421-3
Introduction to Hamiltonian Chaos and Statistical Mechanics

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Canonical Ensemble and Free Energy

The Helmholtz free energy F can be defined as

$$F = -k_B T \ln Z \tag{1}$$

with Z the canonical partition function. Show that this definition is consistent with that given in thermodynamics

$$F =< E > -T < S >, \tag{2}$$

where $< E >$ and $< S >$ are the most probable values of the energy and the entropy in the canonical ensemble, respectively. (Hint: chapter 2.B in Plischke and Bergersen).

Monte Carlo Approach to the Ising Model

Consider the Ising model for a ferromagnet. Its energy is given by

$$E = -\sum_{i<j} J_{ij}\, s_i\, s_j - h \sum_i s_i, \tag{3}$$

where the coupling $J_{ij} = J$ for next neighbors and $J_{ij} = 0$ otherwise. The magnetic field is given by h. By scaling the temperature one can set $J/k_B = 1$.
The goal of this study is to see how such a simple model can exhibit a phase transition and how the signatures of the transition depend on the system size.

1. **Signatures of a Phase Transition in 2d Ising Model**

   (a) Write a Monte-Carlo program for the Ising model in two spatial dimensions[1]. Use periodic boundary conditions.

   (b) For $L = 32$ plot the spatial average $M^{(n)} \equiv \sum_i s_i^{(n)}$ as a function of n. Here n counts the number of Monte Carlo steps *per spin* and $\{s_i^{(n)}\}$ denotes the spin configuration at the n^{th} step. To get a good impression of the behavior of the system, the number of steps n has to be at the very least $5,000$. Compare the "evolution" you obtain for different values of the temperature $2 < T < 5$. Describe the qualitative differences you observe. Do your data suggest a transition between different regimes?

   (c) Determine the ensemble average of the *absolute value* of the magnetization,

$$\mathcal{M}(T) \equiv < |\sum_i s_i| >, \tag{4}$$

[1] See also the hand-out taken from Binder & Heermann.

as a function of the temperature T and of the system size L. Here $< ... >$ denotes the average over sufficiently many configurations $\{s_i\}$. To skip transient behavior do not include the first 1,000 configurations in the average. To judge whether you have included sufficiently many configurations monitor the changes in $\mathcal{M}$ as you increase the number of configurations.

Plot $\mathcal{M}(T)$ for $1 < T < 4$ for increasing values of the system size $L = 8, 16, 32, ...$ For larger values of L focus your efforts on the vicinity of the transition (see also part 1d). Near the transition the transients may be longer than 1,000 and you may have to include more configurations in the average than further away.

(d) The exact solution by Onsager for the two-dimensional Ising model in an infinite system yields a critical temperature of $1/T_c = \frac{1}{2}\ln(1+\sqrt{2})$. The scaling theory of second-order phase transitions predicts that near T_c the magnetization should scale as $\mathcal{M}(T) \propto (T_c - T)^\beta$ for $T < T_c$. According to Onsager's exact solution $\beta = \frac{1}{8}$. Plot your results for $\mathcal{M}$ in a suitable log-log plot. Can you extract a power-law behavior from your data? To see a power law clearly you may have to take a large system and be quite close to the transition.

(e) Switch on the magnetic field h and determine the susceptibility $\chi \equiv \partial_h \mathcal{M}$ at $h = 0$ as a function of the temperature near the transition temperature. Approximate the derivative by $(\mathcal{M}(h) - \mathcal{M}(0))/h$ and choose $h/k_B = 0.005$. Do this for system lengths $L = 16, 32....$ Make sure that you discard transients and average over sufficiently many configurations. Plot χ as a function of T.

2. **Pictures of Spin Configurations**

To get a better impression of the Monte Carlo dynamics for the two-dimensional Ising model run the program *xising* on `scooter.esam.nwu.edu`[2]. Start with a high temperature (clicking at the "thermometer") and decrease the temperature in steps. Use the program *xv* to capture and print pictures of representative spin configurations for $T > T_c$, $T \approx T_c$, and $T < T_c$. Comment on the size of the clusters of spins of like sign. Comment on clusters with $s = +1$ and with $s = -1$ separately. How does the size distribution change as T decreases below T_c?

3. **The One-dimensional Ising Model**

(a) Modify your Monte Carlo code to solve the one-dimensional Ising model. To avoid that the system gets stuck in a "pure" configuration choose non-matching Dirichlet boundary conditions, $s(x = 0) = -1$ and $s(x = L + 1) = +1$.

(b) As for the two-dimensional case, measure and plot $\mathcal{M}$ as a function of the temperature for a range of system sizes, $L = 128, 256, ...$

(c) Generate a space-"time" plot for the "evolution" of the spin-system that shows how the cluster size depends on the temperature.

(d) Compare the results in one dimension with those in two dimensions. Can you find a transition in 1d as you decrease T? If there is a transition its critical temperature $T_c(L)$ has to converge to a non-zero value for $L \to \infty$. Is that the case?

[2] Use the same password as previously.