $x_0 = 0$

1°) $P(x,t) = \psi(t)\, \varphi\left(\frac{x}{\sqrt{t}}\right)$ ; $\int_{-\infty}^{+\infty} P(x,t)\, dx = 1 = \int_{-\infty}^{+\infty} \psi(t)\, \varphi\left(\frac{x}{\sqrt{t}}\right) \sqrt{t}\, \frac{dx}{\sqrt{t}}$

$\tilde{x} = x/\sqrt{t}$ $\qquad = \psi(t)\sqrt{t} \int_{-\infty}^{+\infty} \varphi(\tilde{x})\, d\tilde{x}$

Hence $\psi(t)\sqrt{t}$ is a constant, that can be chosen $= 1$:

$$P(x,t) = \frac{1}{\sqrt{t}}\, \varphi\left(\frac{x}{\sqrt{t}}\right)$$

We next plug into $\partial_t P = D\, \partial_x^2 P$: $-\frac{1}{2\, t^{3/2}}\, \varphi\left(\frac{x}{\sqrt{t}}\right) - \frac{x}{2 t^{3/2} \sqrt{t}}\, \varphi'\left(\frac{x}{\sqrt{t}}\right) = D\, \frac{1}{t^{3/2}}\, \varphi''\left(\frac{x}{\sqrt{t}}\right)$

$$\Rightarrow D\, \varphi''(\tilde{x}) + \frac{1}{2} \tilde{x}\, \varphi'(\tilde{x}) + \frac{1}{2} \varphi(\tilde{x}) = 0$$

$$D\, \varphi''(\tilde{x}) + \frac{1}{2} \frac{d}{d\tilde{x}} \left[ \tilde{x}\, \varphi(\tilde{x}) \right] = 0$$

$$\Rightarrow D\frac{d\varphi}{d\tilde{x}} + \frac{1}{2}\tilde{x}\varphi(\tilde{x}) = \text{Cst} = 0$$ assuming $\varphi$ and $\varphi'$ decay fast enough for $|\tilde{x}| \to \infty$

$$\frac{d\varphi}{\varphi} = -\frac{1}{2D}\tilde{x}\,d\tilde{x}$$

$$\log\varphi(\tilde{x}) = -\frac{1}{4D}\tilde{x}^2 + \text{Cst} \Rightarrow \varphi(\tilde{x}) = \varphi_0\, e^{-\tilde{x}^2/4D}$$ and $\varphi_0 = \frac{1}{\sqrt{4\pi D}}$ follows from normalization of $P$ ie $\int \varphi(\tilde{x})\,d\tilde{x} = 1$.

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

and reintroducing $x_0$ and $t_0$ : $$P(x,t|x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}}\exp\left[-\frac{(x-x_0)^2}{4D(t-t_0)}\right]$$

## 2) Laplace transform method

$$\tilde{P}(x,s) \equiv \int_0^\infty P(x,\tau)\,e^{-s\tau}\,d\tau \quad ; \quad \tau = t - t_0$$

$$\int_0^\infty \frac{\partial P}{\partial \tau}(x,\tau)\,e^{-s\tau}\,d\tau = \int_0^\infty D\frac{\partial^2 P(x,\tau)}{\partial x^2}\,e^{-s\tau}\,d\tau$$

$$\Rightarrow \left[P(x,\tau)e^{-s\tau}\right]_{\tau=0}^{\tau=\infty} + \int_0^\infty P(x,\tau)\,s\,e^{-s\tau}\,d\tau = D\frac{\partial^2}{\partial x^2}\int_0^\infty P(x,\tau)\,e^{-s\tau}\,d\tau$$

$$0 - P(x,\tau=0) + s\tilde{P}(x,s) = D\frac{\partial^2}{\partial x^2}\tilde{P}(x,s) \; ;$$

↳ we assume $\mathrm{Re}(s) > 0$ so that $\exp(-s\tau) \xrightarrow[\tau\to\infty]{} 0$

and we use $P(x,\tau=0) = \delta(x-x_0)$

$$\Rightarrow \boxed{D\frac{\partial^2\tilde{P}(x,s)}{\partial x^2} - s\tilde{P}(x,s) = -\delta(x-x_0)} \qquad (*)$$

$x < x_0$ : $\tilde{P}(x,s) = A_1 e^{\sqrt{\frac{s}{D}}x} + B_1 e^{-\sqrt{\frac{s}{D}}x}$

$\tilde{P}$ does not diverge when $x \to -\infty$, $B_1 = 0$

$$\Rightarrow \tilde{P}(x,s) = A_1\exp\left(\sqrt{\frac{s}{D}}\,x\right) = \tilde{A}_1\exp\left(\sqrt{\frac{s}{D}}\,(x-x_0)\right)$$

$x > x_0$ : same thing $\rightarrow \tilde{P}(x,s) = \tilde{A}_2\exp\left(-\sqrt{\frac{s}{D}}\,(x-x_0)\right)$

the function is continuous at $x = x_0 \Rightarrow \tilde{A}_1 = \tilde{A}_2$

Finally, the $\delta(x-x_0)$ term brings a discontinuity of $\frac{\partial \tilde{P}}{\partial x}$ at $x_0$, like in electrostatics. Integrate $(*)$ from $x_0 - \varepsilon$ to $x_0 + \varepsilon$, then $\varepsilon \to 0^+$.

