Problem Set 2:

Handout: Thu, Nov. 19, 2020; Solutions: Fri, Nov. 27, 2020

Problem 1 Strongly correlated states of matter

(1.a) Consider the *classical* 1D Heisenberg ferromagnet ($J < 0$), with the classical energy

$$E = J \sum_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}. \tag{1}$$

Find all classical ground state configurations $\{\boldsymbol{S}_j\}$ which minimize the energy functional $E[\{\boldsymbol{S}_j\}]$. Determine the ground state energy E_0.

Show that E is invariant under global $SU(2)$ rotations. Are the ground states minimizing $E[\{\boldsymbol{S}_j\}]$ symmetric?

(1.b) Consider the *quantum* 1D Heisenberg ferromagnet ($J < 0$), with the Hamiltonian

$$\hat{\mathcal{H}} = J \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}. \tag{2}$$

Using the variational principle, show that the classical ground states $|\{\boldsymbol{\sigma}_j\}\rangle$, obtained by multiplying the positive-eigenvalue eigenstates of $\boldsymbol{\sigma} \cdot \hat{\boldsymbol{S}}_j$, are true ground (and thus eigen-) states of $\hat{\mathcal{H}}$.

Are these ground states correlated? Are these ground states entangled?

Choose the classical ground state $|\mathrm{FM}_z\rangle$ with all spins pointing along z and define the following set of all states with total magnetization $S^z_{\mathrm{tot}} = L/2 - 1$,

$$\{\hat{S}^-_j |\mathrm{FM}_z\rangle\}_{j=1\ldots L}. \tag{3}$$

Show that the Hamiltonian $\hat{\mathcal{H}}$ is block-diagonal in $S^z_{\mathrm{tot}} = \sum_j \hat{S}^z_j$ and diagonalize the block with $S^z_{\mathrm{tot}} = L/2 - 1$. Show that the resulting one-magnon states have a dispersion relation

$$\omega_k = -2J\left(1 - \cos(k_x)\right) \simeq -J k_x^2 + \mathcal{O}(k_x^4). \tag{4}$$

(1.c) Consider the *classical* 1D Heisenberg antiferromagnet ($J > 0$), with the classical energy

$$E = J \sum_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}. \tag{5}$$

Find all classical ground state configurations $\{\boldsymbol{S}_j\}$ which minimize the energy functional $E[\{\boldsymbol{S}_j\}]$. Determine the ground state energy E_0.

Show that E is invariant under global $SU(2)$ rotations. Are the ground states minimizing $E[\{\boldsymbol{S}_j\}]$ symmetric?

(1.d) Consider the two-site quantum Heisenberg antiferromagnet ($J > 0$), with the Hamiltonian

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

Calculate all eigenstates and eigenenergies. Show that the classical two-site antiferromagnet $|\uparrow_1\downarrow_2\rangle$ is not an eigenstate, and calculate its average energy.

Is the quantum mechanical ground state degenerate? How does the ground state transform under global $SU(2)$ transformations? As an example, calculate explicitly the action of a unitary transformation rotating spins around the y-axis by an angle $\pi/2$.

Show that the ground state is entangled and correlated.

Problem 2 Matrix product states

An important class of variational states is defined by the so-called *matrix product states* (MPS), which form the basis for the numerical DMRG method. In this exercise, we illustrate how MPS's can represent entangled quantum states. For a one-dimensional periodic chain, with lattice sites $j = 1...L$, a general MPS can be written:

$$|\mathrm{MPS}\rangle = \sum_{\{\sigma_j\}} c_{\sigma_1,...,\sigma_L}|\sigma_1....\sigma_L\rangle, \qquad c_{\sigma_1,...,\sigma_L} = \prod_{k=1}^{L}\sum_{m_k=1}^{D} M^{(\sigma_1)}_{m_L,m_1}M^{(\sigma_2)}_{m_1,m_2}...M^{(\sigma_L)}_{m_{L-1},m_L}. \tag{7}$$

Here $\sigma_j = 1...d$ label the local basis states $|\sigma_j\rangle$ at site j. In the second expression, the coefficients $c_{\sigma_1,...,\sigma_L}$ are expressed as a product of $D \times D$ matrices $M^{(\sigma_j)}$ which depend on the respective local states σ_j. Written in matrix notation, we have:

$$c_{\sigma_1,...,\sigma_L} = \mathrm{tr}\left[M^{(\sigma_1)}M^{(\sigma_2)}...\ M^{(\sigma_L)}\right]. \tag{8}$$

The integers d and D denote the local Hilbert space dimension and the bond dimension of the MPS, respectively.

