

## Exercise 2: Swendsen-Wang algorithm for the 2D Ising model

The goal of this exercise is to implement the Swendsen-Wang algorithm for the 2D Ising model. Recall that the update of the Swendsen-Wang algorithm works as follows:

- Assign to each bond  $b$  a weight  $w_b \in \{0, 1\}$ , where 1 means “connected” and 0 means “disconnected”. If the spins connected by the bond  $b = (n, m)$  are antiparallel, always choose  $w_b = 0$ , if the spins are parallel, choose  $w_b = 0$  with probability  $e^{-2\beta J}$ , where  $\beta = \frac{1}{k_B T}$ . In terms of conditional probabilities:

$$\begin{aligned} p(w_b = 0 | \sigma_n \neq \sigma_m) &= 1, & p(w_b = 0 | \sigma_n = \sigma_m) &= e^{-2\beta J}, \\ p(w_b = 1 | \sigma_n \neq \sigma_m) &= 0, & p(w_b = 1 | \sigma_n = \sigma_m) &= 1 - e^{-2\beta J}. \end{aligned}$$

- Interpreting these weights as edges of a graph (where 0 means no edge), find “clusters” of spins, i.e., connected components of the graph.
- Flip each cluster (= connected component) with probability  $p = 0.5$ .

After the update, do a measurement (if the system is already thermalized) and continue with the next update.

- a) Since we need to identify clusters, it is better to label the lattice sites  $(x, y)$  by a single integer number  $n = n(x, y) = x \cdot L_y + y = 0, 1, \dots, N - 1$  where  $N = L_x \cdot L_y$ . The inverse mapping is given by  $x(n) = n // L_y$  (integer division, rounding down) and  $y(n) = n \bmod L_y$ . Create an array that contains each bond  $(n, m)$  of the square lattice with periodic boundary conditions exactly once. The bond array should have shape  $(2N, 2)$ .
- b) Initialize a 1D array for the spin states  $\sigma_n$  (having random entries  $\pm 1$ ).
- c) Write a function that determines the weights  $w_b$  for each of the bonds.
- d) To determine the connected components, you can use the function `scipy.sparse.csgraph.connected_components`. Look up the documentation of the function online. The graph is represented by a sparse matrix of the type `scipy.sparse.csr_matrix`. You can use the initialization of the form `csr_matrix((weights, (bonds[:, 0], bonds[:, 1])), size=(N, N))`. Don't forget to add the transposed to obtain a symmetric graph. Using the result of `connected_components`, flip each of the determined clusters with probability  $p = 0.5$ . Collect the code in a function performing one update with the Swendsen-Wang algorithm.
- e) Write functions to measure the energy and magnetization.
- f) Write a function to run the whole Monte Carlo simulation at given temperature, returning arrays with all measured values  $E$  and  $M$ . Plot the mean values for different temperatures and make sure you get (roughly) the same results as last week. (Begin the comparison with small systems!)

- g) Optionally: Now is a good time to optimize the code with `numba.jit`.
- h) Measure and plot the autocorrelation of the energy

$$C_E(\delta) = \frac{\langle E_{t+\delta} E_t \rangle_t - \langle E_t \rangle_t^2}{\langle (E_t)^2 \rangle_t - \langle E_t \rangle_t^2}$$

versus  $\delta$  (and similarly for the magnetization) for  $T$  right at, above, and below the critical temperature  $T_c$ .

- i) Recreate the the autocorrelation plots for an update function which proposes to flip  $L_x \cdot L_y$  random spins with the Metropolis algorithm.