Computational Many-Body Physics

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Exercise Sheet No. 5

Please upload your solutions to ILIAS until **Thursday, June 23, 16:00**.

Exercise 1: Spin correlations of the one-dimensional Heisenberg model

(11 points)

Here we focus on the isotropic Heisenberg model in dimension $d = 1$ with open boundary conditions

$$H = -J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1} \ ,$$

with $J = -1$ (the antiferromagnetic case). We are interested in the spin correlations between sites 1 and n, $\chi_{1n} = \langle \vec{S}_1 \cdot \vec{S}_n \rangle$, for both zero and finite temperature.

a) Calculate $\chi_{1n} = \langle \psi_{\mathrm{g}} | \vec{S}_1 \cdot \vec{S}_n | \psi_{\mathrm{g}} \rangle$ for the ground state $|\psi_{\mathrm{g}}\rangle$ of a Heisenberg chain with $N = 10$ sites and $n = 1, \ldots, 10$. Note that for an even number of sites N, the ground state of the antiferromagnetic Heisenberg chain is non-degenerate. (5 points)

b) Calculate the temperature dependence of the spin correlation

$$\chi_{1n}(T) = \frac{1}{Z} \sum_l \langle l | \vec{S}_1 \cdot \vec{S}_n | l \rangle e^{-\beta E_l} \ ,$$

with $Z = \sum_l e^{-\beta E_l}$ the partition function, $\beta = 1/(k_{\mathrm{B}} T)$ (k_{B} can be set to 1), and $|l\rangle$ the eigenstates of H with eigenenergies E_l, for temperatures $T = 0.5, 2$, and 10. (4 points)

c) Show numerically that, in the limit $T \to 0$, the finite-temperature spin-correlation $\chi_{1n}(T)$ of part b) corresponds to the zero-temperature spin-correlation of part a). (2 points)

Exercise 2: Reduced density matrix and entanglement entropy

(5 points)

Consider a two-site system (with sites A and B) with a two-dimensional basis for each site: $\{|i\rangle\} = \{|\uparrow\rangle_A, |\downarrow\rangle_A\}$ for site A and $\{|j\rangle\}$ for site B accordingly. A given state $|\psi\rangle$ can be expressed in this basis as

$$|\psi\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2} \psi_{ij}|i\rangle|j\rangle \ . \tag{1}$$

Here we want to calculate the reduced density matrices ρ for the following three states:

$$\begin{aligned}
|\psi\rangle_1 &= |\uparrow\rangle_A|\downarrow\rangle_B \ , \\
|\psi\rangle_2 &= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A|\downarrow\rangle_B - |\downarrow\rangle_A|\uparrow\rangle_B\right) \ , \\
|\psi\rangle_3 &= \frac{1}{2}\left(|\uparrow\rangle_A + |\downarrow\rangle_A\right)\left(|\uparrow\rangle_B + |\downarrow\rangle_B\right) \ .
\end{aligned}$$

a) Write the states $|\psi\rangle_i$ $(i = 1, 2, 3)$ in the form given by eq. (1), i.e. determine the matrix $\bar{\psi}$ with matrix elements $(\bar{\psi})_{ij} = \psi_{ij}$. (1 point)

The reduced density operator $\hat{\rho}$ is defined as

$$\hat{\rho}_{\mathrm{A}} = \mathrm{Tr}_B\left(|\psi\rangle\langle\psi|\right) = \sum_{j=1}^{2}\langle j|\psi\rangle\langle\psi|j\rangle \ ,$$

with the matrix elements $\rho_{ii'} = \langle i|\hat{\rho}|i'\rangle = \sum_j \psi_{ij}\psi_{i'j}$.

b) Calculate the reduced density matrices (i.e. the matrix elements $\rho_{ii'}$) for the states $|\psi\rangle_i$ $(i = 1, 2, 3)$. (3 points)

We can now proceed with calculating the entanglement entropy S_{e}:

$$S_{\mathrm{e}} = -\mathrm{Tr}_{\mathrm{A}}\left[\hat{\rho}_{\mathrm{A}} \ln \hat{\rho}_{\mathrm{A}}\right] = -\sum_{\alpha} w_\alpha \ln w_\alpha \ ,$$

with w_α the eigenvalues of the reduced density matrix. The entanglement entropy is a measure of the entanglement between subsystems A and B of a quantum system; this can now be tested on the three states $|\psi\rangle_i$, $i = 1, 2, 3$, given above.

c) Calculate the entanglement entropy S_{e} for the states $|\psi\rangle_i$. (1 point)