

PHYSICS 210B : NONEQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) Show that for time scales sufficiently greater than γ^{-1} that the solution $x(t)$ to the Langevin equation $\ddot{x} + \gamma\dot{x} = \eta(t)$ describes a Markov process. You will have to construct the matrix M defined in eqns. 2.213 and 2.214 of the lecture notes. You should assume that the random force $\eta(t)$ is distributed as a Gaussian, with $\langle \eta(s) \rangle = 0$ and $\langle \eta(s) \eta(s') \rangle = \Gamma \delta(s-s')$.

Solution:

The probability distribution is

$$P(x_1, t_1; \dots; x_N, t_N) = \det^{-1/2}(2\pi M) \exp\left\{-\frac{1}{2} \sum_{j,j'=1}^N M_{jj'}^{-1} x_j x_{j'}\right\},$$

where

$$M(t, t') = \int_0^t ds \int_0^{t'} ds' G(s-s') K(t-s) K(t'-s'),$$

and $K(s) = (1 - e^{-\gamma s})/\gamma$. Thus,

$$\begin{aligned} M(t, t') &= \frac{\Gamma}{\gamma^2} \int_0^{\min(t, t')} ds (1 - e^{-\gamma(t-s)})(1 - e^{-\gamma(t'-s)}) \\ &= \frac{\Gamma}{\gamma^2} \left\{ t_{\min} - \frac{1}{\gamma} + \frac{1}{\gamma} (e^{-\gamma t} + e^{-\gamma t'}) - \frac{1}{2\gamma} (e^{-\gamma|t-t'|} + e^{-\gamma(t+t')}) \right\}. \end{aligned}$$

In the limit where t, t' , and $|t - t'|$ are all large compared to γ^{-1} , we have $M(t, t') = 2D \min(t, t')$, where the diffusion constant is $D = \Gamma/2\gamma^2$. Thus,

$$M = 2D \begin{pmatrix} t_1 & t_2 & t_3 & t_4 & t_5 & \cdots & t_N \\ t_2 & t_2 & t_3 & t_4 & t_5 & \cdots & t_N \\ t_3 & t_3 & t_3 & t_4 & t_5 & \cdots & t_N \\ t_4 & t_4 & t_4 & t_4 & t_5 & \cdots & t_N \\ t_5 & t_5 & t_5 & t_5 & t_5 & \cdots & t_N \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ t_N & t_N & t_N & t_N & t_N & \cdots & t_N \end{pmatrix},$$

since $t_1 \geq t_2 \geq \dots \geq t_N$. To find the determinant of M , subtract row 2 from row 1, then subtract row 3 from row 2, etc. The result is

$$\widetilde{M} = 2D \begin{pmatrix} t_1 - t_2 & 0 & 0 & 0 & 0 & \cdots & 0 \\ t_2 - t_3 & t_2 - t_3 & 0 & 0 & 0 & \cdots & 0 \\ t_3 - t_4 & t_3 - t_4 & t_3 - t_4 & 0 & 0 & \cdots & 0 \\ t_4 - t_5 & t_4 - t_5 & t_4 - t_5 & t_4 - t_5 & 0 & \cdots & 0 \\ t_5 - t_6 & t_5 - t_6 & t_5 - t_6 & t_5 - t_6 & t_5 - t_6 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ t_N & t_N & t_N & t_N & t_N & \cdots & t_N \end{pmatrix}.$$

Note that the last row is unchanged, since there is no row $N + 1$ to subtract from it. Since \widetilde{M} is obtained from M by consecutive row additions, we have

$$\det M = \det \widetilde{M} = (2D)^N (t_1 - t_2)(t_2 - t_3) \cdots (t_{N-1} - t_N) t_N \quad .$$

