Exercise-sheet 6 (November 30, 2015)

1 In-class exercises

1.1 Analytical continuation of Matsubara Green's functions

In the lecture, the function

$$G(z) = \int dt\, e^{-izt}\, G_R(t), \tag{1}$$

with z a complex variable and $G_R(t)$ the retarded Green's function, was defined. This function

(i) is analytic in the upper half-plane of z,

(ii) decays as z^{-1} when $|z|$ becomes large,

(iii) and has a branch cut on the real axis.

(a) Revisit the arguments behind (i), (ii) and (iii) above.

(b) In the last homework you study some properties of the Matsubara Green function and its Fourier coefficients $\tilde{G}(\omega_l)$. Show that there is a unique function $G(z)$ satisfying (i), (ii) and (iii) which can be reconstructed from the infinite set of Fourier coefficients, such that $G(i\omega_l) = \tilde{G}(\omega_l)$.

1.2 Green's function of an impurity immersed in a fermionic bath (continuation)

Show the complex function

$$G(z) = \frac{1}{z - \epsilon - \sum_{\boldsymbol{k}} \frac{V^2}{z - \epsilon_{\boldsymbol{k}}}}, \tag{2}$$

is the correct analytic continuation of $\tilde{G}(\omega_l)$, which was calculated in the last homework.

1.3 Frequency summations

Let's consider the following sum

$$S = -\frac{1}{\beta}\sum_{\nu_n} \tilde{D}^{(0)}(\boldsymbol{q},\nu_n)\,\tilde{G}^{(0)}(\boldsymbol{k},\omega_n+\nu_n), \tag{3}$$

with ν_n (ω_n) bosonic (fermionic) Matsubara frequencies,

$$\tilde{G}^{(0)}(\boldsymbol{k},\xi_n) = \frac{1}{i\xi_n - \epsilon_{\boldsymbol{k}}}, \tag{4}$$

the free-electron Green's function and

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

the free-phonon Green's function. Transform the infinite sum into a contour integral using the Residue theorem and the fact that the Bose function

$$n_B(\omega_{\boldsymbol{q}}) = \frac{1}{e^{\beta\omega_{\boldsymbol{q}}}-1} = -\frac{1}{2} + \frac{\beta}{\omega_{\boldsymbol{q}}} + \beta\sum_{n=1}^{\infty}\left(\frac{1}{\omega_{\boldsymbol{q}}+i\nu_n} + \frac{1}{\omega_{\boldsymbol{q}}-i\nu_n}\right), \tag{6}$$

with $\nu_n = \dfrac{2\pi n}{\beta}$. Deform the contour and calculate the sum.

2 Homework - due date: December 7, 2015 (25 + 10 points).

2.1 Free-phonon Green's function (15 points)

The Matsubara Green's function for phonons is defined as

$$D(\boldsymbol{q},\tau) = -\langle T_\tau \hat{A}(\boldsymbol{q},\tau)\hat{A}(-\boldsymbol{q},0)\rangle, \tag{7}$$

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) Consider the free phonon Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}}\,\hat{a}^\dagger_{\boldsymbol{q}}\hat{a}_{\boldsymbol{q}}, \tag{8}$$

and calculate $\hat{a}^\dagger_{\boldsymbol{q}}(\tau) = e^{\tau\hat{H}}\hat{a}^\dagger_{\boldsymbol{q}}e^{-\tau\hat{H}}$ using the Baker-Campbell-Hausdorff formula

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \,...\, + \frac{1}{n!}[\hat{A},[\hat{A},...,[\hat{A},\hat{B}]...] + \,...$$

Compute also $\hat{a}_{\boldsymbol{q}}(\tau)$.

(b) Use the expressions you got in (a) to show

$$D^{(0)}(\boldsymbol{q},\tau) = -\theta(\tau)\left((1+N_{\boldsymbol{q}})e^{-\tau\omega_{\boldsymbol{q}}} + N_{\boldsymbol{q}}e^{\tau\omega_{\boldsymbol{q}}}\right) - \theta(-\tau)\left((1+N_{\boldsymbol{q}})e^{\tau\omega_{\boldsymbol{q}}} + N_{\boldsymbol{q}}e^{-\tau\omega_{\boldsymbol{q}}}\right), \tag{9}$$

where $N_{\boldsymbol{q}} = \langle \hat{a}^{\dagger}_{\boldsymbol{q}}\,\hat{a}_{\boldsymbol{q}}\rangle = (e^{\beta\omega_{\boldsymbol{q}}}-1)^{-1}$ is the bosonic occupation number.

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

$$\tilde{D}^{(0)}(\boldsymbol{q},\nu_n) = -\frac{2\omega_{\boldsymbol{q}}}{\nu_n^2+\omega_{\boldsymbol{q}}^2}. \tag{10}$$

2.2 Another frequency summation (10 points)

Show

$$\frac{1}{\beta}\sum_{\omega_n}\tilde{G}^{(0)}(\boldsymbol{p},\omega_n)\,\tilde{G}^{(0)}(\boldsymbol{k},\omega_n+\nu_n) = \frac{n_F(\epsilon_{\boldsymbol{p}})-n_F(\epsilon_{\boldsymbol{k}})}{i\nu_n+\epsilon_{\boldsymbol{p}}-\epsilon_{\boldsymbol{k}}}, \tag{11}$$

where $n_F(\epsilon_{\boldsymbol{p}})$ is the Fermi function and ω_n (ν_n) are fermionic (bosonic) frequencies, using the fact that

$$n_F(\epsilon_{\boldsymbol{p}}) = \frac{1}{2} - \beta\sum_{n=0}^{\infty}\left(\frac{1}{\epsilon_{\boldsymbol{p}}+i\omega_n} + \frac{1}{\epsilon_{\boldsymbol{p}}-i\omega_n}\right), \tag{12}$$

with $\omega_n = \frac{(2n+1)\pi}{\beta}$.

2.3 A representation of the low-energy physics in the Benzene molecule (10 points BONUS)

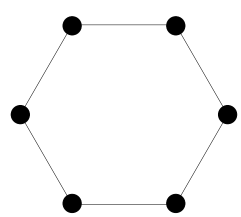

Figure 1: Carbon atoms in Benzene Molecule

Benzene consists of six carbon atoms bounded together in the hexagonal pattern shown in Figure 1, with hydrogen atoms attached to each carbon (not shown in the picture). The low-energy physics of this molecule can be described by a tight-binding model of the "p_z" electrons of each carbon atom. Consider then a tight-binding model with periodic boundary conditions of the 6-atom ring of Fig. 1. Write down explicitly the Hamiltonian in the spatial basis, i.e. the Hamiltonian matrix in the $\{|i\rangle\}$ basis, where "i" labels a lattice site. Do not diagonalize it (i.e. don't Fourier transform $\hat{H}$).