## Several solutions to the diffusion equation (2)

$$D\left[\frac{\partial \tilde{P}}{\partial x}\bigg|_{x_0^+} - \frac{\partial \tilde{P}}{\partial x}\bigg|_{x_0^-}\right] = -1 \quad \Rightarrow -2\tilde{A}_2\sqrt{\frac{s}{D}} = -1$$

$$\tilde{A}_1 = \tilde{A}_2 = \frac{1}{\sqrt{4Ds}}$$

$$\boxed{\tilde{P}(x,s) = \frac{1}{\sqrt{4Ds}}\, e^{-\sqrt{\frac{s}{D}}|x-x_0|}}$$

To conclude, we have to take an inverse Laplace transform. Calculations are in general non trivial, and it is customary to resort to tables.

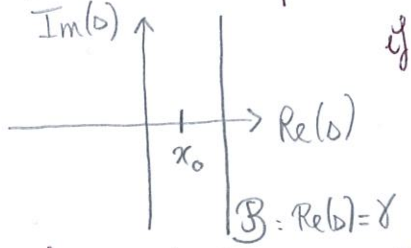
$$\text{Inverse Laplace}\left[\frac{e^{-a\sqrt{s}}}{\sqrt{s}}\right] = \frac{e^{-a^2/4\tau}}{\sqrt{\pi\tau}} \qquad (*)$$

thus $$P(x,\tau) = \text{Inverse Laplace}\left[\frac{1}{\sqrt{4Ds}}\, e^{-\sqrt{\frac{s}{D}}|x-x_0|}\right] = \frac{1}{\sqrt{4\pi D\tau}}\exp\left[-\frac{(x-x_0)^2}{4D\tau}\right]$$

meaning $$\boxed{P(x,t|x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}}\, e^{-\frac{(x-x_0)^2}{4D(t-t_0)}}}$$

Proof of (*) When $\tilde{P}(s) = \int_0^\infty P(\tau)\, e^{-s\tau}\, d\tau$ is known, how do we recover $P(\tau)$?

We have to assume that $\tilde{P}(s)$ is holomorphic for $\text{Re}(s) \geq x_0$, then we define the Bromwich line $\mathcal{B}$ as parallel to $y$ axis (thus in the holomorphic region) and we have,




if $|\tilde{P}(s)|$ is bounded on $\mathcal{B}$:

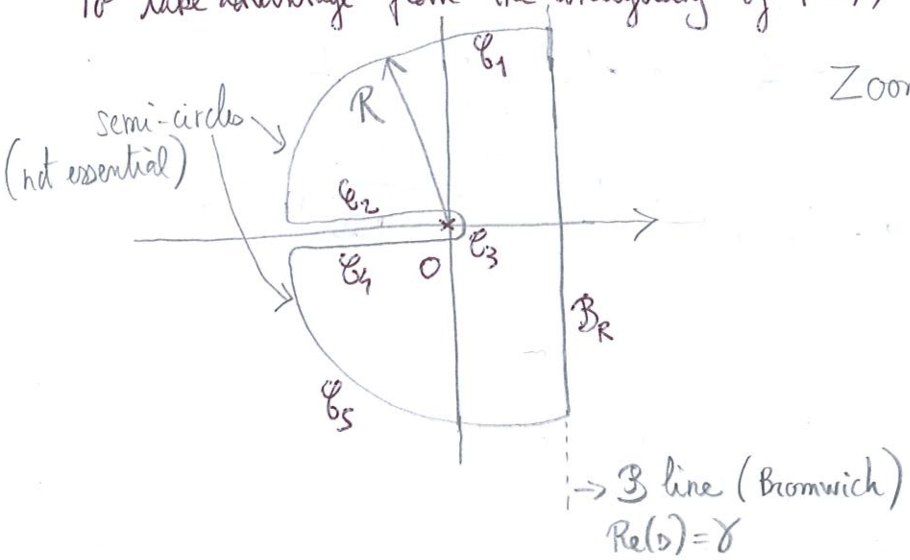
$$P(\tau) = \frac{1}{2i\pi}\int_{\mathcal{B}} \tilde{P}(s)\, e^{s\tau}\, ds$$

