Ito or Stratonovich: multiplicative noise

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Abstract

The issue of diffusion in an inhomogeneous environment and the problem of Ito-Stratonovich will be discussed with simple examples.

1 Paradox of state-dependent diffusion

Imagine a diffusing particle that is moving in a box and suppose that this particle has a position-dependent diffusion coefficient. To address the question of position-dependent diffusion, we further simplify the problem by assuming that a particle's diffusion coefficient can take only two values D_r and D_l, depending on whether it is moving in the right or left-hand halves of the box [2]. For $D_l < D_r$, does this diffusing particle spend more time in the left part of the box? A naive picture based on statistical mechanism suggests that at long times and as the accessible states for the particle on both sides are equal then, the particle should spend equal times on both sides of the box. On the other hand, it seems that the particle is slow in the region with less diffusion coefficient so it should spend more time there. To resolve this ambiguity, we consider some elementary examples.

2 Some examples

To see how position-dependent randomness can be raised in nature, we consider the run and tumble motion of an E. coli bacterium. An E. coli bacterium runs a distance along a straight line then it tumbles. The overall trajectory of bacterium is a repetition of such successive runs and tumbles. Running speed is roughly constant but its duration usually exhibits a Poisson distribution. Tumbling is also a random process, the Bacterium changes its direction by choosing a new random direction. Let's continue with further simplification and consider the case where both time duration and length of successive runs are constant. We denote these time and length increments by τ and ℓ. Instead of time and length increments, equivalently we can work with tumbling rate $\alpha = 1/\tau$ and particle's speed $v = \ell/\tau$.

Denoting by $\rho(\mathbf{r}, t)$, the probability density, we can simply show that for $\delta \to 0$ and $\tau \to 0$, we have:

$$\partial_t \rho + \nabla \cdot \mathbf{J} = 0, \qquad \mathbf{J} = -D\nabla\rho, \tag{1}$$

where the diffusion coefficient is defined by $D = \ell^2/2\tau$. Note that this equation is derived for $v = $ const. and $\alpha = $ const.. As one can see, the long-time steady state in an unbounded system, corresponds to an homogenous equilibrium state with zero current given by $\mathbf{J}_{\text{eq.}} = -D\nabla\rho = 0$. In addition to bacterial diffusion, this equation can describe the self-diffusion of gas molecules in a box.

How can we modify the above equation to consider the position-dependent diffusion coefficient $D(\mathbf{r})$? Shall we replace by $D\nabla\rho$ or $\nabla(D\rho)$, the current density? As a quick answer, we will see that depending on whether v or α or both of them have spatial dependence, the situation differs.

Different physical mechanisms can result in the spatially dependent diffusion coefficient. For a Bacterium the phenomenon of chemotaxis can result in such spatial dependence of the diffusion coefficients. For a system of gas molecules, some interesting cases can be distinguished. Consider a gas container that has an internal dense mesh of solid and fixed obstacles (individually negligible in size). The mesh is so dense that a gas molecule during its motion experiences collision with the obstacles so that its length increment ℓ will be equal to the characteristics distance between adjacent obstacles.

By imposing a spatial gradient to the density of obstacles, length increments will achieve spatial dependence $\ell(\mathbf{r})$. On the other hand, instead of position-dependent density of obstacles, we can impose a temperature gradient on this system. In this case, the average speed of molecules is set to have a spatial dependence $v(\mathbf{r})$.

To see how the diffusion equation works for such cases, an elementary 1-dimensional run and tumble model with spatially dependent $\alpha(x)$ and $v(x)$ can help [1]. Denoting by $P^{\pm}$, the number density of right and left going bacteria, we can write:

$$\partial_t P^{\pm} = \mp \partial_x (v(x) P^{\pm}) \mp (\alpha(x)/2)(P^+ - P^-), \tag{2}$$

or alternatively for total density $\rho = P^+ + P^-$ and total current $J = v(x)(P^+ - P^-)$, we will have:

$$\partial_t^2 \rho = \partial_x \left(v(x) \partial_x (v(x)\rho) + \alpha(x) J \right). \tag{3}$$

