Problem Set 8
Quantum Field Theory and Many Body Physics (SoSe2016)

Due: Thursday, June 16, 2016 at the beginning of the lecture

This problem provides further background on Grassman variables, introduces the frequently used resonant-level model, and familiarizes you with the operator approach to the BCS theory of superconductivity, the latter to complement the functional-integral approach which we will cover later in the class.

Problem 1: Grassmann basics (5+10+10 points)

Read your favorite book (e.g., Negele & Orland) to formulate and prove the following statements:

(a) Linear changes of variables in Grassmann integrals.

(b) Use (a) to prove the most general Gaussian integral for Grassmann variables as given in the class.

(c) Prove the resolution of the identity for fermionic coherent states.

Problem 2: Resonant-level model (10+5+5+5 points)

There are many physical situations in which a localized fermionic level is coupled to a (non-interacting) fermionic many-body system with a continuum of states. For instance, consider an atom placed on a metallic substrate. The atom has a large level spacing so that it can be a good approximation to consider only the atomic level which is closest to the Fermi energy of the substrate. We may then be interested in how the atomic level is influenced by the presence of the surface. Another situation where this model is relevant is a quantum dot coupled to two electronic electrodes. If the quantum dot is sufficiently small, its spectrum will also be discrete with large level spacing so that we can restrict attention to the level which is closest to the Fermi energy in the electrodes.

As it is non-interacting, this problem can of course be solved by elementary means. In this problem, we want to treat it by deriving an effective action for the localized level by integrating out the continuum field. The Hamiltonian of the system takes the form

$$H = \epsilon_d d^\dagger d + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \psi_{\mathbf{k}} + \frac{t}{\sqrt{V}} \sum_{\mathbf{k}} (\psi^\dagger_{\mathbf{k}} d + d^\dagger \psi_{\mathbf{k}}). \tag{1}$$

The first term accounts for the localized fermionic level with energy ϵ_d, the second term of the fermionic continuum with dispersion $\epsilon_{\mathbf{k}}$ and volume V, and the last term allows the fermions to hop between the localized level and the continuum. Note that this hopping is local at the position of the localized level (taken to be at the origin) as reflected in the fact that the hopping amplitudes t (taken as real) are assumed independent of momentum. We need not be very specific about the dispersion $\epsilon_{\mathbf{k}}$ of the continuum. We will simply assume that the continuum has a constant density of states ν_0 and a with bandwidth $-D < \epsilon_{\mathbf{k}} < D$, where D is some large energy. (This is sometimes refered to *wide-band limit.*)

(a) Write down the Grassmann functional integral for the partition function of this model. Integrate out the field $\psi_{\mathbf{k}}$ of the fermionic continuum and show that the effective action for the localized level becomes

$$S = d^*(\partial_\tau + \epsilon_d - \mu + \Sigma)d \tag{2}$$

in compact matrix notation or

$$S = \int \mathrm{d}\tau d^*(\tau)(\partial_\tau + \epsilon_d - \mu)d(\tau) + \int \mathrm{d}\tau \mathrm{d}\tau' d^*(\tau)\Sigma(\tau,\tau')d(\tau') \tag{3}$$

when keeping the explicit time integrals. The self energy in this action is found to be

$$\Sigma(\tau,\tau') = -\frac{1}{V}\sum_{\mathbf{k}} \langle \tau | \frac{t^2}{\partial_\tau + \epsilon_{\mathbf{k}} - \mu} | \tau' \rangle. \tag{4}$$

(b) Show that in Matsubara-frequency representation, the self-energy becomes

$$\Sigma(i\omega_n) = -\frac{1}{V}\sum_{\mathbf{k}} t^2 \mathcal{G}(\mathbf{k}, i\omega_n) \tag{5}$$

with the Green function

$$\mathcal{G}(\mathbf{k}, i\omega_n) = \frac{-1}{i\omega_n - \epsilon_{\mathbf{k}} + \mu} \tag{6}$$

of the fermionic continuum. To evaluate the self energy explicitly, replace the sum over momenta by an integral in the usual way,

$$\frac{1}{V}\sum_{\mathbf{k}} \to \nu_0 \int_{-D}^{D} d\epsilon_{\mathbf{k}} \tag{7}$$

and show that to leading order in μ/D and ω_n/D (i.e., assuming that the bandwidth D is large)

$$\Sigma(i\omega_n) = -\nu_0 t^2 \ln(1 - 2\mu/D) - i\pi\nu_0 t^2 \mathrm{sgn}\omega_n. \tag{8}$$

The real part of the self energy can be interpreted as a small shift in the energy of the localized level. Note that it approaches zero as $D \to \infty$. Let us take this limit in the following and retain only the imaginary part of the self energy in the following.