The inverse is

$$M^{-1} = \frac{1}{2D} \begin{pmatrix} \frac{1}{t_1 - t_2} & -\frac{1}{t_1 - t_2} & 0 & \cdots & & & & & & 0 \\ -\frac{1}{t_1 - t_2} & \frac{t_1 - t_3}{(t_1 - t_2)(t_2 - t_3)} & -\frac{1}{t_2 - t_3} & 0 & \cdots & & & & & \vdots \\ 0 & \vdots & \ddots & & & & & & & \\ \vdots & 0 & & -\frac{1}{t_{n-1} - t_n} & \frac{t_{n-1} - t_{n+1}}{(t_{n-1} - t_n)(t_n - t_{n+1})} & -\frac{1}{t_n - t_{n+1}} & 0 & \cdots & & \\ 0 & \cdots & & & \ddots & & & & & \\ & & & & & & \cdots & 0 & -\frac{1}{t_{N-1} - t_N} & \frac{t_{N-1}}{t_N} \frac{1}{t_{N-1} - t_N} \end{pmatrix} .$$

This yields the general result

$$\sum_{j,j'=1}^N M_{jj'}^{-1}(t_1, \dots, t_N) x_j x_{j'} = \sum_{j=1}^N \left(\frac{1}{t_{j-1} - t_j} + \frac{1}{t_j - t_{j+1}} \right) x_j^2 - \frac{2}{t_j - t_{j+1}} x_j x_{j+1} \quad ,$$

where $t_0 \equiv \infty$ and $t_{N+1} \equiv 0$. Now consider the conditional probability density

$$\begin{aligned} P(x_1, t_1 | x_2, t_2; \dots; x_N, t_N) &= \frac{P(x_1, t_1; \dots; x_N, t_N)}{P(x_2, t_2; \dots; x_N, t_N)} \\ &= \frac{\det^{1/2} 2\pi M(t_2, \dots, t_N) \exp \left\{ -\frac{1}{2} \sum_{j,j'=1}^N M_{jj'}^{-1}(t_1, \dots, t_N) x_j x_{j'} \right\}}{\det^{1/2} 2\pi M(t_1, \dots, t_N) \exp \left\{ -\frac{1}{2} \sum_{k,k'=2}^N M_{kk'}^{-1}(t_2, \dots, t_N) x_k x_{k'} \right\}} \end{aligned}$$

We have

$$\begin{aligned} \sum_{j,j'=1}^N M_{jj'}^{-1}(t_1, \dots, t_N) x_j x_{j'} &= \left(\frac{1}{t_0 - t_1} + \frac{1}{t_1 - t_2} \right) x_1^2 - \frac{2}{t_1 - t_2} x_1 x_2 + \left(\frac{1}{t_1 - t_2} + \frac{1}{t_2 - t_3} \right) x_2^2 + \dots \\ \sum_{k,k'=2}^N M_{kk'}^{-1}(t_2, \dots, t_N) x_k x_{k'} &= \left(\frac{1}{t_0 - t_2} + \frac{1}{t_2 - t_3} \right) x_2^2 + \dots \end{aligned}$$

Subtracting, and evaluating the ratio to get the conditional probability density, we find

$$P(x_1, t_1 | x_2, t_2; \dots; x_N, t_N) = \frac{1}{\sqrt{4\pi D(t_1 - t_2)}} e^{-(x_1 - x_2)^2 / 4D(t_1 - t_2)} \quad ,$$

which depends only on $\{x_1, t_1, x_2, t_2\}$, *i.e.* on the current and most recent data, and not on any data before the time t_2 . Note the normalization:

$$\int_{-\infty}^{\infty} dx_1 P(x_1, t_1 | x_2, t_2; \dots; x_N, t_N) = 1 \quad .$$

(2) Provide the missing steps in the solution of the Ornstein-Uhlenbeck process described in §2.4.3 of the lecture notes. Show that applying the method of characteristics (see appendix IV) to Eqn. 2.61 leads to the solution in Eqn. 2.62.

