Exercise-sheet 5 (November 17, 2017)

1 In-class exercises

1.1 Revisiting Matsubara Green's function (15 points)

The temperature or Matsubara Green's function is defined as follows

$$\begin{aligned} G(\tau,\tau') &= -\langle T_\tau \hat{A}(\tau)\hat{B}(\tau')\rangle \\ &= -\langle \hat{A}(\tau)\hat{B}(\tau')\rangle\theta(\tau-\tau') + \epsilon\langle \hat{B}(\tau')\hat{A}(\tau)\rangle\theta(\tau'-\tau), \end{aligned} \tag{1}$$

where T_τ is the imaginary time-ordering operator, $\theta(\tau-\tau')$ is the Heaviside step function and τ is the imaginary time defined as $\tau = it$, with t the real (physical) time. The brackets $\langle\cdot\rangle$ are to be understood as thermodynamic expectation values. The imaginary time-dependent operators are defined as $\hat{X}(\tau) = e^{\tau\hat{H}}\hat{X}e^{-\tau\hat{H}}$, with $\hat{X} = \{\hat{A},\hat{B}\}$ and $\hat{H}$ the Hamiltonian of the system under study. Finally, if $\hat{A}$ and $\hat{B}$ are bosonic operators ϵ is taken to be (-1), otherwise it is taken to be 1.

(a) Assume $\tau > \tau'$ and use the ciclic properties of the trace to show $G(\tau,\tau') = G(\tau-\tau',0)$.

(b) Consider $G(\tau) \equiv G(\tau,0)$ for $-\beta < \tau < 0$, with β the inverse temperature, and use the cyclic properties of the trace to show

$$G(\tau) = -\epsilon\, G(\tau+\beta). \tag{2}$$

Equation (2) implies that in the interval $-\beta < \tau < \beta$, $G(\tau)$ can be expanded in a Fourier series as follows

$$G(\tau) = \frac{1}{\beta}\sum_l \tilde{G}(\omega_l)e^{-i\omega_l\tau}, \tag{3}$$

with $\tilde{G}(\omega_l) = \displaystyle\int_0^\beta d\tau e^{i\omega_l\tau}G(\tau)$.

(c) What values can take ω_l so that equation (2) holds?

(d) Let's denote by $|m\rangle$ and E_m the exact eigenstates and eigenvalues of the Hamiltonian $\hat{H}$, i.e. $\hat{H}|m\rangle = E_m|m\rangle$. Show that the Fourier transformed Matsubara Green's function $\tilde{G}(\omega_l)$ can be written as

$$\tilde{G}(\omega_l) = -\frac{1}{Z}\sum_{n,m} A_{nm}\, B_{mn}\, \frac{e^{-\beta E_n} + \epsilon\, e^{-\beta E_m}}{E_m - E_n - i\omega_l}, \tag{4}$$

with Z the partition function, $A_{nm} = \langle n|\hat{A}|m\rangle$ and $B_{mn} = \langle m|\hat{B}|n\rangle$.
Since the energies E_m are real numbers, one can rewrite equation (4) as

$$\tilde{G}(\omega_l) = \int_{-\infty}^{\infty} dx\, \frac{A(x)}{i\omega_l - x}, \tag{5}$$

where

$$A(x) = \frac{(1 + \epsilon\, e^{-\beta x})}{Z}\sum_{n,m} e^{-\beta E_n} A_{nm} B_{mn} \delta(x - E_m + E_n), \tag{6}$$

is the spectral function, which was derived in the lecture.

(e) Integrate equation (6) over the entire real line and obtain the corresponding sum rule.

1.2 Analytical continuation of Matsubara Green's functions

In the lecture, the function

$$G(z) = \int dt\, e^{izt}\, G_R(t), \tag{7}$$

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 previous exercise we 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 $G(i\omega_l) = \tilde{G}(\omega_l)$.

2 Homework - due date: November 24, 2017 (30 points).

2.1 Density of states for hybridized bands (10 points)

Consider the situation in which electrons can jump from a broad band $\epsilon(\boldsymbol{k})$ and a narrow energy level ϵ_0. The hybridized energy levels can be computed as

$$\tilde{\epsilon} = \frac{\epsilon + \epsilon_0}{2} \pm \sqrt{\frac{(\epsilon - \epsilon_0)^2}{4} + \Delta}, \tag{8}$$

with Δ a hybridization constant. Assume the ϵ band has a constant DOS $\rho(\epsilon) = \rho_0$ over a bandwidth $W = \epsilon_2 - \epsilon_1$, so that $\rho(\epsilon) = 0$ for $\epsilon < \epsilon_1$ or $\epsilon > \epsilon_2$. Likewise assume that for the narrow band, the DOS peaks sharply at ϵ_0, i.e. $\rho(\epsilon) = \rho_0 W \delta(\epsilon - \epsilon_d)$.

Calculate the DOS for the hybridized band, its bandwidth and where it vanishes using

$$\rho(\tilde{\epsilon}) = \rho(\epsilon)\frac{d\epsilon}{d\tilde{\epsilon}}. \tag{9}$$

2.2 Green's function of an impurity immersed in a fermionic bath (20 points)

Let's consider a single impurity orbital of energy ε_c, coupled with a band of non-interacting electrons through the Hamiltonian

$$\hat{H} = \varepsilon_c \hat{c}^\dagger \hat{c} + \sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) \hat{f}^\dagger_{\boldsymbol{k}} \hat{f}_{\boldsymbol{k}} + V \sum_{\boldsymbol{k}} \left(\hat{c}^\dagger \hat{f}_{\boldsymbol{k}} + \hat{f}^\dagger_{\boldsymbol{k}} \hat{c} \right). \tag{10}$$

(a) Show that the Green's functions

$$G(\tau) = -\langle T_\tau \, \hat{c}(\tau) \hat{c}^\dagger(0) \rangle, \quad F_{\boldsymbol{k}}(\tau) = -\langle T_\tau \hat{f}_{\boldsymbol{k}}(\tau) \hat{c}^\dagger(0) \rangle \tag{11}$$

satisfy the equations of motion

$$\begin{aligned} \left(\frac{\partial}{\partial \tau} + \varepsilon_c \right) G(\tau) &= -\delta(\tau) - V \sum_{\boldsymbol{k}} F_{\boldsymbol{k}}(\tau), \\ \left(\frac{\partial}{\partial \tau} + \varepsilon(\boldsymbol{k}) \right) F_{\boldsymbol{k}}(\tau) &= -V G(\tau). \end{aligned} \tag{12}$$

(b) Using Fourier transforms solve these equations and show that

$$\tilde{G}(\omega_l) = \left\{ i\omega_l - \varepsilon_c - \sum_{\boldsymbol{k}} \frac{V^2}{i\omega_l - \varepsilon(\boldsymbol{k})} \right\}^{-1} \tag{13}$$