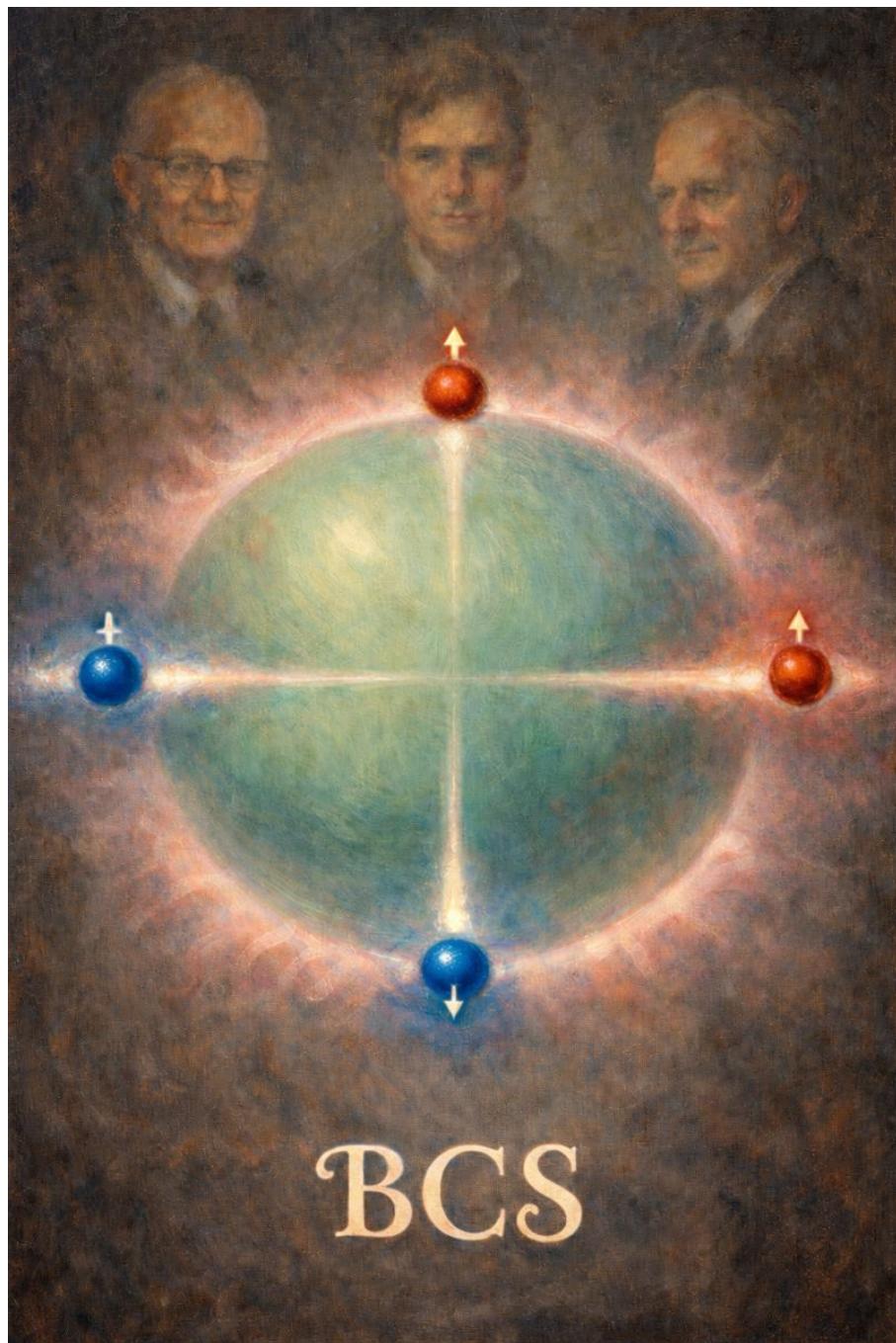


Fermion Pairing and BCS Mean Field

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December 30, 2025



BCS

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1 Interacting Two-Component Fermi Gas and Pairing Instability

1.1 Basic setting: contact interaction and Fermi scales

We consider spin-1/2 fermions with two spin components $\sigma = \uparrow, \downarrow$, and focus on the balanced case

$$n_\uparrow = n_\downarrow \equiv n, \quad n = \frac{k_F^3}{6\pi^2},$$

which defines the Fermi momentum k_F of the noninteracting gas.

