# Sheet 5:

Hand-out: Tuesday, Nov. 21, 2023; Solutions: Tuesday, Nov. 28, 2023

**Problem 1** Super-exchange in a tilted potential

Consider a two-site (pseudo) spin-$1/2$ Hubbard model in the presence of a strong tilt $\Delta$:

$$\hat{\mathcal{H}} = -t \sum_{\sigma=\uparrow,\downarrow} \left( \hat{c}^\dagger_{2,\sigma} \hat{c}_{1,\sigma} + \text{h.c.} \right) + \frac{\Delta}{2} \sum_{\sigma=\uparrow,\downarrow} \left( \hat{c}^\dagger_{1,\sigma} \hat{c}_{1,\sigma} - \hat{c}^\dagger_{2,\sigma} \hat{c}_{2,\sigma} \right) + \\ + U \sum_{n=1}^{2} \hat{n}_{n,\uparrow} \hat{n}_{n,\downarrow} + \frac{U}{2} \sum_{n=1}^{2} \sum_{\sigma=\uparrow\downarrow} \hat{n}_{n,\sigma} \left( \hat{n}_{n,\sigma} - 1 \right) \quad (1)$$

Note that the last sum is identical zero for fermionic particles (Pauli principle). In this problem we will consider the regime:

$$U, \Delta, t > 0, \qquad U, \Delta \gg t, \qquad |U \pm \Delta| \gg t, \quad (2)$$

and we work with *exactly two particles with arbitrary spin*.

(1.a) In the following we will treat $t$ as a perturbation and work with unperturbed states with *exactly one particle per site*. Discuss for which values of $U, \Delta$ such states are ground states when $t = 0$, or metastable excited states respectively.

(1.b) Now consider the particles $\hat{c}_{j,\sigma}$ are *fermions*. Show by an explicit perturbative calculation (degenerate perturbation theory) that the perturbed eigenstates for $t > 0$ are described by the effective Hamiltonian

$$\hat{\mathcal{H}}_{\text{eff}} = J \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 - \frac{J}{4} \hat{n}_1 \hat{n}_2, \quad (3)$$

where $\hat{\boldsymbol{S}}_n$ and $\hat{n}_n$ are the spin and particle number on site $n = 1, 2$. Show that the super-exchange coupling is given by

$$J = \frac{2t^2}{U + \Delta} + \frac{2t^2}{U - \Delta} \quad (4)$$

and discuss under which conditions it is (anti-) ferromagnetic.

1.c) Next, assume that the particles $\hat{c}_{j,\sigma}$ are *bosons*. How do the results from (3.b) change?

(1.d) Finally, discuss how the situation changes if $\hat{c}_{j,\sigma}$ are *bosons* and the Hubbard interaction becomes spin-dependent, i.e.

$$\hat{\mathcal{H}}_U = U_{\uparrow\downarrow} \sum_{n=1}^{2} \hat{n}_{n,\uparrow} \hat{n}_{n,\downarrow} + \frac{1}{2} \sum_{n=1}^{2} \sum_{\sigma=\uparrow\downarrow} U_\sigma \hat{n}_{n,\sigma} \left( \hat{n}_{n,\sigma} - 1 \right) \quad (5)$$

instead of the SU(2)-invariant Hubbard interactions in Eq. (1). Hint: See e.g. Duan et al., Phys. Rev. Lett. 91, 090402 (2003).

**Problem 2** Valence Bond Solid (VBS) and entanglement laws

The ground state of the two-site antiferromagnetic ($J > 0$) Heisenberg spin Hamiltonian,

$$\hat{\mathcal{H}}_2 = J\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2, \tag{6}$$

is given by the spin-singlet, or Bell state

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right). \tag{7}$$

(2.a) Consider a one-dimensional spin chain with an antiferromagnetic Heisenberg term on every second bond:

$$\hat{\mathcal{H}}_{\mathrm{VBS}} = J\sum_n \hat{\boldsymbol{S}}_{2n-1} \cdot \hat{\boldsymbol{S}}_{2n}. \tag{8}$$

Find and describe the unique ground state $|\Psi_{\mathrm{VBS}}\rangle$ of $\hat{\mathcal{H}}_{\mathrm{VBS}}$. ($\hat{\mathcal{H}}_{\mathrm{VBS}}$ is called the parent Hamiltonian of this VBS state.)

(2.b) Assume that the system is realized in the ground state $|\Psi_{\mathrm{VBS}}\rangle$. Calculate the following spin-spin two point correlation functions for distances $d$,

$$C^z(d) = \langle \hat{S}^z_0 \hat{S}^z_d \rangle \tag{9}$$

and the reduced density matrix of the central spin $\hat{\rho}_0 = \mathrm{tr}_{j\neq 0}\left(|\Psi_{\mathrm{VBS}}\rangle\langle\Psi_{\mathrm{VBS}}|\right)$.

Is the pure state $|\Psi_{\mathrm{VBS}}\rangle$ entangled? Is the pure state $|\Psi_{\mathrm{VBS}}\rangle$ correlated?

(2.c) Next, we consider a two-dimensional valence bond solid $|\mathrm{VBS}\rangle$, determined as the ground state of the parent Hamiltonian

$$\hat{\mathcal{H}}^{\mathrm{2d}}_{\mathrm{VBS}} = J\sum_n \sum_{j_y} \hat{\boldsymbol{S}}_{2n-1,j_y} \cdot \hat{\boldsymbol{S}}_{2n,j_y}. \tag{10}$$

Here $\hat{\boldsymbol{S}}_{j_x,j_y}$ denotes the spin operator on site $(j_x, j_y)$ in a 2D square lattice.

Let $A$ be a rectangular region of size $\ell \times \ell$ in the center of the system. Calculate the entanglement entropy $S_{\mathrm{A}}$ of the subsystem. Distinguish between different possible sizes and locations of the rectangular region $A$ relative to the 2D lattice! How does $S_{\mathrm{A}}$ depend on the linear size $\ell$ of the subsystem in the different cases?

(2.d) Now consider a 2D parent Hamiltonian in which every spin $\hat{\boldsymbol{S}}_{\boldsymbol{i}}$ is coupled to *exactly one* other spin $\hat{\boldsymbol{S}}_{\boldsymbol{j}}$ by an antiferromagnetic Heisenberg coupling; denote by $(\boldsymbol{i}, \boldsymbol{j})$ a pair of coupled spins, such that the parent Hamiltonian becomes:

$$\hat{\mathcal{H}} = J\sum_{(\boldsymbol{i},\boldsymbol{j})} \hat{\boldsymbol{S}}_{\boldsymbol{i}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{j}} \tag{11}$$

(i) Assume that no couplings exist between spins at sites $\boldsymbol{i}, \boldsymbol{j}$ further apart than a critical distance $d_c$. Otherwise, assume that the combinations of coupled spins is random. For this situation, how does the entanglement entropy $S_A$ of a rectangular subsystem $A$ of size $\ell \times \ell$ scale with the linear size $\ell$, assuming that $\ell \gg d_c$?

(ii) Next, consider a completely random combination of couplings at arbitrary distances, i.e. $d_c = \infty$. How does the entanglement entropy $S_A$ of a rectangular subsystem $A$ scale with its linear size $\ell$ in this case?