Computational Many-Body Physics

apl. Prof. Dr. R. Bulla

SS 2017

Sheet 4

Exercise 1: spectral function of the one-dimensional Hubbard model

The Hamiltonian of the one-dimensional Hubbard model with N sites and open boundary conditions is given by

$$H = \sum_{i=1}^{N} \sum_{\sigma} \varepsilon c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{i=1}^{N-1} \sum_{\sigma} t \left(c_{i\sigma}^{\dagger} c_{i+1,\sigma} + c_{i+1,\sigma}^{\dagger} c_{i\sigma} \right) + \sum_{i=1}^{N} U c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} \ . \qquad (1)$$

The aim of this exercise is to calculate (numerically) the spectral functions $A_i(\omega)$ of the Green functions $\langle\langle c_{i\sigma}, c_{i\sigma}^{\dagger} \rangle\rangle_z$ for temperature $T = 0$ and particle-hole symmetry ($\varepsilon = -\frac{U}{2}$).

a) As an analytical exercise, calculate the spectral function $A_1(\omega)$ for a single-site Hubbard model.

b) Now set up the Hamilton matrix for the model eq. (1), either as a single matrix ($4^N \times 4^N$), or by taking into account the conservation of total particle number and z-component of the total spin. Calculate the many-particle spectrum for $U = 1$, $t = 1$, and $N = 3$.

We now set $T = 0$, $t = 1$, and N even (this, together with $\varepsilon = -\frac{U}{2}$, guarantees a non-degenerate ground state).

c) Show that in the limit $T \to 0$, and for a non-degenerate ground state $|\psi_{\mathrm{g}}\rangle$, the spectral function $A(\omega)$ takes the form

$$A(\omega) = \sum_{j} \left(|\langle \psi_{\mathrm{g}} | c | j \rangle|^2 \, \delta(\omega + (E_{\mathrm{g}} - E_j)) + |\langle j | c | \psi_{\mathrm{g}} \rangle|^2 \, \delta(\omega + (E_j - E_{\mathrm{g}})) \right) \ .$$

d) Calculate the spectral function $A_1(\omega)$ for $N = 6$ and the following U-values: $U = 0.5, 1, 2, 4$.

Exercise 2: single-impurity Anderson model: impurity Green function, hybridization function, and self energy

The impurity Green function of the single-impurity Anderson model can be written in the following general form:

$$G_\sigma(z) = \frac{1}{z - \varepsilon_\mathrm{f} - \Delta(z) - \Sigma_\sigma^U(z)} \ . \tag{2}$$

The idea of this exercise is to explore the possible structures of the impurity Green function using a specific form of the hybridization function and the self energy.

a) Show that any correlation function defined in the upper complex plane can be represented through its spectral function as

$$X(z) = \int_{-\infty}^{\infty} \mathrm{d}\omega' \ \frac{A(\omega')}{z - \omega'} \ .$$

b) The spectral function of the hybridization function, $A_\Delta(\omega)$, is supposed to be of the following form:

$$A_\Delta(\omega) = e^{-(\omega/10)^2} \ .$$

Calculate (numerically) both real and imaginary part of $\Delta(z = \omega + i\delta)$ with $\delta = 0.01$.

c) Use the result of b) to calculate the impurity spectral function, $A_\mathrm{imp}(\omega)$, for various values of ε_f and $U = 0$.

d) The spectral function of the self energy should take the form

$$A_\Sigma(\omega) = \gamma\omega^2 e^{-\omega^2} \ .$$

Investigate the resulting structures in the impurity Green function for $\varepsilon_\mathrm{f} = 0$ and various values of γ.

Exercise 3: 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 5 on sheet 3. 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 4: the 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

$$|\psi\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2} \psi_{ij}|i\rangle|j\rangle \ . \tag{3}$$

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.