RG Methods in Statistical Field Theory: Problem Set 10 Solution

In this problem set we will use the field theoretical methods developed in class for quantum systems to derive one the most beautiful results in physics: the BCS mean-field solution for superconductivity (in its lattice version). Before we turn to the complexities of the full system, we start with the simple case of non-interacting electrons.

Part I: Non-interacting electrons on a lattice

Consider a d-dimensional hypercubic lattice with N sites at positions $\mathbf{x}_i$ and lattice spacing ℓ. Each site can be empty, singly occupied by a spin-up or spin-down electron, or doubly occupied by two electrons of opposite spin. The operators $c_{i\sigma}^\dagger$, $c_{i\sigma}$ create/destroy an electron with spin σ at site i, where $\sigma = \uparrow$ or $\downarrow$. They satisfy anticommuation relations:

$$\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'}, \qquad \{c_{i\sigma}, c_{j\sigma'}\} = \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0$$

The Hamiltonian we will examine contains only a single physical interaction: the electrons can tunnel to nearest-neighbor sites. It is given by:

$$\mathcal{H} = -t\sum_{\langle ij\rangle}\sum_{\sigma}(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - \mu\sum_{i}\sum_{\sigma} n_{i\sigma}$$

where the operator $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ counts the number of electrons with spin σ at site i. The total particle number operator (which we will label N_p to distinguish it from the number of sites N) is then: $N_p = \sum_i \sum_\sigma n_{i\sigma}$.

(a) To solve this system, we can transform to the momentum representation, where we have a set of operators $c_{\mathbf{k}\sigma}^\dagger$, $c_{\mathbf{k}\sigma}$ that create/destroy an electron of spin σ with momentum $\mathbf{k}$, where $\mathbf{k}$ is one of the N sites in the Brillouin zone of the lattice. These operators are defined through the Fourier transforms of $c_{i\sigma}^\dagger$, $c_{i\sigma}$:

$$c_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}}\sum_i e^{-i\mathbf{k}\cdot\mathbf{x}_i} c_{i\sigma}, \qquad c_{\mathbf{k}\sigma}^\dagger = \frac{1}{\sqrt{N}}\sum_i e^{i\mathbf{k}\cdot\mathbf{x}_i} c_{i\sigma}^\dagger$$

The inverse transforms are:

$$c_{i\sigma} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}\in\mathrm{BZ}} e^{i\mathbf{k}\cdot\mathbf{x}_i} c_{\mathbf{k}\sigma}, \qquad c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}\in\mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{x}_i} c_{\mathbf{k}\sigma}^\dagger$$

Show that the operators $c_{\mathbf{k}\sigma}^\dagger$, $c_{\mathbf{k}\sigma}$ satisfy the anticommutation relations:

$$\{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}^\dagger\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma\sigma'}, \qquad \{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} = \{c_{\mathbf{k}\sigma}^\dagger, c_{\mathbf{k}'\sigma'}^\dagger\} = 0$$

Hint: Remember that $\frac{1}{N}\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}_i} = \delta_{\mathbf{k},\mathbf{k}'}$.

Answer:

$$\{c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'}\} = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}'\cdot\mathbf{x}_j - i\mathbf{k}\cdot\mathbf{x}_i}\{c_{i\sigma}, c^\dagger_{j\sigma'}\} = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}'\cdot\mathbf{x}_j - i\mathbf{k}\cdot\mathbf{x}_i}\delta_{ij}\delta_{\sigma\sigma'} = \frac{1}{N}\sum_{i} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}_i}\delta_{\sigma\sigma'}$$
$$= \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma\sigma'}$$
$$\{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}'\cdot\mathbf{x}_j - i\mathbf{k}\cdot\mathbf{x}_i}\{c_{i\sigma}, c_{j\sigma'}\} = 0$$
$$\{c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'}\} = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}'\cdot\mathbf{x}_j - i\mathbf{k}\cdot\mathbf{x}_i}\{c^\dagger_{i\sigma}, c^\dagger_{j\sigma'}\} = 0$$

Thus we can work easily in momentum space: instead of $2N$ states labeled by site i and spin σ, we have $2N$ states labeled by momentum $\mathbf{k}$ and spin σ. In particular we can define a Fock space in the momentum representation: to describe the total state of the system, we specify whether each of the $2N$ states labeled by $(\mathbf{k}, \sigma)$ is empty or occupied. In other words we have an occupation number $n_{\mathbf{k}\sigma} = 0, 1$ for every $(\mathbf{k}, \sigma)$, and the total state ket can be written as $|\{n_{\mathbf{k}\sigma}\}\rangle$, where $\{n_{\mathbf{k}\sigma}\}$ is the set of all occupation numbers.

(b) Show that the Hamiltonian can be written as:

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \quad \text{where} \quad \xi_{\mathbf{k}} = -2t\sum_{\alpha=1}^{d}\cos(\ell\mathbf{k}\cdot\hat{\mathbf{e}}_\alpha) - \mu$$

Here $\hat{\mathbf{e}}_\alpha$ is the unit vector along the αth direction (so $\mathbf{k}\cdot\hat{\mathbf{e}}_\alpha = k_\alpha$). We can also write $\xi_{\mathbf{k}}$ as $\xi_{\mathbf{k}} = E_{\mathbf{k}} - \mu$, where $E_{\mathbf{k}} = -2t\sum_{\alpha=1}^{d}\cos(\ell\mathbf{k}\cdot\hat{\mathbf{e}}_\alpha)$. Thus $\xi_{\mathbf{k}}$ is the energy of a state with momentum $\mathbf{k}$ minus the chemical potential μ.

Answer:

$$\mathcal{H} = -t\sum_{\langle ij\rangle}\sum_{\sigma}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) - \mu\sum_{i}\sum_{\sigma} n_{i\sigma}$$
$$= -\frac{t}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\langle ij\rangle,\sigma}(e^{i\mathbf{k}'\cdot\mathbf{x}_j - i\mathbf{k}\cdot\mathbf{x}_i} + e^{-i\mathbf{k}\cdot\mathbf{x}_j + i\mathbf{k}'\cdot\mathbf{x}_i})c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma} - \frac{\mu}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{i,\sigma} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}_i}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}$$
$$= -\frac{t}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{i,\sigma}\sum_{\alpha=1}^{d}(e^{i\mathbf{k}'\cdot(\mathbf{x}_i+\ell\hat{\mathbf{e}}_\alpha) - i\mathbf{k}\cdot\mathbf{x}_i} + e^{-i\mathbf{k}\cdot(\mathbf{x}_i+\ell\hat{\mathbf{e}}_\alpha) + i\mathbf{k}'\cdot\mathbf{x}_i})c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma} - \mu\sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$
$$= -\frac{t}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{i,\sigma}\sum_{\alpha=1}^{d} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}_i}(e^{i\ell\mathbf{k}'\cdot\hat{\mathbf{e}}_\alpha} + e^{-i\ell\mathbf{k}\cdot\hat{\mathbf{e}}_\alpha})c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma} - \mu\sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$
$$= -t\sum_{\mathbf{k},\sigma}\sum_{\alpha=1}^{d} 2\cos(\ell\mathbf{k}\cdot\hat{\mathbf{e}}_\alpha)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - \mu\sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} = \sum_{\mathbf{k},\sigma}\xi_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$

