From the Cooper Pair Problem to the BCS Ground State

Contents

1 Introduction

The microscopic theory of superconductivity rests on two conceptual pillars. The first is L. Cooper's observation (1956) that the normal Fermi sea is *unstable* against the formation of bound electron pairs in the presence of an arbitrarily weak attractive interaction. The second is the Bardeen–Cooper–Schrieffer (BCS) construction (1957), which promotes this single-pair instability into a self-consistent many-body ground state in which *all* electrons near the Fermi surface participate in a coherent condensate of pairs.

This document develops both, beginning with the Cooper problem and then generalizing to the full BCS variational treatment, working throughout in the language of second quantization.

2 The Cooper Pair Problem

2.1 Setup

Consider a filled, inert Fermi sea $|\mathrm{FS}\rangle$ of N electrons, and add *two extra* electrons just above the Fermi surface. The Pauli principle forbids these two electrons from occupying any state with $|\mathbf{k}| < k_F$, so they are confined to states with $\epsilon_{\mathbf{k}} > \epsilon_F$. The two added electrons interact through a weak attractive potential, while the sea below is treated as a rigid, non-interacting background whose only role is to block the states it occupies.

For a pair with zero total momentum and a singlet (antisymmetric) spin state, we write the two-particle trial wave function in second-quantized form as

$$|\psi\rangle = \sum_{\mathbf{k}} g_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow}\, c^{\dagger}_{-\mathbf{k}\downarrow}\, |\mathrm{FS}\rangle\,, \qquad g_{\mathbf{k}} = 0 \text{ for } |\mathbf{k}| < k_F, \tag{1}$$

where $g_{\mathbf{k}}$ is the amplitude to find the pair in the momentum configuration $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$. The restriction on $g_{\mathbf{k}}$ enforces the Pauli exclusion of the occupied sea.

2.2 The two-body Schrödinger equation

The relevant Hamiltonian for the two added electrons is

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, c^{\dagger}_{\mathbf{k}'\uparrow} c^{\dagger}_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}. \tag{2}$$

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

$$2\epsilon_{\mathbf{k}}\, g_{\mathbf{k}} + \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, g_{\mathbf{k}'} = E\, g_{\mathbf{k}}, \tag{3}$$

where $2\epsilon_{\mathbf{k}}$ is the kinetic energy of the pair and E is the total energy of the two-electron state.

2.3 The model interaction

Following Cooper, we adopt a constant attractive interaction restricted to a thin shell of width $\hbar\omega_D$ (the Debye energy) above the Fermi surface:

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V & \epsilon_F < \epsilon_{\mathbf{k}},\, \epsilon_{\mathbf{k}'} < \epsilon_F + \hbar\omega_D, \\ 0 & \text{otherwise}, \end{cases} \qquad V > 0. \tag{4}$$

2.4 Solution and the bound-state energy

With this interaction, define the constant

$$C = \sum_{\mathbf{k}'} g_{\mathbf{k}'}. \tag{5}$$

The eigenvalue equation gives

$$g_{\mathbf{k}} = \frac{V\,C}{2\epsilon_{\mathbf{k}} - E}. \tag{6}$$

Summing both sides over $\mathbf{k}$ and cancelling C yields the self-consistency condition

$$1 = V \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}} - E}. \tag{7}$$

Converting the sum to an integral over the density of states per spin $N(0)$, evaluated near the Fermi surface where it is approximately constant, we obtain

$$1 = N(0)\, V \int_{\epsilon_F}^{\epsilon_F + \hbar\omega_D} \frac{d\epsilon}{2\epsilon - E} = \frac{N(0)V}{2} \ln\!\left(\frac{2\epsilon_F - E + 2\hbar\omega_D}{2\epsilon_F - E} \right). \tag{8}$$

Writing the binding energy relative to the two-electron continuum threshold as $\Delta_C = 2\epsilon_F - E > 0$, and taking the weak-coupling limit $N(0)V \ll 1$ (so that $\Delta_C \ll \hbar\omega_D$), this becomes

$$\boxed{E = 2\epsilon_F - 2\hbar\omega_D\, e^{-2/N(0)V}} \tag{9}$$

i.e. the two-electron state has energy *below* $2\epsilon_F$ by an amount

$$\Delta_C = 2\hbar\omega_D\, e^{-2/N(0)V} > 0. \tag{10}$$

2.5 Physical significance

The binding energy Δ_C is nonzero for *any* attraction $V > 0$, however weak. The result is non-analytic in V: the essential singularity $e^{-2/N(0)V}$ cannot be reached by any finite order of perturbation theory. This demonstrates that the normal Fermi sea is unstable: the electrons near ϵ_F will spontaneously bind into pairs. What Cooper's calculation does *not* address is the fate of the sea itself when *all* electrons are allowed to pair simultaneously—this is the problem solved by BCS.

