Problem 1. ***Monte Carlo simulation of the quantum 1D Ising model***

Consider the 1D quantum Ising model in a transverse field:

$$H = -J \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_{i=1}^{L} \sigma_i^x \tag{1}$$

Generalize your simulation of cluster update Monte Carlo from Exercise 6 to an anisotropic square lattice with $L \times M$ spins and coupling constants J_x, J_τ between horizontal and vertical neighbours, respectively. Complete the mapping to the quantum system by identifying

$$\beta_{\mathrm{cl}} J_x = \Delta_\tau J, \quad \beta_{\mathrm{cl}} J_\tau = -\frac{1}{2} \log \Delta_\tau \Gamma, \tag{2}$$

where β_{cl} is the inverse temperature of the classical system and $\Delta_\tau = \beta/M$ the imaginary time discretization of the quantum system. Note that in order to get meaningful results, you have to take $\Delta_\tau \ll 1$ and hence the quantum mechanical model with $|J/\Gamma| \approx 1$ corresponds to an extremely anisotropic classical Ising model. Run your code for different ratios of the coupling constants, plot the results vs. J/Γ and try to locate the quantum phase transition in the model. You can improve your estimate by simulating larger and larger systems. A true phase transition can only happen in the thermodynamic limit $L, M \to \infty$, i.e. for the infinite chain at zero temperature.

Problem 2. ***Hartree-Fock approximation for the attractive Hubbard model***

Consider a two dimensional negative-U Hubbard model on a square lattice:

$$H = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - |U| \sum_i n_{i\uparrow} n_{i\downarrow} \,. \tag{3}$$

To study this problem, we consider a Bogoliubov-de Gennes mean field Hamiltonian:

$$H_{\mathrm{BdG}} = -t \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} - \sum_{i\sigma} \mu_i c_{i\sigma}^\dagger c_{i\sigma} - \sum_i \Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \text{h.c.} \,, \tag{4}$$

where μ_i describes charge ordering and Δ_i is the superconducting pairing term (we have neglected any form of spin ordering). Hamiltonian (4) can be conveniently diagonalized after a particle-hole transformation:

$$\begin{aligned} c_{i\uparrow} &= d_{1i}, \\ c_{i\downarrow} &= d_{2i}^\dagger. \end{aligned} \tag{5}$$

The Hamiltonian reads:

$$\begin{aligned} H_{\mathrm{BdG}} = &- t \sum_{ij} (d_{1i}^\dagger d_{1j} - d_{2i}^\dagger d_{2j} + \text{h.c}) - \sum_i \mu_i (d_{1i}^\dagger d_{1i} - d_{2i}^\dagger d_{2i}) \\ &- \sum_i \Delta_i d_{2i}^\dagger d_{1i} + \text{h.c.} \,, \end{aligned} \tag{6}$$

which can be directly diagonalized.

The non-linear self consistent mean field equations are:

$$\begin{aligned} \Delta_i &= |U| \left\langle c_{i\uparrow} c_{i\downarrow} \right\rangle_{\mathrm{MF}} , \\ \mu_i &= \mu + |U| \sum_\sigma \left\langle c^\dagger_{i\sigma} c_{i\sigma} \right\rangle_{\mathrm{MF}} . \end{aligned} \tag{7}$$

Solve these equations in an iterative scheme:

- Make an initial guess for μ_i and Δ_i.
- Construct the Hamiltonian (6).
- Find the eigenvalues and eigenvectors of the Hamiltonian (6) .
- Compute $\left\langle c_{i\uparrow} c_{i\downarrow} \right\rangle_{\mathrm{MF}} = \left\langle d^\dagger_{2i} d_{1i} \right\rangle$ and $\left\langle c^\dagger_{i\uparrow} c_{i\uparrow} \right\rangle_{\mathrm{MF}} = \left\langle d^\dagger_{1i} d_{1i} \right\rangle$ and $\left\langle c^\dagger_{i\downarrow} c_{i\downarrow} \right\rangle_{\mathrm{MF}} = 1 - \left\langle d^\dagger_{2i} d_{2i} \right\rangle$.
- Recompute the fields μ_i and Δ_i according to Eq. (7).
- Iterate until convergence.

1. Consider a square lattice $N = 20 \times 20$ and $t = 1$. For different values of $|U|$ and $\mu = 2t$, study the evolution of the superconducting gap function $\sum_i \Delta_i / N$. Repeat the same analysis fixing $|U| = 3t$ and varying μ.
2. Consider $|U| = 3t$ and add spatial disorder to μ: $\mu_i = \mu + v_i$, where v_i is drawn from uniform distribution over the interval $[-V, V]$, with $V = 0.5$ and $\mu = 0$. Study the spatial distribution of Δ_i, $n_i = n_{i\uparrow} + n_{i\downarrow}$.