From the Cooper Pair Problem to the BCS Ground State

Outline

Introduction: Two Conceptual Pillars

The microscopic theory of superconductivity rests on two ideas.

- **Cooper (1956):** the normal Fermi sea is *unstable* against the formation of bound electron pairs for an arbitrarily weak attraction.
- **BCS (1957):** this single-pair instability becomes a self-consistent many-body ground state in which *all* electrons near the Fermi surface form a coherent condensate of pairs.

We develop both in second quantization, then compute the spatial size of a Cooper pair from the BCS wave function.

The Cooper Problem: Setup

Take a filled, inert Fermi sea $|\mathrm{FS}\rangle$ and add *two* extra electrons just above ϵ_F.

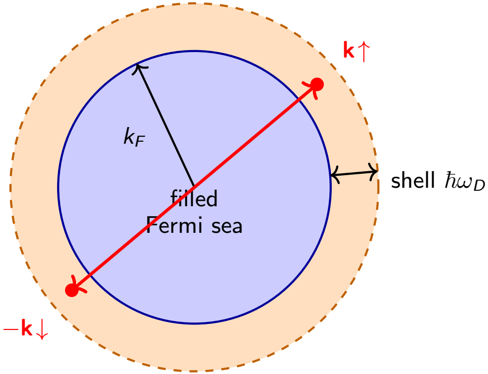
- Pauli principle forbids $|\mathbf{k}| < k_F$: the two electrons live in states $\epsilon_{\mathbf{k}} > \epsilon_F$.
- The sea is a rigid background; its only role is to block occupied states.

Trial state (zero total momentum, spin singlet):

$$|\psi\rangle = \sum_{\mathbf{k}} g_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow}\, c^{\dagger}_{-\mathbf{k}\downarrow}\, |\mathrm{FS}\rangle\,, \qquad g_{\mathbf{k}} = 0 \text{ for } |\mathbf{k}| < k_F.$$

$g_{\mathbf{k}} =$ amplitude for the pair in $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$.

The Cooper Problem: Momentum-Space Picture



Two electrons (red) added above a rigid Fermi sea (blue), scattering only within a shell of width $\hbar\omega_D$ (orange), with zero total momentum and opposite spins.

The Two-Body Schrödinger Equation

Hamiltonian for the two added electrons:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}.$$

Acting on $|\psi\rangle$ and projecting, $H\,|\psi\rangle = E\,|\psi\rangle$ reduces to

$$2\epsilon_{\mathbf{k}}\, g_{\mathbf{k}} + \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, g_{\mathbf{k}'} = E\, g_{\mathbf{k}}.$$

Model interaction (constant attraction in a Debye shell):

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V & \epsilon_F < \epsilon_{\mathbf{k}},\, \epsilon_{\mathbf{k}'} < \epsilon_F + \hbar\omega_D, \\ 0 & \text{otherwise}, \end{cases} \qquad V > 0.$$

Solution: Self-Consistency Condition

Define $C = \sum_{\mathbf{k}'} g_{\mathbf{k}'}$. The eigenvalue equation gives

$$g_{\mathbf{k}} = \frac{V\,C}{2\epsilon_{\mathbf{k}} - E}.$$

Summing over $\mathbf{k}$ and cancelling C:

$$1 = V \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}} - E}.$$

Convert to an integral with density of states per spin $N(0)$:

$$1 = N(0)V \int_{\epsilon_F}^{\epsilon_F + \hbar\omega_D} \frac{d\epsilon}{2\epsilon - E} = \frac{N(0)V}{2} \ln\left(\frac{2\epsilon_F - E + 2\hbar\omega_D}{2\epsilon_F - E}\right).$$

The Bound-State Energy

Let $\Delta_C = 2\epsilon_F - E > 0$ be the binding energy. In the weak-coupling limit $N(0)V \ll 1$ (so $\Delta_C \ll \hbar\omega_D$):

Cooper's result

$$E = 2\epsilon_F - 2\hbar\omega_D \, e^{-2/N(0)V}, \qquad \Delta_C = 2\hbar\omega_D \, e^{-2/N(0)V} > 0.$$

Physical significance:

- Nonzero binding for *any* $V > 0$, however weak.
- Non-analytic in V: the essential singularity $e^{-2/N(0)V}$ is invisible to perturbation theory.
- The normal Fermi sea is unstable $\Rightarrow$ electrons near ϵ_F spontaneously pair.