3 The BCS Hamiltonian

We now let all electrons near the Fermi surface pair on an equal footing. The electron operators obey the fermionic anticommutation relations

$$\{c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'}\} = \delta_{\mathbf{k}\mathbf{k}'}\, \delta_{\sigma\sigma'}, \qquad \{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} = 0. \tag{11}$$

Keeping only the scattering of opposite-momentum, opposite-spin pairs—the channel identified by Cooper as responsible for pairing—gives the *reduced BCS Hamiltonian*

$$\boxed{H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}} \tag{12}$$

Kinetic term. The operator $c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma}$ counts the occupation of the single-particle state $(\mathbf{k}, \sigma)$. It is convenient to measure energies relative to the chemical potential $\mu = \epsilon_F$ by defining

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu, \tag{13}$$

and to work with the grand-canonical operator $H - \mu N$. Then $\xi_{\mathbf{k}} < 0$ below the Fermi surface and $\xi_{\mathbf{k}} > 0$ above it.

Interaction term. The term $c^\dagger_{\mathbf{k}'\uparrow}c^\dagger_{-\mathbf{k}'\downarrow}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$ destroys a pair in the state $(-\mathbf{k}\downarrow, \mathbf{k}\uparrow)$ and creates one in $(\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$: it scatters a Cooper pair from momentum $\mathbf{k}$ to $\mathbf{k}'$. We again use the model interaction

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V & |\xi_{\mathbf{k}}|, |\xi_{\mathbf{k}'}| < \hbar\omega_D, \\ 0 & \text{otherwise,} \end{cases} \qquad V > 0. \tag{14}$$

4 The BCS Trial Wave Function

Because pairs are continually created and destroyed by the interaction, the number of pairs is not sharp. BCS therefore introduced a variational state that does not have a definite particle number, describing each pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ as being empty with amplitude $u_{\mathbf{k}}$ or occupied with amplitude $v_{\mathbf{k}}$:

$$\boxed{|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle} \tag{15}$$

where $|0\rangle$ is the vacuum. Normalization of each factor requires

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1, \tag{16}$$

and for the ground state we may take $u_{\mathbf{k}}, v_{\mathbf{k}}$ real.

Relation to the Cooper amplitude. Factoring out $u_{\mathbf{k}}$ (assumed nonzero),

$$|\Psi_{\mathrm{BCS}}\rangle = \left(\prod_{\mathbf{k}} u_{\mathbf{k}}\right)\prod_{\mathbf{k}}\left(1 + g_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle, \qquad g_{\mathbf{k}} \equiv \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}, \tag{17}$$

where $g_{\mathbf{k}}$ is the amplitude for a pair in $(\mathbf{k}, -\mathbf{k})$ relative to its absence—the direct analogue of Cooper's $g_{\mathbf{k}}$. Projecting onto the sector with exactly $N/2$ pairs recovers the many-pair generalization of the Cooper state,

$$|\Psi_N\rangle \propto \left(\sum_{\mathbf{k}} g_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)^{N/2}|0\rangle. \tag{18}$$

5 Variational Solution

5.1 Expectation value of the energy

Using $\langle n_{\mathbf{k}\sigma}\rangle = v_{\mathbf{k}}^2$ and $\langle c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\rangle = u_{\mathbf{k}}v_{\mathbf{k}}$, the energy functional $W = \langle\Psi_{\mathrm{BCS}}|(H-\mu N)|\Psi_{\mathrm{BCS}}\rangle$ becomes

$$W = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}}\, v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, u_{\mathbf{k}}v_{\mathbf{k}}\, u_{\mathbf{k}'}v_{\mathbf{k}'}. \tag{19}$$

5.2 Minimization

Parametrize the constraint by $u_{\mathbf{k}} = \cos\theta_{\mathbf{k}}$, $v_{\mathbf{k}} = \sin\theta_{\mathbf{k}}$, so that $v_{\mathbf{k}}^2 = \sin^2\theta_{\mathbf{k}}$ and $u_{\mathbf{k}}v_{\mathbf{k}} = \frac{1}{2}\sin 2\theta_{\mathbf{k}}$. Then

$$W = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}}\sin^2\theta_{\mathbf{k}} + \frac{1}{4}\sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\sin 2\theta_{\mathbf{k}}\sin 2\theta_{\mathbf{k}'}. \tag{20}$$

