E8481: Mass on a spring

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The problem:

A balance for measuring weight consists of a sensitive spring which hangs from a fixed point. The spring constant is K. The balance is at temperature T and gravity acceleration is g in the x direction. A small mass m hangs at the end of the spring. There is an option to apply an external force $F(t)$, to which x is conjugate or apply an external vector potential $A(t)$.

(a) Find the partition function Z.

(b) Find $\langle x \rangle$ and $\langle x^2 \rangle$ and $\mathrm{Var}(x)$.

(c) What is the minimal mass that can be meaningfully measured?

(d) Write a Langevin equation for $x(t)$, with friction γ, and a random force $f(t)$.

(e) Assuming $\langle f(t)f(0)\rangle = C\delta(t)$, find $\mathrm{Var}(x)$, and deduce what is C by comparing with the canonical result.

(f) Now, assuming a different force autocorrelation function $\langle g(t)g(0)\rangle = D\frac{sin(at)}{at}$, find the position power spectrum, under what condition will the result found here and (e) agree?

(g) Describe the external force $F(t)$ by a scalar potential and demonstrate FDT.

(h) Describe the external force $F(t)$ by a vector potential and demonstrate FDT.

Note: $\int \frac{d\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2} = \frac{\pi}{\gamma\omega_0^2}$.

The solution:

(a) The Hamiltonian of the system is: $H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 - mgx$, so the partition function Z is

$$Z = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{-\frac{\beta p^2}{2m}}\,dp \int_{-\infty}^{+\infty} e^{-(\frac{\beta K x^2}{2}-mg\beta x)}\,dx$$

This integral can be simplified by changing the integration variable x to $y = \sqrt{\frac{\beta K}{2}}x$

$$Z = \frac{1}{2\pi\hbar}\sqrt{\frac{2m\pi}{\beta}}\int_{-\infty}^{+\infty} e^{-(y^2-\sqrt{\frac{2\beta}{K}}mgy)}\,dy = \frac{1}{\hbar\beta}\sqrt{\frac{m}{K\pi}}\int_{-\infty}^{+\infty} e^{-(y-\sqrt{\frac{\beta}{2K}}mg)^2}\,e^{\frac{\beta m^2 g^2}{2K}}\,dy$$

Finally:

$$Z = \frac{1}{\hbar\beta}\sqrt{\frac{m}{K}}\,e^{\frac{\beta m^2 g^2}{2K}}$$

(b) $\langle x \rangle$ is defined as:

$$\langle x(t)\rangle = \frac{1}{Z}\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-\frac{\beta p^2}{2m}}\, x\, e^{-(\frac{\beta K x^2}{2} - mg\beta x)}\, dxdp$$

This is solved using integration by parts

$$\langle x(t)\rangle = \sqrt{\frac{\beta K}{2\pi}}\, e^{-\frac{\beta m^2 g^2}{2K}} \left[-\frac{1}{\beta K} e^{-(\frac{\beta K x^2}{2} - mg\beta x)}\Big|_{-\infty}^{+\infty} + \frac{mg}{K}\int_{-\infty}^{+\infty} e^{-(\frac{\beta K x^2}{2} - mg\beta x)} dx \right]$$

The first term of the R.H.S. goes to zero and we get

$$\langle x\rangle = \frac{mg}{k}$$

Applying the equipartition theorem $\langle x\frac{\partial H}{\partial x}\rangle = k_B T$ we can find that:

$$\langle x(Kx - mg)\rangle = K\langle x^2\rangle - mg\langle x\rangle = K\langle x^2\rangle - mg(\frac{mg}{K}) = k_B T$$

$$\langle x^2\rangle = \frac{k_B T}{K} + \left(\frac{mg}{K}\right)^2$$

The variance is:

$$\mathrm{Var}(x) = \frac{k_B T}{K}$$

(c) For a meaningful result we want the fluctuation of the spring should be much smaller than the spring length itself, Therefor $\langle x\rangle^2 \gg \langle \delta x^2\rangle$. We define the fluctuations $\langle \delta x^2\rangle = \mathrm{Var}(x) = \frac{k_B T}{K}$. Which results in the following condition for a meaningful measurement:

$$\left(\frac{mg}{K}\right)^2 \gg \frac{k_B T}{K} \quad \rightarrow \quad m \gg \sqrt{\frac{K k_B T}{g^2}}$$