The Reduced BCS Hamiltonian

Now let all electrons pair on equal footing. Fermion algebra:

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

Keeping only opposite-momentum, opposite-spin scattering:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, c^{\dagger}_{\mathbf{k}'\uparrow} c^{\dagger}_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}.$$

Interpreting the BCS Hamiltonian

Kinetic term: $c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma}$ counts occupation. Measure energies from $\mu = \epsilon_F$:

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu, \qquad \text{work with } H - \mu N.$$

So $\xi_{\mathbf{k}} < 0$ below and $\xi_{\mathbf{k}} > 0$ above the Fermi surface.

Interaction term: scatters a Cooper pair $(-\mathbf{k}\downarrow, \mathbf{k}\uparrow) \to (\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$. Model:

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V & |\xi_{\mathbf{k}}|, |\xi_{\mathbf{k}'}| < \hbar\omega_D, \\ 0 & \text{otherwise,} \end{cases} \qquad V > 0.$$

The BCS Trial Wave Function

Pair number is not sharp. Each pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty (amplitude $u_{\mathbf{k}}$) or occupied (amplitude $v_{\mathbf{k}}$):

$$|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \right) |0\rangle \,, \qquad |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1.$$

For the ground state, take $u_{\mathbf{k}}, v_{\mathbf{k}}$ real.

Relation to the Cooper Amplitude

Factor out $u_{\mathbf{k}}$:

$$|\Psi_{\mathrm{BCS}}\rangle = \Big(\prod_{\mathbf{k}} u_{\mathbf{k}}\Big) \prod_{\mathbf{k}} \big(1 + g_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}\big)\, |0\rangle\,, \quad g_{\mathbf{k}} \equiv \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}.$$

$g_{\mathbf{k}}$ is the pair amplitude, the direct analogue of Cooper's $g_{\mathbf{k}}$. Projecting onto exactly $N/2$ pairs recovers the many-pair Cooper state:

$$|\Psi_N\rangle \propto \Big(\sum_{\mathbf{k}} g_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}\Big)^{N/2} |0\rangle\,.$$

Energy Functional and Minimization

With $\langle n_{\mathbf{k}\sigma} \rangle = v_{\mathbf{k}}^2$ and $\langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \rangle = u_{\mathbf{k}} v_{\mathbf{k}}$:

$$W = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}}\, v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, u_{\mathbf{k}} v_{\mathbf{k}}\, u_{\mathbf{k}'} v_{\mathbf{k}'}.$$

Parametrize $u_{\mathbf{k}} = \cos\theta_{\mathbf{k}},\ v_{\mathbf{k}} = \sin\theta_{\mathbf{k}}$:

$$W = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}} \sin^2\theta_{\mathbf{k}} + \frac{1}{4} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k}'}.$$

Set $\partial W / \partial \theta_{\mathbf{k}} = 0$:

$$2\xi_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} + \cos 2\theta_{\mathbf{k}} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sin 2\theta_{\mathbf{k}'} = 0.$$

Gap Parameter and Coherence Factors

Define the gap and quasiparticle energy:

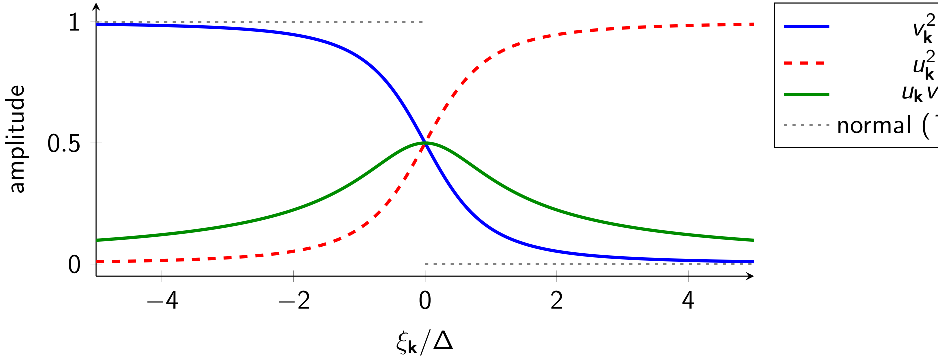
$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, u_{\mathbf{k}'} v_{\mathbf{k}'} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sin 2\theta_{\mathbf{k}'}, \qquad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}.$$