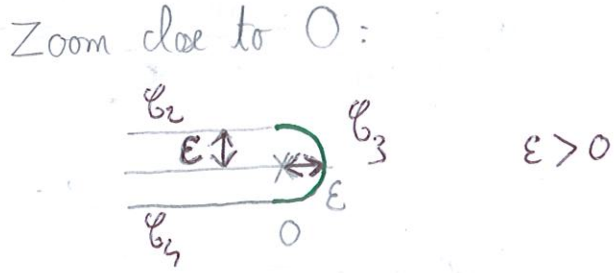
If all the singularities are in the left half-plane, then $\mathcal{B}$ can be taken as the line $\text{Re}(s)=0$, and the formula retrieves the inverse Fourier transform. Hence

$$\mathcal{L}_s^{-1}\left[\frac{e^{-a\sqrt{s}}}{\sqrt{s}}\right] = \frac{1}{2i\pi}\int_{\gamma-i\infty}^{\gamma+i\infty} \frac{e^{-a\sqrt{s}}}{\sqrt{s}}\, e^{s\tau}\, ds$$

The function $\frac{e^{-a\sqrt{s}}}{\sqrt{s}}$ is holomorphic on $\mathbb{C}$, except for $\text{Im}(s)=0$ and $\text{Re}(s) \leq 0$, because of $\sqrt{s}$, when the latter is defined as $\sqrt{\rho}\, e^{i\theta/2}$ for $s = \rho e^{i\theta}$ and $\theta \in [-\pi, \pi]$ : $\underset{\varepsilon>0}{\sqrt{-1+\varepsilon}} \simeq i$ ; $\sqrt{-1-\varepsilon} \simeq -i$

To take advantage from the analyticity of $\bar{F}(s)$, we define the following contour




From Cauchy theorem,

$$\int_{\mathcal{B}_R \cup \mathscr{C}_1 \cup \mathscr{C}_2 \cup \mathscr{C}_3 \cup \mathscr{C}_4 \cup \mathscr{C}_5} \frac{e^{-a\sqrt{s}}}{\sqrt{s}} e^{st}\, ds = 0$$

When $R \to \infty$, $\int_{\mathcal{B}_R} \to \int_{\mathcal{B}}$ is what we are looking for

$$\int_{\mathscr{C}_1} = \int_{\mathscr{C}_5} = 0 \quad ; \quad \left.\begin{array}{l} |e^{st}| \leqslant e^{\gamma t} \text{ fixed} \\ |e^{-a\sqrt{s}}| \leqslant 1 \end{array}\right\}$$

and it can be checked that $\int_{\mathscr{C}_3} \to 0$ for $\varepsilon \to 0$

On $\mathscr{C}_3$ : $s = \rho e^{i\theta}$, $-\pi \leqslant \theta \leqslant \pi$ ; $\rho = \varepsilon$

$$\frac{ds}{\sqrt{s}} = \frac{i\rho\, e^{i\theta}\, d\theta}{\sqrt{\rho}\, e^{i\theta/2}} \xrightarrow[\rho=\varepsilon\to 0]{} 0$$

and therefore, we are left with the integrals over $\mathcal{B}_R$, $\mathscr{C}_2$, $\mathscr{C}_4$ for $\begin{array}{l} R\to\infty \\ \varepsilon \to 0 \end{array}$

$$\int_{\mathcal{B}} = \lim_{R\to\infty} \int_{\mathcal{B}_R} = - \lim_{\substack{R\to\infty \\ \varepsilon\to 0^+}} \left[ \int_{\mathscr{C}_2} + \int_{\mathscr{C}_4} \right]$$

$$\int_{\mathscr{C}_2} = \int_{+\infty}^{0} d(-x)\, \frac{e^{-ia\sqrt{x}}\, e^{-xt}}{i\sqrt{x}} \qquad \text{on } \mathscr{C}_2 : s = -x = x\, e^{i\pi}, \quad \sqrt{s} = i\sqrt{x}$$

$$\int_{\mathscr{C}_4} = \int_{0}^{\infty} d(-x)\, \frac{e^{ia\sqrt{x}}\, e^{-xt}}{-i\sqrt{x}} \qquad \text{on } \mathscr{C}_4 : s = -x = x\, e^{-i\pi}, \quad \sqrt{s} = -i\sqrt{x}$$

$$\frac{1}{2i\pi}\int_{\mathcal{B}} = -\frac{1}{2i\pi}\int_{\mathscr{C}_2 \cup \mathscr{C}_4}$$

$$= -\frac{1}{2i\pi}\int_0^\infty dx\, \frac{e^{-xt}}{i\sqrt{x}} \left( e^{ia\sqrt{x}} + e^{-ia\sqrt{x}} \right)$$

$$\frac{1}{2i\pi}\int_B = \frac{1}{2\pi}\int_0^\infty dx \; \frac{e^{-xt}}{\sqrt{x}} \; 2\cos(a\sqrt{x})$$