Renormalizable contact interaction (contact term).

We model short-range interactions by a zero-range (contact) potential. In momentum space the Hamiltonian can be written as

$$\hat{H} = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \frac{g}{V} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \hat{c}_{\mathbf{k}+\frac{\mathbf{q}}{2}\uparrow}^\dagger \hat{c}_{-\mathbf{k}+\frac{\mathbf{q}}{2}\uparrow}^\dagger \hat{c}_{-\mathbf{k}'+\frac{\mathbf{q}}{2}\downarrow} \hat{c}_{\mathbf{k}'+\frac{\mathbf{q}}{2}\uparrow}, \quad (1)$$

where $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / (2m)$ and V is the volume. Sometimes we denote $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ for short.

We will use the Fermi energy $E_F = \hbar^2 k_F^2 / (2m)$ as the energy unit.

It's beneficial to recall the renormalization of g . In three dimensions, the bare coupling g depends on the ultraviolet (UV) regularization. One trades g for the physical s -wave scattering length a_s via

$$\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{g} + \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}}, \quad (2)$$

so that all low-energy observables are expressed in terms of a_s instead of the cutoff-dependent g .

Why s -wave is the default

At sufficiently low energy, higher partial waves are suppressed by powers of momentum; the contact interaction captures the leading low-energy s -wave channel and is renormalizable in 3D through Eq. (2).

1.2 Two-body problem in vacuum: bound state and renormalization

Two-body ansatz at zero center-of-mass momentum. Consider two fermions with opposite spins in vacuum ($|0\rangle$), and focus on the total-momentum-zero sector. A general state in this sector is

$$|\Psi\rangle = \sum_{\mathbf{k}} \psi_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle, \quad (3)$$

where $\psi_{\mathbf{k}}$ is a (complex) c-number coefficient specifying the wavefunction in momentum space.

Effective Schrödinger equation and self-consistency. In vacuum one may set $\mu = 0$. Solving $\hat{H}|\Psi\rangle = E|\Psi\rangle$ with the contact Hamiltonian (1) yields

$$2\epsilon_{\mathbf{k}}\psi_{\mathbf{k}} + \frac{g}{V} \sum_{\mathbf{k}'} \psi_{\mathbf{k}'} = E \psi_{\mathbf{k}} \quad (4)$$

and hence the self-consistency condition¹

$$\frac{1}{g} = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{E - 2\epsilon_{\mathbf{k}}}. \quad (5)$$

¹To get (5), one can sum over k on both sides of (4).

Because the contact interaction is UV divergent, we eliminate g in favor of the scattering length a_s using Eq. (2), which gives the UV-finite equation

$$\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \sum_{\mathbf{k}} \left(\frac{1}{E - 2\epsilon_{\mathbf{k}}} + \frac{1}{2\epsilon_{\mathbf{k}}} \right). \quad (6)$$

Vacuum bound state and the role of a_s .

A bound state corresponds to $E < 0$. Equation (6) implies:

■ If $a_s > 0$: there exists a two-body bound state with energy

$$E_b = -\frac{\hbar^2}{ma_s^2}. \quad (7)$$

■ If $a_s < 0$: Eq. (6) admits no $E < 0$ solution, i.e., there is no vacuum two-body bound state.

Deriving Eq. (4) by explicit action of \hat{H} on $|\Psi\rangle$

Step 1: split $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$. In vacuum we set $\mu = 0$. The kinetic part is

$$\hat{H}_0 = \sum_{\mathbf{p}, \sigma} \epsilon_{\mathbf{p}} \hat{c}_{\mathbf{p}\sigma}^\dagger \hat{c}_{\mathbf{p}\sigma},$$

and the interaction part is

$$\hat{H}_{\text{int}} = \frac{g}{V} \sum_{\mathbf{pp}'\mathbf{q}} \hat{c}_{\mathbf{p}+\frac{\mathbf{q}}{2}\uparrow}^\dagger \hat{c}_{-\mathbf{p}+\frac{\mathbf{q}}{2}\downarrow}^\dagger \hat{c}_{-\mathbf{p}'+\frac{\mathbf{q}}{2}\downarrow} \hat{c}_{\mathbf{p}'+\frac{\mathbf{q}}{2}\uparrow}.$$

