Statistical Physics IV: Non-equilibrium statistical physics
ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

Solutions to Exercise No.3

Solution: Change of variables of a stochastic function f(X(t)), i.e. Ito's Lemma

1. Assume that we have a stochastic process $x(t)$ of the Ito form:

$$dx = Adt + BdW$$

(for convenience we used $A = A(x(t), t)$ and $B = \sqrt{D(x(t), t)}$). A function $f(x(t), t)$ can be expanded in Taylor series

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial t}dt + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}dx^2 + ...$$

and we can substitute dx to get

$$df = \frac{\partial f}{\partial x}(Adt + BdW) + \frac{\partial f}{\partial t}dt + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}\left(A^2dt^2 + 2ABdt + B^2dW^2\right)$$

For the Wiener increment dW, we know that $dW^2 \longrightarrow dt$ as $dt \longrightarrow 0$. We can delete terms which are $\propto dt^2$ or $\propto dtdW$ (since the latter tends to $dt^{3/2}$ and we are only interested in the first order) and after rearranging we get

$$df = \left(A\frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} + \frac{1}{2}B^2\frac{\partial^2 f}{\partial x^2}\right)dt + B\frac{\partial f}{\partial x}dW$$

which is the desired result.

2. In standard calculus, one would stop at $df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial t}dt$

3. For the Ornstein-Uhlenbeck process:

$$A(X(t), t) = -\frac{X(t)}{\tau}\ ,\ D(X(t), t) = B^2 = c\ .$$

Directly using Ito's lemma we can find:

$$\frac{d}{dt}\left\langle X^2(t)\right\rangle = -\frac{2}{\tau}\left\langle X^2(t)\right\rangle + c$$

Solution: Geometric Brownian motion - multiplicative white noise

1. Directly applying Itô's lemma, we obtain

$$dY = -\frac{c^2}{2}dt + cdW \tag{1}$$

so that

$$\frac{dY}{dt} = -\frac{c^2}{2} + c\Gamma(t). \tag{2}$$

2. We find

$$Y(t) = -\frac{c^2}{2}t + c\left(W(t)\right) + Y_0 \tag{3}$$

so that

$$X(t) = Ce^{-\frac{1}{2}c^2t}e^{cW(t)}. \tag{4}$$

Computing the correlation, we get

$$\langle X(t)X(s)\rangle = X_0^2 e^{-\frac{1}{2}c^2 t}\left\langle e^{c(W(t)+W(s))}\right\rangle \tag{5}$$
$$= X_0^2 e^{-\frac{1}{2}c^2 t} e^{\frac{1}{2}c^2\left\langle (W(t)+W(s))^2\right\rangle} \tag{6}$$
$$= X_0^2 e^{c^2 \min(t,s)} \tag{7}$$

using $\langle \exp z\rangle = \exp\left(\frac{1}{2}\left\langle z^2\right\rangle\right)$ valid for Gaussian variable z, $\langle W^2(t)\rangle = t$ and $\langle W(t)W(s)\rangle = \min(t,s)$.

Solution: Spectral broadening of a laser by phase diffusion

1. From the diffusion process with diffusion constant D, we have the distribution of $\Delta\phi$:

$$\rho(t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{\Delta\phi^2}{4Dt}} \tag{8}$$

From this distribution function we can obtained the expetation value we need (for example, $\langle \Delta\phi^2\rangle = \int_{-\infty}^{+\infty} d\Delta\phi \rho(t) = 2Dt$).
With this distribution function, we have:

$$\begin{aligned}\left\langle e^{i\phi(t_1)-i\phi(t_2)}\right\rangle &= \left\langle e^{i\Delta\phi(|t_1-t_2|)}\right\rangle \\ &= \int_{-\infty}^{+\infty} e^{i\Delta\phi}\rho(\Delta\phi(|t_1-t_2|)) \\ &= \int_{-\infty}^{+\infty} e^{i\Delta\phi}\frac{1}{\sqrt{4\pi D|t_1-t_2|}} e^{-\frac{\Delta\phi^2}{4D|t_1-t_2|}} \\ &= e^{-D|t_1-t_2|}\end{aligned} \tag{9}$$

