0.1 Continuous Diffusion

(Lesson 4 of 14/10/19) Compiled: 14 ottobre 2019

In the last lecture, we discussed the solution of the diffusion equation:

$$W_i(t_n) = \binom{n}{n^+}\frac{1}{2^n} \xrightarrow[l,\epsilon\downarrow 0]{l^2/\epsilon = 2D} \frac{1}{\sqrt{4\pi D t}}\exp\left(-\frac{x^2}{4Dt}\right)$$

with $x_i = li \equiv x$, $t_n = n\epsilon \equiv t$.
This is the solution of the *master equation*:

$$W_i(t_{n+1}) = \frac{1}{2}(W_{i-1}(t_n) + W_{i+1}(t_n))$$

(in the case where the probability to walk to the right P_+ is equal to that for the left P_-).

Then:

$$W_i(t_n) = W(x,t)l$$

and the probability to find a particle in $[a,b] \subset \mathbb{R}$ is given by:

$$\mathbb{P}(x \in [a,b]) = \int_a^b W(x,t)d$$

Substituting the expression for $W_i(t_n)$ in the master equation we have:

$$\cancel{l}W(x,t+\epsilon) = \frac{1}{2}\left[W(x-l,t) + W(x+l,t)\right]\cancel{l}$$

Expanding the first term in series about $\epsilon = 0$:

$$W(x,t+\epsilon) = W(x,t) + \epsilon\dot{W}(x,t) + \frac{\epsilon^2}{2}\ddot{W}(x,t) + O(\epsilon^3)$$

The same expansion can be made for the other terms:

$$W(x \pm l, t) = W(x,t) \pm lW'(x,t) + \frac{l^2}{2}W''(x,t) + O(l^3)$$

(we use $\dot{x}$ for ∂_t and x' for ∂_x (?)).
Summing the two we get:

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

Substituting back:

$$\cancel{W} + \epsilon\dot{W} + \frac{\epsilon^2}{2} = \cancel{W} + \frac{l^2}{2}W'' + O(l^4)$$

Dividing by ϵ:

$$\dot{W} + \frac{\epsilon}{2}\ddot{W} = \underbrace{\frac{l^2}{2\epsilon}}_{D}W'' + O\left(\frac{l^4}{\epsilon}\right)$$

We can now take the limit $\epsilon, l \downarrow 0$, maintaining the ratio $D = l^2/(2\epsilon)$ fixed, $\ddot{W}$ vanishes, but W'' remains:

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

Recall that the solution for the discrete case was:

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

We want now to check if this solution can be derived from the equation in the continuum limit, without having to resort to a discretization.
So, we start from:

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

and we search a solution in the field of reals ($\mathbb{R}$), so that the boundary condition becomes:

$$\lim_{|x|\to\infty} W(x,t) = 0$$

as the probability that the particle is somewhere should be one:

$$\int_{\mathbb{R}} W(x,t)\,\mathrm{d}x = 1$$

If we had a semi-infinite domain, like $[0,\infty)$, we would have to choose a certain boundary condition at 0. For example, one could choose a *reflective* boundary, so that a particle reaching 0 cannot cross it, and remains stationary until it moves right again. Otherwise, an *absorbing* boundary would *remove* every particle that attempts to cross 0.

Note also that $W(x,t)$ needs to be ≥ 0, as it is a probability density. However, it is not clear if the time evolution, given by solving the differential equation, will satisfy $W(x,t) \geq 0 \quad \forall t$, if one start with a $W(x,0) > 0$.
Fortunately, that is guaranteed by the nature of that partial differential equation.

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:

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

And so:

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

and by integrating we arrive at the solution:

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

and finally:

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

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:

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

and the general solution is:

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

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:

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

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:

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

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:

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

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:

$$\langle x(t_2)x(t_1)\rangle = \iint \mathrm{d}x_1\,\mathrm{d}x_2\,\mathbb{P}(x_2,t_2;x_1,t_1)x_2x_1$$

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:

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

we need to use the joint probability:

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

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.