Minimization gives $\tan 2\theta_{\mathbf{k}} = \Delta_{\mathbf{k}}/\xi_{\mathbf{k}}$, hence $\sin 2\theta_{\mathbf{k}} = \Delta_{\mathbf{k}}/E_{\mathbf{k}}$, $\cos 2\theta_{\mathbf{k}} = \xi_{\mathbf{k}}/E_{\mathbf{k}}$:

Coherence factors

$$v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}.$$

Coherence Factors: Plot



$v_{\mathbf{k}}^2$ replaces the sharp normal step by a crossover of width $\sim \Delta$; the pair amplitude $u_{\mathbf{k}} v_{\mathbf{k}} = \Delta/2E_{\mathbf{k}}$ peaks at $\xi_{\mathbf{k}} = 0$.

The Pair Amplitude $g_{\mathbf{k}}$

Using $g_{\mathbf{k}} = v_{\mathbf{k}}/u_{\mathbf{k}} = 2u_{\mathbf{k}}v_{\mathbf{k}}/(2u_{\mathbf{k}}^2)$:

$$g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}/E_{\mathbf{k}}}{1+\xi_{\mathbf{k}}/E_{\mathbf{k}}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}+\xi_{\mathbf{k}}}.$$

$$g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{\xi_{\mathbf{k}}+\sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}}.$$

Peaked at the Fermi surface but regularized by the gap: at $\xi_{\mathbf{k}} = 0$, $g_{\mathbf{k}} = 1$ (pair state exactly half occupied).

The Self-Consistent Gap Equation

Substitute $u_{\mathbf{k}'} v_{\mathbf{k}'} = \Delta_{\mathbf{k}'}/2E_{\mathbf{k}'}$ into $\Delta_{\mathbf{k}}$:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}.$$

For the model interaction $\Delta_{\mathbf{k}} = \Delta$ (constant in the shell):

$$1 = V \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} = N(0)V \int_0^{\hbar\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} = N(0)V \sinh^{-1}\left(\frac{\hbar\omega_D}{\Delta}\right).$$

The Gap in the Weak-Coupling Limit

Therefore

$$\Delta = \frac{\hbar\omega_D}{\sinh\big(1/N(0)V\big)} \xrightarrow{N(0)V \ll 1}$$

BCS gap

$$\Delta \approx 2\hbar\omega_D \, e^{-1/N(0)V}.$$

Note the exponent $1/N(0)V$ vs. $2/N(0)V$ in Cooper's single-pair result: the self-consistent participation of all electrons *strengthens* the effect.

Condensation Energy

Using $\Delta = V \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}$, the interaction energy is $-\Delta^2/V$, and

$$W_s = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right) - \frac{\Delta^2}{V}.$$

Subtract the normal energy $W_n = \sum_{\xi_{\mathbf{k}}<0} 2\xi_{\mathbf{k}}$:

$$W_s - W_n = -\tfrac{1}{2}\, N(0)\, \Delta^2 < 0.$$

The paired state lies *below* the normal sea. The density $\frac{1}{2} N(0)\Delta^2 = H_c^2/8\pi$ (critical-field energy).

The Pair Wave Function

Field operators $\psi_\sigma(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}\sigma}$. The pair (anomalous) correlation function is

$$\Phi(\mathbf{r}_1 - \mathbf{r}_2) = \langle \Psi_{\mathrm{BCS}} | \, \psi_\uparrow(\mathbf{r}_1)\psi_\downarrow(\mathbf{r}_2) \, | \Psi_{\mathrm{BCS}} \rangle \, .$$

Only nonzero anomalous average: $\langle \Psi_{\mathrm{BCS}} | \, c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \, | \Psi_{\mathrm{BCS}} \rangle = u_{\mathbf{k}} v_{\mathbf{k}}$, so with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$:

$$\Phi(\mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \, e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}} \, e^{i\mathbf{k}\cdot\mathbf{r}}.$$

The amplitude $\Delta/2E_{\mathbf{k}}$ is sharply peaked at the Fermi surface (width $\sim \Delta$) $\Rightarrow$ large spatial extent.