There is a fundamental difference between this equation and the previous diffusion equation in the sense that the time derivate here is second order. As a result of this difference, the short time or transient behaviour of this generalized diffusion equation differs from the usual diffusion equation. However, what we are interested in here is the long-time or steady state behaviour. Putting $\partial_t^2 \to 0$, we will see that the steady state (equilibrium) corresponds to

$$J_{\text{eq.}} = -(v/\alpha)\partial_x(v\rho).$$

Different cases can be recognized and summarized as:

$$
\begin{cases}
v = \text{const.,} \ \ \alpha = \text{const.} & \to J = -D\partial_x\rho, \quad D = \frac{v^2}{\alpha} \to \rho_{\text{eq.}} = \rho_0, \\
v = \text{const.,} \ \ \alpha(x) & \to J = -D(x)\partial_x\rho, \quad D(x) = \frac{v^2}{\alpha(x)} \to \rho_{\text{eq.}} = \rho_0, \\
v(x), \ \ \alpha = \text{const.,} & \to J = -D\partial_x\rho - \frac{\rho}{2}\partial_x D, \quad D = \frac{v^2}{\alpha} \to \rho_{\text{eq.}} = \frac{A}{v(x)}, \\
v(x), \ \ \alpha(x), \ \ell = v/\alpha = \text{const.} & \to J = -\partial_x(D(x)\rho), \quad D = \frac{v^2}{\alpha} \to \rho_{\text{eq.}} = \frac{A}{v(x)}.
\end{cases}
\tag{4}
$$

As one can learn from the above cases, different choices for current will result different steady-state distributions for density. In other words, to have a special form for the steady state (equilibrium) density we have to choose a special choice for current.

Now the paradox of state-dependent diffusion is resolved. Actually, by presenting a state-dependent diffusion coefficient, the physical problem is not still completely defined. To put a complete definition of our physical problem, we need to include more information about the system under investigation. As it is shown in the above examples, complete information can be given by specifying both $v(x)$ and $\alpha(x)$. Another alternative way to completely define the physical system is to give simultaneously both $D(x)$ and $\rho_{\text{eq.}}(x)$.

Now we can reconsider the case of gas molecules moving in a container that is filled with obstacles. Particles moving in the presence of an inhomogeneous density of obstacles is a case with constant speed v and position-dependent $\alpha(x)$. For this case, the proper choice for current reads as $J = -D(x)\partial_x\rho$ that corresponds to uniform equilibrium density $\rho_{\text{eq.}} = \rho_0$. On the other hand, for uniform density of obstacles and applied gradient of temperature, we need to choose: $v = v(x)$ and $\alpha = \text{const.}$. In this case current distribution is given by: $J = -D\partial_x\rho - \frac{\rho}{2}\partial_x D$ and it will give an equilibrium density like: $\rho_{\text{eq.}} = \frac{A}{v(x)}$.

3 Stochastic dynamics

We showed that the probability density of a diffusing particle in a uniform medium reads as $\partial_t\rho + \partial_x J = 0$ where the current density has got contributions from drift and fluctuation as: $J = v\rho - D\partial_x\rho$. At the microscopic level, the diffusing particle obeys a stochastic Lengevin differential equation like: $\dot{x} = v + \sqrt{2D}\eta(t)$, where $\eta(t)$ is a Gaussian noise with $<\eta> = 0$ and $<\eta(t)\eta(t')> = \delta(t-t')$. To have a feeling of this noise, one can consider an infinite sequence of kicks with random strength and random intervals between successive events. The duration of each individual kick should be negligibly small otherwise a correlation time equal to this time scale will enter into the system.

Following the Ito calculus, the Langevin equation can be integrated along a small time interval δt to reach a discrete form that is suitable for numerical integration [4]:

$$x_{n+1} = x_n + v_n \delta t + \sqrt{2D}\sqrt{\delta t}\, \gamma, \quad <\gamma> = 0, \quad <\gamma^2> = 1, \tag{5}$$

where γ is a number that needs to be chosen from a set of random numbers with zero average and unit variance.

