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http://www.physik.uni-regensburg.de/forschung/evers/courses/cscn.phtml

Exercise Sheet No. 5
"Computational Condensed Matter Theory"

1 Non-interacting resonant level

We consider a quantum dot (single level) weakly coupled to leads. We model the leads by a one-dimensional tight-binding chain of L atoms and we couple the dot to one of the ends of the chain. The Hamiltonian $\hat{H}$ consists of three parts

$$\hat{H} = \hat{H}^{(l)} + \hat{H}^{(d)} + \hat{H}^{(ld)} \tag{1}$$

$$\hat{H}^{(l)} = t \sum_{\sigma} \sum_{k=1}^{L-1} \left(\hat{c}^{\dagger}_{k,\sigma} \hat{c}_{k+1,\sigma} + \hat{c}^{\dagger}_{k+1,\sigma} \hat{c}_{k,\sigma} \right) \tag{2}$$

$$\hat{H}^{(ld)} = V \sum_{\sigma} \left(\hat{c}^{\dagger}_{L,\sigma} \hat{d}_{\sigma} + \hat{d}^{\dagger}_{\sigma} \hat{c}_{L,\sigma} \right) \qquad \hat{H}^{(d)} = \epsilon_d \sum_{\sigma} \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma}. \tag{3}$$

The first term $\hat{H}^{(l)}$ describes the leads, the term $\hat{H}^{(ld)}$ couples the dot to the leads and the last term gives the on-site potential of the dot. We explicitly include the spin degree of freedom.

To proceed with the problem, let t be the unit of energy ($t > 0$) and let us focus on weak coupling $V = 0.1t$.

(a) The resonant character of the dot level reveals itself in the density of states. Calculate the density of states for the chain lengths $L = 30, 60, 120, 240, 480$ and $\epsilon = -t/2$. When constructing the Hamiltonian, pay attention to the spin degree of freedom.

(b) The density of states projected onto the dot (projected density of states, PDOS) is defined as

$$A_{\mathrm{d},\sigma}(E) = \sum_{n} |\langle n|d,\sigma\rangle|^2 \, \delta(E - E_n) \tag{4}$$

where $|n\rangle, E_n$ are eigenstates and respective eigenvalues, $|d,\sigma\rangle$ is the dot orbital with spin σ. What controls the width of the resonance? Now plot the PDOS with $\epsilon_d = -4t$. What is the physical width of the resonance when $\epsilon_d \ll -2t$?

(c) Assuming zero temperature (micro-canonical ensemble), and $N_{\mathrm{e}} = L+1$ electrons ("half filling"), calculate the ground-state density matrix

$$\langle i', \sigma' | \hat{\varrho} | i\sigma \rangle = \sum_{n} \langle i', \sigma' | n \rangle f_n \langle n | i, \sigma \rangle. \tag{5}$$

The indices i, i' label all sites in the leads and the dot, $|n\rangle, E_n$ are Hamiltonian eigenvectors and eigenvalues and f_n is the occupation number. The density matrix permits to calculate observables of the resonant level: spin $S_z = \left(\langle d,\uparrow | \hat{\varrho} | d,\uparrow \rangle - \langle d,\downarrow | \hat{\varrho} | d,\downarrow \rangle \right)/2$ (units of $\hbar$) and charge $q = \langle d,\uparrow | \hat{\varrho} | d,\uparrow \rangle + \langle d,\downarrow | \hat{\varrho} | d,\downarrow \rangle$ (units of e). Evaluate these quantities for $\epsilon_d = -t, 0, t$; compare and interpret.

[sort eigenvectors and eigenvalues simultaneously: `numpy.argsort`, for the PDOS: `numpy.tensordot`]

2 Non-interacting resonant level at finite temperature

In this exercise we study the system from Problem 1 in a canonical ensemble. In order to calculate observables, first we need to evaluate the chemical potential.

(a) Prepare a routine to calculate the chemical potential μ by solving the equation for the number of electrons $N_{\rm e} = \sum_n 1/[1 + e^{(E_n-\mu)/k_{\rm B}T}]$ at small but finite temperature. What happens in the limit $T \to 0+$?

(b) Use the chemical potential to calculate the density matrix (for $N_e = L + 1$)

$$\langle i', \sigma' | \hat{\varrho} | i\sigma \rangle = \sum_n \langle i', \sigma' | n \rangle \frac{1}{1 + e^{(E_n-\mu)/k_{\rm B}T}} \langle n | i, \sigma \rangle. \tag{6}$$

(c) Evaluate charge on the dot for $\epsilon_d = -t, 0, t$ and discuss the role of the temperature.