(d) We now add friction, denoted as γ that interact with velocity and a random force $f(t)$ such that $\langle f\rangle_t = 0$. The Langevin equation for such a system is:

$$m\ddot{x} + m\gamma\dot{x} + Kx - mg = f(t)$$

(e) We redefine x to be about the mean value so that $X(t) = x(t) - \dfrac{mg}{K}$. Writing Langevin's equation for $X(t)$ and using Fourier transform functional relationships for time derivation we get $\left(-\omega^2 - i\omega\gamma + \frac{K}{m}\right)\tilde{X}(\omega) = \frac{1}{m}f(\omega)$.

$$\tilde{X}(\omega) = \frac{f(\omega)}{m(-\omega^2 - i\omega\gamma + \frac{K}{m})}$$

The expression for $|f(\omega)|^2 = \langle f(\omega) f(-\omega)\rangle = F.T.\left[\tilde{C(\tau)}\right]$ which is the Fourier transform of the given correlation function.

$$F.T.\left[C\delta(t)\right] = C$$

The power spectrum of the X coordinate is:

$$\left|\tilde{X}(\omega)\right|^2 = \frac{C}{(K - m\omega^2)^2 + (\omega m\gamma)^2}$$

The relation of the power spectrum of X to Var(X) is the inverse Fourier transform at $\tau = 0$ (remember this calculation is done at the mean value of x).

$$\text{Var}(X) = \langle X^2(\tau)\rangle = F.T.^{-1}\left[\frac{C}{(K - m\omega^2)^2 + (\omega m\gamma)^2}\right] = \frac{m\pi}{2\gamma K}C$$

This result can now be compared to that found earlier in section (b) that $\langle X^2\rangle = \frac{T}{m}2\gamma$ to find that $C = \frac{T}{m\pi}2\gamma$

(f) We keep $X(t) = x(t) - \frac{mg}{K}$, the Langevin equation for $X(t)$ and use the same methodology as in (e), however the Fourier transform of *sinc* is a window function.

$$F.T.\left[\frac{sin(at)}{at}\right] = \begin{cases} \frac{2\pi}{a} & \text{for } \omega < \frac{a}{2\pi} \\ 0 & \text{for } x > \frac{a}{2\pi} \end{cases}$$

The power spectrum of the X coordinate is:

$$\left|\tilde{X}(\omega)\right|^2 = \begin{cases} \frac{2\pi}{a}\frac{1}{(K - m\omega^2)^2 + (\omega m\gamma)^2} & \text{for } \omega < \frac{a}{2\pi} \\ 0 & \text{for } x > \frac{a}{2\pi} \end{cases}$$

One way for realizing a delta function is by the *sinc* function. For the limit $a \to \infty$ the function's appearance in the time domain becomes very narrow (resembling a delta function) and in the frequency domain becomes very broad (resembling white noise). If in addition to the condition for a we have $C = \frac{\pi}{a}D$ then the position power spectrum found from $f(\omega)$ and $g(\omega)$ will be the same.

(g) An external scalar potential creates the force $F(t)$, with conjugate coordinate $x(t)$ and the interaction term $-F(t)x$ as in the previous sections we will use $X(t)$. The DC response will change the mean value of x, the solution will be the same as in the (b). The AC linear response relation is $\langle X(\omega)\rangle = \chi_X(\omega)F(\omega)$ where we have:

$$\chi_X(\omega) = \frac{1}{m(-\omega^2 - i\omega\gamma + \frac{K}{m})}$$

The imaginary part of $\chi_X(\omega)$ is:

$$\Im\left[\chi_X(\omega)\right] = \frac{\omega\gamma}{m^2(\omega^2 - \frac{K}{m})^2 + \omega^2\gamma^2}$$

In general, the autocorrelation relation here can now be written as:

$$\tilde{C}_{XX}(\omega) = \langle \tilde{X}(\omega)\tilde{X}(-\omega) = \left|\chi_X(\omega)\right|^2 \langle \tilde{F}(\omega)\tilde{F}(-\omega)\rangle$$

