PH 340: Quantum Statistical Field Theory

Problem Set # 6

Total points: 60

Due: Tue. Mar. 19

1. (**10 points**) In class, we argued that we needed 'convergence factors' in order to make certain Mastubara sums converge. What this means is that the integral

$$\frac{\zeta}{2\pi}\oint dz g(z)h(-iz),$$

evaluated along the circular contour with $|z|\to\infty$ employed to compute the sum $\sum_n h(\omega_n)$ with

$$g(z)=\frac{\beta}{e^{\beta z}-\zeta},$$

has to disappear for an appropriate choice of the convergence factor. Show that the integral disappears

   (a) (**5 points**) for

$$h(\omega_n)=\left.\frac{-\zeta T}{i\omega_n e^{-i\omega_n\delta}-\xi}\right|_{\delta=0^+}.$$

   This is the function one needs to calculate the total number of particles. $e^{-i\omega_n\delta}$ is the convergence factor.

   (b) (**5 points**) for

$$h(\omega_n)=\ln\left[\beta\left(i\omega_n-\xi\right)\right]e^{-i\omega_n\delta}\Big|_{\delta=0^+}.$$

   This is the functions one needs to calculate the free energy. Once again, $e^{-i\omega_n\delta}$ is the convergence factor.

2. (**5 points**) While calculating the free energy, we encountered the integral

$$S=\frac{T}{2\pi i}\int_{-\infty}^{\xi}d\epsilon\left[g\left(\epsilon^+\right)\left(\ln(\epsilon^+-\xi)\right)-g\left(\epsilon^-\right)\left(\ln(\epsilon^--\xi)\right)\right].$$

where $g(z)$ is the same as in the above problem. Show that

$$S=\frac{T}{2\pi i}\int_{-\infty}^{\infty}d\epsilon g(\epsilon)\left[\ln(\epsilon^+-\xi)-\ln(\epsilon^--\xi)\right],$$

which was the expression used in class to calculate S.

3. (**10 points**) The Green's function for non-interacting electrons is

$$\mathcal{G}\left(\mathbf{k},\sigma,i\omega_n\right)=\frac{1}{i\omega_n-\xi_{\mathbf{k}}},$$

where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. $\epsilon_{\mathbf{k}}$ is the energy of the electron, $\mathbf{k}$ its momentum, μ is the chemical potential and ω_n is a fermionic Matsubara frequency corresponding to the temperature T. When interacting with phonons, the Green's function gets modified to

$$\mathcal{G}\left(\mathbf{k}, \sigma, i\omega_n\right) = \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \Sigma(\mathbf{k}, \sigma, i\omega_n)},$$

where $\Sigma(\mathbf{k}, i\omega_n)$ is called the self-energy. In the simplest approximation

$$\Sigma(\mathbf{k}, \sigma, i\omega_n) = A \sum_{\mathbf{q}} |M_{\mathbf{q}}|^2 \sum_{\nu_m} \mathcal{G}\left(\mathbf{k} - \mathbf{q}, \sigma, i\omega_n - i\nu_m\right) D\left(\mathbf{q}, i\nu_m\right),$$

where ν_m are bosonic Matsubara frequencies and $\sum_{\mathbf{q}}$ is a sum/integral overall all momenta. The phonon Green's function

$$D\left(\mathbf{q}, i\nu_m\right) = \frac{1}{i\nu_m - \omega_{\mathbf{q}}} - \frac{1}{i\nu_m + \omega_{\mathbf{q}}},$$

where $\omega_{\mathbf{q}}$ is the frequency of a phonon of wavevector $\mathbf{q}$, $M_{\mathbf{q}}$ the matrix element for electron-phonon coupling and A, a constant. Evaluate $\Sigma(\mathbf{k}, i\omega_n)$ by performing the Matsubara sum over ν_m. You can leave your answer as a sum over $\mathbf{q}$ and it can contain the Bose and Fermi distribution functions.

