Exercise 3: Extended Ensemble Simulations

In this third exercise we will employ extended ensemble simulation techniques to (re)investigate the 2D Ising model, now performing an "all-temperature" calculation allowing us to directly estimate the density of states $g(E)$. In the second part we will consider a prototypical system undergoing a first-order phase transition, the Q-state Potts model.

1. Implement the **Wang-Landau algorithm** for the 2D Ising model on the square lattice with periodic boundary conditions. (You should be able to simply expand your single spin-flip Metropolis code.)

2. Calculate estimates for the **density of states** $g(E)$ from Wang-Landau sampling for systems of linear size $L = 8, 16, 32$ in the energy range $E_{\min} = -2N$ to $E_{\max} = 0$. Normalize the calculated density of states such that $g(E_{\min}) = 2$ and plot $\ln g(E)$ for the different system sizes.

3. From the calculated estimate of the density of states calculate the following thermodynamic observables and plot them in the temperature range $T \in [0, 4]$ (showing data for all three system sizes in one plot):

   - the **energy** $U(T) = \frac{1}{Z} \sum_E g(E) E \exp(-\beta E) = \langle E \rangle_T$
   - the **specific heat** $C_v(T) = dU/dT = \left(\langle E^2 \rangle_T - \langle E \rangle_T^2 \right) / T^2$
   - the **free energy** $F(T) = -T \log Z$
   - the **entropy** $S(T) = \left(U(T) - F(T) \right) / T$

   where Z is the partition function $Z = \sum_E g(E) \cdot \exp(-\beta E)$.
   Compare these results to those obtained in the last exercise.

4. Expand the above implementation of the Wang-Landau algorithm to simulate the **Potts model**, which for a Q-state Potts spin $\sigma_i \in \{1, 2, \ldots, Q\}$ we define via the Hamiltonian

$$H = -\sum_{\langle ij \rangle} \delta\left(\sigma_i, \sigma_j\right) ,$$

   where the sum again runs over all nearest-neighbor bonds. Consider a periodic square lattice with $N = L^2$ Potts spins and estimate the density of states $g(E)$ for the 10-state Potts model ($Q = 10$) in the energy range $E_{\min} = -2N$ to $E_{\max} = 0$. This estimate can now be normalized such that $g(E_{\min}) = Q = 10$.

5. For systems of linear size $L = 8, 16, 32$ again plot **thermodynamic averages** for the energy, specific heat, free energy, and entropy as above.

6. Plot the ***canonical* distribution function** $P(E) = g(E)\exp(-\beta E)$ in proximity of the thermal phase transition, which occurs at temperature

$$T^* = \frac{1}{\ln(1+\sqrt{Q})}$$

for the *infinite* system ($L = \infty$). Can you observe a double-peak structure indicative of a first-order phase transition?

7. *Optional exercise I:* From the precise location of the double-peak structure in the canonical distribution function $P(E)$ you can determine estimates of the **finite-size transition temperature** $T^*(L)$ for a given linear system size L. Plot your estimates versus the inverse system size $1/L^2$ and extrapolate your data to the infinite system size limit – can you recover the analytical estimate above? You might want to calculate a few extra system sizes $L = 8, 16, 24, 32, 48, 64, \ldots$ for this extrapolation.

8. *Optional exercise II:* Calculate the **local diffusivity** $D(E)$ of the random walk in energy space for the Ising and Potts model simulations above by running simulations with *fixed* weights $w(E) \approx 1/g(E)$, which you have obtained from Wang-Landau sampling. To obtain an estimate for the local diffusivity

   - Record two histograms during the sampling process – the energy histogram $h(E)$, which is incremented for every step, and the histogram $h^+(E)$, which is incremented only if the last extremal energy you have visited is $E_{\min}$ (and *not* $E_{\max}$).
   - From these two histograms calculate the fraction $f(E) = h^+(E)/h(E)$, which estimates how much time on average the energy random walker spends at a given energy E diffusing towards higher energies. Plot this fraction $f(E)$.
   - Calculate the derivative df/dE of this fraction (and plot it).
   - Plot an estimate of the local diffusivity via

$$D(E) \propto \left(h(E) \cdot \frac{df}{dE} \right)^{-1} .$$