Computational Many-Body Physics

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Sheet 2

Exercise 1: single-particle and many-particle spectra

For a given single-particle spectrum $\{\varepsilon_i\}$, the many-particle energies can be simply calculated via $E = \sum_{i=1}^{N} n_i \varepsilon_i$, with $n_i = 0, 1$. In this project, you are supposed to solve the *reverse* problem: for a given set of many-particle energies $\{E_l\}$:

- find out whether the many-particle spectrum can be represented at all by a single-particle spectrum;
- if this is possible, calculate the single-particle spectrum $\{\varepsilon_i\}$.

As a specific example, consider the following two sets of many-particle energies:

$$\begin{aligned} \{E_l\}_1 &= -2, -1, 0(2), 1(2), 2, 3, \\ \{E_l\}_2 &= -2, -1(2), 0, 1, 2(2), 3 \end{aligned}$$

(The number in brackets indicate the degeneracies). To simplify the calculation, you can assume that the ε_i take integer values only.

Exercise 2: Symmetries

Consider the following two-site model:

$$H_{\rm ts} = \sum_\sigma \varepsilon_{\rm f} f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + V \sum_\sigma \left(f_\sigma^\dagger c_\sigma + c_\sigma^\dagger f_\sigma \right) + \sum_\sigma \varepsilon_{\rm c} c_\sigma^\dagger c_\sigma \ , \qquad (1)$$

which corresponds to a single-impurity Anderson model with only a single bath site.

a) Show that, for the model eq. (1), the total particle number is conserved, i.e. $[H_{\rm ts}, \hat{N}]_- = 0$, with $\hat{N} = \sum_\sigma \left(f_\sigma^\dagger f_\sigma + c_\sigma^\dagger c_\sigma \right)$.

b) Show that, for the model eq. (1), the z-component of the total spin is conserved, i.e. $[H_{\rm ts}, \hat{S}_z]_- = 0$, with $\hat{S}_z = f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow + c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow$.

Now consider a tight-binding model on a finite chain with periodic boundary conditions:

$$H_{\rm tb} = \sum_{i=1}^{N} \epsilon_i c_i^\dagger c_i + \sum_{i=1}^{N-1} t_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + t_N \left(c_N^\dagger c_1 + c_1^\dagger c_N \right) \ . \qquad (2)$$

c) Perform the following two transformations:

$$\begin{aligned} H'_{\rm tb} &= H_{\rm tb}(c_i^\dagger \to c_i, c_i \to c_i^\dagger) \ , \\ H''_{\rm tb} &= H'_{\rm tb}(c_i^\dagger \to -c_i^\dagger, c_i \to -c_i, i \text{ even}) \ . \end{aligned}$$

Under which conditions do we have $H''_{\rm tb} = H_{\rm tb}$?

Exercise 3: tight-binding chain; density of states

The tight-binding model on a finite chain with periodic boundary conditions is defined as (in contrast to eq. (2), the parameters ϵ and t do not depend on i):

$$H_{\rm tb} = \sum_{i=1}^{N} \epsilon c_i^\dagger c_i + \sum_{i=1}^{N-1} t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + t \left(c_N^\dagger c_1 + c_1^\dagger c_N \right) \ . \tag{3}$$

a) Show that the single-particle spectrum of this Hamiltonian can be obtained analytically via the following unitary transformation of the operators c_l:

$$c_l = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{i\frac{2\pi}{N}ml} d_m \ .$$

(The resulting single-particle energies are given by $\varepsilon_m = \epsilon + 2t\cos(\frac{2\pi}{N}m)$).

b) Compare the analytical values for the ε_m obtained in a) with the eigenvalues obtained from a numerical diagonalization of the matrix T (for the definition of T, see Sec. 2.1E in the script).

For a given single-particle spectrum $\{\varepsilon_l\}$, the density of states is defined as

$$\rho(\varepsilon) = \sum_l \delta(\varepsilon - \varepsilon_l) \ ,$$

which is, for a finite system, always a collection of δ-peaks and therefore difficult to visualize. In the following, two common ways of plotting the density of states are used for the single-particle spectrum of the tight-binding chain.

c) One way is to replace each δ-function by a Lorentzian $L_b(\omega, \varepsilon_l)$ of width b and centered at $\omega = \varepsilon_l$:

$$L_b(\omega, \varepsilon_l) = \frac{1}{\pi} \frac{b}{(\omega - \varepsilon_l)^2 + b^2} \ .$$

Write a program which calculates the broadened density of states for the single-particle spectrum of part a) and various values of N and b.

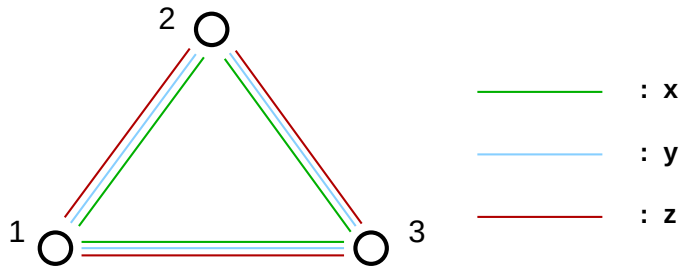
d) The alternative is to divide the interval $[\varepsilon_{\rm min}, \varepsilon_{\rm max}]$ in M equal parts and to count the number of δ-peaks in each of these subintervals. Write a program which calculates the resulting histogram for the single-particle spectrum of part a) and various values of N and M.

Exercise 4: spin-models on a three-site cluster

Consider the following (general) Hamiltonian for a spin-model on a three-site cluster:

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

with $i, j = 1, 2, 3$ ($i < j$ in $\sum_{ij}$) and $\alpha = x, y, z$.



To visualize the model, a colour code for the x, y and z components of the spin-couplings turns out to be useful, see the figure.

a) Rewrite the Hamiltonian using the operators

$$S_i^{\pm} = S_i^x \pm i S_i^y \ , \text{ and } \ S_i^z \ .$$

Now set up (by hand!) the 8×8 Hamilton matrices $\bar{H}$ for the following three special cases:

b) the Ising model, i.e. $J_{ij}^{\alpha} = J\delta_{\alpha z}$,

c) the isotropic Heisenberg model, i.e. $J_{ij}^{\alpha} = J$, and

d) a model with $J_{12}^x = J_{23}^y = J_{31}^z = J$ and all other $J_{ij}^{\alpha} = 0$.

One of the following exercises deals with numerical algorithms to set up these Hamilton matrices.