Superconductivity Part 2 Version 2

Bill Celmaster

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Overview

- In Part 1, we assumed that near $T = 0$, current was carried by Cooper pairs acting as bosons.

- In Part 2, we start with an electron effective Hamiltonian for Cooper pairs and derive the Cooper pair mass-gap (Lancaster).

- In Part 3, we will examine the 2-electron theory of the origin of Cooper pairs and will obtain the effective Hamiltonian (Annett).

The many-body effective Hamiltonian

Section 1

Brief review

Review – previous sessions

- Metals at room temperature – second quantization method:
    - Ground state energy is a perturbation on free-e^- ground state
    - $H = H_K + H_j + H_{el\text{-}j} + H_{el}$ where ions are $\approx$ jellium
    - $H_{el} = \frac{1}{2} \sum_{\mathbf{pkq}} V_{\mathbf{q}} a^\dagger_{\mathbf{p}} a^\dagger_{\mathbf{k}} a_{\mathbf{k+q}} a_{\mathbf{p-q}}$ implicitly summed over spins.

- The semiclassical theory of conductivity:
    - Assumes current is carried by fermions (electrons)
    - Assumes a statistical distribution at room temperature
        - Fermi-Dirac distribution
    - Assumes no electron-electron or ion-ion interactions

- Basic theory of superconductivity = <u>theory of charged superfluid</u>
    - Assumes current is carried by bosons (electron-pairs)
    - Assumes a statistical distribution near $T = 0$
        - Bose-Einstein distribution
    - Assumes most pairs are in the ground state (condensate)
    - Assumes no ion/ion, ion/Cooper-pair or Cooper-pair/Cooper-pair interactions

Section 2

Effective theory

Effective theory – Hamiltonian

▶ Use $c^{\dagger}_{\mathbf{p}\sigma}$ instead of $a^{\dagger}_{\mathbf{p}\sigma}$ for electrons involved in Cooper pairs.

▶ The effective Hamiltonian $\hat{H}$ is

$$\hat{H} = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}} \hat{c}^{\dagger}_{\mathbf{p}\sigma} \hat{c}_{\mathbf{p}\sigma} - \kappa^2 \sum_{\mathbf{p}\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{p}\downarrow} \hat{c}_{-\mathbf{p}\uparrow}$$

where σ labels the spin.

▶ First term is the KE; second is $e^- - e^-$ (not pair-pair) interaction

Effective theory – Candidate ground state

- Define the pair creation operator $\hat{P}_{\mathbf{p}}^{\dagger}$ by $\hat{P}_{\mathbf{p}}^{\dagger} = \hat{c}_{\mathbf{p}\uparrow}^{\dagger}\hat{c}_{-\mathbf{p}\downarrow}^{\dagger}$.

- Define a family of states, parameterized by $\alpha_{\mathbf{p}}$, by

$$|\Psi_{\text{BCS}}^{\alpha}\rangle = \prod_{\mathbf{p}} C_{\mathbf{p}} e^{\alpha_{\mathbf{p}}\hat{P}_{\mathbf{p}}^{\dagger}}|0\rangle$$

  where the $C_{\mathbf{p}}$ will be set by normalization.

- These are known as BCS coherent states.

- Notice that $\hat{P}_{\mathbf{p}}^{\dagger}$ isn't quite a boson operator.

- What matters in our previous analyses is the BCS coherent state

- In general, the ground state is found by $\min_{\Psi}\langle\Psi|\hat{H}|\Psi\rangle$.

- Approximate this by finding $\min_{\alpha}\langle\Psi_{\text{BCS}}^{\alpha}|\hat{H}|\Psi_{\text{BCS}}^{\alpha}\rangle$.

