Project: Many-body approach to superconductivity

In this project, we will derive the Bardeen-Cooper-Schrieffer (BCS) gap equation using the operator method and the path-integral method, respectively. Additionally, we will obtain the effective action for the superconducting order parameter and partially derive the Ginzburg-Landau free energy.

1. **BCS mean-field theory**

   The effective Hamiltonian involving Cooper pairs with opposite momenta and spins is given by

$$\hat{H}_{\text{BCS}} = \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \left(\hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}_{\boldsymbol{k}\uparrow} + \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} \hat{c}_{-\boldsymbol{k}\downarrow} \right) - \sum_{\boldsymbol{k},\boldsymbol{k}'} U_{\boldsymbol{k}\boldsymbol{k}'} \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} \hat{c}_{-\boldsymbol{k}'\downarrow} \hat{c}_{\boldsymbol{k}'\uparrow},$$

   where $\xi_{\boldsymbol{k}} = \varepsilon^{(0)}_{\boldsymbol{k}} - \mu$ and $U_{\boldsymbol{k}\boldsymbol{k}'} = \langle \boldsymbol{k}, -\boldsymbol{k} | \hat{U} | \boldsymbol{k}', -\boldsymbol{k}' \rangle$ describing scattering of a pair of electrons from states $(\boldsymbol{k}' \uparrow, -\boldsymbol{k}' \downarrow)$ to states $(\boldsymbol{k} \uparrow, -\boldsymbol{k} \downarrow)$. Note that $U_{\boldsymbol{k}\boldsymbol{k}'} > 0$ because of the attractive interaction potential.

   (a) In the presence of the pair interaction, operators such as $\hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow}$ can have nonzero expectation values for the ground state. Expressing $\hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} = b_{\boldsymbol{k}} + (\hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} - b_{\boldsymbol{k}})$ where $b_{\boldsymbol{k}} = \langle \hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} \rangle$ and neglecting small fluctuation terms, show that

$$\begin{aligned} \hat{H}_{\text{BCS}} &\approx \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \left(\hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}_{\boldsymbol{k}\uparrow} + \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} \hat{c}_{-\boldsymbol{k}\downarrow} \right) - \sum_{\boldsymbol{k}} \left(\Delta_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} + \Delta^{*}_{\boldsymbol{k}} \hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} - \Delta_{\boldsymbol{k}} b^{*}_{\boldsymbol{k}} \right) \\ &= E_0 + \sum_{\boldsymbol{k}} \Psi^{\dagger}_{\boldsymbol{k}} h(\boldsymbol{k}) \Psi_{\boldsymbol{k}}, \end{aligned}$$

   where $\Psi^{\dagger}_{\boldsymbol{k}} = \left(\hat{c}^{\dagger}_{\boldsymbol{k}\uparrow}, \hat{c}_{-\boldsymbol{k}\downarrow} \right)$. Find $\Delta_{\boldsymbol{k}}$, E_0 and $h(\boldsymbol{k})$.

   (b) For a general two-component Hamiltonian $H = a_0 + \boldsymbol{a} \cdot \boldsymbol{\sigma}$ where $\boldsymbol{\sigma}$ are Pauli matrices, show that H has eigenvalues $\varepsilon_{\pm} = a_0 \pm a$ and the corresponding eigenfunctions are given by (up to a constant)

$$|+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}, |-\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} e^{i\phi} \end{pmatrix},$$

   where $a = \sqrt{a_1^2 + a_2^2 + a_3^2}$, $\tan\theta = \frac{\sqrt{a_1^2 + a_2^2}}{a_3}$ and $\tan\phi = \frac{a_2}{a_1}$.

   $*$ Note that the eigenfunctions are nothing but a rotated spin up and spin down states about the y-axis by θ and subsequently by angle ϕ about the z-axis.

   (c) Note that the Hamiltonian in (a) is a quadratic form in the operators, thus can be diagonalized. For simplicity, assume that $\Delta_{\boldsymbol{k}}$ is real. By diagonalizing the matrix $h(\boldsymbol{k})$, show that the mean-field Hamiltonian can be rewritten as

$$H_{\text{BCS}} = E_{\text{G}} + \sum_{\boldsymbol{k}} E_{\boldsymbol{k}} (\hat{\alpha}^{\dagger}_{\boldsymbol{k}} \hat{\alpha}_{\boldsymbol{k}} + \hat{\beta}^{\dagger}_{\boldsymbol{k}} \hat{\beta}_{\boldsymbol{k}}).$$

   with

$$\hat{c}_{\boldsymbol{k}\uparrow} = u_{\boldsymbol{k}} \hat{\alpha}_{\boldsymbol{k}} + v_{\boldsymbol{k}} \hat{\beta}^{\dagger}_{\boldsymbol{k}} \ , \ \hat{c}_{-\boldsymbol{k}\downarrow} = u_{\boldsymbol{k}} \hat{\beta}_{\boldsymbol{k}} - v_{\boldsymbol{k}} \hat{\alpha}^{\dagger}_{\boldsymbol{k}}.$$

   Find $E_{\boldsymbol{k}}$, E_{G}, $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$. (Here, choose $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ as real.)

