Exercise-sheet 6 (November 23, 2017)

1 In-class exercises

1.1 Free-particle (retarded) Green's, spectral function and the concept of *quasiparticle*

(a) Calculate an explicit expression for the retarded Green's function

$$G^R(\boldsymbol{k},t) = -i\Theta(t)\langle[\hat{c}_{\boldsymbol{k}}(t), \hat{c}^\dagger_{\boldsymbol{k}}]_\varepsilon\rangle, \tag{1}$$

of a (free-particle) system whose dynamics is given by

$$\hat{H} = \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}. \tag{2}$$

(b) Calculate the corresponding spectral function.

(c) How does the spectral function change, if the single-electron Green's function decays exponentially in time with some characteristic time scale?

1.2 Free-phonon Green's function

The Matsubara Green's function for phonons is defined as

$$D(\boldsymbol{q},\tau) = -\langle T_\tau \hat{A}(\boldsymbol{q},\tau)\hat{A}(-\boldsymbol{q},0)\rangle, \tag{3}$$

where $\hat{A}(\boldsymbol{q},\tau) = e^{\tau\hat{H}}(\hat{a}_{\boldsymbol{q}} + \hat{a}^\dagger_{-\boldsymbol{q}})e^{-\tau\hat{H}}$, with $\hat{a}^\dagger_{\boldsymbol{q}}$ and $\hat{a}_{\boldsymbol{q}}$ bosonic operators.
A free-phonon system can be described by the Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}}\, \hat{a}^\dagger_{\boldsymbol{q}} \hat{a}_{\boldsymbol{q}}. \tag{4}$$

Show the Fourier coefficients of the free-phonon Matsubara Green's function are given by

$$\tilde{D}^{(0)}(\boldsymbol{q},\nu_n) = -\frac{2\omega_{\boldsymbol{q}}}{\nu_n^2 + \omega_{\boldsymbol{q}}^2}. \tag{5}$$

2 Homework - due date: December 1, 2017 (30 points).

2.1 Two-site Hubbard model (10 points)

Consider the Hubbard model

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + U \sum_{j} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}. \tag{6}$$

where $\hat{c}^{\dagger}_{i,\sigma}$ ($\hat{c}_{i,\sigma}$) creates (annihilates) an electron with spin σ at the site i of some lattice, $\hat{n}_{i,\sigma} = \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma}$ is the corresponding occupation number operator and the first summation runs over nearest-neighbors only.

In what follows we work with the occupation number representation and we label the sites of a chain of ions as

$$\underbrace{\square}_{L} \cdots \underbrace{\square}_{2} \underbrace{\square}_{1} \underbrace{\square}_{0}, \tag{7}$$

where L is the total number of sites. Each site can have four states, namely, empty, singled occupied ($\uparrow$, $\downarrow$) or doubly occupied ($\uparrow\downarrow$).

Consider the two-site Hubbard model at half-filling, i.e. with two electrons only

(a) How large is the subspace with total spin $S_z = 0$? (with $\hat{S}_z = (1/2) \sum_j (\hat{n}_{j,\uparrow} - \hat{n}_{j,\downarrow})$)

Draw all possible configurations using the convention of equation (7) and placing $\uparrow$ spins to the left of $\downarrow$ spins. Write also the binary representation of all the configurations (assigning, for example, 1 to $\uparrow$ spins and 0 to $\downarrow$ spins).

(b) Write down the matrix representation (in the occupation number basis) of the Hamiltonian (6) in the subspace with $S_z = 0$ and diagonalize it.

2.2 Equation of motion of the Hubbard atom (20 points)

Consider

$$\hat{H} = \sum_{\sigma} (\epsilon_{\sigma} - \mu) \hat{n}_{\sigma} + U \hat{n}_{\uparrow} \hat{n}_{\downarrow}, \tag{8}$$

where σ labels the spin configurations ($\uparrow, \downarrow$), ϵ_{σ} is the orbital energy, μ is the chemical potential and U is the on-site Coulomb repulsion.

Find and solve (using Fourier transforms) the equation of motion for the Hubbard atom problem satisfied by

$$G^R(t) = -i\Theta(t) \langle [\hat{c}_{\sigma}(t), \hat{c}^{\dagger}_{\sigma}]_{\varepsilon} \rangle, \tag{9}$$