Section 3

Ground state energy

Ground state energy – BCS-state Normalization

- This follows Lancaster Section 44.2
- Note that $\left(\hat{P}_\mathbf{p}^\dagger\right)^n = 0$ when $n > 1$.
  - Fermi creation operators anticommute
  - $\hat{c}_{\mathbf{p}\uparrow}^\dagger \hat{c}_{\mathbf{p}\uparrow}^\dagger = 0$ so $\hat{c}_{\mathbf{p}\uparrow}^\dagger \hat{c}_{-\mathbf{p}\downarrow}^\dagger \hat{c}_{\mathbf{p}\uparrow}^\dagger \hat{c}_{-\mathbf{p}\downarrow}^\dagger = 0$ etc.
  - $e^{\alpha_\mathbf{p} \hat{P}_\mathbf{p}^\dagger} = 1 + \alpha_\mathbf{p} \hat{P}_\mathbf{p}^\dagger + \sum_{n>1} \frac{1}{n!} \alpha_\mathbf{p}^n \left(\hat{P}_\mathbf{p}^\dagger\right)^n = 1 + \alpha_\mathbf{p} \hat{P}_\mathbf{p}^\dagger$
- Normalize wave function so $\langle \Psi_{\text{BCS}}^\alpha | \Psi_{\text{BCS}}^\alpha \rangle = 1$
  - First notice that $\langle 0 | \hat{P}_\mathbf{p} \hat{P}_{\mathbf{p}'}^\dagger | 0 \rangle = \delta_{\mathbf{pp}'}$ & $\langle 0 | \hat{P}_\mathbf{p} | 0 \rangle = \langle 0 | \hat{P}_\mathbf{p}^\dagger | 0 \rangle = 0$
  - Set normalization condition

$$1 = \prod_{\mathbf{pp}'} C_\mathbf{p} C_{\mathbf{p}'} \langle 0 | e^{\alpha_\mathbf{p}^* \hat{P}_\mathbf{p}} e^{\alpha_{\mathbf{p}'} \hat{P}_{\mathbf{p}'}^\dagger} | 0 \rangle$$

$$= \prod_{\mathbf{pp}'} C_\mathbf{p} C_{\mathbf{p}'} \langle 0 | \left(1 + \alpha_\mathbf{p}^* \hat{P}_\mathbf{p}\right) \left(1 + \alpha_{\mathbf{p}'} \hat{P}_{\mathbf{p}'}^\dagger\right) | 0 \rangle$$

$$= \prod_\mathbf{p} C_\mathbf{p}^2 \left(1 + |\alpha_\mathbf{p}|^2\right)$$

- Therefore $C_\mathbf{p} = \frac{1}{\left(1 + |\alpha_\mathbf{p}|^2\right)^{\frac{1}{2}}}$

Ground state energy – BCS-state features

▶ Expand exponentials in the definition of $|\Psi_{BCS}^{\alpha}\rangle$

$$|\Psi_{BCS}^{\alpha}\rangle = \prod_{\mathbf{p}} C_{\mathbf{p}} e^{\alpha_{\mathbf{p}} \hat{P}_{\mathbf{p}}^{\dagger}}|0\rangle = \prod_{\mathbf{p}} \left(u_{\mathbf{p}} + v_{\mathbf{p}} \hat{P}_{\mathbf{p}}^{\dagger} \right) |0\rangle$$

where $u_{\mathbf{p}} = \left(1 + |\alpha_{\mathbf{p}}|^2\right)^{-\frac{1}{2}}$ and $v_{\mathbf{p}} = \alpha_{\mathbf{p}} \left(1 + |\alpha_{\mathbf{p}}|^2\right)^{-\frac{1}{2}}$

▶ Note (important later) $|u_{\mathbf{p}}|^2 + |v_{\mathbf{p}}|^2 = 1$.