   $*$ Alternatively, we can use the canonical transformation. Note that $\alpha_{\boldsymbol{k}}$ and $\beta_{\boldsymbol{k}}$ satisfy the fermionic commutation relations.

   (d) Show that

$$\langle \hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} \rangle = u_{\boldsymbol{k}} v_{\boldsymbol{k}} \left\langle 1 - \hat{\alpha}^{\dagger}_{\boldsymbol{k}} \hat{\alpha}_{\boldsymbol{k}} - \hat{\beta}^{\dagger}_{\boldsymbol{k}} \hat{\beta}_{\boldsymbol{k}} \right\rangle = \frac{\Delta_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}} \left[1 - 2f(E_{\boldsymbol{k}}) \right] = \frac{\Delta_{\boldsymbol{k}}}{2E_{\boldsymbol{k}}} \tanh\frac{\beta E_{\boldsymbol{k}}}{2},$$

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where $f(E_{\boldsymbol{k}}) = \left(e^{\beta E_{\boldsymbol{k}}} + 1\right)^{-1}$ and $\beta = \frac{1}{k_{\rm B}T}$. Then show that the gap function $\Delta_{\boldsymbol{k}}$ is given by

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} U_{\boldsymbol{k},\boldsymbol{k}'} \langle \hat{c}_{-\boldsymbol{k}'\downarrow}\hat{c}_{\boldsymbol{k}'\uparrow}\rangle = \sum_{\boldsymbol{k}'} U_{\boldsymbol{k},\boldsymbol{k}'} \frac{\Delta_{\boldsymbol{k}'}}{2E_{\boldsymbol{k}'}} \tanh\frac{\beta E_{\boldsymbol{k}'}}{2}.$$

(e) Assume that $U_{\boldsymbol{k},\boldsymbol{k}'} = \frac{g}{V}$ ($g > 0$) for $|\xi_k|, |\xi_{k'}| < \hbar\omega_{\rm D}$ and zero otherwise, where $\omega_{\rm D}$ is the Debye frequency for phonons. Then, show that the gap function reduces to $\Delta_{\boldsymbol{k}} = \Delta\Theta(\hbar\omega_{\rm D} - |\xi_k|)$ where Δ is a (temperature-dependent) constant which satisfies

$$1 \approx gN_0 \int_0^{\hbar\omega_{\rm D}} d\xi \frac{\tanh\frac{\beta}{2}\left(\xi^2 + \Delta^2\right)^{\frac{1}{2}}}{\left(\xi^2 + \Delta^2\right)^{\frac{1}{2}}}$$

and N_0 is the density of states per spin per volume at the Fermi energy.

∗ Further reading: Tinkham, Ch. 3.5; Fetter and Walecka, §37 and §51.

2. **BCS gap equation**

(a) Show that at $T = 0$, $\Delta(T = 0) \equiv \Delta_0$ is given by

$$\Delta_0 = \frac{\hbar\omega_{\rm D}}{\sinh(1/gN_0)}.$$

(b) At $T = T_{\rm c}$, $\Delta(T = T_{\rm c}) = 0$. Then show that

$$k_{\rm B}T_{\rm c} \approx A\hbar\omega_{\rm D}e^{-\frac{1}{gN_0}}.$$

Note that $\int_0^{x_{\rm c}} dx \frac{\tanh x}{x} \approx \ln(2Ax_{\rm c})$ for large $x_{\rm c}$, where $A = \frac{2e^\gamma}{\pi} \approx 1.13$ and $\gamma \approx 0.577$.

(c) In the weak coupling limit $gN_0 \ll 1$, find the ratio $\frac{\Delta_0}{k_{\rm B}T_{\rm c}}$, which is universal independent of the particular material.

(d) Assuming the weak coupling limit, draw $\Delta(T)/\Delta_0$ numerically as a function of $T/T_{\rm c}$ for $gN_0 = 0.1, 1, 10$, respectively.

