(Lesson 4 of 14/10/19) Compiled: October 29, 2019

Summary of the last lessons. Analysing the dynamics of the Diffusion Problem led to the Master Equation, which in the symmetrical case reduces to:

$$w_i(t_{n+1}) = \frac{1}{2}(w_{i-1}(t_n) + w_{i+1}(t_n)) \tag{1}$$

where $w_i(t_n)$ is the (mass) probability function for a particle, i.e. $w_i(t_n)$ is the probability that a particle will be at position $x_i = i \cdot l$ at time $t_n = n \cdot \epsilon$.
Further evaluation, in terms of the Binomial distribution, leads to the exact solution:

$$w_i(t_n) = \frac{1}{2^n}\binom{n}{n_+} \tag{2}$$

where n_+ is a random variable representing the number of steps in which the particle moves to the *right*.
Then we considered the continuum limit, with $l, \epsilon \downarrow 0$ (keeping $l^2\epsilon^{-1} = 2D$ constant), arriving to:

$$w_i(t_n) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{3}$$

which is the pdf for a particle that starts at $x = 0$ at $t = 0$.

0.1 Continuum limit of the Master Equation

The same result can be obtained by taking directly the continuum limit of the ME (1), which will lead to a differential equation that can *then* be solved.

Not so sure about this part

We start by recalling that, for a fine discretization, $w_i(t_n)$ is approximately equal to the probability of being around a generic (x, t) (i.e. $W(x, t)\Delta x$), up to a normalization constant:

$$W(x_0, t_n)\Delta x = \mathbb{P}(x \in [x_0 - \Delta x/2, x_0 + \Delta x/2]) \approx \frac{\Delta x}{2l} w_{i_0}(t_n) \qquad i_0 = \lfloor \Delta x/l \rceil$$

And so, with a slight abuse of notation:

$$w_i(t_n) \approx 2lW(x, t) \qquad i = \lfloor x/l \rceil, n = \lfloor t/\epsilon \rceil$$

Substituting in (1) leads to:

$$\cancel{2l}W(x, t + \epsilon) = \cancel{2l}\frac{1}{2}(W(x - l, t) + W(x + l, t)) \tag{4}$$

which means that an analogous Master Equation holds even for $W(x, t)$, which is a continuous pdf, and thus can be differentiated. In particular, we can compute $W(x, t + \epsilon)$ in terms of $W(x, t)$ (and derivatives) by expanding around $\epsilon = 0$:

$$W(x, t + \epsilon) = W(x, t) + \epsilon \frac{\partial}{\partial \tau} W(\chi, \tau)\Big|_{(x,t)} + \frac{\epsilon^2}{2} \frac{\partial^2}{\partial \tau^2} W(\chi, \tau)\Big|_{(x,t)} + O(\epsilon^3) \tag{5}$$

And also $W(x \pm l, t)$ by expanding around $l = 0$:

$$W(x \pm l, t) = W(x,t) \pm l \frac{\partial}{\partial \chi} W(\chi, \tau)\Big|_{(x,t)} + \frac{l^2}{2} \frac{\partial^2}{\partial \chi^2} W(\chi, \tau)\Big|_{x,t} + O(l^3) \tag{6}$$

We then introduce the following notation for the space and time derivatives:

$$\dot{W}(x,t) = \frac{\partial}{\partial \tau} W(\chi, \tau)\Big|_{(x,t)} \qquad W'(x,t) = \frac{\partial}{\partial \chi} W(\chi, \tau)\Big|_{(x,t)}$$

so that a space derivative is denoted with a' (a'' for the second derivative), and a time derivative with $\dot{a}$ ($\ddot{a}$ for the second derivative).
We can now substitute back in (4). We start with the right side:

$$W(x+l,t) + W(x-l,t) = 2W(x,t) + l^2 W''(x,t) + O(l^4)$$

where the $O(l^4)$ is given by the cancellation of the odd powers (including l^3). Equating to the left side of (4) leads to:

$$\cancel{W(x,t)} + \epsilon \dot{W}(x,t) + \frac{\epsilon^2}{2} = \cancel{W(x,t)} + \frac{l^2}{2} W''(x,t) + O(l^4)$$

