Solid State Theory
Exercise 13

Exercise 13.1 Two site hubbard model

We consider a two site Hubbard model, i.e., the Hamiltonian

$$\mathcal{H} = -t \sum_s \left(c^\dagger_{1,s} c_{2,s} + \text{h.c.} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \tag{1}$$

with the hopping energy t, the on-site energy U and where the first sum runs over the two z-projected spin states and the second sum runs over the two sites.

a) The cases of 0, 1, 3, and 4 particles are trivial (think about it for a moment). We therefore concentrate on the case of 2 particles. Only six two-particle states are allowed by symmetry. Find them, classify them by their spin- and orbital symmetry and determine the matrix of the Hamiltonian. Show that the spin-singlet and spin-triplet sectors separate and that the latter is trivial.

b) Diagonalize the Hamiltonian and determine in particular the triplet-excitation gap. Analyze the limits $U \to 0$ and $U/t \gg 1$. For all Eigenstates, determine $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle$, the expectation value for double occupancy.

c) We now add an electric field $E(t)$ which leads to a perturbation

$$\mathcal{H}' = V(n_1 - n_2) = \frac{eE(t)d}{2}(n_1 - n_2). \tag{2}$$

Determine the susceptibility $\chi(\omega)$, $P(\omega) = \chi(\omega)E(\omega)$, with the polarisation $P(t) = e\langle n_1(t) - n_2(t) \rangle$. For this, use the Kubo formula in the form

$$\chi(\omega) = \frac{e^2 d}{2} \sum_{n,n'} \frac{e^{-\beta\varepsilon_n}}{Z} |\langle n|n_1 - n_2|n'\rangle|^2 \times \left(\frac{1}{\hbar\omega - \varepsilon_{n'} + \varepsilon_n + i\hbar\eta} - \frac{1}{\hbar\omega - \varepsilon_n + \varepsilon_{n'} + i\hbar\eta} \right), \tag{3}$$

where the sum runs over all Eigenstates $|n\rangle$ of the unperturbed system, and take the limit $T \to 0$. Plot the resulting real part of $\chi(\omega)$ in the limits $U \to 0$ and $U/t \gg 1$. The "conductivity" can be defined as

$$\sigma(\omega) = \frac{i\omega}{8}\chi(\omega). \tag{4}$$

Calculate $\int_0^\infty d\omega \sigma_1(\omega)$, where $\sigma_1(\omega)$ is the real part of $\sigma(\omega)$, and relate the result to the f-sum rule.