(c) Now use the resulting effective action to obtain the thermal Green function $\mathcal{G}(i\omega_n)$ of the localized level and show that it becomes

$$\mathcal{G}(i\omega_n) = \frac{-1}{i\omega_n - \epsilon_d + \mu + i\pi\nu_0 t^2 \mathrm{sgn}\omega_n}. \tag{9}$$

Show that the corresponding spectral function is

$$\rho(\omega) = \frac{\Gamma/2\pi}{(\omega - \epsilon_d)^2 + (\Gamma/2)^2}, \tag{10}$$

where we introduced $\Gamma = 2\pi t^2 \nu_0$, i.e.,

$$\mathcal{G}(i\omega_n) = -\int d\omega' \frac{\rho(\omega')}{i\omega_n - \omega'}. \tag{11}$$

Thus, we see that the imaginary part of the self energy broadens the delta-like spectral function of the uncoupled localized level into a Lorentzian, with the broadening given by $\Gamma/2$. Remembering Fermi's golden rule, interpret the explicit expression for Γ.

(d) To further interpret the imaginary part of the self energy, perform the appropriate analytical continuation to obtain the retarded Green function and Fourier transform your result to real time. How does the broadening Γ enter into the real-time retarded Green function?

Problem 3: Operator approach to BCS theory (10+15 points)

In class, we will discuss the functional integral approach to BCS theory. In this exercise, we derive the same mean field theory in the operator formalism and derive the fermionic excitation spectrum of the superconductor more explicitly.

Consider the Hamiltonian of a uniform electron system with an effectively attractive and local interaction,

$$\mathcal{H} = \int d\mathbf{r} \sum_{\sigma} \psi^{\dagger}_{\sigma}(\mathbf{r}) \left[\epsilon(-i\hbar\nabla) - \mu\right] \psi_{\sigma}(\mathbf{r}) - g \int d\mathbf{r} \psi^{\dagger}_{\uparrow}(\mathbf{r}) \psi^{\dagger}_{\downarrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}). \tag{12}$$

(a) The mean field approximation consists of writing

$$-g\psi_{\downarrow}(\mathbf{r})\psi_{\uparrow}(\mathbf{r}) = \Delta(\mathbf{r}) + [-g\psi_{\downarrow}(\mathbf{r})\psi_{\uparrow}(\mathbf{r}) - \Delta(\mathbf{r})], \tag{13}$$

where $\Delta(\mathbf{r})$ will turn out to be the complex-valued gap function, and neglecting quadratic terms in the fluctuations $[-g\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) - \Delta(\mathbf{r})]$ about the mean field $\Delta(\mathbf{r})$. Make this approximation and derive the mean field Hamiltonian

$$\mathcal{H} \simeq \int \mathrm{d}\mathbf{r} \sum_\sigma \psi_\sigma^\dagger(\mathbf{r})\left[\epsilon(-i\hbar\nabla) - \mu\right]\psi_\sigma(\mathbf{r}) + \int \mathrm{d}\mathbf{r}\Delta^*(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \Delta(\mathbf{r})\psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) + \int \mathrm{d}\mathbf{r}\frac{1}{g}|\Delta(\mathbf{r})|^2. \quad (14)$$

Write this Hamiltonian more compactly by introducing the Nambu spinor

$$\phi(\mathbf{r}) = [\psi_\uparrow(\mathbf{r}), \psi_\downarrow^\dagger(\mathbf{r})]^T. \quad (15)$$