Dividing by ϵ:

$$\begin{aligned} \dot{W}(x,t) + \frac{\epsilon}{2} \ddot{W}(x,t) &= \underbrace{\frac{l^2}{2\epsilon}}_{D} W''(x,t) + O\left(\frac{l^4}{\epsilon}\right) \\ &= DW''(x,t) + O(4\epsilon D^2) \end{aligned}$$

If we now take the continuum limit, then $\epsilon, l \to 0$ with the ratio $D = l^2/(2\epsilon)$ fixed, both $\ddot{W}(x,t)$ and the error term vanish, leading to the **diffusion equation**:

$$\dot{W}(x,t) = DW''(x,t) \tag{7}$$

0.1.1 Solution of the Continuous Master Equation

We want now to solve (7), and show that the solution will be the same we previously derived in (3).
So, we start from:

$$\partial_t W(x,t) = D \partial_x^2 W(x,t)$$

This is a second order partial differential equation. To be able to solve it, we must first define its **boundary conditions**. In this case, we suppose that the particle is unconstrained, and so the spatial domain coincides with $\mathbb{R}$.
As $W(x,t)$ is a pdf, the following conditions must hold:

$$W(x,t) \geq 0 \quad \forall (x,t) \qquad \int_{\mathbb{R}} W(x,t) = 1$$

From the normalization, it follows that $W(x,t)$ - and its spatial derivative $W'(x,t)$ - must vanish as $|x| \to \infty$, so that the integral does not diverge:

$$\lim_{|x|\to\infty} W(x,t) = 0 \qquad \lim_{|x|\to\infty} W'(x,t) = 0$$

However, it is not obvious that $W(x,t) \geq 0$ will always hold, assuming we choose an initial condition $W(x,t_0) \geq 0$. This will be obvious *a posteriori* - and in fact can justified by the peculiar properties of this differential equation.

To solve (7), as the spatial domain is all $\mathbb{R}$, one standard technique is that of Fourier integral transform. This is in fact suggested by the spatial translational invariance of solutions of (7), i.e. if $W(x,t)$ is a solution, then also $\tilde{W}$
Note that the equation is translationally invariant, meaning that if $W(x,t)$ is a solution, also $W(x+y,t)$ is a solution. This is because the space coordinate appears only in a *second-order derivative*.
This suggests a way to solve the equation, by starting from the eigenfunctions of the laplacian, i.e. the solutions of the eigenvalue equation:

$$\partial_x^2 \varphi_k(x) = \lambda_k \varphi_k(x) \qquad \lambda_k \equiv -k^2$$

which are:

$$\varphi_k(x) = A_k e^{\pm ikx} \qquad k \in \mathbb{R}$$

as can easily be checked by substitution.
Note that, as $k \in \mathbb{R}$, the $\pm$ is redundant and can be removed:

$$\varphi_k(x) = A_k e^{ikx}$$

These eigenfunctions are the basis of the Fourier transform - that is every function can be expressed as a (infinite) linear combination of these $\varphi_k(x)$.
We choose $A_k = 1$ for simplicity, and then:

$$W(x,t) = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikx} c_k(t)$$

where the 2π factor is inserted by convention (as in Fourier transforms).
Recall the orthogonality relation:

$$\int_{\mathbb{R}} \mathrm{d}x\, \varphi_k(x)^* \varphi_{k'}(x) = \int_{\mathbb{R}} \mathrm{d}x\, e^{i(k'-k)x} = 2\pi\delta(k-k')$$

and also:

$$\int_{\mathbb{R}} \frac{\mathrm{d}k}{2\pi} \varphi_k(x)^* \varphi_k(x') = \cdots = \delta(x-x')$$