4. (**10 points**) The polarizability of an electron gas at wavevector $\mathbf{q}$ is given by the formula

$$\chi\left(\mathbf{q}, i\nu_n\right) = T \sum_{\omega_n} \frac{1}{V} \sum_{\mathbf{k}\sigma} \mathcal{G}\left(\mathbf{k} + \mathbf{q}, \sigma, i\omega_n + i\nu_n\right) \mathcal{G}\left(\mathbf{k}, \sigma, i\omega_n\right),$$

where $\mathbf{k}$ labels the momentum and σ, the spin of the electrons. T is the temperature and V, the volume of the system. ν_n is a bosonic Matsubara frequency and ω_n a fermionic Matsubara frequency. The Green's function

$$\mathcal{G}\left(\mathbf{k}, \sigma, i\omega_n\right) = \frac{1}{i\omega_n - \xi_{\mathbf{k}}},$$

where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$. $\epsilon_{\mathbf{k}}$ is the energy of an electron of momentum $\mathbf{k}$ and μ is the chemical potential.

(a) (**4 points**) Show that

$$\chi\left(\mathbf{q}, i\nu_n\right) = \frac{1}{V} \sum_{\mathbf{k}} \frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{i\nu_n + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}},$$

where $n_F(\epsilon)$ is the Fermi distribution function at temperature T and chemical potential μ.

(b) (**2 points**) The wavevector $\mathbf{q}$ and frequency ω dependent polarizability $\chi\left(\mathbf{q}, \omega\right)$ can be obtained by making the substitution

$$\chi\left(\mathbf{q}, i\nu_n\right) \to \chi\left(\mathbf{q}, \omega + i\delta\right),$$

where δ is an infinitesimal. Write down the expressions for the real and imaginary part of $\chi\left(\mathbf{q}, \omega\right)$.

(c) (**4 points**) The dissipation of the electron gas is proportional to $-\mathrm{Im}(\chi\left(\mathbf{q}, \omega\right))$. For a 1D electron gas at $T = 0$ with dispersion $\epsilon_k = k^2/2m$ and Fermi energy ϵ_F with corresponding Fermi momentum k_F, indicate the region in the $(\omega,\, q)$ plane where the dissipation in non-zero.

5. (**15 points)** Electrons (whose spins can be ignored) in a certain band have a dispersion $\epsilon(\mathbf{k})$. The electrons in these levels can hybridize with matrix element $V_{\mathbf{k}}$ with an electron in an "impurity" level of energy ϵ_d. This is captured by a "hybridization function"

$$\Delta(z) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{z - \epsilon_k},$$

where $\sum_{\mathbf{k}}$ is shorthand for an integral over the continuous values of $\mathbf{k}$. The Green's function of the impurity level is

$$\mathcal{G} = \frac{1}{z - (\epsilon_d - \mu) - \Delta(z)}.$$

μ is the chemical potential.

(a) (**2 point**) Argue that $\Delta(z)$ has a branch cut along the real axis.

(b) (**3 points**) Calculate $\Gamma(\epsilon) = \pm i\Delta(z \to \epsilon \pm i0^+)$.

(c) (**3 points**) Show that

$$\Delta(z) = \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} \frac{\Gamma(\epsilon)}{z - \epsilon}.$$

(d) (**4 points**) Now, assume that $\Gamma(\epsilon) = \Gamma$ for $|\epsilon| < W$ and 0 otherwise. Show that for $|z| < W$,

$$\Delta(z) = -i\Gamma \text{sgn}[\text{Im}(z)].$$

(e) (**3 points**) Calculate the density of states of the impurity level

$$\rho_{\text{imp}}(\epsilon) = -\frac{1}{\pi} \text{Im } \mathcal{G}(\epsilon + i0^+),$$

for $|\epsilon| < W$.

6. (**10 points**) Now, for the above system, the change in total electron number in the band due to the impurity can be shown to be

$$\Delta N = T \sum_n \mathcal{G}(i\omega_n) \left[1 + \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{1}{(i\omega_n - \epsilon_{\mathbf{k}})^2} \right],$$

where the summation is over the fermionic Matsubara frequencies at temperature T.

(a) (**4 points**) Show that

$$\Delta N = T \sum_n \frac{\partial}{\partial(i\omega_n)} \ln \left(i\omega_n - (\epsilon_d - \mu) - \Delta(i\omega_n) \right).$$

(b) (**6 points**) Evaluate the above Matsubara sum utilizing the arguments employed in problem 1 to show that

$$\Delta N = \int_{-\infty}^{\infty} d\epsilon \; n_F(\epsilon) \rho_{\text{imp}}(\epsilon),$$

where $n_F(\epsilon)$ is the Fermi distribution function at temperature T and chemical potential μ, assuming $T \ll |W|/k_B$.