Statistical Mechanics 2014/2015 Problem Set 6

Submission date: 3.2.15

6.1 Fluctuations and dissipation of a damped oscillator (50 points)

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 $\chi(\omega)$. Plot its real and imaginary parts, respectively χ' and χ'', for three cases: $\lambda \ll \omega_0$, $\lambda = 2\omega_0$ and $\lambda \gg \omega_0$.

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

(c) 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). You can use the following integral:

$$\int_{-\infty}^{\infty} d\omega \frac{1}{\left(\omega^2-\omega_0^2\right)^2+\lambda^2\omega^2} = \frac{\pi}{\lambda\omega_0^2}. \tag{2}$$

6.2 Monte Carlo simulation of the fluctuation-dissipation theorem (50 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

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - H(t)\sum_i s_i, \tag{3}$$

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 previous 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

$$H(t) = \begin{cases} H_0 & \text{when } t < 0 \\ 0 & \text{when } t > 0 \end{cases}. \tag{4}$$

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 send your code by email to ronen.vosk@gmail.com.