So, by multiplying both sides by $e^{-ik'x}$ and integrate over x we get:

$$\int_{\mathbb{R}} W(x,t) e^{-ik'x}\, \mathrm{d}x = \int_{\mathbb{R}} \frac{\mathrm{d}k}{2\pi} \int_{\mathbb{R}} \mathrm{d}x\, e^{i(k-k')x} c_k(t)$$

and we can apply the orthogonality relation, arriving to:

$$\int_{\mathbb{R}} W(x,t)e^{-ik'x}\,\mathrm{d}x = \int_{\mathbb{R}} \mathrm{d}k\,\delta(k-k')c_k(t) = c_{k'}(t)$$

and so:

$$c_k(t) = \int_{\mathbb{R}} \mathrm{d}x\, e^{-ikx}W(x,t)$$

Differentiating wrt t:

$$\begin{aligned}\dot{c}_k(t) &= \int_{\mathbb{R}} \mathrm{d}x\, e^{-ikx}\dot{W}(x,t) = D\int_{-\infty}^{\infty} e^{-ikx}W''(x,t)\,\mathrm{d}x = \\ &= DW'(x,t)e^{-ikx}\Big|_{-\infty}^{\infty} - D\int_{-\infty}^{\infty}\partial_x(e^{-ikx})W'(x,t)\,\mathrm{d}x = \\ &= -D\underbrace{(\partial_x e^{-ikx})}_{-ike^{-ikx}}W(x,t)\Big|_{-\infty}^{\infty} + D\int_{\mathbb{R}}\underbrace{\partial_x^2(e^{-ikx})}_{-k^2e^{-ikx}}W(x,t)\,\mathrm{d}x\end{aligned}$$

And so:

$$\dot{c}_k(t) = \int_{\mathbb{R}} \mathrm{d}x\, e^{-ikx}\dot{W}(x,t) = -Dk^2c_k(t)$$

and by integrating we arrive at the solution:

$$c_k(t) = e^{-Dk^2t}c_{k\_}(0) = e^{-Dk^2t}\int \mathrm{d}x_0\, e^{-ikx}W(x_0,0)$$

and finally:

$$\begin{aligned}W(x,t) &= \int \frac{\mathrm{d}k}{2\pi}e^{ikx-Dk^2t}\int \mathrm{d}x_0\, e^{-ikx_0}W(x_0,0) = \\ &= \int \mathrm{d}x_0\left[\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}e^{-Dk^2t+i(k(x-x_0))}\right]W(x_0,0)\end{aligned}$$

This integral can be computed with the Cauchy residual theorem, by shifting the integral path by $ik(x-x_0)$ on the complex plane. We then arrive to:

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

and the general solution is:

$$W(x,t) = \int \mathrm{d}x_0\,\frac{\exp\left(-\frac{(x-x_0)^2}{4Dt}\right)}{\sqrt{4\pi Dt}}W(x_0,0)$$

If we choose an infinite density for the initial condition:

$$W(x_0,0) = \delta(x_0)$$

then the solution (given that the particle was at x_0 at $t=0$) will be:

$$W(x,t|x_0,0) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right)$$

More generally:

$$W(x,t|x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left(-\frac{(x-x_0)^2}{4D(t-t_0)}\right) \qquad W(x,t|x_0,t_0) = \delta(x-x_0)$$

We will refer to this as a **propagator**.
Note that we can rewrite it as:

$$W(x,t|x_0,t_0) = \int \mathrm{d}x_0 \, W(x,t|x_0,t_0)W(x_0,t_0)$$

Let $x_0 = 0 = t_0$, leading to:

$$W(x,t|0,0) = (4\pi Dt)^{-1/2} \exp\left(-\frac{x^2}{4Dt}\right)$$

We will now talk about the concept of **scale invariance**.
We start from:

$$\partial_t W(x,t) = D\partial_x^2 W(x,t); \qquad x' = \lambda x, t' = \lambda^2 t$$

so that:

$$\frac{\partial}{\partial t'} = \frac{1}{\lambda^2}\frac{\partial}{\partial t}; \qquad \frac{\partial}{\partial x'} = \frac{1}{\lambda}\frac{\partial}{\partial x}$$

By rearranging, we can write the differential equation as the action of an operator:

$$(\partial_t - D\partial_x^2)W(x,t) = 0$$

which satisfies:

$$\frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2} = \frac{1}{\lambda^2}\left(\frac{\partial}{\partial t'} - D\frac{\partial^2}{\partial x'^2}\right)$$