∗ Express the gap equation in Prob. 1(e) in terms of $\Delta(T)/\Delta(0)$ and $T/T_{\rm c}$ using the result of (a) and (b).

∗ In the weak coupling limit $gN_0 \ll 1$, $\Delta(T)/\Delta_0$ as a function of $T/T_{\rm c}$ in the BCS theory exhibits a universal curve. Note that $T_{\rm c}$ relation in (b) is valid only for large $x_{\rm c}$ or small $T_{\rm c}$, i.e. for weak coupling limit. In principle, for large gN_0, you should find $T_{\rm c}$ numerically using the condition $\Delta(T_{\rm c}) = 0$ in the gap function.

∗ Further reading: Tinkham, Ch. 3.6; Fetter and Walecka, §37 and §51.

3. **Path integral method: Effective action for the bosonic field**

Consider a coordinate representation of the BCS Hamiltonian ignoring vector and scalar potentials:

$$\hat{H}_{\rm BCS} = \int d^dx \left[\sum_\sigma \hat{\psi}^\dagger_\sigma(\boldsymbol{x})K_0(\boldsymbol{x})\hat{\psi}_\sigma(\boldsymbol{x}) - g\hat{\psi}^\dagger_\uparrow(\boldsymbol{x})\hat{\psi}^\dagger_\downarrow(\boldsymbol{x})\hat{\psi}_\downarrow(\boldsymbol{x})\hat{\psi}_\uparrow(\boldsymbol{x})\right]$$

where $K_0(\boldsymbol{x}) = -\frac{\hbar^2}{2m}\nabla^2 - \mu$. From now on, we will set $\hbar = 1$ for simplicity.

(a) Using the coherent state path integral, show that the quantum partition function is given by $Z = \int D\bar{\psi}D\psi e^{-S[\bar{\psi},\psi]}$ where

$$S[\bar{\psi},\psi] = \int_0^\beta d\tau \int d^dx \left[\sum_\sigma \bar{\psi}_\sigma(\boldsymbol{x},\tau)\left(\partial_\tau + K_0(\boldsymbol{x})\right)\psi_\sigma(\boldsymbol{x},\tau) - g\bar{\psi}_\uparrow(\boldsymbol{x},\tau)\bar{\psi}_\downarrow(\boldsymbol{x},\tau)\psi_\downarrow(\boldsymbol{x},\tau)\psi_\uparrow(\boldsymbol{x},\tau)\right].$$

(b) Using a Hubbard-Stratonovich transformation, express

$$e^{g\int d\tau \int d^dx \bar{\psi}_\uparrow\bar{\psi}_\downarrow\psi_\downarrow\psi_\uparrow}$$

by introducing a bosonic field Δ to decouple the quartic interaction.

(c) Show that the partition function can be expressed as

$$Z = \int D\bar{\psi} D\psi D\bar{\Delta} D\Delta e^{-S[\bar{\psi},\psi,\bar{\Delta},\Delta]}$$

where

$$\begin{aligned} S[\bar{\psi},\psi,\bar{\Delta},\Delta] &= \int d\tau \int d^d x \left[\sum_\sigma \bar{\psi}_\sigma \left(\partial_\tau + K_0\right) \psi_\sigma - \Delta \bar{\psi}_\uparrow \bar{\psi}_\downarrow - \bar{\Delta} \psi_\downarrow \psi_\uparrow + \frac{\bar{\Delta}\Delta}{g} \right] \\ &= \int d\tau d^d x \left(\frac{\bar{\Delta}\Delta}{g} - \bar{\Psi} \mathbb{g}^{-1} \Psi \right) \end{aligned}$$

with $\Psi = \begin{pmatrix} \psi_\uparrow \\ \bar{\psi}_\downarrow \end{pmatrix}$ and $\mathbb{g}^{-1} = \begin{pmatrix} -\partial_\tau - K_0 & \Delta \\ \bar{\Delta} & -\partial_\tau + K_0 \end{pmatrix}$.

(d) Since the action is quadratic in the fermion field ψ, we can carry out the Gaussian integral over the fermionic field to obtain an effective action for Δ. Show that

$$Z = \int D\bar{\Delta} D\Delta e^{-S_{\text{eff}}[\bar{\Delta},\Delta]},$$

where

$$S_{\text{eff}}[\bar{\Delta},\Delta] = \int d\tau \int d^d x \left(\frac{\bar{\Delta}\Delta}{g} \right) - \ln \operatorname{Det}\left(-\mathbb{g}^{-1}\right).$$

∗ Further reading: Altland and Simons, Ch. 6.4; Coleman, Ch. 14.6.