Solution:

We solve

$$\frac{\partial \hat{P}}{\partial t} + \beta k \frac{\partial \hat{P}}{\partial k} = -Dk^2 \hat{P} \quad (1)$$

using the method of characteristics, writing $t = t_\zeta(s)$ and $k = k_\zeta(s)$, where s parameterizes the curve $(t_\zeta(s), k_\zeta(s))$, and ζ parameterizes the initial conditions, which are $t(s=0) = 0$ and $k(s=0) = \zeta$. The above PDE in two variables is then equivalent to the coupled system

$$\frac{dt}{ds} = 1 \quad , \quad \frac{dk}{ds} = \beta k \quad , \quad \frac{d\hat{P}}{ds} = -Dk^2 \hat{P} \quad .$$

Solving, we have

$$t_\zeta = s \quad , \quad k_\zeta = \zeta e^{\beta s} \quad , \quad \frac{d\hat{P}}{ds} = -D \zeta^2 e^{2\beta s} \hat{P} \quad ,$$

and therefore

$$\hat{P}(s, \zeta) = f(\zeta) \exp \left\{ -\frac{D\zeta^2}{2\beta} (e^{2\beta s} - 1) \right\} \quad .$$

We now identify $f(\zeta) = \hat{P}(k e^{-\beta t}, t=0)$, hence

$$\hat{P}(k, t) = \exp \left\{ -\frac{D}{2\beta} (1 - e^{-2\beta t}) k^2 \right\} \hat{P}(k, 0) \quad .$$

(3) Consider a discrete one-dimensional random walk where the probability to take a step of length 1 in either direction is $\frac{1}{2}p$ and the probability to take a step of length 2 in either direction is $\frac{1}{2}(1-p)$. Define the generating function

$$\hat{P}(k, t) = \sum_{n=-\infty}^{\infty} P_n(t) e^{-ikn} \quad ,$$

where $P_n(t)$ is the probability to be at position n at time t , with $P_n(0) = \delta_{n,0}$. Solve for $\hat{P}(k, t)$ and provide an expression for $P_n(t)$. Evaluate $\sum_n n^2 P_n(t)$.

Solution:

We have the master equation

$$\frac{dP_n}{dt} = \frac{1}{2}(1-p)P_{n+2} + \frac{1}{2}pP_{n+1} + \frac{1}{2}pP_{n-1} + \frac{1}{2}(1-p)P_{n-2} - P_n.$$

Upon Fourier transforming,

$$\frac{d\hat{P}(k,t)}{dt} = \left[(1-p)\cos(2k) + p\cos(k) - 1 \right] \hat{P}(k,t),$$

with the solution

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

where

$$\lambda(k) = 1 - p\cos(k) - (1-p)\cos(2k).$$

One then has

$$P_n(t) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikn} \hat{P}(k,t).$$

The average of n^2 is given by

$$\langle n^2 \rangle_t = - \left. \frac{\partial^2 \hat{P}(k,t)}{\partial k^2} \right|_{k=0} = \left[\lambda''(0)t - \lambda'(0)^2 t^2 \right] = (4-3p)t.$$

Note that $\hat{P}(0,t) = 1$ for all t by normalization.

(4) Numerically simulate the one-dimensional Wiener and Cauchy processes discussed in §2.6.1 of the lecture notes, and produce a figure similar to Fig. 2.3.

Hint: To generate normal (Gaussian) deviates with a distribution $p(y) = (4\pi D\varepsilon)^{-1/2} \exp(-y^2/4D\varepsilon)$, we must invert the relation

$$x(y) = \frac{1}{\sqrt{4\pi D\varepsilon}} \int_{-\infty}^y ds e^{-s^2/4D\varepsilon} = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left(\frac{y}{\sqrt{4D\varepsilon}}\right).$$

This is somewhat unpleasant. A slicker approach is to use the *Box-Muller method*, which you can read about on Wikipedia.