▶ The number operator $\hat{N}$ for pairs is $\sum_{\mathbf{p}} \left(\hat{N}_{\mathbf{p}\uparrow} + \hat{N}_{\mathbf{p}\downarrow} \right)$

  ▶ $\hat{N}_{\mathbf{p}\uparrow} = c_{\mathbf{p}\uparrow}^{\dagger} c_{\mathbf{p}\uparrow}$
  ▶ $\hat{N}_{\mathbf{p}\downarrow} = c_{\mathbf{p}\downarrow}^{\dagger} c_{\mathbf{p}\downarrow}$

▶ Evaluate $\langle \Psi_{BCS}^{\alpha} | \hat{N}_{\mathbf{p}\downarrow} | \Psi_{BCS}^{\alpha}\rangle$ noting that $c_{\mathbf{p}\downarrow} \hat{P}_{\mathbf{p}'}^{\dagger}|0\rangle = 0$ if $\mathbf{p} \neq -\mathbf{p}'$

$$\langle \Psi_{BCS}^{\alpha} | \hat{N}_{\mathbf{p}\downarrow} | \Psi_{BCS}^{\alpha}\rangle = |v_{\mathbf{p}}|^2 \langle 0| \hat{P}_{-\mathbf{p}} c_{\mathbf{p}\downarrow}^{\dagger} c_{\mathbf{p}\downarrow} \hat{P}_{-\mathbf{p}}^{\dagger}|0\rangle$$
$$= |v_{\mathbf{p}}|^2 \langle 0| \hat{c}_{\mathbf{p}\downarrow} \hat{c}_{-\mathbf{p}\uparrow} c_{-\mathbf{p}\uparrow}^{\dagger} c_{\mathbf{p}\downarrow} \hat{c}_{-\mathbf{p}\uparrow}^{\dagger} \hat{c}_{\mathbf{p}\downarrow}^{\dagger}|0\rangle = |v_{\mathbf{p}}|^2$$

▶ Similarly with $\hat{N}_{\mathbf{p}\uparrow}$ so $N = \langle \Psi_{BCS}^{\alpha} | \hat{N} | \Psi_{BCS}^{\alpha}\rangle = 2 \sum_{\mathbf{p}} |v_{\mathbf{p}}|^2$

▶ N is a constraint of the theory.

Ground state energy – Minimizing the BCS energy

▶ The BCS finite-temperature "Hamiltonian"[1] is
$\hat{H}_T = \hat{H} - \mu \left(\hat{N} - N \right)$ where μ is a constraint parameter for N.

▶ The BCS finite-temperature energy is

$$E_T(\alpha, \mu) = \langle \Psi_{\mathrm{BCS}}^\alpha | \hat{H}_T | \Psi_{\mathrm{BCS}}^\alpha \rangle$$

$$= \langle \Psi_{\mathrm{BCS}}^\alpha | \left(\sum_{\mathbf{p}\sigma} (\epsilon_{\mathbf{p}} - \mu) \, \hat{c}_{\mathbf{p}\sigma}^\dagger \hat{c}_{\mathbf{p}\sigma} - \kappa^2 \sum_{\mathbf{pk}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{\mathbf{p}\downarrow} \hat{c}_{-\mathbf{p}\uparrow} \right) | \Psi_{\mathrm{BCS}}^\alpha \rangle$$

▶ Expand $|\Psi_{\mathrm{BCS}}^\alpha\rangle$ as before. See Lancaster Sec. 44.3 (& exercise 44.5)

▶ $E_T(\alpha, \mu) = \mu N + \sum_{\mathbf{p}} 2 (\epsilon_{\mathbf{p}} - \mu) |v_{\mathbf{p}}|^2 - \kappa^2 \sum_{\mathbf{pk}} v_{\mathbf{p}}^* v_{\mathbf{k}} u_{\mathbf{k}}^* u_{\mathbf{p}}$
  ▶ $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ are functions of α so we can vary E w.r.t. α

▶ Alternatively (Lancaster) vary E w.r.t. $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ constrained s.t.
$|u_{\mathbf{p}}|^2 + |v_{\mathbf{p}}|^2 = 1$, with constraint parameter $E_{\mathbf{p}}$.