2. We have

$$S_{EE}(\omega) = E_0^2 \int_{-\infty}^{+\infty} d\tau e^{-i(\omega_0-\omega)\tau}\left\langle e^{i\phi(t+\tau)-i\phi(t)}\right\rangle \tag{10}$$
$$= E_0^2 \int_{-\infty}^{+\infty} d\tau e^{-i(\omega_0-\omega)\tau} e^{-D\tau} \tag{11}$$
$$= 2E_0^2 \operatorname{Re}\frac{1}{-i(\omega_0-\omega) - D} \tag{12}$$
$$= 2E_0^2 \frac{D}{(\omega_0-\omega)^2 - D^2} \tag{13}$$

The width is given by the diffusion constant D.

3. For a large number of uncorrelated phase-shifting events, the central limit theorem allows one to use the Gaussian probability distribution as used above. From which we have:

$$\left\langle e^{i\Delta\phi}\right\rangle = e^{-\frac{1}{2}\langle\Delta\phi^2\rangle} \tag{14}$$

Therefore:

$$\begin{aligned}S_{EE}(\omega) &= E_0^2 \int e^{-i(\omega_0-\omega)\tau}\left\langle e^{i\Delta\phi(\tau)}\right\rangle \\ &= E_0^2 \int e^{-i(\omega_0-\omega)\tau} e^{-\frac{1}{2}\langle\Delta\phi^2\rangle} \\ &= E_0^2 \int e^{-i(\omega_0-\omega)\tau} e^{-\frac{1}{2}\left(\tau^2\frac{k}{\pi}\left(a+\log\left(\frac{aT^2k}{\pi}\right)\right)\right)} \\ &= E_0^2 \frac{\sqrt{2}\pi \exp\left(-\frac{\pi(\omega-\omega_0)^2}{2k\left(\log\left(\frac{akT^2}{\pi}\right)+a\right)}\right)}{\sqrt{k\left(\log\left(\frac{akT^2}{\pi}\right)+a\right)}}\end{aligned} \tag{15}$$

Solution: Johnson noise in an RLC circuit

1. The equation of motion for the (forced) RLC circuit is given by:

$$V(t) = RI(t) + \frac{Q(t)}{C} + L\frac{dI(t)}{dt} .$$

It can be reexpressed using only the charge on the capacitor and the fact that the applied voltage is a stochastic function:

$$L\frac{d^2Q(t)}{dt^2} = \sqrt{c}\Gamma(t) - \frac{Q(t)}{C} - R\frac{dQ(t)}{dt} .$$

2. We solve the above equation in Fourier space.

$$Q[\omega] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} Q(t)e^{i\omega t}dt$$

Define

$$\chi[\omega] = [L(\omega_R^2 - \omega^2 - i\omega\gamma)]^{-1} \; ; \; \omega_R = \frac{1}{\sqrt{LC}} \text{ and } \gamma = \frac{R}{L} \; ;$$

so that the solution to the above equation in Fourier space takes the following form:

$$Q[\omega] = V[\omega]\chi[\omega] .$$

We can calculate $\langle V[\omega_1]V^*[\omega_2]\rangle = c\delta(\omega_1 - \omega_2)$ to obtain[1] $\left\langle |V[\omega]|^2 \right\rangle = c$.
So

$$S_{QQ}[\omega] = \langle |Q[\omega]^2| \rangle = \langle |V[\omega]^2| \rangle \, |\chi[\omega]|^2 = \frac{c/L^2}{(\omega_R^2 - \omega^2)^2 + \omega^2\gamma^2}$$

To find c we can use multiple methods (integration in the complex plane, admittance of circuit...), we choose here the results of the fluctuation dissipation theorem.

$$L\gamma = \frac{1}{k_B T} \int_{0}^{\infty} \langle V(t)V(t+t_0)\rangle \, e^{-i\omega t_0} dt_0 = \frac{c}{2k_B T}$$

So[2]

$$S_{QQ}[\omega] = \frac{2k_B T\gamma/L}{(\omega_R^2 - \omega^2)^2 + \omega^2\gamma^2}$$

3. $S_{II}(\omega) = \omega^2 S_{QQ}(\omega)$

Brownian motion as a Markov jump process and the two force hypothesis

The solution here is adapted from the provided reference.