(c) Note that the Hamiltonian in part (b) is diagonal in the momentum Fock space:

$$\mathcal{H}|\{n_{\mathbf{k}\sigma}\}\rangle = \left(\sum_{\mathbf{k},\,\sigma} \xi_{\mathbf{k}} n_{\mathbf{k}\sigma}\right) |\{n_{\mathbf{k}\sigma}\}\rangle$$

Using standard methods, show that the partition function Z is given by:

$$Z = \sum_{\{n_{\mathbf{k}\sigma}=0,1\}} \langle\{n_{\mathbf{k}\sigma}\}|e^{-\beta\mathcal{H}}|\{n_{\mathbf{k}\sigma}\}\rangle = \prod_{\mathbf{k},\,\sigma} \left(1 + e^{-\beta\xi_{\mathbf{k}}}\right)$$

where $\sum_{\{n_{\mathbf{k}\sigma}=0,1\}}$ denotes the sum over all possible sets of occupation numbers $\{n_{\mathbf{k}\sigma}\}$. *Hint:* Remember that $\sum_{\{n_{\mathbf{k}\sigma}=0,1\}} \prod_{\mathbf{k},\,\sigma} = \prod_{\mathbf{k},\,\sigma} \sum_{n_{\mathbf{k}\sigma}=0,1}$.

Answer:

$$\begin{aligned} Z &= \sum_{\{n_{\mathbf{k}\sigma}=0,1\}} \langle\{n_{\mathbf{k}\sigma}\}|e^{-\beta\mathcal{H}}|\{n_{\mathbf{k}\sigma}\}\rangle = \sum_{\{n_{\mathbf{k}\sigma}=0,1\}} e^{-\beta\sum_{\mathbf{k},\,\sigma}\xi_{\mathbf{k}} n_{\mathbf{k}\sigma}} = \sum_{\{n_{\mathbf{k}\sigma}=0,1\}} \prod_{\mathbf{k},\,\sigma} e^{-\beta\xi_{\mathbf{k}} n_{\mathbf{k}\sigma}} \\ &= \prod_{\mathbf{k},\,\sigma} \sum_{n_{\mathbf{k}\sigma}=0,1} e^{-\beta\xi_{\mathbf{k}} n_{\mathbf{k}\sigma}} = \prod_{\mathbf{k},\,\sigma} (1 + e^{-\beta\xi_{\mathbf{k}}}) \end{aligned}$$

(d) Calculate the average total particle number $\langle N_p\rangle = -\partial A/\partial\mu$, where $A = -(1/\beta)\ln Z$ is the free energy. You should find:

$$\langle N_p\rangle = \sum_{\mathbf{k},\,\sigma} \frac{1}{e^{\beta\xi_{\mathbf{k}}} + 1} \equiv \sum_{\mathbf{k},\,\sigma} f_F(\xi_{\mathbf{k}})$$

where the function $f_F(x)$ is the Fermi distribution. Note that in the limit $T \to 0$ ($\beta \to \infty$), we have $f_F(\xi_{\mathbf{k}}) = 1$ if $\xi_{\mathbf{k}} < 0$ and $f_F(\xi_{\mathbf{k}}) = 0$ if $\xi_{\mathbf{k}} > 0$. This means that at zero temperature all the states with momenta $\mathbf{k}$ satisfying $E_{\mathbf{k}} < \mu$ are occupied, and all those with $E_{\mathbf{k}} > \mu$ are empty. In order words at $T = 0$ the chemical potential μ equals the Fermi energy E_F, which is defined as the maximum occupied energy level.

Answer:

$$\begin{aligned} A &= -\frac{1}{\beta}\ln Z = -\frac{1}{\beta}\sum_{\mathbf{k},\,\sigma} \ln(1 + e^{-\beta\xi_{\mathbf{k}}}) \\ \langle N_p\rangle &= -\frac{\partial A}{\partial\mu} = -\sum_{\mathbf{k},\,\sigma} \frac{e^{-\beta\xi_{\mathbf{k}}}\frac{\partial\xi_{\mathbf{k}}}{\partial\mu}}{1 + e^{-\beta\xi_{\mathbf{k}}}} = \sum_{\mathbf{k},\,\sigma} \frac{e^{-\beta\xi_{\mathbf{k}}}}{1 + e^{-\beta\xi_{\mathbf{k}}}} = \sum_{\mathbf{k},\,\sigma} \frac{1}{e^{\beta\xi_{\mathbf{k}}} + 1} \end{aligned}$$

Conclusion: non-interacting electrons on a lattice behave almost exactly the same as the ideal Fermi gas you are familiar with from statistical mechanics. At $T = 0$ all the states below a certain energy E_F are occupied. The states with the smallest momenta have the lowest energies, and so are occupied first. The only difference is that the kinetic energy of a Fermi gas electron is $E_{\mathbf{k}} = \mathbf{k}^2/2m$ (i.e. $\mathbf{p}^2/2m$ with $p = \hbar\mathbf{k}$ and $\hbar$ set to 1), while on the lattice the energy $E_{\mathbf{k}} = -2t\sum_{\alpha=1}^{d}\cos(\ell\mathbf{k}\cdot\hat{\mathbf{e}}_\alpha)$.

