Statistical Mechanics 2012/2013 Problem Set 6

Submission date: 4.2.13, total of 120 points!

6.1 Noise in phase space and Langevin equations (25 points)

Consider a system with phase space coordinates $\mathbf{p}, \mathbf{q}$, having an internal potential energy $\tilde{V}(\mathbf{q})$. The system is coupled linearly to a thermal reservoir with temperature T. The Hamiltonian is then

$$\mathcal{H} = \frac{p^2}{2M} + \tilde{V}(\mathbf{q}) + \mathcal{H}_{\text{bath}}(y_1, y_2, y_3, \ldots) - \mathbf{q} \cdot \mathbf{F}(y_1, \ldots) \ . \tag{1}$$

Here, $y_1, y_2, \ldots$ denote the degrees of freedom of the bath, $\mathcal{H}_{\text{bath}}$ is its Hamiltonian, and the last term describes the coupling between the system and the bath. Assume that without the coupling, the bath would contribute an external noise $\mathbf{f}(t)$ with mean zero. With coupling, the force develops a non-zero mean value

$$\langle \mathbf{F}(t) \rangle = \int_{-\infty}^{t} dt' \alpha(t - t') \mathbf{q}(t') \ . \tag{2}$$

where $\alpha(t - t')$ is the susceptibility of the reservoir to the motion of the system described by $\mathbf{q}(t')$. Our system then has the following equation of motion:

$$\dot{\mathbf{p}} = M\ddot{\mathbf{q}} = -\partial_{\mathbf{q}} \tilde{V} + \mathbf{f} + \int_{-\infty}^{t} dt' \alpha(t - t') \mathbf{q}(t') \ . \tag{3}$$

The correlation function of the noise in the absence of the system, is defined to be $C_b(t-t') \equiv \langle \mathbf{f}(t) \cdot \mathbf{f}(t') \rangle$.

(a) Use the fluctuation-dissipation theorem to show that the equation of motion of the system has the form

$$M\ddot{\mathbf{q}} = -\partial_{\mathbf{q}} V + \mathbf{f} - \beta \int_{-\infty}^{t} dt' C_b(t - t') \dot{\mathbf{q}}(t') \ , \tag{4}$$

and find V in terms of $\tilde{V}$ and C_b.

(b) Assume that the time scale at which the bath de-correlates is short compared to the time scales of the system. Show that the equation is then that of a Brownian particle. Derive the friction coefficient λ.

(c) Following the derivation leading up to equation (223) of the lecture notes, derive the Fokker-Planck equation for the probability distribution in phase space $P(\mathbf{p}, \mathbf{q})$ of a Brownian particle in the potential $V(\mathbf{q})$ (this is known as the Kramers problem). Show that $P(\mathbf{q}, \mathbf{p}) = \frac{1}{Z} \exp[-\beta(V(\mathbf{q}) + p^2/2m)]$ is a stationary solution.

6.2 Fluctuations and dissipation of a damped oscillator (30 points)

A damped harmonic oscillator moving under the action of an external force $f(t)$ obeys the equation of motion

$$\frac{d^2 x}{dt^2} = -\omega_0^2 x - \lambda \frac{dx}{dt} + f(t) \ . \tag{5}$$

Assume that the friction coefficient satisfies $\lambda > 0$.

(a) Find the susceptibility $\hat{\alpha}(\omega)$. Plot its real and imaginary parts, respectively α' and α'', for three cases: $\lambda \ll \omega_0$, $\lambda = 2\omega_0$ and $\lambda \gg \omega_0$.

(b) Check that $\hat{\alpha}(\omega)$ is causal, i.e., $\alpha(t) = 0$ for $t < 0$. Examine the singularities of $\alpha(\omega)$ in the complex ω plane. At what value of λ do the poles begin to sit on the imaginary axis. What does it mean physically?

(c) Given a periodic forcing $f(t) = A\cos(\omega t)$, find $x(t)$. Calculate the average power dissipated $p(\omega)$ by integrating your resulting formula for $f dx/dt$. Compare your expressions for the power and for α'' with the general formula $p(\omega) = \frac{\omega|f(\omega)|^2}{2}\alpha''$ which was derived in class.