We now calculate the linear response for the coordinate $V = \dot{X}$ for which we have $X_\omega = \frac{i}{\omega}V_\omega$. We will find $\chi_V(\omega)$ from the modified force equation: $\langle \frac{i}{\omega}V(\omega)\rangle = \chi_X(\omega)F(\omega)$, such that the velocity autocorrelation function is:

$$\tilde{C}_{VV}(\omega) = \langle \frac{i}{\omega}\tilde{V}(\omega)\frac{-i}{\omega}\tilde{V}(-\omega)\rangle = \frac{1}{\omega^2}\left|\chi_X(\omega)\right|^2 \langle \tilde{F}(\omega)\tilde{F}(-\omega)\rangle$$

We can now see that the relation between the position (X) and velocity (V) autocorrelation functions is $\omega^2\tilde{C}_{XX}(\omega) = \tilde{C}_{VV}(\omega)$. We can calculate the fluctuation of X and V using the FD relation:

$$\tilde{C}_{XX}(\omega) = \hbar cotgh\left(\frac{\hbar\omega}{2T}\right)\mathrm{Im}\left[\chi(\omega)\right] = \hbar cotgh\left(\frac{\hbar\omega}{2T}\right)\frac{\omega\gamma}{m^2(\omega^2 - \frac{K}{m})^2 + \omega^2\gamma^2}$$

We can now transform back to the time domain to have:

$$C_{XX}(\tau) = \hbar\int\limits_{-\infty}^{+\infty} d\omega cotgh\left(\frac{\hbar\omega}{2T}\right)\frac{\omega\gamma e^{-i\omega\tau}}{m^2(\omega^2 - \frac{K}{m})^2 + \omega^2\gamma^2}$$

And the fluctuation of V are simply:

$$\tilde{C}_{VV}(\tau) = \hbar\int\limits_{-\infty}^{+\infty} d\omega\hbar cotgh\left(\frac{\hbar\omega}{2T}\right)\frac{\omega^3\gamma e^{-i\omega\tau}}{m^2(\omega^2 - \frac{K}{m})^2 + \omega^2\gamma^2}$$

(h) An external vector potential creates the force $\epsilon(t) = -\frac{d}{dt}\vec{F}$, with conjugate coordinate $V(t)$ and the interaction term $-\vec{F}(t)V$ as in the previous sections we will use $X(t)$ which is $X(t) = x(t) - \langle x(t)\rangle$. The DC linear response $(\omega = 0)$ relation is $\langle V\rangle = \mu\epsilon$ which describes the drift motion. In general we have the linear response relation $\langle X(\omega)\rangle = \chi_X(\omega)\epsilon(\omega)$ where we have:

$$-i\omega V(\omega) + \gamma V(\omega) + \frac{K}{m}\frac{i}{\omega}V(\omega) = \frac{-i\omega}{m}\epsilon(\omega)$$

The susceptibility is:

$$\chi_V(\omega) = \frac{i\omega}{\frac{m}{\omega}(\gamma\omega - i\left(\omega^2 - \frac{K}{m}\right))}$$

And the autocorrelation function is:

$$\tilde{C}_{VV}(\omega) = \langle \tilde{V}(\omega)\tilde{V}(-\omega)\rangle = |\chi_V(\omega)|^2 \langle \tilde{\epsilon}(\omega)\tilde{\epsilon}(-\omega)\rangle$$

We now use again the relation $V = \dot{X} \to V_\omega = -i\omega X_\omega$, the autocorrelation relation here is thus:

$$\tilde{C}_{XX}(\omega) = \langle (-i\omega)\tilde{V}(\omega)(i\omega)\tilde{V}(-\omega) = \omega^2 |\chi_V(\omega)|^2 \langle \tilde{F}(\omega)\tilde{F}(-\omega)\rangle$$

Once again we relate the autocorrelation functions of the position and the velocity by the ω^2 factor. In the case where the external force creates a DC component we can relate the mobility of a particle to the spectral density of the force. this is gives by the relation : $\langle \tilde{F}(0)\tilde{F}(0)\rangle = 2D = 2\mu T$ where D is the diffusion coefficient and μ is the mobility.