Part II: Attractive Hubbard Model

Let us add an interaction term to the Hamiltonian: electrons of opposite spin sitting on the same site i lower their energy by a constant factor g. This attractive interaction between negatively charged particles may seem a little strange, but it exists in real materials as a consequence of phonons. Consider the resulting Hamiltonian, known as the *attractive Hubbard model*:

$$\mathcal{H} = -t\sum_{\langle ij\rangle}\sum_{\sigma}(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - \mu\sum_{i}\sum_{\sigma} n_{i\sigma} - g\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

(e) Before we attack the problem with all our field theoretical tools, let us first see what this attractive interaction looks like in momentum space. Show that:

$$\begin{aligned} -g\sum_i n_{i\uparrow}n_{i\downarrow} &= -\frac{g}{N}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_2\downarrow}^\dagger c_{\mathbf{k}_3\downarrow}c_{\mathbf{k}_4\uparrow}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \\ &= -\frac{g}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c_{\mathbf{k}'\uparrow}^\dagger c_{\mathbf{q}-\mathbf{k}'\downarrow}^\dagger c_{\mathbf{q}-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} \end{aligned}$$

where in the second line we have introduced momenta $\mathbf{k} = \mathbf{k}_4$, $\mathbf{k}' = \mathbf{k}_1$, and $\mathbf{q} = \mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$. Thus the interaction describes scattering in momentum space: a pair of up and down spin electrons with momenta $\mathbf{k}$ and $\mathbf{q}-\mathbf{k}$ is destroyed, and another pair with momenta $\mathbf{k}'$ and $\mathbf{q}-\mathbf{k}'$ is created. In this process the total momentum $\mathbf{q}$ of the pair is conserved.

Answer:

$$\begin{aligned} -g\sum_i n_{i\uparrow}n_{i\downarrow} &= -g\sum_i c_{i\uparrow}^\dagger c_{i\uparrow}c_{i\downarrow}^\dagger c_{i\downarrow} = -g\sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow}c_{i\uparrow} \\ &= -\frac{g}{N^2}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4}\sum_i e^{i(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{x}_i} c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_2\downarrow}^\dagger c_{\mathbf{k}_3\downarrow}c_{\mathbf{k}_4\uparrow} \\ &= -\frac{g}{N}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4} c_{\mathbf{k}_1\uparrow}^\dagger c_{\mathbf{k}_2\downarrow}^\dagger c_{\mathbf{k}_3\downarrow}c_{\mathbf{k}_4\uparrow}\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \end{aligned}$$

We would like to write the Hamiltonian as a path integral, in the same way we did it for the spinless fermion system discussed in class. The details are almost exactly the same, but we will be working in the momentum representation, where we have $2N$ sets of creation/destruction operators $c_{\mathbf{k}\sigma}^\dagger$, $c_{\mathbf{k}\sigma}$. We associate with each creation operator $c_{\mathbf{k}\sigma}^\dagger$ a Grassmann number function $\bar{\psi}_{\mathbf{k}\sigma}(\tau)$, and with each destruction operator $c_{\mathbf{k}\sigma}$ a Grassmann number function $\psi_{\mathbf{k}\sigma}(\tau)$. We use the shorthand notation that $\psi(\tau)$ and $\bar{\psi}(\tau)$ without indices represent $2N$-component Grassmann vectors whose components are $\psi_{\mathbf{k}\sigma}(\tau)$ and $\bar{\psi}_{\mathbf{k}\sigma}(\tau)$ respectively.

Thus for example the inner product $\bar{\psi}(\tau)\cdot\psi(\tau) = \sum_{\mathbf{k},\sigma} \bar{\psi}_{\mathbf{k}\sigma}(\tau)\psi_{\mathbf{k}\sigma}(\tau)$. The partition function is given by:

$$Z = \int e^S\, \mathcal{D}\bar{\psi}\mathcal{D}\psi \quad \text{where} \quad S = \int_0^\beta d\tau\, \left(-\bar{\psi}(\tau)\cdot\frac{\partial}{\partial\tau}\psi(\tau) - \mathcal{H}[\bar{\psi}(\tau),\psi(\tau)]\right)$$

and:

$$\mathcal{H}[\bar{\psi}(\tau),\psi(\tau)] = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\sigma}(\tau)\psi_{\mathbf{k}\sigma}(\tau) - \frac{g}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \bar{\psi}_{\mathbf{k}'\uparrow}(\tau)\bar{\psi}_{\mathbf{q}-\mathbf{k}'\downarrow}(\tau)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)\psi_{\mathbf{k}\uparrow}(\tau)$$

The Grassmann functions $\bar{\psi}_{\mathbf{k}\sigma}(\tau)$ and $\psi_{\mathbf{k}\sigma}(\tau)$ over which we are integrating satisfy antiperiodic boundary conditions: $\bar{\psi}_{\mathbf{k}\sigma}(\beta) = -\bar{\psi}_{\mathbf{k}\sigma}(0)$, $\psi_{\mathbf{k}\sigma}(\beta) = -\psi_{\mathbf{k}\sigma}(0)$.

Let us separate the action S into quadratic and quartic parts, $S = S_0 + S_{\text{int}}$, where:

$$S_0 = \int_0^\beta d\tau\, \sum_{\mathbf{k},\sigma} \bar{\psi}_{\mathbf{k}\sigma}(\tau)\left(-\frac{\partial}{\partial\tau} - \xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\tau)$$

$$S_{\text{int}} = \frac{g}{N}\int_0^\beta d\tau\, \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \bar{\psi}_{\mathbf{k}'\uparrow}(\tau)\bar{\psi}_{\mathbf{q}-\mathbf{k}'\downarrow}(\tau)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)\psi_{\mathbf{k}\uparrow}(\tau)$$

The whole difficulty of the problem resides in the quartic interaction term S_{int}. If $g = 0$, we would have $S = S_0$, and you could do the quadratic Grassmann integrals directly, leading (with some work) to the same answer found in part (c). How do we deal with the interaction term?

(f) As a first step, prove the following results for a Gaussian integral over the complex number z:

$$Z = \int dz^* dz\, e^{-az^*z + h_1 z + h_2 z^*} \propto \exp\left(\frac{h_1 h_2}{a}\right)$$

$$\langle z\rangle = \frac{1}{Z}\int dz^* dz\, z e^{-az^*z + h_1 z + h_2 z^*} = \frac{h_2}{a}$$

where $a > 0$. To show these, write z in terms of its real and imaginary components, $z = x+iy$. The integration measure $dz^*\, dz \propto dx\, dy$ (up to a constant that does not interest us).