$x = u^2$
$dx = 2u\,du$

$$= \frac{1}{\pi}\int_0^\infty du \; 2\, e^{-u^2 t}\cos(au)$$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} du \; e^{-u^2 t}\cos(au)$$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} du \; \underbrace{e^{-u^2 t}\, e^{iau}}_{e^{-t\left(u-\frac{ia}{2t}\right)^2}\; e^{-a^2/4t}}$$

$$= \frac{1}{\pi}\, e^{-a^2/4t}\sqrt{\frac{\pi}{t}}$$

$$= \frac{1}{\sqrt{\pi t}}\, e^{-a^2/4t} \quad \square$$

3°) <u>Third method</u> Irrespective of the specific form for the operator $\hat{H}$, we consider the eigenfunctions $\psi_\lambda(x)$ s.t $\hat{H}\psi_\lambda = \lambda\,\psi_\lambda$. Note that $\hat{H}$ is self-adjoint

They are orthogonal: $\int dx\, \psi_\lambda(x)\,\psi^*_{\lambda'}(x') = \delta_{\lambda,\lambda'}$

Once we know these eigenfunctions: to solve $\boxed{\partial_t P = -\hat{H} P}$, we seek for

$$P(x,0) = \sum_\lambda a_\lambda(0)\psi_\lambda(x)$$

$$\text{with } a_\lambda(0) = \int_{-\infty}^{+\infty} \underbrace{P(x,0)}_{\delta(x-x_0)}\,\psi^*_\lambda(x)\,dx = \psi^*_\lambda(x_0)$$

$$\text{ie } \delta(x-x_0) = \sum_\lambda \psi_\lambda(x)\,\psi^*_\lambda(x_0)$$

Then $P(x,t) = \sum_\lambda a_\lambda(t)\,\psi_\lambda(x) \Rightarrow \dfrac{da_\lambda}{dt} = -\lambda a_\lambda \Rightarrow a_\lambda(t) = \underbrace{a_\lambda(0)}_{\psi^*_\lambda(x_0)} e^{-\lambda t}$

$$P(x,t) \equiv P(x,t|x_0,t_0) = \sum_\lambda e^{-\lambda(t-t_0)}\,\psi_\lambda(x)\,\psi^*_\lambda(x_0)$$

<u>Rk</u> Another way to proceed is to use the bra-ket notation of quantum mechanics:

$$\langle x|\lambda\rangle = \psi_\lambda(x)$$

Starting from the initial condition $|x_0\rangle$, such that $\langle x|x_0\rangle = \delta(x-x_0)$, we apply $e^{-\hat{H}t}$ to evolve it by a time $t$. The formal solution to the diffusion equation is $\langle x|\,e^{-\hat{H}t}\,|x_0\rangle$

$$\langle x | e^{-\hat{H}t} | x_0 \rangle = \sum_{\lambda,\lambda'} \langle x | \lambda \rangle \langle \lambda | e^{-\hat{H}t} | \lambda' \rangle \langle \lambda' | x_0 \rangle$$

where we use $\sum_\lambda |\lambda\rangle\langle\lambda| = \mathbb{1}$

$$= \sum_{\lambda,\lambda'} \psi_\lambda(x) \; e^{-\lambda t} \delta_{\lambda\lambda'} \; \psi^*_{\lambda'}(x_0)$$

$$= \sum_\lambda \psi_\lambda(x) e^{-\lambda t} \psi^*_\lambda(x_0)$$

Here, we have $\hat{H} = -D\partial_x^2$. The eigenfunctions are plane waves

$$\hat{H}\psi_\lambda(x) = -D\frac{d^2\psi_\lambda}{dx^2} = \lambda\,\psi_\lambda(x) \quad ; \quad \psi_\lambda(x) = \underset{\substack{\downarrow \\ \text{normalization}}}{\mathcal{N}} e^{ikx} \quad ; \quad \lambda = Dk^2 \quad k = \sqrt{\lambda/D}$$

We index the eigenfunctions by $k$; they need to be normalized.
Here, $k$ is a continuous variable, and the orthonormalization condition reads

$$\delta(k-k') = \int dx \;\; \psi_k(x)\,\psi^*_{k'}(x)$$

$$= \mathcal{N}^2 \int dx \;\; \exp[ix(k-k')] = \mathcal{N}^2 \, 2\pi \; \delta(k-k')$$

$$\Rightarrow \psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

Then, $P(x,t|x_0,0) = \sum_\lambda \psi_\lambda(x) e^{-\lambda t} \psi^*_\lambda(x_0) \longrightarrow \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \, e^{ikx} \, e^{-Dk^2t} \, e^{-ikx_0}$

$$= \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) \qquad \square$$

Note that if we had computed from the outset the Fourier Transform of the diffusion equation, we would have gotten, for the Fourier components in space

$$\hat{P}(k,t) \equiv \int dx \;\; e^{ikx} P(x,t)$$

$$\partial_t \hat{P} = -Dk^2 \hat{P}(k,t)$$

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

and $P(x,t=0) = \delta(x-x_0)$

$$\Rightarrow \hat{P}(k,t=0) = e^{ikx_0}$$

Thus

$$P(x,t) = \int \frac{dk}{2\pi} \hat{P}(k,t) e^{-ikx}$$

$$= \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \; e^{-Dk^2 t} \; e^{-ik(x-x_0)}$$

with the same conclusion as above.