(2.a) Show that the entangled Bell state $|\Psi^-\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ in a two-site chain $L = 2$ can be represented by an MPS with the following matrices:

$$M^{(\uparrow_1)} = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix},\ M^{(\uparrow_2)} = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix},\ M^{(\downarrow_1)} = \begin{pmatrix}0 & -1\\ 0 & 0\end{pmatrix},\ M^{(\downarrow_2)} = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}. \tag{9}$$

How do the matrices have to be changed to obtain a normalized state?

(2.b) Show that a general product state

$$|\Phi\rangle = \prod_j \left(\sum_{\sigma_j=1}^{d} \phi_{\sigma_j}|\sigma_j\rangle\right) \tag{10}$$

can be represented by a MPS with bond dimension $D = 1$. Give explicit expressions for the corresponding matrices M^{σ_j}!

(2.c) Describe the physical state of $L = 4$ spin-$1/2$ represented by:

$$M^{(\uparrow_j)} = \begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 0\\ 1/\sqrt{2} & 0 & 0\end{pmatrix}, \qquad M^{(\downarrow_j)} = \begin{pmatrix}0 & 0 & 1\\ -1/\sqrt{2} & 0 & 0\\ 0 & 0 & 0\end{pmatrix} \tag{11}$$

Problem 3 Entanglement spectrum

The entanglement of a subsystem V can be characterized by the structure of its reduced density matrix, $\hat{\rho}_V = \mathrm{tr}_{\overline{V}} |\Psi\rangle\langle\Psi|$. The entanglement spectrum is defined by the eigenvalues λ_n of $-\log \hat{\rho}_V$ – i.e. one writes

$$\hat{\rho}_V = e^{-\hat{h}}, \qquad \hat{h} = \hat{U}^\dagger \,\mathrm{diag}\,(\lambda_1, ..., \lambda_d)\ \hat{U}. \tag{12}$$

(3.a) Assume that $|\Psi\rangle$ is the ground state of a Hamiltonian $\hat{\mathcal{H}}$, which satisfies the following global conservation law:

$$[\hat{\mathcal{H}}, \hat{\mathcal{O}}] = 0, \qquad \hat{\mathcal{O}} = \hat{\mathcal{O}}_V + \hat{\mathcal{O}}_{\overline{V}}, \qquad \hat{\mathcal{O}}^\dagger = \hat{\mathcal{O}}, \tag{13}$$

where $\hat{\mathcal{O}}_V$ is defined only on the subsystem V and $\hat{\mathcal{O}}_{\overline{V}}$ on its complement $\overline{V}$.

Show that the reduced density matrix $\hat{\rho}_V$ commutes with $\hat{\mathcal{O}}_V$:

$$[\hat{\rho}_V, \hat{\mathcal{O}}_V] = 0. \tag{14}$$

Discuss how this implies that the entanglement spectrum can be calculated separately for the different eigenvalues o_n of $\hat{\mathcal{O}}_V$:

$$\hat{\rho}_V = \bigoplus_n e^{-\hat{h}_n}, \qquad \hat{h}_n = \hat{U}_n^\dagger \,\mathrm{diag}\,(\lambda_1(n), ..., \lambda_{d_n}(n))\ \hat{U}_n. \tag{15}$$

(3.b) Calculate the $\hat{S}^z_A$-resolved entanglement spectrum $h_{-1/2}$ and $h_{+1/2}$ for a spin-singlet state shared by Alice (A) and Bob (B).

(3.c) Now consider the following Hamiltonian on a $L = 4$-site chain:

$$\hat{\mathcal{H}} = J\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_4 + J\hat{\boldsymbol{S}}_2 \cdot \hat{\boldsymbol{S}}_3 \tag{16}$$

Show that $\hat{S}^z_{\mathrm{tot}}$ is conserved and qualifies as an observable $\hat{\mathcal{O}}$ in (3.a).

Find the ground state for $J > 0$ and calculate the $\hat{S}^z$-resolved entanglement spectrum if the system is cut in two in the middle ($A : j = 1, 2$ and $B : j = 3, 4$).