Computational Many-Body Physics

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SS 2020

Sheet 4 - please submit your solutions via e-mail to Chae-Yeun Park until Monday, July 6, 2020, 12:00.

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 $\chi_{1n} = \langle \psi_{\rm g} | \vec{S}_1 \cdot \vec{S}_n | \psi_{\rm g} \rangle$ for the ground state $|\psi_{\rm g}\rangle$ 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, $\beta = 1/(k_{\rm B} T)$ ($k_{\rm B}$ 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

(4 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

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

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)

The entanglement between sites A and B can be directly calculated from these reduced density matrices (see the following exercise).

Exercise 3: Reduced density matrix and entanglement entropy

(11 points)

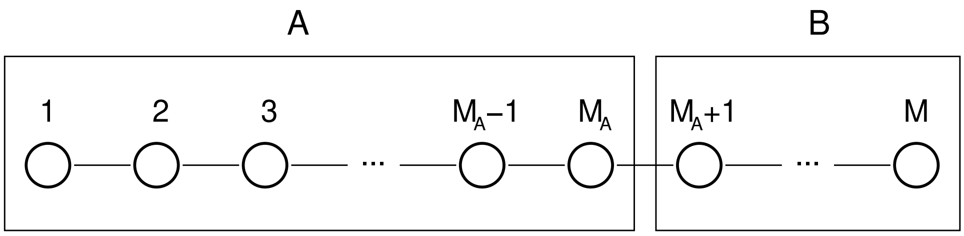
With the definition of the reduced density matrix given in the previous exercise, we can now proceed with calculating the entanglement entropy S_e:

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

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 in exercise 2.

a) Calculate the entanglement entropy S_e for the states $|\psi\rangle_i$. (1 point)

We now extend the analysis to larger systems, in particular one-dimensional spin systems with a bi-partitioning into parts A and B as shown in the figure:



The number of sites in parts A (B) is M_A (M_B), with $M_\mathrm{A} + M_\mathrm{B} = M$. The state of the total system in expressed in the standard basis $\{|l\rangle\}$, $l = 1, \ldots, 2^M$, with $\{|l\rangle\} = \{|\downarrow\downarrow \ldots \downarrow\rangle, |\uparrow\downarrow \ldots \downarrow\rangle, \ldots\}$:

$$|\psi\rangle = \sum_{l=0}^{2^M - 1} a_l |l\rangle \ .$$

b) Consider a random state $|\psi\rangle_\mathrm{r}$ with $\bar{a}_l$ random numbers in the range $[-1, 1]$, and $a_l = \bar{a}_l / \sqrt{\sum_l \bar{a}_l^2}$. Calculate S_e for different values of M_A and $M = 10$. (4 points)

c) The following state has a much simpler structure:

$$|\psi\rangle_\mathrm{afm} = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\uparrow\downarrow \ldots\rangle - |\downarrow\uparrow\downarrow\uparrow \ldots\rangle\right) \ .$$

Calculate S_e for different values of M_A and $M = 10$. (3 points)

d) In the following state, site 1 is entangled with site 5:

$$|\psi\rangle_{1-5} = \frac{1}{2^{(M-1)/2}} \left(|\uparrow\rangle_1 |\downarrow\rangle_5 - |\downarrow\rangle_1 |\uparrow\rangle_5\right) \prod_{i=2}^{4} \left(|\uparrow\rangle_i + |\downarrow\rangle_i\right) \prod_{i=6}^{M} \left(|\uparrow\rangle_i + |\downarrow\rangle_i\right) \ .$$

How does this entanglement show up in the entanglement entropy S_e as a function of M_A ($M = 10$)? (3 points)