Step 2: action of \hat{H}_0 . Using $\hat{c}_{\mathbf{p}\sigma}|0\rangle = 0$ and the canonical anticommutation relations,

$$\hat{H}_0 \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle = (\epsilon_{\mathbf{k}} + \epsilon_{-\mathbf{k}}) \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle = 2\epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle.$$

Step 3: action of \hat{H}_{int} and why only $\mathbf{q} = 0$ survives. Consider one basis state $|\mathbf{k}\rangle \equiv \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle$. When \hat{H}_{int} acts on $|\mathbf{k}\rangle$, the annihilation operators must remove exactly the two particles present. This forces

$$\mathbf{p}' + \frac{\mathbf{q}}{2} = \mathbf{k}, \quad -\mathbf{p}' + \frac{\mathbf{q}}{2} = -\mathbf{k},$$

which together imply $\mathbf{q} = 0$ and $\mathbf{p}' = \mathbf{k}$. Concretely, using

$$\hat{c}_{\mathbf{p}\uparrow} \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle = \delta_{\mathbf{p},\mathbf{k}} |0\rangle, \quad \hat{c}_{\mathbf{p}\downarrow} \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle = \delta_{\mathbf{p},-\mathbf{k}} |0\rangle,$$

one finds

$$\begin{aligned} \hat{H}_{\text{int}} |\mathbf{k}\rangle &= \frac{g}{V} \sum_{\mathbf{pp}'\mathbf{q}} \hat{c}_{\mathbf{p}+\frac{\mathbf{q}}{2}\uparrow}^\dagger \hat{c}_{-\mathbf{p}+\frac{\mathbf{q}}{2}\downarrow}^\dagger \hat{c}_{-\mathbf{p}'+\frac{\mathbf{q}}{2}\downarrow} \hat{c}_{\mathbf{p}'+\frac{\mathbf{q}}{2}\uparrow} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle \\ &= \frac{g}{V} \sum_{\mathbf{p}} \hat{c}_{\mathbf{p}\uparrow}^\dagger \hat{c}_{-\mathbf{p}\downarrow}^\dagger |0\rangle, \end{aligned}$$

where the $\mathbf{q} \neq 0$ terms vanish because they cannot annihilate both particles consistently.

Step 4: assemble $\hat{H}|\Psi\rangle$ and project onto the basis. Putting Steps 2–3 together,

$$\hat{H} |\Psi\rangle = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} \psi_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle + \frac{g}{V} \left(\sum_{\mathbf{k}'} \psi_{\mathbf{k}'} \right) \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle.$$

Now project onto the coefficient of each basis vector $\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle$. Equating $\hat{H}|\Psi\rangle = E|\Psi\rangle$ gives

$$2\epsilon_{\mathbf{k}}\psi_{\mathbf{k}} + \frac{g}{V} \sum_{\mathbf{k}'} \psi_{\mathbf{k}'} = E\psi_{\mathbf{k}},$$

which is Eq. (4).

1.3 Two-body problem on top of a Fermi sea: Cooper problem

Now consider two additional fermions placed on top of a filled Fermi sea $|\text{FS}\rangle$. The Fermi sea is

$$|\text{FS}\rangle = \prod_{|\mathbf{k}| < k_F} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}^\dagger |0\rangle. \quad (8)$$

Pauli exclusion forbids using already occupied momentum states, so the two-body ansatz becomes

$$|\Psi\rangle = \sum_{|\mathbf{k}| > k_F} \psi_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |\text{FS}\rangle. \quad (9)$$

Here we ignore the back-reaction (distortion) of $|\text{FS}\rangle$ caused by adding the two particles, and take $\mu = E_F$ as the reference chemical potential.