So if $W(x,t)$ is a solution, then also $W(\lambda x, \lambda^2 t)$ is a solution. For a general integral:

$$\begin{aligned} W(x,t|0,0) &= (4\pi Dt)^{-1/2} \exp\left(-\frac{x^2}{4Dt}\right) \\ W(\lambda x, \lambda^2 t|0,0) &= (4\pi D\lambda^2 t)^{-1/2} \exp\left(-\frac{\cancel{\lambda^2} x^2}{4Dt\cancel{\lambda^2}}\right) \\ &= \frac{1}{\lambda} W(x,t|0,0) \end{aligned}$$

But why are we getting an extra factor of λ?
Recall that $W(x,t)$ is a probability density, so that it is normalized:

$$1 = \int_{-\infty}^{\infty} \mathrm{d}x\, W(x,t)$$

So, if we rearrange:

$$\lambda W(\lambda x, \lambda^2 t|0,0) = W(x,t|0,0)$$

and then integrate both sides:

$$\int \mathrm{d}x\, \lambda W(\lambda x, \lambda^2 t|0,0) = \int \mathrm{d}z\, W(z, \lambda^2 t|0,0) = 1$$

The two integrals are the same up to a change of variables: $x' = \lambda x$, $\mathrm{d}x' = \lambda\, \mathrm{d}x$.
By choosing $\lambda = 1/\sqrt{t}$ we get:

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

Note that this property can be derived even if we do not know the explicit solution:

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

In fact, by an argument of dimensional analysis, note that $[D] = L^2/t$, and so $[Dt] = [x^2]$. Recall that $[W] = 1/x$, as it is a pdf, and $W\,\mathrm{d}x$ is a pure number. So:

$$W(x,t|0,0) = \frac{1}{x}\frac{x}{\sqrt{Dt}}) = \frac{1}{\sqrt{Dt}} \underbrace{\frac{\sqrt{Dt}}{x} F\left(\frac{x}{\sqrt{Dt}}\right)}_{f(x/\sqrt{Dt})}$$

where F is dimensionless, and $1/x$ restores the correct dimensions.
But if we consider also the initial conditions, we have an extra parameter that can be added to the function:

$$W(x,t|x_0,t_0)$$

However, by translational invariance, we can simply translate time and space:

$$W(x-x_0, t-t_0|0,0)$$

Now, we start again from:

$$\begin{aligned} W(x,t) &= \int \mathrm{d}x_0\, \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left(-\frac{(x-x_0)^2}{4D(t-t_0)}\right) W(x_0,t_0) = \\ &= \int d\,\mathrm{d}x_0\, W(x,t|x_0,t_0) W(x_0,t_0) \end{aligned}$$

and ask what is the probability that a particle will be at position x_2 at $t = t_2$, given that the initial condition was x_1 at t_1.
We now that:

$$\mathbb{P}(x, t|x_0, t_0) \equiv W(x, t|x_0, t_0)$$

But can we derive the same result by using the propagator?

$$\begin{aligned} W(x_2, t_2) &= \int \mathrm{d}x_0\, W(x_2, t_2|x_0, t_0) W(x_0, t_0) \\ W(x_1, t_1) &= \int \mathrm{d}x_0\, W(x_1, t_1|x_0, t_0) W(x_0, t_0) \end{aligned}$$

In principle, we can also write what happens at t_2 in terms of what happens at t_1:

$$W(x_2, t_2) = \int \mathrm{d}x_1\, W(x_2, t_2|x_1, t_1) W(x_1, t_1)$$

If we substitute $W(x_1, t_1)$ in there:

$$W(x_2, t_2) = \iint \mathrm{d}x_1\, \mathrm{d}x_0\, W(x_2, t_2|x_1, t_1) W(x_1, t_1|x_0, t_0) W(x_0, t_0)$$

By comparing with the previous integrals, we find that:

$$W(x_2, t_2|x_0, t_0) = \int \mathrm{d}x_1\, W(x_2, t_2|x_1, t_1) W(x_1, t_1|x_0, t_0)$$

This is the **ESCK** property of the propagator.
Then, using gaussian integration:

$$W(x, t|x_0, t_0) = \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp\left(-\frac{(x - x_0)^2}{4D(t - t_0)}\right)$$

(verify it as exercise).