$$E_T(u_{\mathbf{p}}, v_{\mathbf{p}}, \mu, E_{\mathbf{p}}) = \mu N + \sum_{\mathbf{p}} (\epsilon_{\mathbf{p}} - \mu) \left(|v_{\mathbf{p}}|^2 - |u_{\mathbf{p}}|^2 - 1 \right) -$$

$$\kappa^2 \sum_{\mathbf{pk}} v_{\mathbf{p}}^* v_{\mathbf{k}} u_{\mathbf{k}}^* u_{\mathbf{p}} + E_{\mathbf{p}} \left(|u_{\mathbf{p}}|^2 + |v_{\mathbf{p}}|^2 - 1 \right)$$

▶ Solve $\frac{\partial E_T}{\partial u_{\mathbf{p}}} = 0$ and $\frac{\partial E_T}{\partial v_{\mathbf{p}}} = 0$.

▶ Note the constraint equations.

    ▶ $\frac{\partial E_T}{\partial \mu} = 0 \implies N = 2\sum_{\mathbf{p}} |v_{\mathbf{p}}|^2$.

    ▶ $\frac{\partial E_T}{\partial E_{\mathbf{p}}} = 0 \implies |u_{\mathbf{p}}|^2 + |v_{\mathbf{p}}|^2 = 1$.

▶ Calculations are done in Lancaster 44.3 or Annett 6.6

▶ We assume (see references for intuitive justification)

    ▶ The chemical potential μ is $\approx \epsilon_F$, the Fermi energy

    ▶ $\epsilon_{\mathbf{p}}$ is the band-structure energy dispersion

    ▶ Cooper pairs only involve electrons near the Fermi surface

    ▶ Electron interactions are mediated by phonons

    ▶ The maximum phonon energy is ω_D, the Debye frequency

    ▶ So Cooper-electron energies have $|\epsilon_{\mathbf{p}} - \mu| < \omega_D$

▶ For later convenience, express some results in terms of $\epsilon'_{\mathbf{p}} \equiv \epsilon_{\mathbf{p}} - \mu$

Ground state energy – Results II

- Define $\Delta \equiv \kappa^2 \sum_{\mathbf{p}} u_{\mathbf{p}}^* v_{\mathbf{p}}$

- Then $E_{\mathbf{p}} = \pm \left[(\epsilon_{\mathbf{p}}')^2 + \Delta^2 \right]^{\frac{1}{2}}$ (Nb: $|E_{\mathbf{p}}| > \Delta$)

- The positive branch $E_{\mathbf{p}} = + \left[(\epsilon_{\mathbf{p}}')^2 + \Delta^2 \right]^{\frac{1}{2}}$ gives the lowest energy.

- From minimization we can derive[2] the BCS energy gap equation

$$\Delta = \kappa^2 \sum_{\mathbf{p}} \frac{\Delta}{2E_{\mathbf{p}}}$$

- Then $|\Delta| \approx \omega_D e^{-\frac{1}{\Lambda}}$ where $\Lambda = \kappa^2 g(\epsilon_F)$, and $g(\epsilon_F)$ is the density of states at the Fermi energy

- $|\Omega_{\text{BCS}}\rangle = \prod_{\mathbf{p}} \left(u_{\mathbf{p}}^* + v_{\mathbf{p}}^* c_{\mathbf{p}\uparrow}^{\dagger} c_{-\mathbf{p}\downarrow}^{\dagger} \right) |0\rangle$

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[2] See Lancaster Eqs.44

Section 4

The Energy Gap

Energy Gap – The mean field Hamiltonian

▶ There are justifications etc. for a mean field Hamiltonian
  ▶ Lancaster – read secs. 43.1, 43.3 and 44.4
    ▶ Lancaster is sloppy with some errors and hard to follow
    ▶ Should say that normal ordering is defined w.r.t. a vacuum.
    ▶ Sec. 43.1 makes sense only by realizing that $N[a_k^\dagger a_p] \neq a_k^\dagger a_p$ unless a_p annihilates the vacuum (not true for $|\Omega_{BCS}\rangle$).
    ▶ Eq. (44.28) interaction term should sum over $\mathbf{p}$ and $\mathbf{p}'$
    ▶ Few explanations of what approximations are being done.
  ▶ Annett – read secs 6.5 and 6.6
    ▶ Explains why certain terms are dropped
    ▶ Discusses validity of the mean field approximation
  ▶ A complete but less abstract derivation is in Feynman Statistical Mechanics Chptr 10
  ▶ If you still have questions, ask ChatGPT (as I've done)