<u>Answer:</u>

$$Z = \int dz^* dz\, e^{-az^*z + h_1 z + h_2 z^*} \propto \int dx \int dy\, e^{-ax^2 - ay^2 + (h_1+h_2)x + i(h_1-h_2)y}$$

$$= \frac{\pi}{a} e^{(h_1+h_2)^2/4a} e^{-(h_1-h_2)^2/4a} = \frac{\pi}{a} e^{h_1 h_2/a}$$

$$\langle z\rangle = \frac{1}{Z}\frac{\partial Z}{\partial h_1} = \frac{h_2}{a}$$

(g) The result of part (f) naturally generalizes to the following path integral, where we are integrating over a complex-valued function $\phi(\tau)$:

$$\int \mathcal{D}\phi^*\mathcal{D}\phi\, e^{\int d\tau\,[-a\phi^*(\tau)\phi(\tau)+h_1(\tau)\phi(\tau)+h_2(\tau)\phi^*(\tau)]} \propto \exp\left(\frac{1}{a}\int d\tau\, h_1(\tau)h_2(\tau)\right)$$

This is true because in the path integral each $\phi(\tau)$, $\phi^*(\tau)$ for different τ is an independent variable you are integrating over. Why is this result useful? Define two Grassmann-valued functions $\bar{\rho}_{\mathbf{q}}(\tau)$ and $\rho_{\mathbf{q}}(\tau)$ as follows:

$$\bar{\rho}_{\mathbf{q}}(\tau) = \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}\uparrow}(\tau)\bar{\psi}_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)$$
$$\rho_{\mathbf{q}}(\tau) = \sum_{\mathbf{k}} \psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)\psi_{\mathbf{k}\uparrow}(\tau)$$

Note that since $\bar{\rho}_{\mathbf{q}}(\tau)$ and $\rho_{\mathbf{q}}(\tau)$ are made from products of two Grassmann numbers, they commute with everything and we can treat them in most cases like ordinary numbers. The quartic interaction part of the action can be written as:

$$S_{\text{int}} = \frac{g}{N}\int_0^\beta d\tau \sum_{\mathbf{q}} \bar{\rho}_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(\tau)$$

Now let us introduce a different complex-valued function $\Delta_{\mathbf{q}}(\tau)$ for every $\mathbf{q}$. Using the path integral result above, show that $e^{S_{\text{int}}}$ can be written as a product of path integrals over all the $\Delta_{\mathbf{q}}(\tau)$:

$$e^{S_{\text{int}}} \propto \int \exp\left(\int_0^\beta d\tau \sum_{\mathbf{q}}\left[-\frac{N}{g}\Delta^*_{\mathbf{q}}(\tau)\Delta_{\mathbf{q}}(\tau) + \Delta_{\mathbf{q}}(\tau)\bar{\rho}_{\mathbf{q}}(\tau) + \Delta^*_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(\tau)\right]\right)\mathcal{D}\Delta^*\mathcal{D}\Delta$$

where $\mathcal{D}\Delta^*\mathcal{D}\Delta \equiv \prod_{\mathbf{q}}\mathcal{D}\Delta^*_{\mathbf{q}}\mathcal{D}\Delta_{\mathbf{q}}$. Note that since $\bar{\rho}_{\mathbf{q}}(0) = \bar{\rho}_{\mathbf{q}}(\beta)$ and $\rho_{\mathbf{q}}(0) = \rho_{\mathbf{q}}(\beta)$, the functions $\Delta_{\mathbf{q}}(\tau)$ also satisfy periodic boundary conditions: $\Delta_{\mathbf{q}}(0) = \Delta_{\mathbf{q}}(\beta)$.

Answer:

$$\begin{aligned}
\exp(S_{\text{int}}) &= \exp\left(\frac{g}{N}\int_0^\beta d\tau\sum_{\mathbf{q}}\bar{\rho}_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(\tau)\right) = \prod_{\mathbf{q}}\exp\left(\frac{g}{N}\int_0^\beta d\tau\,\bar{\rho}_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(\tau)\right)\\
&\propto \prod_{\mathbf{q}}\int\exp\left(\int_0^\beta d\tau\left[-\frac{N}{g}\Delta^*_{\mathbf{q}}(\tau)\Delta_{\mathbf{q}}(\tau) + \Delta_{\mathbf{q}}(\tau)\bar{\rho}_{\mathbf{q}}(\tau) + \Delta^*_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(\tau)\right]\right)\mathcal{D}\Delta^*_{\mathbf{q}}\mathcal{D}\Delta_{\mathbf{q}}\\
&= \int\exp\left(\int_0^\beta d\tau\sum_{\mathbf{q}}\left[-\frac{N}{g}\Delta^*_{\mathbf{q}}(\tau)\Delta_{\mathbf{q}}(\tau) + \Delta_{\mathbf{q}}(\tau)\bar{\rho}_{\mathbf{q}}(\tau) + \Delta^*_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}(\tau)\right]\right)\mathcal{D}\Delta^*\mathcal{D}\Delta
\end{aligned}$$

We have done something quite remarkable: the quartic interaction $e^{S_{\text{int}}}$ has been rewritten as a path integral involving only quadratic Grassmann terms like $\bar{\rho}_{\mathbf{q}}(\tau)$ and $\rho_{\mathbf{q}}(\tau)$. This trick is known as a *Hubbard-Stratonovich transformation*, similar to the one used in Problem Set 1. However, it comes at a price: we have introduced new complex fields $\Delta_{\mathbf{q}}(\tau)$, which we now have to include in the partition function. The full expression for Z looks like:

$$Z = \int e^S \, \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}\Delta^*\mathcal{D}\Delta$$

where

$$S = \int_0^\beta d\tau \left[\sum_{\mathbf{k},\sigma} \bar{\psi}_{\mathbf{k}\sigma}(\tau) \left(-\frac{\partial}{\partial \tau} - \xi_{\mathbf{k}} \right) \psi_{\mathbf{k}\sigma}(\tau) - \frac{N}{g} \sum_{\mathbf{q}} \Delta^*_{\mathbf{q}}(\tau)\Delta_{\mathbf{q}}(\tau) \right.$$
$$\left. + \sum_{\mathbf{q},\mathbf{k}} \Delta_{\mathbf{q}}(\tau)\bar{\psi}_{\mathbf{k}\uparrow}(\tau)\bar{\psi}_{\mathbf{q}-\mathbf{k}\downarrow}(\tau) + \sum_{\mathbf{q},\mathbf{k}} \Delta^*_{\mathbf{q}}(\tau)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)\psi_{\mathbf{k}\uparrow}(\tau) \right]$$

(h) Before we proceed, let us pause to try to give a physical interpretation to this new field $\Delta_{\mathbf{q}}(\tau)$. From the second result of part (f), we can guess that the average

$$\langle \Delta_{\mathbf{q}}(\tau) \rangle \propto \langle \rho_{\mathbf{q}}(\tau) \rangle = \sum_{\mathbf{k}} \langle \psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)\psi_{\mathbf{k}\uparrow}(\tau) \rangle$$

But what is the meaning of the Grassmann average on the right? Since $\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)$ is associated with the operator $c_{\mathbf{q}-\mathbf{k}\downarrow}$ and $\psi_{\mathbf{k}\uparrow}(\tau)$ is associated with the operator $c_{\mathbf{k}\uparrow}$, we can make the further guess:

$$\langle \Delta_{\mathbf{q}}(\tau) \rangle \propto \sum_{\mathbf{k}} \langle c_{\mathbf{q}-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$$