4. **Path integral method: Saddle-point or mean-field solution**

A variation of the action with respect to Δ generates a mean-field equation for Δ. Assume that configurations extremizing the action is homogeneous in space and time.

(a) Show that

$$\operatorname{Det}\left(-\mathbb{g}^{-1}\right) = \prod_{\boldsymbol{k},\omega_n} \left[(i\omega_n)^2 - \xi_{\boldsymbol{k}}^2 - |\Delta|^2 \right]$$

and thus, the effective action for Δ is given by

$$S_{\text{eff}}[\bar{\Delta},\Delta] \approx \beta V \left(\frac{\bar{\Delta}\Delta}{g} \right) - \sum_{\boldsymbol{k},\omega_n} \ln \left[(i\omega_n)^2 - \xi_{\boldsymbol{k}}^2 - \Delta_{\boldsymbol{k}}^2 \right].$$

(b) From the frequency summation $\frac{1}{\beta\hbar} \sum_{\omega_n} \frac{1}{i\omega_n - \omega_{\boldsymbol{k}}} = f(\omega_{\boldsymbol{k}})$ where $f(\omega) = \left(e^{\beta\hbar\omega} + 1\right)^{-1}$ for fermions, prove that

$$\frac{1}{\beta\hbar} \sum_{\omega_n} \frac{1}{\omega_n^2 + \omega_{\boldsymbol{k}}^2} = \frac{1}{2\omega_{\boldsymbol{k}}} \tanh \frac{\beta\hbar\omega_{\boldsymbol{k}}}{2}.$$

(c) The saddle-point solution can be obtained from $\frac{\partial}{\partial\bar{\Delta}} S_{\text{eff}}[\bar{\Delta},\Delta] = 0$. Then, show that

$$\frac{1}{g} = \frac{1}{\beta V} \sum_{\boldsymbol{k},\omega_n} \frac{1}{\hbar^2\omega_n^2 + \xi_{\boldsymbol{k}}^2 + |\Delta|^2} = \int \frac{d^d k}{(2\pi)^d} \frac{1}{2E_k} \tanh \frac{\beta E_k}{2}$$

where $E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + |\Delta|^2}$, which gives the gap equation in Prob. 1(d) or 1(e).

∗ Further reading: Altland and Simons, Ch. 6.4; Coleman, Ch. 14.6.

5. **Path integral method: Gaussian fluctuation**

In the vicinity of the phase transition, Δ is small in comparison with the temperature, thus we can perturbatively expand the action in powers of Δ.

(a) Show that the effective action in Prob. 3(d) can be rewritten as

$$S_{\text{eff}}[\bar{\Delta},\Delta] = \int d\tau \int d^d x \left(\frac{\bar{\Delta}\Delta}{g} \right) - \operatorname{Tr} \ln \left(-\mathbb{g}^{-1}\right).$$

(b) Let us define $\mathbb{g}^{-1} = \mathbb{g}_0^{-1} + \mathbb{\Delta}$ with $\mathbb{g}_0^{-1} = \mathbb{g}^{-1}\big|_{\Delta=0}$ and $\mathbb{\Delta} = \begin{pmatrix} 0 & \Delta \\ \bar{\Delta} & 0 \end{pmatrix}$, and expand $\mathrm{Tr}\ln\left(-\mathbb{g}^{-1}\right)$ in powers of Δ. Then, show that

$$\mathrm{Tr}\ln\left(-\mathbb{g}^{-1}\right) = \mathrm{Tr}\ln\left(-\mathbb{g}_0^{-1}\right) + \mathrm{Tr}\left(\mathbb{g}_0\mathbb{\Delta}\right) - \frac{1}{2}\mathrm{Tr}\left(\mathbb{g}_0\mathbb{\Delta}\right)^2 + \cdots.$$

(c) Explain that the first and second terms in (b) do not contribute to $S_{\text{eff}}[\bar{\Delta}, \Delta]$.