The motion of $V(t)$ over its allowed states $\{v_n\}$ consists of random steps of size $\pm\Delta$, these steps being taken at random times and in a past-forgetting (Markovian) manner. Such behavior can be characterized by two "stepping functions" $W_+(v)$ and $W_-(v)$, which are defined so that

$$W_\pm(v_n)dt \equiv \text{the probability, given } V(t) = v_n \text{, that } V(t+dt) \text{ will equal } v_{n\pm1}. \quad (16)$$

[1]This piece of mathematical trickery can be properly justified by taking the appropriate limit of a bounded Fourier transform

[2]A factor two in the answer here could simply be due to different integration bounds depending on whether we take a full spectrum or only a positive spectrum.

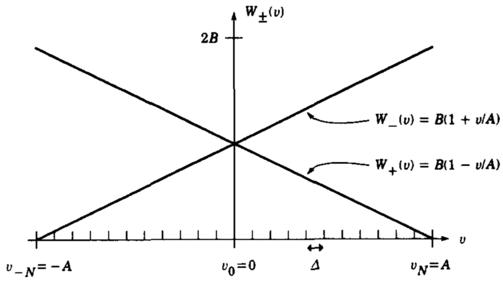

Figure 1: Graphs of the stepping functions $W_{\pm}(v)$.

Our first task will be to find forms for these two functions that characterize in a plausible way the effect on the particle's velocity of the naturally occurring molecular impingements. Since symmetry considerations dictate that

$$W_-(-v) = W_+(v), \tag{17}$$

then we may focus our efforts on finding a form for the function $W_+(v)$.

Suppose first that the particle is at rest. Then in the next infinitesimal time interval dt, there will be a certain probability that some molecule will strike the particle's backside sufficiently hard to increase the particle's velocity from zero to $v_1 = \Delta$. Let us assume that this probability can be written in the form Bdt, where B is some positive constant:

$$\begin{aligned} Bdt \equiv &\text{the probability that the particle, at rest at time} t, \text{ will acquire velocity } v_1 = \Delta \\ &\text{in the next infinitesimal time interval } [t, t + dt) \end{aligned} \tag{18}$$

We may reasonably expect B to be an increasing function of the average kinetic energy of the bath molecules, and a decreasing function of the particle's mass M and the velocity step size Δ; however, we shall be content here to let B be phenomenologically defined by the statement Eq. 18. Comparison with the definition Eq. 16 shows that

$$W_+(0) = B. \tag{19}$$

Since our model assumes that the velocity of the particle can never exceed the value A, then we must have

$$W_+(A) = 0. \tag{20}$$

And it is clear on physical grounds that, for any $v < A$, $W_+(v)$ must be a *steadily* decreasing function of v; because, if the particle's forward speed is increased, then the likelihood that the particle will be struck from behind by a gas molecule hard enough to further augment its forward speed by Δ should surely decrease. To keep our model simple, let us assume that $W_+(v)$ is a *linearly* decreasing function of v. This linearity assumption an the conditions Eq. 19 and Eq. 20 suffice to determine $W_+(v)$ completely

$$W_+(v) = B(1 - v/A), \quad (-A <\leq v \leq A). \tag{21}$$

The symmetry relation Eq. 17 then gives

$$W_-(v) = B(1 + v/A), \quad (-A <\leq v \leq A). \tag{22}$$

Plots of these functions are shown in Fig. 1.

We now have a fully defined jump Markov process model for the particle's velocity $V(t)$. Our model contains two parameters A and B, and we shall later have to decide how these parameters should depend upon the parameter N that controls the total number of velocity states. For now, though, let us deduce the consequences of this model.