Returning to the integral we found:

$$\mathbb{P}(x_2, t_2; x_1, t_1; x_0, t_0) = W(x_2, t_2|x_1, t_1) W(x_1, t_1|x_0, t_0) W(x_0, t_0)$$

This is the joint probability that the particle arrives at x_1 at t_1 and then at x_2 at t_2, given that it started in x_0 at t_0.
We can then compute:

$$\langle x(t_2) x(t_1) \rangle = \iint \mathrm{d}x_1\, \mathrm{d}x_2\, \mathbb{P}(x_2, t_2; x_1, t_1) x_2 x_1$$

Let's do an example. Consider:

$$\mathbb{P}(x_2, t_2; x_1, t_1|0, 0) = \mathbb{P}(x_2, t_2; x_1, t_1; 0, 0) \frac{1}{W(0, 0)} = W(x_2, t_2|x_1, t_1) W(x_1, t_1|0, 0)$$

we want to compute $\langle x(t_2)x(t_1)\rangle$:

$$\langle x(t_2)x(t_1)\rangle = \iint \mathrm{d}x_1\,\mathrm{d}x_2\,x_1x_2\frac{\exp\left(-\frac{(x_2-x_1)^2}{4D(t_2-t_1)}\right)}{\sqrt{4\pi D(t_2-t_1)}}\frac{\exp\left(-\frac{x_1^2}{4Dt_1}\right)}{\sqrt{4\pi Dt_1}}$$

Changing variables ($x_1 = y_1$, $x_2 - x_1 = y_2$) we get:

$$= \frac{1}{\sqrt{4\pi D(t_2-t_1)}}\frac{1}{\sqrt{4\pi Dt_1}}\iint \mathrm{d}y_1\,\mathrm{d}y_2\,y_1(y_1+y_2)\exp\left(-\frac{y_2^2}{4D(t_2-t_1)}-\frac{y_1^2}{4Dt_1}\right)$$

Notice that the exponential is an even function, and y_1y_2 is odd, so only the term with y_1^2 remains. We arrive at:

$$\begin{aligned}\langle x(t_2)x(t_1)\rangle &= \frac{1}{\sqrt{4\pi D(t_2-t_1)}}\frac{1}{\sqrt{4\pi Dt_1}}\int \mathrm{d}y_1\,y_1^2\exp\left(-\frac{y_1^2}{4Dt_1}\right)\cdot\int \mathrm{d}y_2\exp\left(-\frac{y_2^2}{4\pi D(t_2-t_1)}\right) = \\ &= 2Dt_1\end{aligned}$$

Here we supposed $t_1 < t_2$. In the general case, we would have:

$$\langle x(t)x(t')\rangle = 2D\min(t,t')$$

Generalizing:

$$\begin{aligned}\mathbb{P}(x_i,t_i;i=0,\dots,n) &= \mathbb{P}(x_n,t_n;x_{n-1},t_{n-1};\dots;x_1,t_1;x_0,t_0) = \\ &= \prod_{i=1}^{n}W(x_i,t_i|x_{i-1},t_{i-1})W(x_0,t_0)\end{aligned}$$

This is the joint probability for a *discrete trajectory*, meaning that we care only about what happens at certain discrete times.
For the average value of a generic function f of the trajectory points:

$$\langle f(x(t_n),x(t_{n-1}),\dots,x(t_0))\rangle$$

we need to use the joint probability:

$$= \int\prod_{i=0}^{n}W(x_i,t_i;i=0,\dots,n)\cdot f(x_n,x_{n-1},\dots,x_0)$$

In the next lecture we will try to see how to generalize this kind of calculation to a function that also depends on the *inbetween points*, that is on a *infinite set of values of the trajectory*. For example:

$$\langle\exp\left(-\int_0^t a(\tau)x(\tau)\,\mathrm{d}\tau\right)\rangle$$

depends on the *whole* trajectory.