(d) Show that

$$\frac{1}{2}\mathrm{Tr}\left(\mathbb{g}_0\mathbb{\Delta}\right)^2 = -\sum_q \bar{\Delta}(-q)\Pi_0(q)\Delta(q),$$

where $q = (\boldsymbol{q}, i\nu_m)$ with an even m and $\Pi_0(\boldsymbol{q}, i\nu_m)$ is given by

$$\hbar\Pi_0(\boldsymbol{q}, i\nu_m) = \frac{1}{\beta\hbar}\sum_{\omega_n}\int\frac{d^dk}{(2\pi)^d}g_0(\boldsymbol{k}, i\omega_n)g_0(-\boldsymbol{k}+\boldsymbol{q}, -i\omega_n + i\nu_m) = -\int\frac{d^dk}{(2\pi)^d}\frac{1 - f(\xi_{\boldsymbol{k}}) - f(\xi_{\boldsymbol{k}+\boldsymbol{q}})}{i\nu_m - \omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}}}.$$

Here $f(\xi_{\boldsymbol{k}}) = \left(e^{\beta\xi_{\boldsymbol{k}}} + 1\right)^{-1}$ is the Fermi distribution function.

(e) Show that the effective action $S_{\text{eff}}[\bar{\Delta}, \Delta]$ becomes

$$S_{\text{eff}}[\bar{\Delta}, \Delta] \approx \frac{1}{\beta\hbar}\sum_{\nu_m}\int\frac{d^dq}{(2\pi)^d}\bar{\Delta}(-\boldsymbol{q}, -i\nu_m)\Gamma^{-1}(\boldsymbol{q}, i\nu_m)\Delta(\boldsymbol{q}, i\nu_m)$$

where $\Gamma^{-1}(\boldsymbol{q}, i\nu_m) = \frac{1}{g} - \Pi_0(\boldsymbol{q}, i\nu_m)$.

(f) Note that $\Gamma^{-1}(0,0) \to 0$ corresponds to an instability of the $\Delta(0,0)$ mode with a sign change in action, which occurs at $T = T_{\text{c}}$. Show that

$$\frac{1}{g} \approx \Pi_0(0,0)|_{T=T_{\text{c}}} \approx N_0\int_{-\hbar\omega_{\text{D}}}^{\hbar\omega_{\text{D}}} d\xi\, \frac{1 - 2f(\xi)}{2\xi}\bigg|_{T=T_{\text{c}}},$$

which gives the equation for the critical temperature in Prob. 2(b).

(g) For $r(T) \equiv \Gamma^{-1}(0,0)$, show that

$$r(T) \approx N_0\int_{-\hbar\omega_{\text{D}}}^{\hbar\omega_{\text{D}}} d\xi\frac{f(\xi)|_T - f(\xi)|_{T_{\text{c}}}}{\xi} \approx N_0\left(\frac{T - T_{\text{c}}}{T_{\text{c}}}\right),$$

which changes sign at $T = T_{\text{c}}$.

∗ Note that $f(\xi)|_T - f(\xi)|_{T_{\text{c}}} \approx (\beta\xi - \beta_{\text{c}}\xi)\left(\frac{\partial f}{\partial\beta\xi}\right) = \left(\frac{T-T_{\text{c}}}{T_{\text{c}}}\right)\xi\left(-\frac{\partial f}{\partial\xi}\right)$ where $\beta = \frac{1}{k_{\text{B}}T}$ and $\beta_{\text{c}} = \frac{1}{k_{\text{B}}T_{\text{c}}}$.

(h) For $T < T_{\text{c}}$, justify that $S_{\text{eff}}[\bar{\Delta}, \Delta]$ near T_{c} can be expanded as

$$S_{\text{eff}}[\bar{\Delta}, \Delta] = \int d\tau dx\left[r(T)\bar{\Delta}\Delta + \frac{u}{2}(\bar{\Delta}\Delta)^2 + \frac{c}{2}(\nabla\Delta)^2 + \cdots\right]$$

with $u > 0$ and $c > 0$, leading to the Ginzburg-Landau theory.

∗ Further reading: Altland and Simons, Ch. 6.4; Nagaosa, Ch. 5.1.

∗ Considering symmetries of the order parameter, we can construct the Ginzburg-Landau free energy phenomenologically even without the corresponding microscopic theory. From it, we can derive various physical properties, for example, the Meissner effect and fluxoid quantization in superconductors. For further reading, refer to Coleman, Ch. 11.5, Tinkham, Ch. 4 and Annet, Ch. 4.3-11.

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[1] M. Tinkham, *Introduction to Superconductivity* (2nd ed.), McGraw-Hill, Inc (1996).
[2] A. Fetter and J. Walecka, *Quantum theory of many-particle systems*, Dover (2003).
[3] A. Altland and B. Simons, *Condensed matter field theory* (2nd ed.), Cambridge University Press (2010).
[4] Piers Coleman, *Introduction to Many-Body Physics*, Cambridge University Press (2016).
[5] Naoto Nagaosa, *Quantum Field Theory in Condensed Matter Physics*, Springer (1999).