Show that

$$\mathcal{H} \simeq \int \mathrm{d}\mathbf{r}\phi^\dagger(\mathbf{r})\begin{bmatrix} \xi(-i\hbar\nabla) & \Delta \\ \Delta^* & -\xi(-i\hbar\nabla) \end{bmatrix}\phi(\mathbf{r}) + \int \mathrm{d}\mathbf{r}\frac{1}{g}|\Delta(\mathbf{r})|^2 + \sum_\mathbf{k} \xi_\mathbf{k}, \quad (16)$$

where $\xi(-i\hbar\nabla) = \epsilon(-i\hbar\nabla) - \mu$. The last two terms are merely constants which are important for computing the ground-state energy, but not for diagonalizing the Hamiltonian. We will drop them in the following.

The Hamiltonian

$$H = \begin{bmatrix} \xi(-i\hbar\nabla) & \Delta \\ \Delta^* & -\xi(-i\hbar\nabla) \end{bmatrix} \quad (17)$$

is referred to as Bogoliubov-de Gennes Hamiltonian. The corresponding eigenvalue equation is known as Bogoliubov-de Gennes equation, which describes the energies and wavefunctions of fermionic excitations of the superconductor (see below) and which is widely used in the theory of superconductivity. Note that $\Delta(\mathbf{r})$ need not be uniform in space.

(b) We now need to diagonalize Hamiltonians with terms of the sort $\psi\psi$ and $\psi^\dagger\psi^\dagger$. This is done by means of a Bogoliubov transformation (which we already encoutered earlier in the class when we were studying the transverse field Ising model). Let us assume that the superconductor is translationally invariant, so that

$$\mathcal{H} = \sum_\mathbf{k} \phi_\mathbf{k}^\dagger \begin{bmatrix} \xi_\mathbf{k} & \Delta \\ \Delta^* & -\xi_\mathbf{k} \end{bmatrix}\phi_\mathbf{k}, \quad (18)$$

where $\phi_\mathbf{k} = [c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^\dagger]^T$. This Hamiltonian can be diagonalized by a suitable linear combination of annihilation and creation operators, termed Bogoliubov transformation,

$$\begin{bmatrix} \gamma_{\mathbf{k},\uparrow} \\ \gamma_{-\mathbf{k},\downarrow}^\dagger \end{bmatrix} = \begin{bmatrix} \cos\theta_\mathbf{k} & \sin\theta_\mathbf{k} \\ \sin\theta_\mathbf{k} & -\cos\theta_\mathbf{k} \end{bmatrix}\phi_\mathbf{k}. \quad (19)$$

Show that the newly introduced operators (termed Bogoliubov quasiparticle operators) are fermions. Rewrite the Hamiltonian (for real Δ for simplicity) in terms of the new operators and show that it becomes diagonal when choosing

$$\xi_\mathbf{k}\sin 2\theta_\mathbf{k} - \Delta\cos 2\theta_\mathbf{k} = 0. \quad (20)$$

Show that this implies

$$u_\mathbf{k} = \cos\theta_\mathbf{k} = \frac{1}{2}\sqrt{1 - \frac{\xi_\mathbf{k}}{E_\mathbf{k}}} \quad (21)$$

$$v_\mathbf{k} = \sin\theta_\mathbf{k} = \frac{1}{2}\sqrt{1 + \frac{\xi_\mathbf{k}}{E_\mathbf{k}}} \quad (22)$$

with the quasiparticle energy $E_\mathbf{k} = \sqrt{\xi_\mathbf{k}^2 + \Delta^2}$ and the standard notation of $u_\mathbf{k}$ (electron wavefucntion) and $v_\mathbf{k}$ (hole wavefunction). Finally show that when written in terms of the new operators, the Hamiltonian takes the form

$$\mathcal{H} = \sum_\mathbf{k} E_k(\gamma_{\mathbf{k}\uparrow}^\dagger\gamma_{\mathbf{k}\uparrow} - \gamma_{-\mathbf{k}\downarrow}\gamma_{-\mathbf{k}\downarrow}^\dagger). \quad (23)$$

Discuss the excitation spectrum described by this Hamiltonian.

(If you are ambitious, you may also want to continue this discussion and derive the gap equation and compute the condensation energy of the superconducting state.)