We will study the formal details of how to go from Grassmann averages to operator averages next lecture, but for now we can accept the above result as sensible. Transform back to position space, and show that:

$$\sum_{\mathbf{k}} \langle c_{\mathbf{q}-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = \sum_i e^{-i\mathbf{q}\cdot\mathbf{x}_i} \langle c_{i\downarrow} c_{i\uparrow} \rangle$$

<u>**Answer:**</u>

$$\sum_{\mathbf{k}} \langle c_{\mathbf{q}-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = \frac{1}{N} \sum_{i,j} \sum_{\mathbf{k}} e^{-i(\mathbf{q}-\mathbf{k})\cdot\mathbf{x}_i - i\mathbf{k}\cdot\mathbf{x}_j} \langle c_{i\downarrow} c_{j\uparrow} \rangle$$
$$= \frac{1}{N} \sum_{i,j} \sum_{\mathbf{k}} e^{-i\mathbf{q}\cdot\mathbf{x}_i} e^{i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)} \langle c_{i\downarrow} c_{j\uparrow} \rangle = \sum_i e^{-i\mathbf{q}\cdot\mathbf{x}_i} \langle c_{i\downarrow} c_{i\uparrow} \rangle$$

The quantity $\langle c_{i\downarrow} c_{i\uparrow} \rangle$ is just the expectation value for destroying a pair of opposite spin electrons at site i, and the above result is just the Fourier transform of this expectation value. In other words, $\langle \Delta_{\mathbf{q}}(\tau) \rangle$ is associated with a pair of opposite spin electrons having total momentum $\mathbf{q}$. The electron pair behaves like a single bosonic particle, and thus the field that describes them is not Grassmann, but a complex number $\Delta_{\mathbf{q}}(\tau)$. These are the famous *Cooper pairs* responsible for superconductivity.

(i) The functions $\Delta_{\mathbf{q}}(\tau)$, $\bar{\psi}_{\mathbf{k}\sigma}(\tau)$, and $\psi_{\mathbf{k}\sigma}(\tau)$ over the continuous variable τ can be Fourier transformed to a discrete frequency representation. This will make performing the integrals in the partition function easier. Let us define the expansions:

$$\begin{aligned}
\bar{\psi}_{\mathbf{k}\sigma}(\tau) &= \sum_{n=-\infty}^{\infty} e^{i\omega_n\tau}\bar{\psi}_{\mathbf{k}\sigma}(\omega_n) \\
\psi_{\mathbf{k}\sigma}(\tau) &= \sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\psi_{\mathbf{k}\sigma}(\omega_n) \\
\Delta_{\mathbf{q}}(\tau) &= \sum_{n=-\infty}^{\infty} e^{-i\nu_n\tau}\Delta_{\mathbf{q}}(\nu_n)
\end{aligned}$$

Since $\bar{\psi}_{\mathbf{k}\sigma}(\beta) = -\bar{\psi}_{\mathbf{k}\sigma}(0)$ and $\psi_{\mathbf{k}\sigma}(\beta) = -\psi_{\mathbf{k}\sigma}(0)$, the ω_n are fermionic Matsubara frequencies:

$$\omega_n = \frac{(2n+1)\pi}{\beta}, \qquad n = 0, \pm1, \pm2, \ldots$$

On the other hand, $\Delta_{\mathbf{q}}(\beta) = \Delta_{\mathbf{q}}(0)$, so the ν_n are bosonic Matsubara frequencies:

$$\nu_n = \frac{2n\pi}{\beta}, \qquad n = 0, \pm1, \pm2, \ldots$$

Note the orthogonality relations:

$$\int_0^\beta d\tau\, e^{i(\omega_n-\omega_m)\tau} = \beta\delta_{mn}, \qquad \int_0^\beta d\tau\, e^{i(\nu_n-\nu_m)\tau} = \beta\delta_{mn}$$

Show that:

$$\begin{aligned}
S = \beta\sum_n\sum_{\mathbf{k},\sigma}\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\left(i\omega_n-\xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\omega_n) - \frac{\beta N}{g}\sum_m\sum_{\mathbf{q}}\Delta^*_{\mathbf{q}}(\nu_m)\Delta_{\mathbf{q}}(\nu_m) \\
+ \beta\sum_{n,m}\sum_{\mathbf{q},\mathbf{k}}\Delta_{\mathbf{q}}(\nu_m)\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{\mathbf{q}-\mathbf{k}\downarrow}(\nu_m-\omega_n) + \beta\sum_{n,m}\sum_{\mathbf{q},\mathbf{k}}\Delta^*_{\mathbf{q}}(\nu_m)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\nu_m-\omega_n)\psi_{\mathbf{k}\uparrow}(\omega_n)
\end{aligned}$$

<u>**Answer:**</u> Let us transform each term in the action separately:

$$\begin{aligned}
\int_0^\beta d\tau\sum_{\mathbf{k},\sigma}\bar{\psi}_{\mathbf{k}\sigma}(\tau)\left(-\frac{\partial}{\partial\tau}-\xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\tau) &= \sum_{n,n'}\sum_{\mathbf{k},\sigma}\int_0^\beta d\tau\, e^{i(\omega_n-\omega_{n'})\tau}\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\left(i\omega_{n'}-\xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\omega_{n'}) \\
&= \beta\sum_n\sum_{\mathbf{k},\sigma}\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\left(i\omega_n-\xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\omega_n)
\end{aligned}$$

$$-\frac{N}{g}\int_0^\beta d\tau\sum_{\mathbf{q}}\Delta^*_{\mathbf{q}}(\tau)\Delta_{\mathbf{q}}(\tau) = -\frac{N}{g}\sum_{m,m'}\sum_{\mathbf{q}}\int_0^\beta d\tau\, e^{i(\nu_m-\nu_{m'})\tau}\Delta^*_{\mathbf{q}}(\nu_m)\Delta_{\mathbf{q}}(\nu_{m'})$$

$$= -\frac{\beta N}{g} \sum_m \sum_{\mathbf{q}} \Delta^*_{\mathbf{q}}(\nu_m) \Delta_{\mathbf{q}}(\nu_m)$$

$$\begin{aligned}
\int_0^\beta d\tau \sum_{\mathbf{q},\,\mathbf{k}} \Delta_{\mathbf{q}}(\tau)\bar{\psi}_{\mathbf{k}\uparrow}(\tau)\bar{\psi}_{\mathbf{q}-\mathbf{k}\downarrow}(\tau) &= \sum_{m,n,n'} \sum_{\mathbf{q},\,\mathbf{k}} \int_0^\beta d\tau\, e^{i(\omega_n+\omega_{n'}-\nu_m)\tau} \Delta_{\mathbf{q}}(\nu_m)\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{\mathbf{q}-\mathbf{k}\downarrow}(\omega_{n'}) \\
&= \beta \sum_{n,m} \sum_{\mathbf{q},\,\mathbf{k}} \Delta_{\mathbf{q}}(\nu_m)\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{\mathbf{q}-\mathbf{k}\downarrow}(\nu_m-\omega_n)
\end{aligned}$$