# Ornstein-Uhlenbeck process, linear response, and fluctuation-dissipation theorem

$$\dot{x}(t) = -\mu K x + \mu f(t) + \sqrt{2D}\, \xi(t)$$

1°) $D$ is the diffusion coefficient, $\mu$ is the mobility. Since the suspending fluid is at equilibrium, $D = \mu kT$

2°) $$\boxed{x(t) = x_0\, e^{-K\mu(t-t_0)} + \int_{t_0}^{t} e^{-K\mu(t-t')}\left[\mu f(t') + \sqrt{2D}\,\xi(t')\right] dt'} \quad (1)$$

as found by "variation of the constant".

$$\Rightarrow \boxed{\langle x(t)\rangle = x_0\, e^{-K\mu(t-t_0)} + \int_{t_0}^{t} e^{-K\mu(t-t')}\mu f(t')\,dt'} \quad (2)$$

3°) We have already done this calculation for $\langle v(0)v(t)\rangle_{eq}$ in the process $\dot{v} = -\gamma v + R(t)$.

Method 1 : we use the trajectory solution (1), with $t_0 \to -\infty$, to leave time to the p to be equilibrated:

$$x(t) = \int_{-\infty}^{t} e^{-K\mu(t-t')}\sqrt{2D}\,\xi(t')\,dt' \qquad \text{since } f = 0$$

$$\Rightarrow \langle x(0)x(t)\rangle_{eq} = \int_{-\infty}^{0} dt' \int_{-\infty}^{t} dt''\, e^{-K\mu(0-t'+t-t'')}\, 2D \underbrace{\langle \xi(t')\xi(t'')\rangle}_{\delta(t'-t'')}$$

Take here $t>0$:

$$\langle x(0)\,x(t)\rangle_{eq} = \int_{-\infty}^{0} dt'\, e^{-K\mu(t-2t')}\, 2D$$

$$= \frac{2D}{2K\mu}\, e^{-K\mu t}\left[e^{2K\mu t'}\right]_{-\infty}^{0}$$

$$= \frac{D}{K\mu}\, e^{-K\mu t} \qquad \text{and } D = \mu kT$$

By parity of $\langle x(0)x(t)\rangle_{eq}$, we know then that for $t$ of arbitrary sign

$$\boxed{\langle x(0)\,x(t)\rangle_{eq} = \frac{kT}{K}\, e^{-K\mu|t|}}$$

Method 2

$$\frac{d}{dt}\langle x(t')x(t)\rangle_{eq} = \langle x(t')\,\dot{x}(t)\rangle_{eq} = -K\mu\,\langle x(t')x(t)\rangle_{eq} + \sqrt{2D}\underbrace{\langle x(t')\,\xi(t)\rangle}_{0 \text{ for } t>t'}$$

$$\Rightarrow \langle x(t)x(t')\rangle = A(t')\,e^{-K\mu t} \qquad \text{for } t > t'$$

Since we know, by equipartition, that $\langle x^2(t)\rangle_{eq} = \langle x^2(t')\rangle_{eq} = \frac{kT}{K}$, we deduce $A(t')$ : $\frac{kT}{K} = A(t')\,e^{-K\mu t'}$

Thus $\langle x(t)\,x(t')\rangle_{eq} = \frac{kT}{K}\, e^{-K\mu(t-t')}$ for $t > t'$

$= \frac{kT}{K}\, e^{-K\mu|t-t'|}$ by parity.

4°) If a static force is applied since prehistoric times: $f = K\langle x\rangle$ ; $\boxed{\langle x\rangle = \frac{f}{K}}$
(behavior of a spring of stiffness $K$). We can check this from (2), with $t_0 \to -\infty$:

$$\langle x\rangle = 0 + \int_{-\infty}^{t} e^{-K\mu(t-t')}\,\mu f\,dt' = \frac{\mu f}{K\mu} = \frac{f}{K}$$

But we can also invoke

$$\langle x\rangle = f\int_{-\infty}^{t} \chi(t-t')\,dt' = f\int_0^{\infty} \chi(\tau)\,d\tau \qquad \tau = t-t'$$

and $\chi(\tau) = -\beta\,\theta(\tau)\,\frac{d}{d\tau}\langle x(\tau)\,x(0)\rangle_{eq} \Rightarrow \int_0^{\infty}\chi(\tau)\,d\tau = \beta\langle x^2\rangle_{eq}$

