0.1 Homework 7

0.1.1 Stretched String

A string of length l is stretched, under a constant tension F, between two fixed points A and B. Show that the mean square (fluctuational) displacement $y(x)$ at point P, distant x from A, is given by

$$\overline{\{y(x)\}^2} = \frac{kT}{Fl}x(l-x)$$

Further show that, for $x_2 \geq x_1$,

$$\overline{y(x_1)y(x_2)} = \frac{kT}{Fl}x_1(l-x_2).$$

[Hint : Calculate the energy, Φ, associated with the fluctuation in question; the desired probability distribution is then given by $p \propto$ exp$(-\Phi/kT)$, from which the required averages can be readily evaluated.]

Boundary conditions: $y(0) = y(l) = 0$. Energy of the fluactuation: $\Phi[y(x)] = \frac{F}{2}\int_0^l \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 \mathrm{d}x$.

Therefore $P[y(x)] \propto \exp\left(-\frac{\Phi[y(x)]}{kT}\right) = \exp\left[-\frac{F}{2kT}\int_0^l \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 \mathrm{d}x\right]$.

Expand $y(x)$ in eigenmodes which satisfies the boundary conditions: $y(x) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{l}\right)$,

so the derivative becomes $\frac{\mathrm{d}y}{\mathrm{d}x} = \sum_{n=1}^{\infty} a_n \frac{n\pi}{l}\cos\left(\frac{n\pi x}{l}\right)$.

Substitute into the energy: $\Phi = \frac{F}{2}\int_0^l \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2 \mathrm{d}x = \frac{F}{2}\sum_{n=1}^{\infty} a_n^2 \left(\frac{n\pi}{l}\right)^2 \frac{l}{2} = \sum_{n=1}^{\infty} \frac{F\pi^2 n^2}{4l}a_n^2$.

The probability distribution is $p(\{\}) \propto \exp\left[-\sum_{n=1}^{\infty}\frac{F\pi^2 n^2}{4l}a_n^2\right]$, which is a product of independent Gaussian distribution for each a_n. And the variance of each a_n can be extracted from the exponent term: $\overline{a_n^2} = \frac{2kT}{Fl}\left(\frac{l}{n\pi}\right)^2 = \frac{2kTl}{F\pi^2 n^2}$.

Fourier expand $\overline{y(x)^2} = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \overline{a_n a_m}\sin\left(\frac{n\pi x}{l}\right)\sin\left(\frac{m\pi x}{l}\right)$. Since $\overline{a_n a_m} = \overline{a_n^2}\delta_{nm}$, $\overline{y(x)^2} = \frac{2kTl}{F\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin^2\left(\frac{n\pi x}{l}\right)$.

Use the indentity $\sum_{n=1}^{\infty}\frac{\cos 2n\theta}{n^2} = \frac{\pi^2}{6} - \frac{\pi\theta}{2} + \frac{\theta^2}{2}$ and $\sin^2\theta = \frac{1-\cos(2\theta)}{2}$, the summation term:

$$\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\left(\frac{n\pi x}{l}\right) = \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n^2} - \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n^2}\cos\left(\frac{2n\pi x}{l}\right) = \frac{\pi^2}{12} - \frac{1}{2}\left(\frac{\pi^2}{6} - \frac{\pi^2 x}{2l} + \frac{\pi^2 x^2}{2l^2}\right) = \frac{\pi^2 x}{2l} - \frac{\pi^2 x^2}{2l^2} = \frac{\pi^2}{2l^2}x(l-x)$$

Substitute it back into the expansion to get $\overline{y(x)^2} = \frac{2kTl}{F\pi^2}\times\frac{\pi^2}{2l^2}x(l-x) = \boxed{\frac{kT}{Fl}x(l-x)}$

Similarly, $\overline{y(x_1)y(x_2)} = \sum_{n=1}^{\infty}\overline{a_n^2}\sin\left(\frac{n\pi x_1}{l}\right)\sin\left(\frac{n\pi x_2}{l}\right) = \frac{2kTl}{F\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\left(\frac{n\pi x_1}{l}\right)\sin\left(\frac{n\pi x_2}{l}\right)$.

Use the indentity $\sum_{n=1}^{\infty}\frac{\cos(n\theta)}{n^2} = \frac{\pi^2}{6} - \frac{\pi\theta}{2} + \frac{\theta^2}{4}$ and $\sin A\sin B = \frac{\cos(A-B) - \cos(A+B)}{2}$, the summation term:

$$\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\left(\frac{n\pi x_1}{l}\right)\sin\left(\frac{n\pi x_2}{l}\right) = \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n^2}\cos\left[\frac{n\pi(x_1-x_2)}{l}\right] - \frac{1}{2}\sum_{n=1}^{\infty}\frac{1}{n^2}\cos\left[\frac{n\pi(x_1+x_2)}{l}\right]$$

