Magnetism: Part 3

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We work with the Ising model in two dimensions. In practice, this means that you have a square lattice of $N = L \times L$ spins. For a configuration of spins

$$S = (s_1, \ldots, s_N) , \tag{1}$$

the energy is given by

$$\boxed{E(S) = -\frac{1}{2} J \sum_{i=1}^{N} \sum_{j \in \text{neighbors of } i} s_i s_j - B \sum_{i=1}^{N} s_i} , \tag{2}$$

with $s_i = \pm 1$, J the exchange interaction, and B an external field.

We continue to work with a ferromagnet ($J > 0$) in the absence of a magnetic field ($B = 0$). For simplicity, we set $J = 1$ and vary the inverse temperature β. Recall that, for the two-dimensional Ising model in the thermodynamic limit, the exact critical point is at $J\beta_c = 0.4407$ (see lecture notes, Eq. 46).

1. Set $L = 10$ and $B = 0$.

   Consider $\beta = 0.3$, 0.4, and 0.6 and, for $\beta = 0.4$ (closest to the critical point), perform a somewhat longer run (at least 10^4 "unit" steps).

   a) Compute $m(S_k)$ in the three cases, describe what you observe, and compare the three cases.

   b) Based on your observations, draw a rough sketch of the probability densities, $P(m)$, for the three values of β. Explain the physical meaning of your sketches.

      Hint: If you struggle to come up with the sketches, histogram $m(S_k)$.

2. $P(m)$ depends however not only on β but also on L.

   a) Consider the following lattices with $L = 5$, 10, 15, and 20. Perform a Monte Carlo run for each lattice size and estimate how $P(m)$ varies with the size of lattice for the values of $\beta = 0.3$ and 0.5, namely, in the paramagnetic and magnetic phase, respectively.

   b) As L increases, are you more likely or less likely to observe in practice symmetry breaking for $\beta > \beta_c$? Explain your answer.

3. Let us now consider the average energy

$$\langle E \rangle = \frac{1}{Z} \sum_{I=1}^{K} E(S_I) e^{-\beta E(S_I)}, \tag{3}$$

and its fluctuations.

   a) Set $L = 10$ and $B = 0$. Vary the parameter β in the range $0 \leq \beta \leq 1$. Compute and plot the average energy per spin $\langle E \rangle / N$.

      Based on the expression of $E(S)$, explain the limits you obtain for $\langle E \rangle / N$ for low and high temperatures.

   b) Similarly to the relation between $\langle m \rangle$ and χ, it is possible to write the heat capacity in terms of the fluctuations of the energy. Recall that the heat capacity (at constant field) is the response of the energy of the system to a change in temperature

$$C_B = \frac{\partial \langle E \rangle}{\partial T}. \tag{4}$$

      Show that C_B can be expressed as

$$C_B = k_B \beta^2 \left[\langle E^2 \rangle - \langle E \rangle^2 \right]. \tag{5}$$

   c) Zoom in close to the critical point with $0.2 \leq \beta \leq 0.6$ and consider the two lattices with $L = 5$ and 20. Plot $C_B/(k_B N)$ and describe your finding.

4. **Optional exercise on correlation function**. The spin-spin correlation function quantifies the correlation among spins and is defined as

$$g(r) = \langle s_k s_{k+r} \rangle - \langle s_k \rangle \langle s_{k+r} \rangle = \langle s_k s_{k+r} \rangle - \langle m \rangle^2. \tag{6}$$

   At very high temperatures, the spins are essentially random and $g(r) = 0$. At finite temperatures, close spin are correlated and we expect $g(r)$ to decrease as $r \to \infty$. The behavior of $g(r)$ is approximately given by

$$g(r) \sim \exp[-r/\xi(\beta)], \tag{7}$$

   where the correlation length $\xi(\beta)$ is temperature dependent.

   a) Set $L = 20$. Compute and plot $g(r)$ for $\beta = 0.3$, 0.4, and 0.5.

      Hint: Compute $g(r)$ for $r = 1, \ldots, L/2$. This means that, for one value of r, you must average over all k. For simplicity, you can only calculate $g(r)$ horizontally but you must be careful about the periodic boundary conditions. Finally, you must of course average over the Monte Carlo steps.

   b) Explain what happens to the correlation length at the different temperatures.

      Note: The correlation length ξ is the typical size of clusters of spins pointing in the same direction. As these regions grow in size in the vicinity of the critical point, the Metropolis algorithm suffers from a so-called *critical slowing down*, namely, it becomes more and more difficult to flip a spin at random as this is likely to be coupled to neighboring spins pointing in the same direction. One then needs to use more sophisticated Monte Carlo moves (than one spin flip) to efficiently sample configuration space near the critical temperature.