Hence $\langle x\rangle = \frac{f}{K} = f\beta\langle x^2\rangle_{eq}$. $\Rightarrow \boxed{\langle x^2\rangle_{eq} = \frac{kT}{K}}$

5°) For $t_0 \to -\infty$, we compare Eq.(2) with $\langle x(t)\rangle = \int_{-\infty}^{t} \chi(t-t')\,f(t')\,dt'$, and we get

$$\chi(\tau) = \mu\, e^{-K\mu\tau} \quad \text{for } \tau > 0$$
$$= 0 \quad \text{for } \tau < 0 \quad \text{(from causality)}$$

$$\frac{d}{d\tau}\underbrace{\langle x(\tau)\,x(0)\rangle_{eq}}_{\mathcal{C}(\tau)} = \frac{kT}{K}(-K\mu)\,e^{-K\mu\tau} \quad \text{for } \tau > 0$$
$$= -\mu kT\, e^{-K\mu\tau}$$

$$\boxed{\chi(\tau) = -\beta\,\theta(\tau)\,\frac{d\mathcal{C}}{d\tau}}$$

Fluctuation-dissipation theorem is obeyed

6°) For every finite $K$, no matter how small, FDT is obeyed; an equilibrium exists.
Yet, it takes longer and longer to equilibrate: characteristic time $\frac{1}{K\mu} \to \infty$.
When $K = 0$ from the outset: $\chi(\tau) = \mu\,\theta(\tau)$

$$\langle x(\tau)\,x(0)\rangle = 2D\tau \quad \text{for } \tau > 0$$

and thus $\chi(\tau) \neq -\beta\,\theta(\tau)\,\frac{d}{d\tau}\langle x(\tau)\,x(0)\rangle$

The reason for the breakdown of fluctuation-dissipation is that there is here no equilibrium. The fluctuation-dissipation theorem is an equilibrium result.

# 11 Generalized Feynman-Kac relations

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

$t_0 \ll t$

$$Q(x_0,t,t_0) = \left\langle f(x(t),t)\, e^{-\int_{t_0}^{t} V(x(\tau),\tau)\,d\tau} \right\rangle$$

average fixing $x(t_0)=x_0$

does not depend on $\Omega_0$.

1°) the propagator $p(x,\Omega,t|x_0,\Omega_0,t_0)$ obeys

$$\partial_{t_0} p = -V(x_0,t_0)\,\partial_{\Omega_0} p - \mu F(x_0,t_0)\,\partial_{x_0} p - D\,\partial_{x_0}^2 p$$

and we have: $$Q(x_0,t,t_0) = \int dx\, d\Omega\; f(x,t)\, e^{-(\Omega-\Omega_0)}\, p(x,\Omega,t|x_0,\Omega_0,t_0)$$

$$\Rightarrow \partial_{t_0} Q = \int dx\, d\Omega\; f(x,t)\, e^{-(\Omega-\Omega_0)}\, \partial_{t_0} p$$

$$= -e^{\Omega_0}\, V(x_0,t_0)\, \underbrace{\partial_{\Omega_0} \underbrace{\int dx\, d\Omega\, f(x,t)\, e^{-(\Omega)}}_{e^{-\Omega_0} Q}}_{= -e^{-\Omega_0} Q} - \mu F(x_0,t_0)\,\partial_{x_0} Q - D\,\partial_{x_0}^2 Q$$

$$\Rightarrow \boxed{\partial_{t_0} Q + D\,\partial_{x_0}^2 Q + \mu F(x_0,t_0)\,\partial_{x_0} Q - V(x_0,t_0)\, Q = 0}$$

$$Q(x_0,t_0,t_0) = \langle f(x_0,t_0) \rangle_{\to \text{fixing } x_0} = f(x_0,t_0).$$

When $V=0$, we already get a non trivial equation for $Q(x_0,t,t_0) = \langle f(x(t),t) \rangle$ at fixed $x(0)=x_0$

2°) We consider another functional, related to the previous one:

$$\mathcal{Q}(x_0,t,t_0) = \int_{t_0}^{t} dt'\, Q(x_0,t',t_0)$$

$$\Rightarrow \partial_{t_0} \mathcal{Q} = -Q(x_0,t_0,t_0) + \int_{t_0}^{t} dt'\, \partial_{t_0} Q(x_0,t',t_0)$$

$$= -f(x_0,t_0) + \int_{t_0}^{t} dt' \left[ -D\,\partial_{x_0}^2 Q - \mu F(x_0,t_0)\,\partial_{x_0} Q + V(x_0,t_0)\, Q \right]$$

$$= -f(x_0,t_0) - D\,\partial_{x_0}^2 \mathcal{Q} - \mu F(x_0,t_0)\,\partial_{x_0} \mathcal{Q} + V(x_0,t_0)\,\mathcal{Q} \quad \square$$