Solution:

Most computing languages come with a random number generating function which produces uniform deviates on the interval $x \in [0, 1]$. Suppose we have a prescribed function $y(x)$. If x is distributed uniformly on $[0, 1]$, how is y distributed? Clearly

$$|p(y) dy| = |p(x) dx| \quad \Rightarrow \quad p(y) = \left| \frac{dx}{dy} \right| p(x),$$

where for the uniform distribution on the unit interval we have $p(x) = \Theta(x)\Theta(1-x)$. For example, if $y = -\ln x$, then $y \in [0, \infty]$ and $p(y) = e^{-y}$ which is to say y is exponentially distributed. Now suppose we want to specify $p(y)$. We have

$$\frac{dx}{dy} = p(y) \quad \Rightarrow \quad x = F(y) = \int_{y_0}^y ds p(s) \quad ,$$

where y_0 is the minimum value that y takes. Therefore, $y = F^{-1}(x)$, where F^{-1} is the inverse function.

To generate normal (Gaussian) deviates with a distribution $p(y) = (4\pi D\varepsilon)^{-1/2} \exp(-y^2/4D\varepsilon)$, we have

$$x = F(y) = \frac{1}{\sqrt{4\pi D\varepsilon}} \int_{-\infty}^y ds e^{-s^2/4D\varepsilon} = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left(\frac{y}{\sqrt{4D\varepsilon}}\right) \quad .$$

We now have to invert the error function, which is slightly unpleasant.

A slicker approach is to use the *Box-Muller* method, which used a two-dimensional version of the above transformation,

$$p(y_1, y_2) = p(x_1, x_2) \left| \frac{\partial(x_1, x_2)}{\partial(y_1, y_2)} \right| \quad .$$

This has an obvious generalization to higher dimensions. The transformation factor is the Jacobian determinant. Now let x_1 and x_2 each be uniformly distributed on $[0, 1]$, and let

$$\begin{aligned} x_1 &= \exp\left(-\frac{y_1^2 + y_2^2}{4D\varepsilon}\right) & y_1 &= \sqrt{-4D\varepsilon \ln x_1} \cos(2\pi x_2) \\ x_2 &= \frac{1}{2\pi} \tan^{-1}(y_2/y_1) & y_2 &= \sqrt{-4D\varepsilon \ln x_1} \sin(2\pi x_2) \end{aligned}$$

Then

$$\begin{aligned} \frac{\partial x_1}{\partial y_1} &= -\frac{y_1 x_1}{2D\varepsilon} & \frac{\partial x_2}{\partial y_1} &= -\frac{1}{2\pi} \frac{y_2}{y_1^2 + y_2^2} \\ \frac{\partial x_1}{\partial y_2} &= -\frac{y_2 x_1}{2D\varepsilon} & \frac{\partial x_2}{\partial y_2} &= \frac{1}{2\pi} \frac{y_1}{y_1^2 + y_2^2} \end{aligned}$$

and therefore the Jacobian determinant is

$$J = \left| \frac{\partial(x_1, x_2)}{\partial(y_1, y_2)} \right| = \frac{1}{4\pi D\varepsilon} e^{-(y_1^2 + y_2^2)/4D\varepsilon} = \frac{e^{-y_1^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} \cdot \frac{e^{-y_2^2/4D\varepsilon}}{\sqrt{4\pi D\varepsilon}} \quad ,$$

which says that y_1 and y_2 are each independently distributed according to the normal distribution $p(y) = (4\pi D\varepsilon)^{-1/2} \exp(-y^2/4D\varepsilon)$. Nifty!

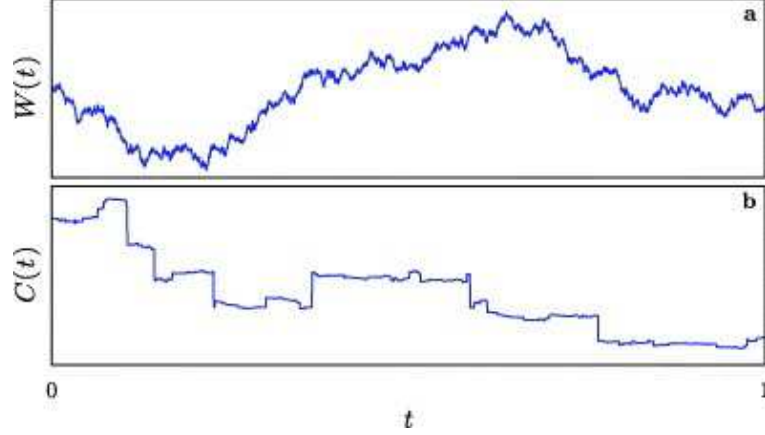


Figure 1: (a) Wiener process sample path $W(t)$. (b) Cauchy process sample path $C(t)$. From K. Jacobs and D. A. Steck, *New J. Phys.* **13**, 013016 (2011).

