

Computational Many-Body Physics

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Sheet 2: return on: Monday, May 2, 2016, 14:00

Exercise 1: single-particle and many-particle spectra

(10 bonus points)

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:

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

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

- Show that, for the model eq. (1), the total particle number is conserved, i.e. $[H_{\text{ts}}, \hat{N}]_{-} = 0$, with $\hat{N} = \sum_{\sigma} (f_{\sigma}^{\dagger} f_{\sigma} + c_{\sigma}^{\dagger} c_{\sigma})$. (3 points)
- Show that, for the model eq. (1), the z -component of the total spin is conserved, i.e. $[H_{\text{ts}}, \hat{S}_z]_{-} = 0$, with $\hat{S}_z = f_{\uparrow}^{\dagger} f_{\uparrow} - f_{\downarrow}^{\dagger} f_{\downarrow} + c_{\uparrow}^{\dagger} c_{\uparrow} - c_{\downarrow}^{\dagger} c_{\downarrow}$. (3 points)

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

$$H_{\text{tb}} = \sum_{i=1}^N \varepsilon_i c_i^{\dagger} c_i + \sum_{i=1}^{N-1} t_i (c_i^{\dagger} c_{i+1} + c_{i+1}^{\dagger} c_i) + t_N (c_N^{\dagger} c_1 + c_1^{\dagger} c_N). \quad (2)$$

c) Perform the following two transformations:

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

Under which conditions do we have $H''_{\text{tb}} = H_{\text{tb}}$? (3 points)

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):

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

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 $\epsilon_m = \epsilon + 2t \cos(\frac{2\pi}{N}m)$). (3 points)

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). (3 points)

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

$$\rho(\epsilon) = \sum_l \delta(\epsilon - \epsilon_l) ,$$

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 $L_b(\omega, \epsilon_l)$ of width b and centered at $\omega = \epsilon_l$:

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

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 . (4 points)

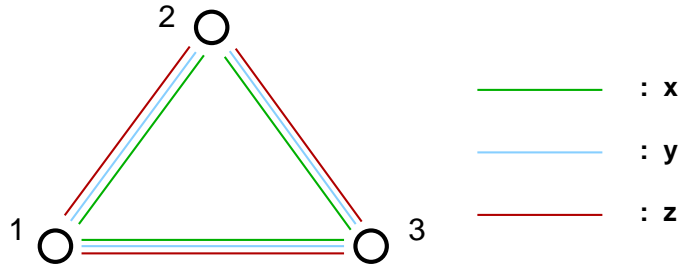
d) The alternative is to divide the interval $[\epsilon_{\min}, \epsilon_{\max}]$ in M equal parts and to count the number of δ -peaks in each of these subintervals. Write a program which calculates the resulting histogram for the single-particle spectrum of part a) and various values of N and M . (4 bonus points)

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

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

(3 points)

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

- b) the Ising model, i.e. $J_{ij}^\alpha = J\delta_{\alpha z}$, (4 points)
- c) the isotropic Heisenberg model, i.e. $J_{ij}^\alpha = J$, (5 bonus points) and
- d) a model with $J_{12}^x = J_{23}^y = J_{31}^z = J$ and all other $J_{ij}^\alpha = 0$. (5 bonus points)

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