Computational Many-Body Physics

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Sheet 2 - tutorial of Monday, May 6, 14:00

Exercise 1: Hamilton matrices for spin models

Consider a spin model of the form

$$H = -\sum_{ij\alpha} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha} \ ,$$

with $i, j = 1, \ldots, N$ and $\alpha = x, y, z$.

a) Write a program which sets up the Hamilton matrix for a model with arbitrary N and an arbitrary list of couplings $\{J_{ij}^{\alpha}\}$. As discussed in the lecture, the x-, y- and z-links should be treated separately. For each link of the form $-J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha}$, the action of $S_i^{\alpha} S_j^{\alpha}$ on the basis state $|n\rangle$ gives another basis state $|l\rangle$ (times a prefactor). With the equation of l given in the lecture, the Hamiltonian matrix can be set up very efficiently.

b) Set up the Hamilton matrices for the three models discussed in exercise 3 on sheet 1 (the three-site clusters).

c) Calculate the eigenenergies and corresponding eigenstates for these three models.

Exercise 2: Spin correlations of one-dimensional spin models

Here we focus on one-dimensional spin models of the form

$$H = -\sum_{i=1}^{N-1} \sum_{\alpha} J_i^{\alpha} S_i^{\alpha} S_{i+1}^{\alpha} \ ,$$

which is just a special case of the spin models for which the Hamiltonian matrix has been set up in exercise 1. We are interested in the spin correlations between sites l and m in the ground state $|\psi_{\mathrm{g}}\rangle$ of the system:

$$C_{lm} = \langle \psi_{\mathrm{g}} | \vec{S}_l \cdot \vec{S}_m | \psi_{\mathrm{g}} \rangle \ .$$

(For a degenerate ground state, the C_{lm} is defined as the average over the different ground states.)

Calculate the distance dependence of the spin correlations, i.e. the correlation between site 1 and site m: C_{1m} $(m = 2, \ldots, N)$, for the following three models:

a) $J_i^\alpha = J\delta_{\alpha z}$,

b) $J_i^\alpha = J$,

c) $J_i^\alpha = \begin{cases} J\delta_{\alpha x} & : i \text{ even}, \\ J\delta_{\alpha z} & : i \text{ odd}. \end{cases}$

The number of sites can be chosen as $N = 6, 8$, and 10; consider both $J = +1$ and $J = -1$.

Exercise 3: Entropy

The many-particle spectrum of a system (classical or quantum mechanical) is assumed to be of the following form:

$$E_l = \sqrt{l} \quad , \quad l = 1, 2, \ldots, L \ .$$

Here we want to investigate how the temperature dependence of the entropy $S(T)$ is affected by L, the number of many-particle states.

The entropy can be calculated in the following way:

$$S(T) = -\frac{\partial F}{\partial T},$$

with the free energy

$$F = -k_{\mathrm{B}} T \ln Z \ ,$$

and the partition function

$$Z = \sum_{l=1}^{L} e^{-\beta E_l} \ , \ \beta = \frac{1}{k_{\mathrm{B}} T} \ .$$

(k_{B} can be set to 1.) Write a program which calculates the entropy $S(T)$ in this way. Compare the numerical results for different values of L (such as $L = 10, 100, 1000$).

Exercise 4: Reduced density matrix

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. (3), i.e. determine the matrix $\bar{\psi}$ with matrix elements $(\bar{\psi})_{ij} = \psi_{ij}$.

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

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

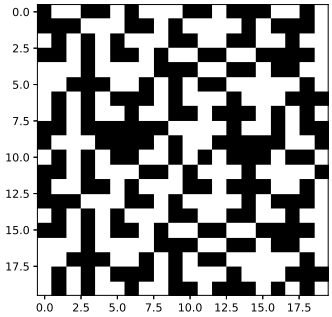
with the matrix elements $\rho_{ii'} = \langle i|\hat{\rho}|i'\rangle = \sum_j \psi_{ij}\psi_{i'j}$.

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

The entanglement between sites A and B can be directly calculated from these reduced density matrices – this will be discussed in one of the following exercises, together with the extension to spin models on small clusters/chains.

Exercise 5: Rule N

The figure below shows 20 generations (at times $t = 0, 1, \ldots, 19$) of rule N, starting from a random initial configuration at time $t = 0$. The number of cells is $M = 20$ with periodic boundary conditions.



a) What is the value of N?

b) Find the error!