

Computational Many-Body Physics

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Sheet 3: return on: Monday, May 23, 2016, 14:00

Exercise 1: Hamilton matrix of the tight-binding chain

(10 points)

The idea of this exercise is to calculate the many-particle spectrum of the tight-binding chain via diagonalization of the *full* Hamilton matrix, and to check whether the result agrees with the many-particle spectrum constructed from the single-particle levels. The model is the tight-binding chain with open boundary conditions:

$$H_{\text{tb}} = \sum_{i=1}^{N-1} t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) . \quad (1)$$

- Set up a program which calculates the full $2^N \times 2^N$ -matrix $H_{lm} = \langle l | H_{\text{tb}} | m \rangle$. One option here, which is not required, is to split up the Hilbert space into subspaces with different particle numbers. (6 points)
- Show that the eigenvalues of the Hamilton matrix agree with the many-particle energies constructed from the single-particle levels. ($N = 3, 4$ and 5 is sufficient.) (4 points)

Exercise 2: Hamilton matrix of the two-site Anderson model

(6 points)

Consider again (see exercise 2 on sheet 2) the single-impurity Anderson model with a single bath site only:

$$H_{\text{ts}} = \sum_{\sigma} \varepsilon_f f_{\sigma}^\dagger f_{\sigma} + U f_{\uparrow}^\dagger f_{\uparrow} f_{\downarrow}^\dagger f_{\downarrow} + V \sum_{\sigma} (f_{\sigma}^\dagger c_{\sigma} + c_{\sigma}^\dagger f_{\sigma}) + \sum_{\sigma} \varepsilon_c c_{\sigma}^\dagger c_{\sigma} , \quad (2)$$

The basis of the Hilbert space of H_{ts} can be written as:

$$\{|0\rangle_f, |\uparrow\rangle_f, |\downarrow\rangle_f, |\uparrow\downarrow\rangle_f\} \otimes \{|0\rangle_c, |\uparrow\rangle_c, |\downarrow\rangle_c, |\uparrow\downarrow\rangle_c\} .$$

- Due to the conservation of the total particle number N and the z -component of the total spin S_z , the Hilbert space can be decomposed into subspaces (N, S_z) . Determine the dimensions of these subspaces. (2 points)
- Calculate (analytically) the matrix elements of the Hamilton matrix for the subspace $(N = 2, S_z = 0)$. (4 points)

Exercise 3: imaginary-time Green function and spectral function

(6 points)

The imaginary-time Green function $G(\tau)$ and the spectral function $A(\omega)$ are related by

$$G(\tau) = - \int_{-\infty}^{\infty} d\omega \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} A(\omega) .$$

Derive this relation starting from the definitions given in the lecture. For this it is useful to derive the following relations first:

$$\begin{aligned} C^<(t) &= C^>(t') \text{ with } it' = it + \beta , \\ C^>(\omega) &= \frac{1}{1 + e^{-\beta\omega}} [C^>(\omega) + C^<(\omega)] , \\ A(\omega) &= \frac{1}{2\pi} [C^>(\omega) + C^<(\omega)] . \end{aligned}$$

Exercise 4: analytic continuation

(5 points + 8 bonus points)

The imaginary-time Green function $G(\tau)$ and the spectral function $A(\omega)$ are related by

$$G(\tau) = - \int_{-\infty}^{\infty} d\omega \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} A(\omega) .$$

In this exercise, we assume $G(\tau)$ to be given by $G(\tau) = -\frac{1}{70}(\tau - 6)^2 - 0.1$, $0 \leq \tau < \beta = 10$, and that the corresponding spectral function can be written as a sum of δ -peaks: $A(\omega) = \sum_{i=1}^N a_i \delta(\omega - \varepsilon_i)$, with $a_i \geq 0$.

- a) We set $N = 3$ and $a_1 = 0.4$, $\varepsilon_1 = -0.6$, $a_2 = 0.3$, $\varepsilon_2 = 0.35$, and $a_3 = 0.3$. Write a program which determines the optimal value for ε_3 (the value which gives the best fit to the given $G(\tau)$). (5 points)
- b) With $N = 3$, we now regard all a_i and ε_i as parameters. Write a program which locates minima of the function $f(a_1, a_2, a_3, \varepsilon_1, \varepsilon_2, \varepsilon_3)$ (see the lecture for a definition) in the 6-dimensional parameter space spanned by the a_i and ε_i . The result of part a) can be used as a starting point, but to investigate whether there are other local minima of the function f which give better estimates for the spectral function, it is useful to repeat the calculation for other starting points as well. (8 bonus points)

Exercise 5: Hamilton matrices for spin models

(11 points + 3 bonus points)

The aim of this exercise is to develop an algorithm which sets up the Hamilton matrix for spin models of the form

$$\begin{aligned} H &= - \sum_{ij\alpha} J_{ij}^\alpha S_i^\alpha S_j^\alpha \\ &= - \sum_{ij} \left[\frac{1}{4} (J_{ij}^x - J_{ij}^y) (S_i^+ S_j^+ + S_i^- S_j^-) + \frac{1}{4} (J_{ij}^x + J_{ij}^y) (S_i^+ S_j^- + S_i^- S_j^+) + J_{ij}^z S_i^z S_j^z \right]. \end{aligned}$$

- a) Write a program which sets up the matrices for the individual terms in the Hamiltonian, i.e. $\langle i | S_n^+ S_m^- | j \rangle$ etc.; one possible strategy is to go through all the states labeled by $j = 1, \dots, 2^N$, apply the operator $S_n^+ S_m^-$ on the state $|j\rangle$, ($S_n^+ S_m^- |j\rangle = \alpha |i\rangle$) and extract from this the prefactor α and the index i .
(4 points)
- b) Now write a code which can deal with arbitrary N and an arbitrary list of couplings $\{J_{ij}^\alpha\}$.
(4 points)
- c) Set up the Hamilton matrices for the three models discussed in exercise 4 on sheet 2 (the three-site clusters). Of course, we expect the results to agree with the construction by hand.
(3 points)
- d) Calculate the spectrum of many-particle energies for these three models.
(3 bonus points)