For the Cauchy distribution, with

$$p(y) = \frac{1}{\pi} \cdot \frac{\varepsilon}{y^2 + \varepsilon^2} \quad ,$$

we have

$$F(y) = \frac{1}{\pi} \int_{-\infty}^y ds \frac{\varepsilon}{s^2 + \varepsilon^2} = \frac{1}{2} + \frac{1}{\pi} \tan^{-1}(y/\varepsilon) \quad ,$$

and therefore

$$y = F^{-1}(x) = \varepsilon \tan \left(\pi x - \frac{\pi}{2} \right) \quad .$$

(5) Due to quantum coherence effects in the backscattering from impurities, one-dimensional wires don't obey Ohm's law in the limit where the 'inelastic mean free path' is greater than the sample dimensions, which you may assume here. Rather, let $\mathcal{R}(L) = e^2 R(L)/h$ be the dimensionless resistance of a quantum wire of length L , in units of $h/e^2 = 25.813 \text{ k}\Omega$. The dimensionless resistance of a quantum wire of length $L + \delta L$ is then given by

$$\begin{aligned} \mathcal{R}(L + \delta L) &= \mathcal{R}(L) + \mathcal{R}(\delta L) + 2\mathcal{R}(L)\mathcal{R}(\delta L) \\ &\quad + 2\cos\alpha \sqrt{\mathcal{R}(L)[1 + \mathcal{R}(L)]\mathcal{R}(\delta L)[1 + \mathcal{R}(\delta L)]} \quad , \end{aligned}$$

where α is a *random phase* uniformly distributed over the interval $[0, 2\pi)$. Here,

$$\mathcal{R}(\delta L) = \frac{\delta L}{2\ell} \quad ,$$

is the dimensionless resistance of a small segment of wire, of length $\delta L \lesssim \ell$, where ℓ is the 'elastic mean free path'.

(a) Show that the distribution function $P(\mathcal{R}, L)$ for resistances of a quantum wire obeys the equation

$$\frac{\partial P}{\partial L} = \frac{1}{2\ell} \frac{\partial}{\partial \mathcal{R}} \left\{ \mathcal{R} (1 + \mathcal{R}) \frac{\partial P}{\partial \mathcal{R}} \right\}.$$

(b) Show that this equation may be solved in the limits $\mathcal{R} \ll 1$ and $\mathcal{R} \gg 1$, with

$$P(\mathcal{R}, z) = \frac{1}{z} e^{-\mathcal{R}/z}$$

for $\mathcal{R} \ll 1$, and

$$P(\mathcal{R}, z) = (4\pi z)^{-1/2} \frac{1}{\mathcal{R}} e^{-(\ln \mathcal{R} - z)^2/4z}$$

for $\mathcal{R} \gg 1$, where $z = L/2\ell$ is the dimensionless length of the wire. Compute $\langle \mathcal{R} \rangle$ in the former case, and $\langle \ln \mathcal{R} \rangle$ in the latter case.