(d) Using the fluctuation-dissipation theorem, find the correlation function $\langle x(0)x(t)\rangle$ at a given temperature T when no external force is applied. Check that $\langle x^2\rangle$ satisfies the equipartition theorem (for that you need to recall what is the potential energy here).

6.3 Monte Carlo simulation of the fluctuation-dissipation theorem (25 points)

In this question you will examine in a numerical experiment the relation between fluctuations and dissipation in a two-dimensional Ising model with Metropolis dynamics. Consider a two-dimensional Ising model on an $L \times L$ square lattice with periodic boundary conditions. The Hamiltonian of the system in a time-dependent external field is

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - H(t)\sum_i s_i, \tag{6}$$

where $s_i = \pm 1$ are spins, and $\sum_{\langle ij\rangle}$ denotes a sum over all nearest-neighbor pairs.

Below, an average in the equilibrium state with $H = 0$ is denoted by $\langle\cdots\rangle_0$, while an average over repeated stochastic evolutions of the system with a given protocol $H(t)$ is denoted by $\langle\cdots\rangle_{H(t)}$. Use the previously implementation of the metropolis algorithm with the maximal system size you can simulate which should be around $L = 200$.

(a) Begin with no magnetic field, $H = 0$, and measure the correlation function for the magnetization: $C(t) = \big\langle (M(0) - \langle M\rangle_0)(M(t) - \langle M\rangle_0)\big\rangle_0$, where the magnetization is $M(t) = \sum_i s_i(t)$. Work at $T = 3J$. This is above the critical temperature, which is known from Onsager's exact solution to be $T_c = 2J/\log(1+\sqrt{2}) \approx 2.27J$. Verify that indeed $\langle M\rangle_0 = 0$ at $T = 3J$. Note that this was already measured in one of the previous homework exercises.

(b) Next, consider the time-dependent magnetic field

$$H(t) = \begin{cases} H_0 & \text{when } t < 0 \\ 0 & \text{when } t > 0 \end{cases}. \tag{7}$$

Determine how long it takes the system to equilibrate at $T = 3J$ with a small magnetic field H_0. Allow the system to equilibrate at this magnetic field, and then, at time $t = 0$, turn off the field and measure $M(t)$. Repeat this protocol many times to find $\langle M(t)\rangle_{H(t)}$. Compare your results for $C(t)$ and $\langle M(t)\rangle_{H(t)}$ on a semi-logarithmic plot.

(c) Use the fluctuation-dissipation theorem to deduce the relation between $C(t)$ and $\langle M(t)\rangle_{H(t)}$. Compare your theoretical predictions with the numerical results. In particular, how does your analytical ratio between $C(t)$ and $\langle M(t)\rangle_{H(t)}$ compare with the numerical ratio at $t = 0$?

Note: Please attach your code to your answer.

6.4 Alphabet (15 points)

A source produces a character x from the alphabet $\{0, 1, \ldots, 9, a, b, \ldots, z\}$. With probability $1/3$, x is a numeral; with probability $1/3$, x is a vowel (a,e,i,o,u); with probability $1/3$, x is one of 21 consonants. All numerals are equiprobable, and the same goes for vowels and consonants. Estimate the entropy of the source or the mean information per character in bits.

6.5 Large Deviation theory (25 points)

In class we considered the large deviation principle for the average one N independent identically distributed variables, y_i (see section 8.4 in the lecture notes). We now consider the case where each variable can assume M possible values with probablity p_m,

$$P(y_i = v_m) = p_m \qquad \forall m = 1, \ldots, M. \tag{8}$$

We define the empirical vector as the average number of times the value m appears in the set of N varaibles,

$$L_m = \sum_{i=1}^{N} \delta_{y_i - v_m}. \tag{9}$$

Show that probability distribution of the empirical vector, $P_N(\vec{L})$ where $\vec{L} = \{L_1, L_2, \ldots L_M\}$, obeys a large deviation principle in the limit $N \gg 1$ and find its rate function. One way to compute it is to consider the generating function of $P_N(\vec{L})$, and to compute it using the Laplace method. How is the resulting rate function related to the concept of relative entropy (also known as the Kullback-Leibler divergence)? Can you explain it intuitively?