Exercise-sheet 5 (November 23, 2015)

1 Homework - due date: November 30, 2015 (30 points).

1.1 Matsubara Green's function (15 points)

During the lecture the temperature or Matsubara Green's function was 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 $\tilde{G}(\omega_l) = \int_0^\beta d\tau e^{i\omega_l\tau}G(\tau)$.

(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 Green's function of an impurity immersed in a fermionic bath (15 points)

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

$$\hat{H} = \varepsilon_c\, \hat{c}^\dagger \hat{c} \; + \sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) \hat{f}^\dagger_{\boldsymbol{k}} \hat{f}_{\boldsymbol{k}} + V \sum_{\boldsymbol{k}} \left(\hat{c}^\dagger \hat{f}_{\boldsymbol{k}} + \hat{f}^\dagger_{\boldsymbol{k}} \hat{c} \right). \tag{7}$$

(a) Show that the Green's functions

$$G(\tau) = -\langle T_\tau\, \hat{c}(\tau) \hat{c}^\dagger(0)\rangle, \quad F_{\boldsymbol{k}}(\tau) = -\langle T_\tau \hat{f}_{\boldsymbol{k}}(\tau) \hat{c}^\dagger(0)\rangle \tag{8}$$

satisfy the equations of motion

$$\begin{aligned} \left(\frac{\partial}{\partial \tau} + \varepsilon_c\right) G(\tau) &= -\delta(\tau) - V \sum_{\boldsymbol{k}} F_{\boldsymbol{k}}(\tau), \\ \left(\frac{\partial}{\partial \tau} + \varepsilon(\boldsymbol{k})\right) F_{\boldsymbol{k}}(\tau) &= -V G(\tau). \end{aligned} \tag{9}$$

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

$$\tilde{G}(\omega_l) = \left\{ i\omega_l - \varepsilon_c - \sum_{\boldsymbol{k}} \frac{V^2}{i\omega_l - \varepsilon(\boldsymbol{k})} \right\}^{-1} \tag{10}$$