Proceeding as in vacuum but restricting intermediate states to $|\mathbf{k}| > k_F$, one obtains the renormalized equation

$$\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \left[\sum_{|\mathbf{k}| > k_F} \frac{1}{E - 2(\epsilon_{\mathbf{k}} - \mu)} + \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}} \right]. \quad (10)$$

Comparison between Fermi Sea and Vacuum

Key difference from vacuum.

- Vacuum: the allowed virtual states extend down to $\mathbf{k} = 0$ and the equation admits a bound state only for $a_s > 0$.
- Cooper: Pauli blocking removes $|\mathbf{k}| < k_F$ and changes the infrared structure near the Fermi surface; this modification is responsible for the existence of a bound-state-like solution even when $a_s < 0$.

1.4 Two scattering-length regimes and pairing instability

Unified dimensionless form. Using E_F as energy unit and k_F^{-1} as length unit, both the vacuum equation (6) and the Cooper equation (10) can be cast into

$$\frac{1}{k_F a_s} = f\left(\frac{E}{E_F}\right), \quad (11)$$

where the function f differs between vacuum and Fermi-sea backgrounds.

Behavior of f in vacuum (qualitative facts used for conclusions)

For the vacuum two-body problem, the corresponding $f_{\text{vac}}(E/E_F)$ satisfies:

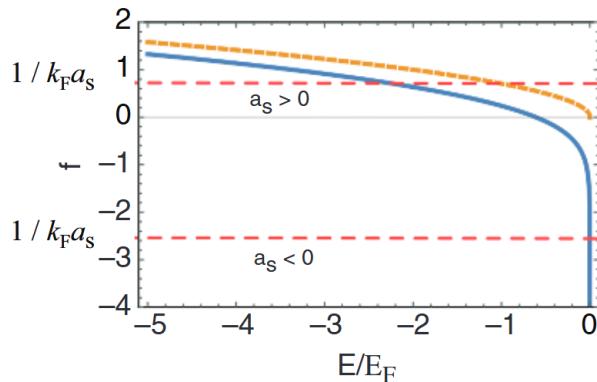
- For $E < 0$, $f_{\text{vac}}(E/E_F) > 0$ and $f_{\text{vac}}(E/E_F) \rightarrow 0$ as $E \rightarrow 0^-$.
- Therefore, for $a_s < 0$ (left-hand side negative), Eq. (11) has no $E < 0$ solution: no vacuum bound state.

- For $a_s > 0$, Eq. (11) has a bound state solution consistent with $E_b = -\hbar^2/(ma_s^2)$.

Behavior of f in the Cooper problem (qualitative facts used for conclusions)

For the Cooper problem above a Fermi sea, the corresponding $f_{FS}(E/E_F)$ obeys:

- $f_{FS}(E/E_F) \rightarrow -\infty$ as $E \rightarrow 0^-$ due to the singular phase space near the Fermi surface in the presence of Pauli blocking.
- Hence Eq. (11) always has an $E < 0$ solution for any a_s , including $a_s < 0$.



Physical conclusion in the two regimes.

■ **Regime $a_s < 0$: no vacuum bound state, but a Cooper bound state exists.** Two particles cannot form a bound state in vacuum, yet can form a bound state on top of a Fermi sea. This indicates that, for any attractive interaction, the free Fermi sea has a two-particle excitation with *negative* excitation energy, i.e., the free Fermi sea is unstable toward pairing. The many-body ground state must be reconstructed to incorporate pairing, leading to the Bardeen–Cooper–Schrieffer (BCS) state.

■ **Regime $a_s > 0$: molecules and BEC limit.** A two-body bound state exists already in vacuum. When a_s is small and positive, the bound state size $\sim a_s$ is much smaller than the interparticle spacing $\sim k_F^{-1}$, so the many-body environment matters little for the internal structure of the pair; the bound state behaves as a diatomic bosonic molecule, which can undergo Bose–Einstein condensation (BEC) at low temperature.

Pairing instability vs “bound state”. In a Fermi sea, the appearance of an $E < 0$ solution of the Cooper equation means a two-particle excitation lowers the energy of the free Fermi sea; this invalidates the free Fermi-liquid ansatz and signals an instability toward a paired many-body state.