Solution:

(a) From the composition rule for series quantum resistances, we derive the phase averages

$$\begin{aligned} \langle \delta \mathcal{R} \rangle &= \left(1 + 2 \mathcal{R}(L) \right) \frac{\delta L}{2\ell} \\ \langle (\delta \mathcal{R})^2 \rangle &= \left(1 + 2 \mathcal{R}(L) \right)^2 \left(\frac{\delta L}{2\ell} \right)^2 + 2 \mathcal{R}(L) \left(1 + \mathcal{R}(L) \right) \frac{\delta L}{2\ell} \left(1 + \frac{\delta L}{2\ell} \right) \\ &= 2 \mathcal{R}(L) \left(1 + \mathcal{R}(L) \right) \frac{\delta L}{2\ell} + \mathcal{O}((\delta L)^2), \end{aligned}$$

whence we obtain the drift and diffusion terms

$$F_1(\mathcal{R}) = \frac{2\mathcal{R} + 1}{2\ell}, \quad F_2(\mathcal{R}) = \frac{2\mathcal{R}(1 + \mathcal{R})}{2\ell}.$$

Note that $2F_1(\mathcal{R}) = dF_2/d\mathcal{R}$, which allows us to write the Fokker-Planck equation as

$$\frac{\partial P}{\partial L} = \frac{\partial}{\partial \mathcal{R}} \left\{ \frac{\mathcal{R} (1 + \mathcal{R})}{2\ell} \frac{\partial P}{\partial \mathcal{R}} \right\}.$$

(b) Defining the dimensionless length $z = L/2\ell$, we have

$$\frac{\partial P}{\partial z} = \frac{\partial}{\partial \mathcal{R}} \left\{ \mathcal{R} (1 + \mathcal{R}) \frac{\partial P}{\partial \mathcal{R}} \right\}.$$

In the limit $\mathcal{R} \ll 1$, this reduces to

$$\frac{\partial P}{\partial z} = \mathcal{R} \frac{\partial^2 P}{\partial \mathcal{R}^2} + \frac{\partial P}{\partial \mathcal{R}},$$

which is satisfied by $P(\mathcal{R}, z) = z^{-1} \exp(-\mathcal{R}/z)$. For this distribution one has $\langle \mathcal{R} \rangle = z$.

In the opposite limit, $\mathcal{R} \gg 1$, we have

$$\frac{\partial P}{\partial z} = \frac{\partial}{\partial \mathcal{R}} \left(\mathcal{R}^2 \frac{\partial}{\partial \mathcal{R}} \right) = \frac{\partial^2 P}{\partial \nu^2} + \frac{\partial P}{\partial \nu},$$

where $\nu \equiv \ln \mathcal{R}$. This is solved by the log-normal distribution,

$$P(\mathcal{R}, z) = (4\pi z)^{-1/2} e^{-(\nu+z)^2/4z}.$$

Note that

$$P(\mathcal{R}, z) d\mathcal{R} = \tilde{P}(\nu, z) d\nu = \frac{1}{\sqrt{4\pi z}} e^{-(\nu-z)^2/4z} d\nu,$$

One then obtains $\langle \nu \rangle = \langle \ln \mathcal{R} \rangle = z$. Furthermore,

$$\langle \mathcal{R}^n \rangle = \langle e^{n\nu} \rangle = \frac{1}{\sqrt{4\pi z}} \int_{-\infty}^{\infty} d\nu e^{-(\nu-z)^2/4z} e^{n\nu} = e^{k(k+1)z}$$

Note then that $\langle \mathcal{R} \rangle = \exp(2z)$, so the mean resistance grows *exponentially* with length. However, note also that $\langle \mathcal{R}^2 \rangle = \exp(6z)$, so

$$\langle (\Delta \mathcal{R})^2 \rangle = \langle \mathcal{R}^2 \rangle - \langle \mathcal{R} \rangle^2 = e^{6z} - e^{4z},$$

and so the standard deviation grows as $\sqrt{\langle \mathcal{R}^2 \rangle} \sim \exp(3z)$ which grows faster than $\langle \mathcal{R} \rangle$. In other words, the resistance \mathcal{R} itself is not a *self-averaging* quantity, meaning the ratio of its standard deviation to its mean doesn't vanish in the thermodynamic limit – indeed it diverges. However, $\nu = \ln \mathcal{R}$ is a self-averaging quantity, with $\langle \nu \rangle = z$ and $\sqrt{\langle \nu^2 \rangle} = \sqrt{2z}$.