▶ The mean field Hamiltonian $\hat{H}_{MF}$ is

$$\hat{H}_{MF} = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}}' c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} - $$
$$\kappa^2 \sum_{\mathbf{p}\mathbf{p}'} \left(\langle c_{\mathbf{p}\uparrow}^\dagger c_{-\mathbf{p}\downarrow}^\dagger \rangle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} + c_{\mathbf{p}\uparrow}^\dagger c_{-\mathbf{p}\downarrow}^\dagger \langle c_{-\mathbf{p}'\downarrow} c_{\mathbf{p}'\uparrow} \rangle \right)$$

where $\langle \hat{A} \rangle$ denotes $\langle \Omega_{BCS} | \hat{A} | \Omega_{BCS} \rangle$.

Energy Gap – Diagonalizing $\hat{H}_{MF}$

- $\hat{H}_{MF}$ is quadratic in operators.

- $\langle\Omega_{BCS}|c_{-\mathbf{p'}\downarrow}c_{\mathbf{p'}\uparrow}|\Omega_{BCS}\rangle = u_{\mathbf{p'}}v_{\mathbf{p'}}^*$ & $\langle\Omega_{BCS}|c_{\mathbf{p}\uparrow}^\dagger c_{-\mathbf{p}\downarrow}^\dagger|\Omega_{BCS}\rangle = u_{\mathbf{p}}^* v_{\mathbf{p}}$

- Recall $\Delta = \kappa^2 \sum_{\mathbf{p}} u_{\mathbf{p}}^* v_{\mathbf{p}}$ so

$$\hat{H}_{MF} = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}}' c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} - \sum_{\mathbf{p}} \left(\Delta^* c_{-\mathbf{p}\downarrow}c_{\mathbf{p}\uparrow} + \Delta c_{\mathbf{p}\uparrow}^\dagger c_{-\mathbf{p}\downarrow}^\dagger \right)$$

- Now perform a Bogoliubov transformation

$$c_{\mathbf{p}\uparrow} = u_{\mathbf{p}}^* b_{\mathbf{p}\uparrow} + v_{\mathbf{p}} b_{-\mathbf{p}\downarrow}^\dagger$$
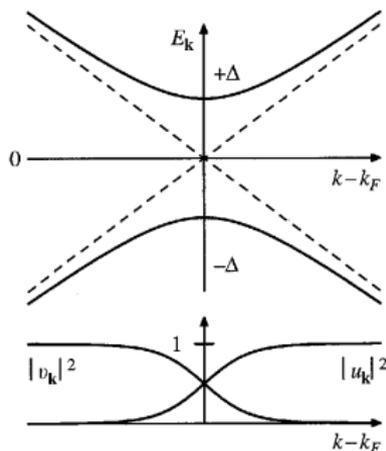$$c_{-\mathbf{p}\downarrow}^\dagger = -v_{\mathbf{p}}^* b_{\mathbf{p}\uparrow} + u_{\mathbf{p}} b_{-\mathbf{p}\downarrow}^\dagger$$

  where the b's are quasiparticle[3] $|\Omega_{BCS}\rangle$-annih/creation operators

$$\{b_{\mathbf{p}_1\sigma_1}, b_{\mathbf{p}_2\sigma_2}^\dagger\} = \delta_{\mathbf{p}_1\mathbf{p}_2}\delta_{\sigma_1\sigma_2}$$
$$\{b_{\mathbf{p}_1\sigma_1}^\dagger, b_{\mathbf{p}_2\sigma_2}^\dagger\} = \{b_{\mathbf{p}_1\sigma_1}, b_{\mathbf{p}_2\sigma_2}\} = 0$$