Our analysis will focus on the function

$$P\left(v_n, t\right) \equiv \text{the probability that } V(t)=v_n, \text{ given that } V(0)=V_0. \tag{23}$$

To derive a time-evolution equation for this function, we begin by using the definitions Eq. 23 and Eq. 16, along with the multiplication and addition laws of probability, to infer the following expression for the probability that $V(t+dt)$ will equal v_n :

$$\begin{aligned} P\left(v_n, t+dt\right)= & P\left(v_{n-1}, t\right) \times W_{+}\left(v_{n-1}\right) dt \\ & +P\left(v_{n+1}, t\right) W_{-}\left(v_{n+1}\right) dt \\ & +P\left(v_n, t\right)\left\{1-\left[W_{+}\left(v_n\right) dt+W_{-}\left(v_n\right) dt\right]\right\}. \end{aligned} \tag{24}$$

The first term on the right is the probability that $V(t)=v_{n-1}$ and then an up-going step occurs in the next dt; the second term is the probability that $V(t)=v_{n+1}$ and then a down-going step occurs in the next dt; and the third term is the probability that $V(t)=v_n$ and then no step occurs in the next dt. All other routes to $V(t+dt)=v_n$ from time t involve more than one velocity jump in time $[t, t+dt)$, and consequently will be of order >1 in dt. Upon transposing the term $P\left(v_n, t\right)$, dividing through by dt and then passing to the limit $dt \rightarrow 0^{+}$, we obtain

$$\begin{aligned} \frac{\partial}{\partial t} P\left(v_n, t\right)= & P\left(v_{n+1}, t\right) W_{-}\left(v_{n+1}\right)-P\left(v_n, t\right) W_{+}\left(v_n\right) \\ & +P\left(v_{n-1}, t\right) W_{+}\left(v_{n-1}\right)-P\left(v_n, t\right) W_{-}\left(v_n\right). \end{aligned} \tag{25}$$

Substitution of the formulas Eq. 21 and Eq. 22 for the functions $W_{\pm}(v)$, followed by some simple algebraic rearrangement, then gives

$$\begin{aligned} \frac{\partial}{\partial t} P\left(v_n, t\right)= & (B / A)\left[v_{n+1} P\left(v_{n+1}, t\right)-v_{n-1} P\left(v_{n-1}, t\right)\right] \\ & +B\left[P\left(v_{n-1}, t\right)-2 P\left(v_n, t\right)+P\left(v_{n+1}, t\right)\right] \\ & (-N \leqslant n \leqslant N). \end{aligned} \tag{26}$$

In preparation for taking the limit $N \rightarrow \infty$, we use the fact that $\Delta=A / N$ to write Eq. Eq. 26 as

$$\begin{aligned} \frac{\partial}{\partial t} P\left(v_n, t\right)= & \frac{2 B}{N}\left(\frac{v_{n+1} P\left(v_{n+1}, t\right)-v_{n-1} P\left(v_{n-1}, t\right)}{2 \Delta}\right) \\ & +\frac{B A^2}{N^2}\left(\frac{P\left(v_{n-1}, t\right)-2 P\left(v_n, t\right)+P\left(v_{n+1}, t\right)}{\Delta^2}\right) \\ & (-N \leqslant n \leqslant N). \end{aligned} \tag{27}$$

Now, as mentioned earlier, we intend to arrange things so that $\Delta \rightarrow 0$ and $A \rightarrow \infty$ when $N \rightarrow \infty$. Assuming that those conditions are fulfilled, then the limit $N \rightarrow \infty$ brings Eq. 27 into the form of the partial differential equation

$$\frac{\partial}{\partial t} P(v, t)=C_1 \frac{\partial}{\partial v}[v P(v, t)]+C_2 \frac{\partial^2}{\partial v^2} P(v, t) \quad(-\infty \leqslant v \leqslant \infty), \tag{28}$$

where we have put

$$C_1 \equiv \lim_{N\to\infty} \frac{2B}{N}, \tag{29a}$$

$$C_2 \equiv \lim_{N\to\infty} \frac{BA^2}{N^2}. \tag{29b}$$

As may be verified by direct differentiation, the solution to Eq. 27 that satisfies the required initial condition $P(v,0) = \delta(v - V_0)$ is

$$P(v,t) = \left[2\pi (C_2/C_1)\left(1 - e^{-2C_1 t}\right)\right]^{-1/2} \times \exp\left(-\frac{\left(v - V_0 e^{-C_1 t}\right)^2}{2(C_2/C_1)(1 - e^{-2C_1 t})}\right). \tag{30}$$