2 BCS Mean-Field Theory

2.1 Self-consistent mean-field scheme and the role of fluctuations

General structure $g\hat{A}^\dagger\hat{A}$ and mean-field decomposition. Consider an interaction term $g\hat{A}^\dagger\hat{A}$. Write

$$\hat{A} = \langle \hat{A} \rangle + \delta\hat{A}, \quad \hat{A}^\dagger = \langle \hat{A}^\dagger \rangle + \delta\hat{A}^\dagger.$$

Then

$$g\hat{A}^\dagger \hat{A} = g\langle \hat{A}^\dagger \rangle \hat{A} + g\hat{A}^\dagger \langle \hat{A} \rangle - g|\langle \hat{A} \rangle|^2 + g\delta\hat{A}^\dagger \delta\hat{A}. \quad (12)$$

Mean-field approximation as neglecting a fluctuation term. The self-consistent mean-field approximation consists of dropping the fluctuation term

$$g\delta\hat{A}^\dagger \delta\hat{A} = g(\hat{A}^\dagger - \langle \hat{A}^\dagger \rangle)(\hat{A} - \langle \hat{A} \rangle),$$

and keeping only the first three terms in Eq. (12). One then determines $\langle \hat{A} \rangle$ self-consistently from the mean-field ground state (or by minimizing the mean-field energy).

What is gained and what is lost. The mean-field Hamiltonian is quadratic (quasi-free / Gaussian), enabling exact diagonalization and Wick factorization. The price is that interaction-driven higher-body correlations beyond the chosen order parameter are neglected through the dropped fluctuation term.

2.2 BCS mean-field Hamiltonian from the $q = 0$ sector

Keeping only $q = 0$ scatterings.² In the contact Hamiltonian (1), focus on the $q = 0$ sector:

$$\frac{g}{V} \sum_{\mathbf{k}\mathbf{k}'} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} = \frac{g}{V} \left(\sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \right) \left(\sum_{\mathbf{k}'} \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \right).$$

Introduce

$$\hat{A} = - \sum_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow}.$$

Applying the mean-field scheme yields the BCS mean-field Hamiltonian

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger - \Delta^* \sum_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} - \frac{V|\Delta|^2}{g}, \quad (13)$$

where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, and the order parameter is

$$\Delta = -\frac{g}{V} \sum_{\mathbf{k}} \langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle. \quad (14)$$

By a global $U(1)$ gauge choice one may take Δ to be real and positive. Under this convention:

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger - \Delta \sum_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} - \frac{V\Delta^2}{g}, \quad (15)$$

2.3 Bogoliubov diagonalization

Nambu spinor and 2×2 BdG form. Define the Nambu spinor $\hat{\Psi}_{\mathbf{k}} = (\hat{c}_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}^\dagger)^T$. Then Eq. (39) can be written (up to a constant) as

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k}} \hat{\Psi}_{\mathbf{k}}^\dagger \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\Delta & -\xi_{\mathbf{k}} \end{pmatrix} \hat{\Psi}_{\mathbf{k}} + \sum_{\mathbf{k}} \xi_{\mathbf{k}} - \frac{V\Delta^2}{g}.$$

The quasiparticle dispersion is

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}. \quad (16)$$

²The reason is left for latter chapters.

Explicit 2×2 diagonalization and fermionic Bogoliubov rotation

Eigenvalues and coherence factors.

The matrix

$$h_{\mathbf{k}} = \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\Delta & -\xi_{\mathbf{k}} \end{pmatrix}$$

has eigenvalues $\pm E_{\mathbf{k}}$ with $E_{\mathbf{k}}$ in Eq. (16). Choose real $u_{\mathbf{k}}, v_{\mathbf{k}} > 0$ satisfying $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ and

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right). \quad (17)$$

Then define quasiparticles

$$\hat{\alpha}_{\mathbf{k}} = u_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}^\dagger, \quad \hat{\beta}_{\mathbf{k}}^\dagger = v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow} + u_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}^\dagger. \quad (18)$$

Why this is “unitary” for fermions (contrast with bosons).

