Computational Many-Body Physics

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Sheet 1: return on: Monday, Apr 18, 2016, 14:00

Exercise 1: single-particle and many-particle spectra

We consider a Hamiltonian of the form

$$H = \sum_{i=1}^{N} \varepsilon_i c_i^\dagger c_i \ , \tag{1}$$

with $N = 6$ and energies $\varepsilon_i = 0.1 \cdot (i - 3.5)$. The many-particle energies of this system are given by $E = \sum_{i=1}^{N} n_i \varepsilon_i$, with $n_i = 0, 1$.

a) Write a program which translates the integer $j = 0, \ldots, 2^N - 1$ into the bit pattern $(n_1, n_2, \ldots, n_N)$, with $j = \sum_{i=1}^{N} n_i 2^{i-1}$. (3 points)

b) With the algorithm of part a), write a program which calculates the many-particle spectrum $\{E_l\}$ of the Hamiltonian eq. (1). (3 points)

Exercise 2: entropy

(7 points)

The many-particle spectrum of a system (classical or quantum mechanical) is assumed to be of the following form:

$$E_l = \sqrt{l} \ \ , \ \ l = 1, 2, \ldots, L \ .$$

Here we want to investigate how the temperature dependence of the entropy $S(T)$ is affected by L, the number of many-particle states.

The entropy can be calculated in the following way:

$$S(T) = -\frac{\partial F}{\partial T},$$

with the free energy

$$F = -k_{\mathrm{B}} T \ln Z \ ,$$

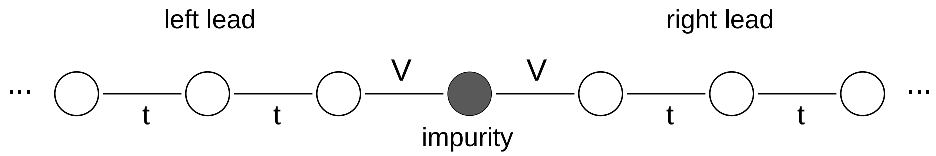
and the partition function

$$Z = \sum_{l=1}^{L} e^{-\beta E_l} \ , \ \beta = \frac{1}{k_{\mathrm{B}} T} \ .$$

(k_{B} can be set to 1.) Write a program which calculates the entropy $S(T)$ in this way. Compare the numerical results for different values of L (such as $L = 10, 100, 1000$).

Exercise 3: single-impurity Anderson model: even/odd basis

(5 points)



The figure shows a sketch of the single-impurity Anderson model, with coupling of the impurity to left and right 'leads', both represented by tight-binding chains. The Hamiltonian is of the form

$$H = H_{\rm imp} + H_{\rm imp-bath} + H_{\rm bath} \ ,$$

with the individual parts given by

$$\begin{aligned} H_{\rm imp} &= \sum_\sigma \varepsilon_{\rm f} f^\dagger_\sigma f_\sigma + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow \ , \\ H_{\rm imp-bath} &= V \sum_{\alpha=l,r} \sum_\sigma \left(f^\dagger_\sigma c_{\alpha 1 \sigma} + c^\dagger_{\alpha 1 \sigma} f_\sigma \right) \ , \\ H_{\rm bath} &= t \sum_{\alpha=l,r} \sum_{i=1}^{\infty} \sum_\sigma \left(c^\dagger_{\alpha i \sigma} c_{\alpha i+1 \sigma} + c^\dagger_{\alpha i+1 \sigma} c_{\alpha i \sigma} \right) \ . \end{aligned}$$

The impurity in this model seems to couple to two 'channels'. Show that with the following transformation to an even/odd basis, the impurity only couples to a single channel (the even channel), with the odd channel decoupled from the impurity:

$$\begin{aligned} c^e_{i\sigma} &= \frac{1}{\sqrt{2}} \left(c_{li\sigma} + c_{ri\sigma} \right) \ , \\ c^o_{i\sigma} &= \frac{1}{\sqrt{2}} \left(c_{li\sigma} - c_{ri\sigma} \right) \ . \end{aligned}$$

Exercise 4: matrix diagonalization

Consider the $N \times N$ matrix T with matrix elements

$$(T)_{ij} = \varepsilon_i \delta_{ij} + \delta_{i,j+1} + \delta_{i+1,j} \ .$$

The parameters ε_i are given by $\varepsilon_i = w x_i$, with x_i random numbers drawn from a flat distribution in the interval $[-1, 1]$.

a) For a fixed set of $\{x_i\}$, plot the eigenvalues of T as a function of w ($0 \le w \le 5$). (Recommended values for N are $N = 10, 20, 30$). (3 points)

b) Pick out the eigenvector corresponding to the lowest eigenvalue. Visualize the development of the eigenvector for increasing w. (3 points)