$$\begin{aligned}
\int_0^\beta d\tau \sum_{\mathbf{q},\,\mathbf{k}} \Delta^*_{\mathbf{q}}(\tau)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\tau)\psi_{\mathbf{k}\uparrow}(\tau) &= \sum_{m,n,n'} \sum_{\mathbf{q},\,\mathbf{k}} \int_0^\beta d\tau\, e^{i(\nu_m-\omega_{n'}-\omega_n)\tau} \Delta^*_{\mathbf{q}}(\nu_m)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\omega_{n'})\psi_{\mathbf{k}\uparrow}(\omega_n) \\
&= \beta \sum_{n,m} \sum_{\mathbf{q},\,\mathbf{k}} \Delta^*_{\mathbf{q}}(\nu_m)\psi_{\mathbf{q}-\mathbf{k}\downarrow}(\nu_m-\omega_n)\psi_{\mathbf{k}\uparrow}(\omega_n)
\end{aligned}$$

The partition function is obtained by integrating over all the Fourier components $\Delta^*_{\mathbf{q}}(\nu_m)$, $\Delta_{\mathbf{q}}(\nu_m)$, $\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)$, and $\psi_{\mathbf{k}\sigma}(\omega_n)$:

$$Z = \int e^S \left[\prod_{m,\mathbf{q}} d\Delta^*_{\mathbf{q}}(\nu_m)\, d\Delta_{\mathbf{q}}(\nu_m)\right] \left[\prod_{n,\mathbf{k},\sigma} d\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\, d\psi_{\mathbf{k}\sigma}(\omega_n)\right]$$

The action S above describes a complicated theory, and it is not possible to solve the partition function exactly. Thus we are forced to make some approximation. The simplest one is mean-field theory: we look for paths that maximize the action S, since these contribute most to the partition function Z. Let us concentrate on the $\Delta_{\mathbf{q}}(\tau)$ field, since we saw above that it is related to the presence of Cooper pairs in the system. Typically fluctuations cost energy, so it is reasonable to assume that the field configuration that maximizes S will be uniform in space and "time" τ. Thus we will focus only on the static part of the action S, i.e. the part involving the $\mathbf{q} = 0$, $\nu_m = 0$ component of the field. This we can do by setting $\Delta_{\mathbf{q}}(\nu_m) = 0$ if $\mathbf{q}, \nu_m \neq 0$. Let us denote the $\Delta_{\mathbf{q}=\mathbf{0}}(\nu_m = 0)$ component as Δ. The resulting simplified action and partition function look like:

$$\begin{aligned}
S &= \beta \sum_n \sum_{\mathbf{k},\sigma} \bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\,(i\omega_n - \xi_{\mathbf{k}})\,\psi_{\mathbf{k}\sigma}(\omega_n) - \frac{\beta N}{g}\Delta^*\Delta \\
&\quad + \beta \sum_n \sum_{\mathbf{k}} \Delta\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n) + \beta \sum_n \sum_{\mathbf{k}} \Delta^*\psi_{-\mathbf{k}\downarrow}(-\omega_n)\psi_{\mathbf{k}\uparrow}(\omega_n) \\
Z &= \int e^S\, d\Delta^*\, d\Delta \left[\prod_{n,\mathbf{k},\sigma} d\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\, d\psi_{\mathbf{k}\sigma}(\omega_n)\right]
\end{aligned}$$

From this action we can derive the mean-field theory of superconductivity, first studied in a different form by Bardeen, Cooper, and Schrieffer.

(j) Show the simplified action S can be written in the following matrix product form:

$$S = -\frac{\beta N}{g}\Delta^*\Delta + \beta\sum_n\sum_{\mathbf{k}}\begin{pmatrix}\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n) & \psi_{-\mathbf{k}\downarrow}(-\omega_n)\end{pmatrix}\begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta \\ \Delta^* & i\omega_n + \xi_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}\psi_{\mathbf{k}\uparrow}(\omega_n) \\ \bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n)\end{pmatrix}$$

__**Answer:**__

$$\begin{aligned}
S = &-\frac{\beta N}{g}\Delta^*\Delta + \beta\sum_n\sum_{\mathbf{k},\sigma}\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\left(i\omega_n - \xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\sigma}(\omega_n) \\
&+ \beta\sum_n\sum_{\mathbf{k}}\Delta\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n) + \beta\sum_n\sum_{\mathbf{k}}\Delta^*\psi_{-\mathbf{k}\downarrow}(-\omega_n)\psi_{\mathbf{k}\uparrow}(\omega_n) \\
= &-\frac{\beta N}{g}\Delta^*\Delta + \beta\sum_n\sum_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\left(i\omega_n - \xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\uparrow}(\omega_n) \\
&+ \beta\sum_n\sum_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\downarrow}(\omega_n)\left(i\omega_n - \xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\downarrow}(\omega_n) \\
&+ \beta\sum_n\sum_{\mathbf{k}}\Delta\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n) + \beta\sum_n\sum_{\mathbf{k}}\Delta^*\psi_{-\mathbf{k}\downarrow}(-\omega_n)\psi_{\mathbf{k}\uparrow}(\omega_n)
\end{aligned}$$

Note that since the sum over n runs from $-\infty$ to ∞, and $\omega_n = (2n+1)\pi/\beta$, the following identity is true: $\sum_n f(\omega_n) = \sum_n f(-\omega_n)$ for any function f. Similarly, since $\mathbf{k} \in$ B.Z. implies that $-\mathbf{k} \in$ B.Z., we have: $\sum_{\mathbf{k}} f(\mathbf{k}) = \sum_{\mathbf{k}} f(-\mathbf{k})$. Thus we can write:

$$\begin{aligned}
\beta\sum_n\sum_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\downarrow}(\omega_n)\left(i\omega_n - \xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\downarrow}(\omega_n) &= \beta\sum_n\sum_{\mathbf{k}}\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n)\left(-i\omega_n - \xi_{-\mathbf{k}}\right)\psi_{-\mathbf{k}\downarrow}(-\omega_n) \\
&= \beta\sum_n\sum_{\mathbf{k}}\psi_{-\mathbf{k}\downarrow}(-\omega_n)\left(i\omega_n + \xi_{\mathbf{k}}\right)\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n)
\end{aligned}$$