12 - Martingales for the asymmetric random walk

The jump at step $i$ is $\eta_i$ $\begin{cases} \to 1, \text{ proba } p \\ \to -1, \text{ proba } q = 1-p \end{cases}$

Position after $n$ steps: $X_n = \sum_{i=1}^{n} \eta_i$ ; $X_0 = 0$ is the starting point

$$M_n \equiv \left(\frac{q}{p}\right)^{X_n} \quad ; \quad \langle M_n | X_{n-1} \rangle = p \left(\frac{q}{p}\right)^{X_{n-1}+1} + q \left(\frac{q}{p}\right)^{X_{n-1}-1}$$

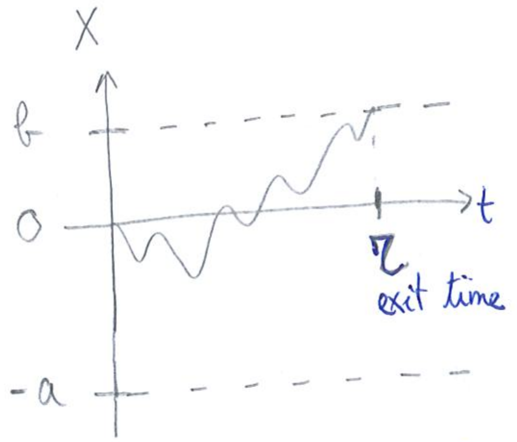
$$= \left(\frac{q}{p}\right)^{X_{n-1}} \left[ p \frac{q}{p} + q \frac{p}{q} \right] = \left(\frac{q}{p}\right)^{X_{n-1}}$$

$= M_{n-1}$ and $M_n$ is thus a martingale

$$M'_n \equiv X_n - n(p-q) \; ; \; \langle M'_n | X_{n-1} \rangle = X_{n-1} + p - q - n(p-q)$$

$$= X_{n-1} - (n-1)(p-q) = M'_{n-1}$$

Since $X_n = X_{n-1} + \eta_n$ ; $\langle \eta_n \rangle = p - q$




Since $M_n$ is a martingale, and $\tau$ is a stopping time that is bounded on average

$$\langle M_\tau \rangle = M_0 = 1$$

$$\Rightarrow \left\langle \left(\frac{q}{p}\right)^{X_\tau} \right\rangle = 1$$

and $X_\tau$ only takes 2 values, $b$ or $-a$, with (splitting) probabilities $\Pr[X_\tau = b]$ and $\Pr[X_\tau = -a]$:

$$\left\langle \left(\frac{q}{p}\right)^{X_\tau} \right\rangle = \left(\frac{q}{p}\right)^{b} \Pr[X_\tau = b] + \left(\frac{q}{p}\right)^{-a} \Pr[X_\tau = -a]$$

Besides: $\Pr[X_\tau = b] + \Pr[X_\tau = -a] = 1$

$$\Rightarrow 1 = \left[ \left(\frac{q}{p}\right)^{b} - \left(\frac{q}{p}\right)^{-a} \right] \Pr[X_\tau = b] + \left(\frac{q}{p}\right)^{-a}$$

$$\boxed{\Pr[X_\tau = b] = \frac{1 - (q/p)^a}{1 - (q/p)^{a+b}} \; ; \; \Pr[X_\tau = -a] = \frac{1 - (p/q)^b}{1 - (p/q)^{a+b}}}$$

and we check that these 2 probab are symmetric upon $a \Leftrightarrow b$, $p \Leftrightarrow q$

In a second step, we use the martingale $M'_n = X_n - n(p-q)$, to which we also apply Doob's stopping theorem:

$$\langle M'_\tau \rangle = M'_0 = 0$$

$$\Rightarrow \langle X_\tau \rangle = \langle \tau \rangle (p-q)$$

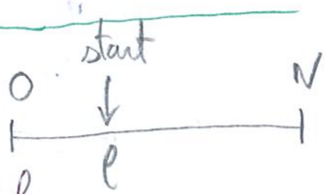
$$\Rightarrow \langle \tau \rangle = \frac{1}{p-q}\left[ b \cdot P_r[X_\tau = b] - a\, P_r[X_\tau = -a] \right]$$

$$= \frac{1}{p-q}\left[ b\,\frac{1-\left(\frac{q}{p}\right)^a}{1-\left(\frac{q}{p}\right)^{a+b}} - a\,\frac{\left(\frac{q}{p}\right)^{a+b} - \left(\frac{q}{p}\right)^a}{\left(\frac{q}{p}\right)^{a+b} - 1} \right]$$

$$= \frac{1}{p-q}\left[\frac{1}{1-\left(\frac{q}{p}\right)^{a+b}}\right]\left[ b - b\left(\frac{q}{p}\right)^a + a\left(\frac{q}{p}\right)^{a+b} - a\left(\frac{q}{p}\right)^a \right]$$

$$= \frac{1}{p-q}\,\frac{1}{1-\left(\frac{q}{p}\right)^{a+b}}\left[ a+b - b\left(\;\right)^a + a\left[\left(\frac{q}{p}\right)^{a+b} - 1\right] - a\left(\frac{q}{p}\right)^a \right]$$

