Statistical Mechanics 2011–12 — Problem Set 5

due: January 19, 2012

5.1 Fluctuations and dissipation of a damped oscillator

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

$$\frac{d^2x}{dt^2} = -\omega_0^2 x - \lambda \frac{dx}{dt} + f(t) \ . \tag{1}$$

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).

5.2 Noise in phase space and Langevin equations

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

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

Here, $y_1, y_2, \ldots$ denote the degrees of freedom of the bath, $\mathcal{H}_{\mathrm{bath}}$ 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

$$\langle \mathbf{F}(t) \rangle = \int_{-\infty}^{t} dt' \alpha(t-t') \mathbf{q}(t') \ . \tag{3}$$

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:

$$\dot{\mathbf{p}} = M\ddot{\mathbf{q}} = -\partial_{\mathbf{q}} \tilde{V} + \mathbf{f} + \int_{-\infty}^{t} dt' \alpha(t-t') \mathbf{q}(t') \ . \tag{4}$$

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

$$M\ddot{\mathbf{q}} = -\partial_{\mathbf{q}} V + \mathbf{f} - \beta \int_{-\infty}^{t} dt' C_b(t-t') \dot{\mathbf{q}}(t') \ , \tag{5}$$

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 (188) 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.

5.3 Markov processes and detailed balance

Markov processes constitute convenient, and often quite accurate, models for the dynamics of noisy systems. A Markov process is considered to be an equilibrium process if it obeys the detailed balance criterion, while Markov processes that do not obey it are considered to be nonequilibrium systems. In this question we will explore the relation between detailed balance and equilibrium.

Throughout the question we consider a system with a finite number of microstates, labeled $\alpha = 1, \ldots, N$ (e.g., a two-dimensional Ising model of length L, which has $N = 2^{L^2}$ states). A Markov dynamics is defined on this state space by the rates to jump from one state to another. These rates are given by a matrix $W_{\alpha \to \beta}$, such that the probability to be at state β at time $t + dt$ given that the system was at state $\alpha \neq \beta$ at time t is $W_{\alpha \to \beta} dt$.

(a) Write down the differential equation which describes the evolution of the probability $P_\alpha(t)$ to be in state α at time t (it may be convenient to begin with discrete time-steps of duration dt, and then take the limit $dt \to 0$). Show that this equation can be written as a continuity equation of the form $\dot{P}_\alpha = J_{\rm in}(\alpha) - J_{\rm out}(\alpha)$, where $J_{\rm in/out}(\alpha)$ are the probability fluxes into and out of state α. This equation is known as the *master equation*.

If the Markov process is ergodic (i.e., one in which every two states are connected by a path), the probability distribution tends as $t \to \infty$ towards a unique stationary distribution, which will be denoted P^*_α. The Markov process is said to obey detailed balance if $P^*_\alpha W_{\alpha\to\beta} = P^*_\beta W_{\beta\to\alpha}$ holds for every α and β.

(b) What is the net probability flux at time t between states α and β? What does the detailed balance condition imply for the probability fluxes in the steady state?

(c) Since the matrix W determines the steady state P^*, the condition of detailed balance is in fact a condition only on W. We now show this explicitly. Show that detailed balance is equivalent to the following condition:

$$\begin{aligned} &W_{\alpha_1\to\alpha_2} W_{\alpha_2\to\alpha_3} \dots W_{\alpha_{n-1}\to\alpha_n} W_{\alpha_n\to\alpha_1} = \\ &\qquad\qquad = W_{\alpha_1\to\alpha_n} W_{\alpha_n\to\alpha_{n-1}} \dots W_{\alpha_3\to\alpha_2} W_{\alpha_2\to\alpha_1} \end{aligned} \tag{6}$$

holds for every n and every cycle of states $\alpha_1, \alpha_2, \dots, \alpha_n, \alpha_1$.

Hint: If (6) is satisfied, assume that the stationary distribution has the Boltzmann form $P^*_\alpha = \frac{1}{Z} e^{-E(\alpha)}$. Arbitrarily assign $E(1) = 0$, and then proceed to construct the "energy" function E by assigning energies to the neighbors of state 1 in such a way that detailed balance is satisfied. Continue this process until P^* is defined everywhere. Be sure to take care of loops!

(d) Explain why detailed balance is a condition of time reversal symmetry. Give an example of a a Markov chain with three states which does not obey detailed balance, and explain why it is not time-reversal symmetric.

Bonus: (Optional) The Kullback-Leibler divergence (also known as the relative entropy) of the distributions $P(t)$ and P^* is given by $D(P(t)||P^*) \equiv \sum_\alpha P_\alpha(t) \log \frac{P_\alpha(t)}{P^*_\alpha}$. This is an information-theoretic measure of how different the two distributions are. Show that if P^* is given by a Boltzmann form, $D(P(t)||P^*)$ can be interpreted as the free energy of the system. Assume that the rates W satisfy detailed balance. Show that this free energy is a monotonically decreasing function of time, and that it tends towards its minimum value which is obtained when $P(t) = P^*$. Hint: It might be easier to work with discrete time. The convexity of the function $x \log x$ and Jensen's inequality might also be useful.

5.4 Monte Carlo simulation of the fluctuation-dissipation theorem

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.

Note that although the Metropolis dynamics is probably not a realistic model of the dynamics of real magnets (as was stressed in class), it is nonetheless instructive from a theoretical perspective to explore this 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

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - H(t) \sum_i s_i, \tag{7}$$

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 $\langle \cdots \rangle_{H(t)}$.

Implement the metropolis algorithm in your favorite programming language. Work with the largest system for which you can collect enough statistics. In C, Fortran, Java and similar languages you should be able to reach systems of size $L = 200$, while in Matlab you will probably be limited to $L \lesssim 10$. Therefore, it is preferable that you do not run the simulation in Matlab if possible.

(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 $T = 3J$.

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

$$H(t) = \begin{cases} H_0 & \text{when } t < 0 \\ 0 & \text{when } t > 0 \end{cases}. \tag{8}$$

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. Also, make sure to save your code, as it might be useful for future homework assignments.