Comparing the form of this solution to the form of a normal distribution, we immediately deduce that

$$V(t) = \mathbf{N}\left(V_0 e^{-C_1 t}, (C_2/C_1)\left(1 - e^{-2C_1 t}\right)\right). \tag{31}$$

We now observe that this solution will be physically sensible only if C_1 and C_2 are both finite, positive numbers. But according to Eq. 29a, C_1 can be finite and positive only if $B \propto N$ as $N \to \infty$. And given that, Eq. 29b tells us that C_2 can be finite and positive only if $A^2 \propto N$ as $N \to \infty$. Thus we conclude that our two model parameters A and B must scale with N according to

$$N \to \infty : \left\{ \begin{array}{l} A = aN^{1/2} \\ B = bN \end{array} \right. , \tag{32}$$

where the positive constants a and b are now our new model parameters.

Before proceeding, let us verify that these scaling formulas are satisfactory. First, Eq. 32 implies that A does indeed satisfy the required condition $A \to \infty$ as $N \to \infty$. Second, Eq. 32 and $\Delta = A/N$ together give, for $N \to \infty$,

$$\Delta = aN^{-1/2}, \tag{33}$$

which in turn implies that Δ satisfies the required condition $\Delta \to 0$ as $N \to \infty$. And finally, the implication of Eq. 32 that B increases with N is entirely plausible; because, increasing N decreases the step size Δ, and that in turn should increase the probability Eq. 18.

Substituting Eq. 32 into Eqs. 14, we find that

$$C_1 = 2b; \quad C_2 = ba^2. \tag{34}$$

Therefore, our formula (40) for $V(t)$ becomes

$$V(t) = \mathbf{N}\left(V_0 e^{-2bt}, (a^2/2)\left(1 - e^{-4bt}\right)\right). \tag{35}$$

This is the solution of our jump Markov process model of Brownian motion in the continuum limit of $\Delta \to 0$ and $A \to \infty$.

When we compare our model solution Eq. 35 with the solution of the Langevin, we observe that the two solutions will be identical provided that

$$2b = \frac{\gamma}{M}; \quad \frac{a^2}{2} = \frac{f^2}{2\gamma M}. \tag{36}$$

Solving these two relations simultaneously for γ and f, we conclude that our jump Markov process model, in the continuum limit, predicts the existence of a dissipative drag force $-\gamma V(t)$

and a zero-mean fluctuating force $f\Gamma(t)$, where γ and f are given in terms of our model parameters a and b by

$$\gamma = 2Mb, \tag{37}$$
$$f = Ma(2b)^{1/2}. \tag{38}$$

To this point, we have not invoked the thermodynamic requirement. To do so, we first note that the $t \to \infty$ limit of Eq. 35 gives

$$V(\infty) = \mathrm{N}\left(0, a^2/2\right). \tag{39}$$

So satisfaction of the equipartition theorem demands that $a^2/2 = k_B T/M$, or

$$a = (2k_B T/M)^{1/2}. \tag{40}$$

With this result, our formulas Eq. 36 for γ and f become

$$\gamma = 2Mb, \tag{41}$$
$$f = (4Mbk_B T)^{1/2}. \tag{42}$$

Now only the single model parameter $b(= B/N)$ remains. The fact that γ and f both increase with b, and vanish only when $b = 0$, is an expression of the fluctuation-dissipation theorem: the dissipative drag force and the zero-mean fluctuating force are concomitants.

Solution: Computer simulation of Brownian motion

See the supplementary Mathematica notebook