So define $\theta_1 = \frac{\pi(x_1-x_2)}{l}$, $\quad\theta_2 = \frac{\pi(x_1+x_2)}{l}$, the summation term becomes

$$\sum_{n=1}^{\infty}\frac{\cos(n\theta_1)}{n^2} = \frac{\pi^2}{6} - \frac{\pi|\theta_1|}{2} + \frac{\theta_1^2}{4}, \quad \sum_{n=1}^{\infty}\frac{\cos(n\theta_2)}{n^2} = \frac{\pi^2}{6} - \frac{\pi\theta_2}{2} + \frac{\theta_2^2}{4}.$$ Therefore

$$\begin{aligned}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin\left(\frac{n\pi x_1}{l}\right)\sin\left(\frac{n\pi x_2}{l}\right) &= \frac{1}{2}\left[\frac{\pi^2}{6} - \frac{\pi^2|x_1-x_2|}{2l} + \frac{\pi^2(x_1-x_2)^2}{4l^2}\right] - \frac{1}{2}\left[\frac{\pi^2}{6} - \frac{\pi^2(x_1+x_2)}{2l} + \frac{\pi^2(x_1+x_2)^2}{4l^2}\right] \\ &= \frac{\pi^2(x_1+x_2-|x_1-x_2|)}{4l} + \frac{\pi^2[(x_1-x_2)^2-(x_1+x_2)^2]}{8l^2} \overset{x_2\geq x_1}{=} \frac{\pi^2(2x_1)}{4l} + \frac{\pi^2(-4x_1x_2)}{8l^2}\end{aligned}$$

Substitute it back into the expansion to get $\overline{y(x_1)y(x_2)} = \dfrac{2kTl}{F\pi^2} \times \left(\dfrac{\pi^2 x_1}{2l} - \dfrac{\pi^2 x_1 x_2}{2l^2}\right) = \boxed{\dfrac{kT}{Fl} x_1(l - x_2)}$

0.1.2 Derive the Onsager's Reciprocal Relations

Derive for the Onsager's reciprocity relation. [Refer to Section 15.7 @ Pathria& Beale]

Forces X_i and the current $\dot{x}_i$: $\dot{x}_i = \gamma_{ij} X_j$.

$$S(x_i) = S(\widetilde{x}_i) + \cancel{\left(\frac{\partial S}{\partial x_i}\right)_{x_i=\widetilde{x}_i} (x_i - \widetilde{x}_i)} + \frac{1}{2}\left(\frac{\partial^2 S}{\partial x_i \partial x_j}\right)_{x_{i,j}=\widetilde{x}_{i,j}} (x_i - \widetilde{x}_i)(x_j - \widetilde{x}_j), \quad \left(\frac{\partial S}{\partial x_i}\right)_{x_i=\widetilde{x}_i} = 0$$

$$\Delta S \equiv S(x_i) - S(\widetilde{x}_i) = -\frac{1}{2}\beta_{ij}(x_i - \widetilde{x}_i)(x_j - \widetilde{x}_j), \quad \beta_{ij} = -\left(\frac{\partial^2 S}{\partial x_i \partial x_j}\right)_{x_{i,j}=\widetilde{x}_{i,j}} = \beta_{ji}$$

The driving forces X_i can be defined as the second law of thermodynamics: $X_i = \left(\dfrac{\partial S}{\partial x_i}\right) = -\beta_{ij}(x_j - \widetilde{x}_j)$

$$\langle x_i X_j \rangle = \frac{\displaystyle\int_{-\infty}^{+\infty} (x_i X_j)\exp\left\{-\frac{1}{2k}\beta_{ij}(x_i - \widetilde{x}_i)(x_j - \widetilde{x}_j)\right\}\prod_i \mathrm{d}x_i}{\displaystyle\int_{-\infty}^{+\infty} \exp\left\{-\frac{1}{2k}\beta_{ij}(x_i - \widetilde{x}_i)(x_j - \widetilde{x}_j)\right\}\prod_i \mathrm{d}x_i}, \text{ where}$$

$$\langle x_i \rangle = \frac{\displaystyle\int_{-\infty}^{+\infty} x_i\exp\left\{-\frac{1}{2k}\beta_{ij}(x_i - \widetilde{x}_i)(x_j - \widetilde{x}_j)\right\}\prod_i \mathrm{d}x_i}{\displaystyle\int_{-\infty}^{+\infty} \exp\left\{-\frac{1}{2k}\beta_{ij}(x_i - \widetilde{x}_i)(x_j - \widetilde{x}_j)\right\}\prod_i \mathrm{d}x_i} = \widetilde{x}_i, \quad \frac{\partial \langle x_i \rangle}{\partial x_j} = \delta_{ij} \Rightarrow \langle x_i X_j \rangle = -k\delta_{ij}.$$

According to time reversal symmetry(in microscopic process),

$\langle x_i(0)x_j(s)\rangle = \langle x_i(0)x_j(-s)\rangle, \quad \langle x_i(0)x_j(-s)\rangle = \langle x_i(s)x_j(0)\rangle \Rightarrow \langle x_i(0)x_j(s)\rangle = \langle x_i(s)x_j(0)\rangle.$

Let $s \to 0$ to get: $\langle x_i(0)\dot{x}_j(0)\rangle = \langle \dot{x}_i(0)x_j(0)\rangle$.

Substitute the force-current relation, and get $\begin{cases} \langle x_i(0)\gamma_{jl}X_l(0)\rangle = -k\gamma_{jl}\delta_{il} = -k\gamma_{ji} \\ \langle \gamma_{il}X_l(0)x_j(0)\rangle = -k\gamma_{il}\delta_{jl} = -k\gamma_{ij} \end{cases} \Rightarrow \boxed{\gamma_{ij} = \gamma_{ji}}.$