where we have used the fact that $\xi_{-\mathbf{k}} = \xi_{\mathbf{k}}$ and the anticommutation of Grassmann-valued functions. Plugging this back into the action we have:

$$\begin{aligned}
S = &-\frac{\beta N}{g}\Delta^*\Delta + \beta\sum_n\sum_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\left(i\omega_n - \xi_{\mathbf{k}}\right)\psi_{\mathbf{k}\uparrow}(\omega_n) \\
&+ \beta\sum_n\sum_{\mathbf{k}}\psi_{-\mathbf{k}\downarrow}(-\omega_n)\left(i\omega_n + \xi_{\mathbf{k}}\right)\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n) \\
&+ \beta\sum_n\sum_{\mathbf{k}}\Delta\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n)\bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n) + \beta\sum_n\sum_{\mathbf{k}}\Delta^*\psi_{-\mathbf{k}\downarrow}(-\omega_n)\psi_{\mathbf{k}\uparrow}(\omega_n) \\
= &-\frac{\beta N}{g}\Delta^*\Delta + \beta\sum_n\sum_{\mathbf{k}}\begin{pmatrix}\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n) & \psi_{-\mathbf{k}\downarrow}(-\omega_n)\end{pmatrix}\begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta \\ \Delta^* & i\omega_n + \xi_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}\psi_{\mathbf{k}\uparrow}(\omega_n) \\ \bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n)\end{pmatrix}
\end{aligned}$$

(k) If $\bar{\eta}$ and χ are vectors of Grassmann numbers, we know the basic identity:

$$\int e^{-\bar{\eta}^T M\chi}d\bar{\eta}\,d\chi = \det M$$

Using this identity, simplify Z by performing the integrals over the Grassmann variables $\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)$ and $\psi_{\mathbf{k}\sigma}(\omega_n)$ for all $\mathbf{k}$, σ, and n. You should find the following result:

$$Z = \int e^{\tilde{S}(\Delta^*,\Delta)} d\Delta^*\, d\Delta$$

where the effective action $\tilde{S}$ depending only on Δ^* and Δ is given by:

$$\tilde{S}(\Delta^*,\Delta) = -\frac{\beta N}{g}|\Delta|^2 + \sum_{n,\,\mathbf{k}} \ln(-\beta^2\omega_n^2 - \beta^2\xi_{\mathbf{k}}^2 - \beta^2|\Delta|^2)$$

Show that $\tilde{S}(\Delta^*,\Delta)$ can be written:

$$\tilde{S}(\Delta^*,\Delta) = \tilde{S}(0,0) - \frac{\beta N}{g}|\Delta|^2 + \sum_{n,\,\mathbf{k}} \ln\left(\frac{\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)$$

where $\tilde{S}(0,0)$ is a constant independent of Δ or Δ^*.

Answer:

$$\begin{aligned}
Z &= \int e^{S}\, d\Delta^*\, d\Delta \left[\prod_{n,\mathbf{k},\sigma} d\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\, d\psi_{\mathbf{k}\sigma}(\omega_n)\right] \\
&= \int e^{-\frac{\beta N}{g}|\Delta|^2} \prod_{n,\mathbf{k}} \exp\left[\beta \begin{pmatrix}\bar{\psi}_{\mathbf{k}\uparrow}(\omega_n) & \psi_{-\mathbf{k}\downarrow}(-\omega_n)\end{pmatrix} \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta \\ \Delta^* & i\omega_n + \xi_{\mathbf{k}}\end{pmatrix} \begin{pmatrix}\psi_{\mathbf{k}\uparrow}(\omega_n) \\ \bar{\psi}_{-\mathbf{k}\downarrow}(-\omega_n)\end{pmatrix}\right] \\
&\qquad \cdot \left[\prod_{n,\mathbf{k},\sigma} d\bar{\psi}_{\mathbf{k}\sigma}(\omega_n)\, d\psi_{\mathbf{k}\sigma}(\omega_n)\right] d\Delta^*\, d\Delta \\
&= \int e^{-\frac{\beta N}{g}|\Delta|^2} \prod_{n,\mathbf{k}} \det\left[\beta \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta \\ \Delta^* & i\omega_n + \xi_{\mathbf{k}}\end{pmatrix}\right] d\Delta^*\, d\Delta \\
&= \int e^{-\frac{\beta N}{g}|\Delta|^2} \prod_{n,\mathbf{k}} \left(-\beta^2\omega_n - \beta^2\xi_{\mathbf{k}}^2 - \beta^2|\Delta|^2\right) d\Delta^*\, d\Delta \\
&= \int e^{-\frac{\beta N}{g}|\Delta|^2 + \sum_{n,\mathbf{k}} \ln\left(-\beta^2\omega_n - \beta^2\xi_{\mathbf{k}}^2 - \beta^2|\Delta|^2\right)} d\Delta^*\, d\Delta = \int e^{\tilde{S}(\Delta^*,\Delta)} d\Delta^*\, d\Delta
\end{aligned}$$

Now we write:

$$\begin{aligned}
\tilde{S}(\Delta^*,\Delta) &= -\frac{\beta N}{g}|\Delta|^2 + \sum_{n,\,\mathbf{k}} \ln(-\beta^2\omega_n^2 - \beta^2\xi_{\mathbf{k}}^2 - \beta^2|\Delta|^2) \\
&= -\frac{\beta N}{g}|\Delta|^2 + \sum_{n,\,\mathbf{k}} \ln\left[\left(-\beta^2\omega_n^2 - \beta^2\xi_{\mathbf{k}}^2\right)\left(1 + \frac{|\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)\right] \\
&= \sum_{n,\,\mathbf{k}} \ln\left(-\beta^2\omega_n^2 - \beta^2\xi_{\mathbf{k}}^2\right) - \frac{\beta N}{g}|\Delta|^2 + \sum_{n,\,\mathbf{k}} \ln\left(1 + \frac{|\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)
\end{aligned}$$

$$= \tilde{S}(0,0) - \frac{\beta N}{g}|\Delta|^2 + \sum_{n,\mathbf{k}} \ln\left(\frac{\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)$$

where $\tilde{S}(0,0) = \sum_{n,\mathbf{k}} \ln\left(-\beta^2\omega_n^2 - \beta^2\xi_{\mathbf{k}}^2\right)$.