Mean-Square Radius

Define the pair size by

$$\xi_0^2 \equiv \langle r^2 \rangle = \frac{\int d^3r \; r^2 \, |\Phi(\mathbf{r})|^2}{\int d^3r \; |\Phi(\mathbf{r})|^2}.$$

Using $\int d^3r \, r^2 e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = -(2\pi)^3 \nabla_{\mathbf{k}}^2 \delta(\mathbf{k}-\mathbf{k}')$ and Parseval, with $f_{\mathbf{k}} \equiv u_{\mathbf{k}} v_{\mathbf{k}} = \Delta/2E_{\mathbf{k}}$:

$$\langle r^2 \rangle = \frac{\sum_{\mathbf{k}} |\nabla_{\mathbf{k}} f_{\mathbf{k}}|^2}{\sum_{\mathbf{k}} |f_{\mathbf{k}}|^2}.$$

Evaluation

Since $f_{\mathbf{k}}$ depends on $\mathbf{k}$ only through $\xi_{\mathbf{k}}$:

$$\nabla_{\mathbf{k}} f_{\mathbf{k}} = \frac{df_{\mathbf{k}}}{d\xi_{\mathbf{k}}}\,\hbar \mathbf{v}_{\mathbf{k}}, \quad |\mathbf{v}_{\mathbf{k}}| \approx v_F, \quad \frac{df_{\mathbf{k}}}{d\xi} = -\frac{\Delta\,\xi}{2E_{\mathbf{k}}^3}.$$

Convert to ξ-integrals ($N(0)$ cancels), extend to $\pm\infty$:

$$\int_{-\infty}^{\infty} \left|\tfrac{df}{d\xi}\right|^2 d\xi = \frac{\Delta^2}{4}\int \frac{\xi^2\,d\xi}{(\xi^2+\Delta^2)^3} = \frac{\Delta^2}{4}\cdot\frac{\pi}{8\Delta^3} = \frac{\pi}{32\Delta},$$

$$\int_{-\infty}^{\infty} |f|^2 d\xi = \frac{\Delta^2}{4}\int \frac{d\xi}{\xi^2+\Delta^2} = \frac{\Delta^2}{4}\cdot\frac{\pi}{\Delta} = \frac{\pi\Delta}{4}.$$

The Coherence Length

Therefore

$$\langle r^2 \rangle = \hbar^2 v_F^2 \, \frac{\pi/(32\Delta)}{\pi\Delta/4} = \frac{\hbar^2 v_F^2}{8\,\Delta^2},$$

Cooper pair size

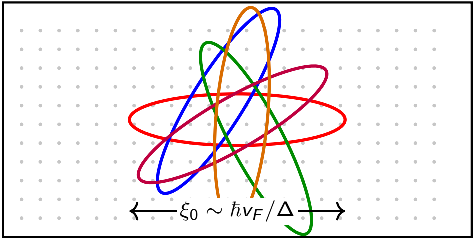
$$\xi_0 = \sqrt{\langle r^2 \rangle} = \frac{\hbar v_F}{2\sqrt{2}\,\Delta} \;\sim\; \frac{\hbar v_F}{\Delta}.$$

(Convention-dependent prefactor; the Pippard/BCS length is often written $\xi_0 = \hbar v_F/\pi\Delta$.)

Pairs Overlap Massively

Since $\Delta \sim k_B T_c \ll \epsilon_F \sim \hbar v_F k_F$:

$$k_F \, \xi_0 \sim \frac{\epsilon_F}{\Delta} \gg 1, \qquad \xi_0 \sim 10^2\text{–}10^4 \text{ Å}.$$



$\sim (k_F \xi_0)^3 \sim 10^6$–$10^9$ pairs overlap in one pair volume $\Rightarrow$ coherent BCS mean field, unlike BEC of small molecules.

Summary

- **Cooper:** two electrons bind for any attraction, $\Delta_C = 2\hbar\omega_D e^{-2/N(0)V} \Rightarrow$ Fermi sea unstable.
- **BCS state:** $\prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}) |0\rangle$ with fluctuating pair number.
- **Variation:** coherence factors $u_{\mathbf{k}}^2, v_{\mathbf{k}}^2$; pair amplitude $g_{\mathbf{k}} = \Delta/(\xi_{\mathbf{k}} + E_{\mathbf{k}})$.
- **Gap:** $\Delta \approx 2\hbar\omega_D e^{-1/N(0)V}$; condensation energy $-\frac{1}{2}N(0)\Delta^2$.
- **Pair size:** $\xi_0 \sim \hbar v_F/\Delta$ with $k_F\xi_0 \gg 1 \Rightarrow$ massive overlap, coherence of the condensate.