Our discussion in the previous section revealed the mystery behind the state (position) dependent diffusion coefficient at the deterministic level. Here we want to reconsider the same problem at the stochastic level where the Langevin equation governs the dynamics. Are we allowed to simply write an equation like: $\dot{x} = v + \sqrt{2D(x)}\eta(t)$? Mathematically thinking, we can simply realize that such an equation has ambiguity in its definition. The problem is due to the so called multiplicative noise term $\sqrt{2D(x)}\eta(t)$. As we discussed before, $\eta(t)$ can be realized as a sequence of random kicks. Now we note that following each kick the particle will jump to its new position. How do we deal with $\sqrt{D(x(t))}$? Do we replace the position before or after the jump or even its average in between the jump? Similar to the physical picture that we had provided for the deterministic case, the above stochastic equation is not still completely defined. Ito and Stratonovich have different choices for the multiplicative noise term. In Ito's prescription, the noise term is assumed to be evaluated before the jump as $\sqrt{D(x_n)}$. Stratonovich has different choice where the average position of the particle is used to evaluate the noise term as: $\sqrt{D(\frac{x_{n+1}+x_n}{2})}$. Implementing Ito's case numerically is as simple as the case of constant D. For Ito's case, the discrete equation reads as:

$$\text{Ito:} \qquad x_{n+1} = x_n + v_n\delta t + \sqrt{2D_n}\sqrt{\delta t}\,\gamma, \quad <\gamma>=0, \quad <\gamma^2>=1,$$
$$\partial_t\rho + \partial_x\left(v\rho - \partial_x(D\rho)\right) = 0. \tag{6}$$

For comparison, the corresponding deterministic diffusion equation is written. Compared with our previous discussion, we can see that Ito's choice corresponds to a physical problem with $v = \text{const.}$ and $\alpha = \alpha(x)$.

In Stratonovich's case, the situation is slightly different. Following the techniques of stochastic calculus, it is easy to show that the Stratonovich case is equivalent to Ito's case with an additional drift term given by $(1/2)\partial_x D(x)$. So the discrete equation is given by:

$$\text{Strat.:} \qquad x_{n+1} = x_n + \left(v_n + \frac{1}{2}\partial_x D(x_n)\right)\delta t + \sqrt{2D_n}\sqrt{\delta t}\,\gamma, \quad <\gamma>=0, \quad <\gamma^2>=1,$$
$$\partial_t\rho + \partial_x\left((v+\frac{1}{2}\partial_x D)\rho - \partial_x(D\rho)\right) = 0. \tag{7}$$

This Stratonovich's choice corresponds to a physical system with $\alpha = \text{const.}$ and $v = v(x)$.

In addition to Ito and Stratonovich's cases, we can define a new class of stochastic multiplicative noise. In this case the value of the noise after a jump is replaced as $\sqrt{D(x_{n+1})}$ [3]. Here it can be shown that the isothermal case is equivalent to an Ito problem with additional drift given by $\partial_x D(x)$. The discrete equation is given by:

$$\text{IsoTher.:} \qquad x_{n+1} = x_n + (v_n + \partial_x D(x_n))\delta t + \sqrt{2D_n}\sqrt{\delta t}\,\gamma, \quad <\gamma>=0, \quad <\gamma^2>=1,$$
$$\partial_t\rho + \partial_x\left((v+\partial_x D)\rho - \partial_x(D\rho)\right) = 0. \tag{8}$$

To see the origin of this name isothermal", note that in this case the probability current reads as: $J = (v_n + \partial_x D)\rho - \partial_x(D\rho)$. Note that the particle in external potential U with friction coefficient ζ, experience a drift term given by $v = -\zeta^{-1}\partial_x U$ and at local thermal equilibrium $D\zeta = k_B T$. Now the long time equilibrium corresponds to a distribution like $\rho_{\text{eq}} \sim \exp(-U(x)/k_B T(x))$. We conclude that this isothermal case corresponds to a case where a temperature gradient is applied to physical system.

References

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