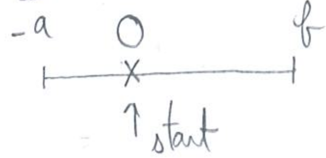
$$\boxed{\langle \tau \rangle = \frac{1}{p-q}\left[ -a + (a+b)\,\frac{1-\left(\frac{q}{p}\right)^a}{1-\left(\frac{q}{p}\right)^{a+b}} \right]}$$




This has to be compared to where we got the mean escape time $\langle T(\ell)\rangle$, starting from site $\ell$

$$\langle T(\ell)\rangle = \frac{1}{p-q}\left[ -\ell + N\,\frac{1-(q/p)^\ell}{1-(q/p)^{a+b}} \right]$$

see Tutorial




↳ same result, since $N \Leftrightarrow a+b$

$\ell \Leftrightarrow a \quad (>0)$

# Algebraic area enclosed by a random walk

1°) For a given closed walk with $n$ steps, and $k$ steps made along $x$ (horizontal) there are $\binom{n}{k}$ choices of these "horizontal" steps; the remaining $n-k$ steps are along $y$. We have $0 \leqslant k \leqslant n$. For a given $k$, $k/2$ steps have to be to the right, and $k/2$ to the left, for a total of $\binom{k}{k/2}$ walks. Likewise, there are $\binom{n-k}{\frac{n-k}{2}}$ possible sequences of up-down moves (vertical)

The number of closed path is then

$$\sum_{\substack{k=0\\k\text{ even}}}^{n} \binom{n}{k}\binom{k}{k/2}\binom{n-k}{\frac{n-k}{2}} = \sum_{\substack{k=0\\k\text{ even}}} \frac{n!}{\cancel{k!(n-k)!}} \frac{\cancel{k!}}{\left[(k/2)!\right]^2} \frac{\cancel{(n-k)!}}{\left[\left(\frac{n-k}{2}\right)!\right]^2}$$

$$= \frac{n!}{\left[\left(\frac{n}{2}\right)!\right]^2} \underbrace{\sum_{\substack{k=0\\k\text{ even}}}^{n} \binom{n/2}{k/2}^2}$$

$$= \sum_{j=0}^{n/2} \binom{n/2}{j}^2 = \binom{n}{n/2}$$

Indeed, we can form $\binom{2p}{p}$ teams of $p$ players among a group of $2p$. We put a cap to $p$ players, the others have no cap. Denoting $j$ the number of players with a cap, there are $\binom{p}{j}$ choices of players with cap, $\binom{p}{p-j}$ choices of players without a cap, and then

$$\binom{2p}{p} = \sum_{j=0}^{p} \binom{p}{j}\binom{p}{p-j} = \sum_{j=0}^{p} \binom{p}{j}^2$$

$$= \boxed{\binom{n}{n/2}^2 \quad \text{closed random walks}}$$

2°) Consider the path  with $n = 4$, ie $r u r^{-1} u^{-1}$ and we replace $ru$ by $Qur$ : we get $Q u r r^{-1} u^{-1} = Q$. Similarly, for 

$$u r u^{-1} r^{-1} = \frac{1}{Q} r u u^{-1} r^{-1} = Q^{-1} .$$

In a sequence of $u, u^{-1}, r, r^{-1}$ associated to a closed path, there are as many $u$ and $u^{-1}$ (up/down moves) and as many $r$ and $r^{-1}$ (right/left moves).

The goal is to replace $ur$ by $\frac{1}{Q} ru$ or $ru$ by $Qur$ or $u$ by $\frac{1}{Q} r u r^{-1}$ ...
so that the walk "simplifies", from $u u^{-1} = u^{-1} u = 1 = r r^{-1} = r^{-1} r$.

Take a plaquette with $A = 4$:

 $\Leftrightarrow$ $u^{-1} u^{-1} r \underbrace{\boxed{r u}}_{Qur} u r^{-1} r^{-1}$

$\downarrow$

$Q u^{-1} u^{-1} r u \underbrace{\boxed{r u}}_{Qur} r^{-1} r^{-1}$ $\Leftrightarrow$ 

$\downarrow$

$Q^2 u^{-1} u^{-1} r u u \underbrace{r r^{-1}}_{1} r^{-1}$ $\Leftrightarrow$ 


etc until we get $Q^4$.

When we trade a $ru$  for a $ur$ , we get a factor $Q$ and this keeps track of the unit cell that is removed. We end up with $Q^A \times$ a trivial sequence ie a sequence like $\underbrace{\underbrace{r r^{-1}}_{1} r \underbrace{u u^{-1}}_{1} r^{-1}}_{1}$