Computational Many-Body Physics

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Sheet 3

Exercise 1: Hamilton matrix of the tight-binding chain

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:

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

a) Set up a program which calculates the full $2^N \times 2^N$-matrix $H_{lm} = \langle l | H_{\mathrm{tb}} | m \rangle$. One option here, which is not required, is to split up the Hilbert space into subspaces with different particle numbers.

b) 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.)

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

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

$$H_{\mathrm{ts}} = \sum_\sigma \varepsilon_{\mathrm{f}} f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + V \sum_\sigma \left(f_\sigma^\dagger c_\sigma + c_\sigma^\dagger f_\sigma \right) + \sum_\sigma \varepsilon_{\mathrm{c}} c_\sigma^\dagger c_\sigma \ , \tag{2}$$

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

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

a) 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.

b) Calculate (analytically) the matrix elements of the Hamilton matrix for the subspace $(N = 2, S_z = 0)$.

Exercise 3: imaginary-time Green function and spectral function

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

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

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

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

Exercise 4: analytic continuation

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

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

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 $G(\tau)$).

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.

Exercise 5: Hamilton matrices for spin models

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 $j = 1, \ldots, 2^N$, 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.

b) Now write a code which can deal with arbitrary N and an arbitrary list of couplings $\{J_{ij}^{\alpha}\}$.

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.

d) Calculate the spectrum of many-particle energies for these three models.