(l) Ignoring any overall constant factors multiplying the partition function, show that you can write:

$$Z = \int e^{-\beta F(|\Delta|)} d\Delta^* d\Delta$$

where:

$$F(|\Delta|) = \frac{N}{g}|\Delta|^2 - \frac{1}{\beta}\sum_{n,\mathbf{k}} \ln\left(\frac{\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)$$

Mean-field theory tells us the free energy $A = -(1/\beta)\ln Z$ is approximately given by F evaluated at $|\Delta| = |\Delta|_{\text{min}}$, where F has its minimum value:

$$Z \approx e^{-\beta F(|\Delta|_{\text{min}})} \qquad \Rightarrow \qquad A = -\frac{1}{\beta}\ln Z \approx F(|\Delta|_{\text{min}})$$

To see how $|\Delta|_{\text{min}}$ behaves, let us expand $F(|\Delta|)$ around $|\Delta| = 0$. Show that up to order $|\Delta|^4$, the expansion is given by:

$$F = \frac{1}{2}r(T)|\Delta|^2 + u(T)|\Delta|^4 + \cdots$$

$$r(T) = \frac{2N}{g} - 2k_BT\sum_{n,\mathbf{k}} \frac{1}{\omega_n^2 + \xi_{\mathbf{k}}^2} \equiv \frac{2N}{g} - C(T)$$

$$u(T) = \frac{k_BT}{2}\sum_{n,\mathbf{k}} \frac{1}{(\omega_n^2 + \xi_{\mathbf{k}}^2)^2} \equiv D(T)$$

where clearly the functions $C(T)$ and $D(T)$ are both positive. (Remember that the Matsubara frequencies ω_n depend on β, which is why the sums $C(T)$ and $D(T)$ are functions of temperature). It is possible to evaluate the Matsubara and Brillouin zone sums and find these functions (using techniques we will discuss in lecture), but here we do not need the precise values. It is enough to know that the function $r(T)$ changes sign from positive to negative as T is decreased. To demonstrate this, argue that $C(T) \to \infty$ as $T \to 0$ and $C(T) \to 0$ as $T \to \infty$.

Answer: Ignoring the overall factor of $e^{\tilde{S}(0,0)}$ in front, we have:

$$Z = \int \exp\left[-\frac{\beta N}{g}|\Delta|^2 + \sum_{n,\mathbf{k}} \ln\left(\frac{\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)\right] d\Delta^*\, d\Delta$$

$$= \int \exp\left[-\beta\left(\frac{N}{g}|\Delta|^2 - \frac{1}{\beta}\sum_{n,\mathbf{k}} \ln\left(\frac{\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2}\right)\right)\right] d\Delta^*\, d\Delta = \int e^{-\beta F(|\Delta|)} d\Delta^* d\Delta$$

Note the Taylor expansion:

$$\ln\left(\frac{\omega_n^2+\xi_{\mathbf{k}}^2+|\Delta|^2}{\omega_n^2+\xi_{\mathbf{k}}^2}\right)=\ln\left(1+\frac{|\Delta|^2}{\omega_n^2+\xi_{\mathbf{k}}^2}\right)\approx\frac{|\Delta|^2}{\omega_n^2+\xi_{\mathbf{k}}^2}-\frac{1}{2}\frac{|\Delta|^4}{(\omega_n^2+\xi_{\mathbf{k}}^2)^2}$$

Plugging this into $F(|\Delta|)$ immediately gives us $r(T)$ and $u(T)$ in the form quoted above. Now let us look at $C(T)$:

$$C(T)=2k_BT\sum_{n,\mathbf{k}}\frac{1}{\omega_n^2+\xi_{\mathbf{k}}^2}=2k_BT\sum_{\mathbf{k}}\frac{\tanh(\xi_{\mathbf{k}}/2k_BT)}{2\xi_{\mathbf{k}}k_BT}=\sum_{\mathbf{k}}\frac{\tanh(\xi_{\mathbf{k}}/2k_BT)}{\xi_{\mathbf{k}}}$$

For $T\to\infty$, we have $\tanh(\xi_{\mathbf{k}}/2k_BT)\approx\xi_{\mathbf{k}}/2k_BT$, and

$$C(T\to\infty)\approx\sum_{\mathbf{k}}\frac{1}{2k_BT}\to 0$$

For $T\to 0$, we have $\tanh(\xi_{\mathbf{k}}/2k_BT)\to 1$, and

$$C(T\to 0)\approx\sum_{\mathbf{k}}\frac{1}{\xi_{\mathbf{k}}}$$

This sum is dominated by the region near the Fermi surface, where $E_{\mathbf{k}}\approx\mu$ and $\xi_{\mathbf{k}}=E_{\mathbf{k}}-\mu\approx 0$. Thus $C(T\to 0)\to\infty$.

(m) For $r(T)>0$ the minimum of F occurs at $|\Delta|_{\min}=0$, while for $r(T)<0$ the minimum is at some $|\Delta|_{\min}\neq 0$. We have a very familiar result: a second-order phase transition with a complex order parameter Δ, whose magnitude $|\Delta|$ gets a nonzero value below a certain temperature T_c, defined by the condition $r(T_c)=0$. For temperatures just below T_c, where $|\Delta|$ is small, show that $|\Delta|\propto(T_c-T)^{\beta}$. Find β.

Answer: Expanding $r(T)$ and $u(T)$ to lowest-order around $T=T_c$, and using the fact that $r(T_c)=0$, we have:

$$r(T)\approx r'(T_c)(T-T_c)+\cdots\qquad u(T)\approx u(T_c)+\cdots$$

where from the results of part (l) we can assume $r'(T_c),\ u(T_c)>0$. Plugging these expansions into the free energy, we get:

$$F=\frac{1}{2}r'(T_c)(T-T_c)|\Delta|^2+u(T_c)|\Delta|^4+\cdots$$

The minimum occurs at

$$\frac{\partial F}{\partial|\Delta|}=0\qquad\Rightarrow\qquad r'(T_c)(T-T_c)|\Delta|+4u(T_c)|\Delta|^3=0$$

For $T<T_c$ this has a nonzero solution at:

$$|\Delta|=\sqrt{\frac{r'(T_c)(T_c-T)}{4u(T_c)}}\propto(T_c-T)^{1/2}$$

Thus $\beta = 1/2$, the typical mean-field result.

In conclusion, we have started from the microscopic Hamiltonian of a lattice electron gas with a local attractive interaction, and derived an effective field theory in terms of a complex order parameter Δ, where $|\Delta|^2$ is proportional to the density of Cooper pairs. As we saw in part (l), this field theory has the form of a Landau-Ginzburg Hamiltonian near T_c, where $|\Delta|^2$ is small. We have already studied the Landau-Ginzburg theory for superconductors in Problem Set 4, but here we can see directly how such a theory is derived. We can even find exact expressions for the coefficients $r(T), u(T), \ldots$ in terms of the parameters in the microscopic Hamiltonian.