Magnetism: Part 2

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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.

You will now adapt your code to treat also a **ferromagnet**, namely, introduce $\boxed{J > 0}$.

- **Note 1**: β, J, and B enter in $\beta E(S)$ through the products βB and βJ. For simplicity, set $J = 1$ and vary β and B.
- **Note 2**: Always use the "unit" Monte Carlo time of a sweep over N spin flips.
- **Periodic boundary conditions**. Since spins interact and you have a finite $L \times L$ lattice, the spins living close to the edge of the lattice will see a different environment than the ones in the middle of the lattice. To reduce these so-called "finite-size effects", we impose "periodic boundary conditions". This means that, for instance, a spin sitting at (L, L) will interact with four spin at $(L-1, L)$, $(1, L)$, $(L, L-1)$, and $(L, 1)$ as shown in Fig. 1. Therefore, the lattice is periodically repeated.

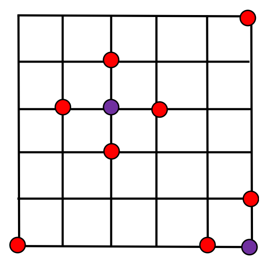

Figure 1: Periodic boundary conditions for a 6×6 lattice. The purple spin interacts with its so-called nearest "images" neighbors.

A possible (not the only) way to program periodic boundary conditions is to setup four vectors (called here "above, below, right, and left") at the beginning to tell you with which neighbors a spin at (x, y) interacts so that its contribution to the interaction energy is

```
e = -J * S[x,y] * ( S[right[x],y] + S[left[x],y]
                    + S[x,above[y]] + S[x,below[y]] )
```

1. Before programming, do some thinking, go back to point 4.a) of Part 1, and answer the same question for $J > 0$.

2. Set $L = 10$ and explore the parameters of your simulations.

   a) Set $\beta = 1$ and $B = 0$.

      i) Perform a Monte Carlo run and compute $m(S_k)$ along the run. Repeat the calculation ten times starting every time with a different random configuration, S_0, and explain what you find. In particular, describe and explain what happens in the runs which clearly differ from each other.

      Hint: It might help to also look at the last configuration with `pcolor` or `surf`.

      Note: You should try to keep the number of the "unit" steps less than 1000.

      ii) Estimate the equilibration time κ and the number of steps needed to obtain a reasonable estimate of $\langle m \rangle$.

      Note: If this is difficult for some runs, think about the next question.

      iii) In the absence of a magnetic field, which value of $\langle m \rangle$ would you obtain if you could run your Monte Carlo simulation for many, many steps?

   b) Set $\beta = 1$ and consider the case of a strong and a weak field, namely, $B \approx 1$ and $B \approx 0.05$, respectively.

      How does the magnetization behave if you repeat the calculations of point a.i) in the presence of these external fields? Give a qualitative explanation of what you observe.

   c) Set $\beta = 0.2$ and $B = 0$.

      Also for this case, repeat the calculations of point a.i) and estimate κ and a reasonable length of the run. In which part of the phase diagram are $\beta = 1$ and $\beta = 0.2$ located?

3. Set $L = 10$ and $B = 0$. Vary the parameter β in the range $0 \leq \beta \leq 1$. For each value of β, repeat the calculation a few (at least 5) times.

   a) Plot the values of $\langle m \rangle$ from all your runs as a function of β.

      The behavior of the $m(\beta)$ is clearly different on the left and on the right of a critical point β_c. What happens before, around, and after β_c? Give a physical interpretation.

   b) In the mean field treatment of the Ising model,[1]

$$J\,\beta = \frac{1}{8m} \ln\left(\frac{1+m}{1-m}\right) , \tag{3}$$

[1] In the Statistical Physics course, you have already encountered the mean field solution of the Ising model, where a spin s_i interacts with the mean value of its neighbors as $e_{ij} = -J s_i \langle s_j \rangle$. With such an assumption, it is easy to derive that $\langle s_i \rangle = \tanh(z\beta J \langle s_j \rangle)$, where z is the number of nearest neighbors ($z = 4$ in two dimensions). Since all spins see the same environment, $\langle s_i \rangle = \langle s_j \rangle = \langle m \rangle$ and $\langle m \rangle$ satisfies the self-consistent equation $\langle m \rangle = \tanh(z\beta J \langle m \rangle)$. Using $\text{arctanh}(x) = \frac{1}{2} \ln\left(\frac{1+x}{1-x}\right)$, one obtains Eq. 3.

where m denotes here for simplicity $\langle m \rangle$. Compare this expression with what you have computed. How does this theory perform?

Hint: Use the formula to compute $\beta(m)$ for $0 \leq m \leq 1$ but plot $m(\beta)$.

c) Plot the values of $\chi(\beta)$ from all your runs as a function of β. To compute χ, use the expression of χ in terms of the fluctuations of m.

   The presence of a critical point is also clear in the plot of $\chi(\beta)$. Explain what you observe around β_c.

   Hint: In your plot, you might have some scatter of $\chi(\beta)$ at large β. If this is the case, try to increase the equilibration time κ.

d) **Optional exercise on modified susceptibility**. Define a modified susceptibility χ' in terms of $\langle |m| \rangle$ as

$$\frac{\chi'}{N} = N\beta[\langle m^2 \rangle - \langle |m| \rangle^2] \,, \tag{4}$$

   Compute χ' from your runs as a function of β. Describe your findings and the advantages (if any) with respect to the simulation of χ.