Exercise 12: Stochastic Series Expansion (SSE)

This exercise uses the provided file `sse.py`, which implements the SSE algorithm.

a) Read the file `sse.py`.

b) Formally, the series expansions of the exponential $e^{-\beta H}$ requires an infinte sum over all n (=the number of (non-identity) operators in the operator string). Yet, this code works with a fixed length of the operator string, which is only increased during the warm-up in `thermalize`. To justify this, generate histograms showing the distribution of n for simulations of 3 different inverse temperatures $\beta \in \{ 0.1, 1, 64 \}$ for a lattice of 8×8 spins.

   Hint: Use the function `init_SSE_square` for initialization. Call the functions `thermalize` and `measure` for each temperature, and use the function `matplotlib.pyplot.hist` to plot a histogram.

c) Use the function `run_simulation` to measures the energy for various temperatures $0 < T \leq 2$ and $L \times L$ systems of increasing system sizes $L = 4, 8, 16$. Plot the energy versus temperature T.

   Hint: In all your simulations, start from high temperatures (small β) and cool down to smaller temperatures (large β). This makes the thermalization more efficient and actually runs faster (The code does only increase the length of the operator string during thermalization, but never decreases it).

d) Extend the function `run_simulation` to also measure the specific heat $C_v = \partial_T \langle E \rangle = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$ per site. Measure and plot it for $L = 8$ versus T, including error bars. What do you observe at low temperatures? Can you explain the behaviour?

Since we simulate an anti-ferromagnet favoring anti-alignment of the spins, the relevant order parameter is the staggered magnetization

$$M_s = \frac{1}{L^2} \sum_{x,y} (-1)^{x+y} \; \hat{\sigma}^z_{x,y}. \tag{1}$$

The Heisenberg model has a continuous SU(2) symmetry. In the thermodynamic limit $L \to \infty$, the Mermin-Wagner theorem rules out a spontaneous symmetry breaking in 2D at any finite $T > 0$; the basic idea behind the theorem are Goldstone modes, in this case magnons. Thus, at any fixed temperature T, the magnetization $\langle |M_s| \rangle \to 0$ with increasing L.
However, the ground state has a finite expectation value $M_s = 0.3074(1)$ for the staggered magnetization [arXiv:0807.0682]. Since finite systems have an energy gap which vanishes only for $L \to \infty$, one can extract the ground state magnetization by simulating large enough β for a given L and only then extrapolate to $L \to \infty$. In other words, one can exploit that the limits $L \to \infty$ and $T \to 0$ do not commute to extract ground state properties from finite-temperature simulations.

e) Write a function to calculate the staggered magnetization from the configuration of the `spins`.

   Hint: The function `site` defines the ordering of the `spins`. Calculate a 1D array with the phases `stag` $= (-1)^{x+y}$ in the same ordering as the spins and store it separately (like the bonds), such that a single measurement only involves the calculation `sum(stag * spins)`.

f) Measure and plot the absolute value of the staggered magnetization $\langle |M_s| \rangle$ for $L = 4, 8, 16$ versus temperature. What is your estimate of the ground state staggered magnetization?

Bonus Write a function `init_SSE_honeycomb` similar to `init_SSE_square`, but initializing the `bonds` array to simulate a Honeycomb lattice. What staggered magnetization do you find in the ground state?

   Hint: The honeycomb lattice has a two-site unit cell of A and B sites and 3 bonds per unit cell. You don't need to modify the update functions of the diagonal or loop updates. You can choose `stag` to be $+1$ on A sites and -1 on B sites.