Setting $\partial W/\partial\theta_{\mathbf{k}} = 0$,

$$2\xi_{\mathbf{k}}\sin 2\theta_{\mathbf{k}} + \cos 2\theta_{\mathbf{k}}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\sin 2\theta_{\mathbf{k}'} = 0. \tag{21}$$

5.3 The gap parameter and coherence factors

Define the superconducting gap

$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\, u_{\mathbf{k}'} v_{\mathbf{k}'} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sin 2\theta_{\mathbf{k}'}. \tag{22}$$

The minimization condition then reads

$$\tan 2\theta_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{\xi_{\mathbf{k}}}. \tag{23}$$

Introducing the quasiparticle energy

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}, \tag{24}$$

we find $\sin 2\theta_{\mathbf{k}} = \Delta_{\mathbf{k}}/E_{\mathbf{k}}$ and $\cos 2\theta_{\mathbf{k}} = \xi_{\mathbf{k}}/E_{\mathbf{k}}$, hence the coherence factors

$$\boxed{v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \qquad u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \qquad u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}.} \tag{25}$$

The occupation $v_{\mathbf{k}}^2$ interpolates smoothly from 1 (occupied) far below ϵ_F to 0 (empty) far above, with the crossover smeared over an energy $\sim \Delta$ about the Fermi surface—the hallmark of pairing.

5.4 The pair amplitude $g_{\mathbf{k}}$

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

$$g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}/E_{\mathbf{k}}}{1 + \xi_{\mathbf{k}}/E_{\mathbf{k}}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}} + \xi_{\mathbf{k}}}, \tag{26}$$

that is,

$$\boxed{g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{\xi_{\mathbf{k}} + \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}}} \tag{27}$$

As in the Cooper problem, $g_{\mathbf{k}}$ is peaked at the Fermi surface, but here it is regularized by the gap: at $\xi_{\mathbf{k}} = 0$ one has $g_{\mathbf{k}} = 1$, so the pair state is exactly half occupied.

6 The Gap Equation and Condensation Energy

6.1 Self-consistent gap equation

Substituting $u_{\mathbf{k}'}v_{\mathbf{k}'} = \Delta_{\mathbf{k}'}/2E_{\mathbf{k}'}$ back into the definition of $\Delta_{\mathbf{k}}$ gives the BCS gap equation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}. \tag{28}$$

For the model interaction, $\Delta_{\mathbf{k}} = \Delta$ is constant within the shell, and cancelling Δ yields

$$1 = V\sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} = N(0)V \int_0^{\hbar\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} = N(0)V\, \sinh^{-1}\!\left(\frac{\hbar\omega_D}{\Delta}\right). \tag{29}$$

Hence

$$\Delta = \frac{\hbar\omega_D}{\sinh\bigl(1/N(0)V\bigr)}, \tag{30}$$

and in the weak-coupling limit $N(0)V \ll 1$,

$$\boxed{\Delta \approx 2\hbar\omega_D\, e^{-1/N(0)V}} \tag{31}$$

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

6.2 Condensation energy

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

$$W_s = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right) - \frac{\Delta^2}{V}. \tag{32}$$

Subtracting the normal-state energy $W_n = \sum_{\xi_{\mathbf{k}}<0} 2\xi_{\mathbf{k}}$ and converting to an integral, one finds the compact result

$$\boxed{W_s - W_n = -\tfrac{1}{2}\, N(0)\, \Delta^2} \tag{33}$$

The negative sign confirms that the paired state lies below the normal Fermi sea: the normal metal is unstable and condenses into the superconducting ground state. The condensation energy density $\frac{1}{2}N(0)\Delta^2$ equals $H_c^2/8\pi$, the energy density of the critical field that destroys superconductivity.

7 Summary

Cooper's calculation shows that two electrons above a filled sea bind for any attraction, with binding energy $\Delta_C = 2\hbar\omega_D e^{-2/N(0)V}$, signalling the instability of the normal state. BCS turns this instability into a genuine ground state: the coherent trial function $\prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow})\,|0\rangle$ allows a fluctuating pair number, and variational minimization yields the coherence factors $u_{\mathbf{k}}^2, v_{\mathbf{k}}^2$, the pair amplitude $g_{\mathbf{k}} = \Delta/(\xi_{\mathbf{k}} + E_{\mathbf{k}})$, the self-consistent gap $\Delta \approx 2\hbar\omega_D e^{-1/N(0)V}$, and a condensation energy $-\frac{1}{2}N(0)\Delta^2$ proving that the superconducting state is the true ground state.