- Then $\hat{H}_{MF} = \sum_{\mathbf{p}} E_{\mathbf{p}} \left(b_{\mathbf{p}\uparrow}^\dagger b_{\mathbf{p}\uparrow} + b_{-\mathbf{p}\downarrow}^\dagger b_{-\mathbf{p}\downarrow} \right) = \sum_{\mathbf{p}} E_{\mathbf{p}} \left(N_{\mathbf{p}}^b + N_{-\mathbf{p}}^b \right)$
  - Some non-operator (constant) terms have been dropped

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[3] Lancaster refers to these as bogolons, but they are fermion versions

Energy Gap – Figure (Annett)

Fig. 6.8 Top: Energy eigenvalues $E_{\mathbf{k}}$ as a function of $\mathbf{k}$ near the Fermi wave vector $\mathbf{k}_F$. The dashed lines show the electron and hole energy levels $\epsilon_{\mathbf{k}} - \epsilon_F$ and $-\epsilon_{\mathbf{k}} + \epsilon_F$ in the normal metal. In the superconductor these states become hybridized, and the resulting eigenvalues are $\pm E_{\mathbf{k}}$ relative to ϵ_F. One can see that there are no states with energy less than $\pm\Delta$ near the Fermi energy. **Bottom:** The BCS wave function parameters $|u_{\mathbf{k}}|^2$ and $|v_{\mathbf{k}}|^2$ for $\mathbf{k}$ near to the Fermi surface. The state is predominantly electron like well below k_F ($|v_{\mathbf{k}}|^2 \approx 1$) and predominantly hole like far above the Fermi surface, ($|u_{\mathbf{k}}|^2 \approx 1$). But near to $\mathbf{k}_F$ the quasiparticle has mixed electron and hole character.

Energy Gap – Cooper-pair ionization

- We've shown that the physical ground state involves pairs of paired electrons.

- Insert energy into the system by raising the temperature.
    - Ionization of a Cooper pair requires
        - Annihilate a pair
        - Create two quasiparticles
    - Each contributes $E_{\mathbf{p}} > \Delta$ so ionization energy is $> 2\Delta$.

- Superconductivity goes away **only** if the energy exceeds 2Δ.

- Derive temperature dependence
    - Recall $\kappa^2 \langle \Omega_{\text{BCS}} | c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} | \Omega_{\text{BCS}} \rangle = \Delta^*$
    - Then expand c operators in terms of quasiparticle b operators.
    - For general temperature

    $$\langle \Omega_{\text{BCS}} | b_{\mathbf{p}\uparrow}^{\dagger} b_{\mathbf{p}\uparrow} | \Omega_{\text{BCS}} \rangle = \langle \Omega_{\text{BCS}} | N_{\mathbf{p}} | \Omega_{\text{BCS}} \rangle = f(T, E_{\mathbf{p}})$$
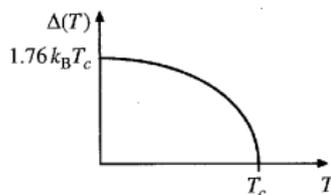
    where $f(T, E) = \frac{1}{e^{\frac{E}{kT}} - 1}$ is the Fermi-Dirac distribution.
    - Leads to $\Delta(T) = \kappa^2 \sum_{\mathbf{p}} u_{\mathbf{p}}^* v_{\mathbf{p}} \left(1 - 2f(T, E_{\mathbf{p}})\right)$

Energy Gap – Critical temperature

- Annett derives (Eq. 6.90) the T-dependent energy gap equation

$$\Delta(T) = \kappa^2 \sum_{\mathbf{p}} \frac{\Delta}{2E_{\mathbf{p}}} \tanh(\frac{E_{\mathbf{p}}}{2kT})$$

Fig. 6.9 Δ as a function of temperature in the BCS theory.

- At T_C the gap is 0 so superconductivity ceases.
- BCS derived $2\Delta(0) = 3.52kT_c$
    - Obeyed accurately for many superconductors