The map $(\hat{c}_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}^\dagger) \mapsto (\hat{\alpha}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}}^\dagger)$ is a unitary rotation in the two-dimensional Nambu space because it preserves the canonical anticommutation relations (CAR): $\{\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}_{\mathbf{k}}^\dagger\} = 1$, $\{\hat{\beta}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}}^\dagger\} = 1$, and mixed anticommutators vanish. For bosons, a similar mixing must preserve commutators and requires a *paraunitary* structure; this is the technical origin of the fermion–boson difference.

Diagonal form. In terms of $\hat{\alpha}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}}$,

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k}} E_{\mathbf{k}} (\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}) + \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) - \frac{V\Delta^2}{g}. \quad (19)$$

2.4 Physical consequences: ground state, gap equation, and excitations

(i) Quasiparticle vacuum and factorized BCS structure.

After Bogoliubov diagonalization, the mean-field Hamiltonian takes the form

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k}} E_{\mathbf{k}} (\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}) + E_0(\mu, \Delta), \quad (20)$$

with $E_0(\mu, \Delta) = \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) - \frac{V\Delta^2}{g}$.³

Therefore the ground state $|\Psi_{\text{BCS}}\rangle$ is the quasiparticle vacuum:

$$\hat{\alpha}_{\mathbf{k}} |\Psi_{\text{BCS}}\rangle = 0, \quad \hat{\beta}_{\mathbf{k}} |\Psi_{\text{BCS}}\rangle = 0, \quad \forall \mathbf{k}, \quad (21)$$

and can be written in the standard product form

$$|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle, \quad u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad (22)$$

where we take $u_{\mathbf{k}}, v_{\mathbf{k}} \geq 0$ and Δ real by a phase convention.

³Note that $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} > 0$ and $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, and thus E_0 is a function of μ and Δ . We will solve for these two parameters with intrinsic constraints later.

Quasiparticle vacuum and the BCS product state

Part I: verify that (22) satisfies $\hat{\alpha}_k|\Psi_{\text{BCS}}\rangle = \hat{\beta}_k|\Psi_{\text{BCS}}\rangle = 0$.

Fix a momentum pair $(\mathbf{k}, -\mathbf{k})$. For notational brevity write $u \equiv u_{\mathbf{k}}$, $v \equiv v_{\mathbf{k}}$, and define the \mathbf{k} -sector factor

$$|\phi_{\mathbf{k}}\rangle \equiv (u + v \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle_{\mathbf{k}}.$$

Take the standard fermionic Bogoliubov modes

$$\hat{\alpha}_{\mathbf{k}} = u \hat{c}_{\mathbf{k}\uparrow} - v \hat{c}_{-\mathbf{k}\downarrow}^\dagger, \quad \hat{\beta}_{\mathbf{k}} = u \hat{c}_{-\mathbf{k}\downarrow} + v \hat{c}_{\mathbf{k}\uparrow}^\dagger,$$

with $\{\hat{c}, \hat{c}^\dagger\} = 1$ within each mode and all different modes anticommute.

Check $\hat{\alpha}_k|\phi_k\rangle = 0$. Compute directly:

$$\begin{aligned} \hat{\alpha}_{\mathbf{k}}|\phi_{\mathbf{k}}\rangle &= (u \hat{c}_{\mathbf{k}\uparrow} - v \hat{c}_{-\mathbf{k}\downarrow}^\dagger)(u + v \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle_{\mathbf{k}} \\ &= uv \hat{c}_{\mathbf{k}\uparrow} \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} - uv \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} \quad (\text{the other two terms vanish}) \\ &= uv (1 - \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow}) \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} - uv \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} \\ &= uv \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} - uv \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} = 0, \end{aligned}$$

where we used $\hat{c}_{\mathbf{k}\uparrow}|0\rangle_{\mathbf{k}} = 0$.

Check $\hat{\beta}_k|\phi_k\rangle = 0$. Similarly,

$$\begin{aligned} \hat{\beta}_{\mathbf{k}}|\phi_{\mathbf{k}}\rangle &= (u \hat{c}_{-\mathbf{k}\downarrow} + v \hat{c}_{\mathbf{k}\uparrow}^\dagger)(u + v \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle_{\mathbf{k}} \\ &= uv \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} + uv \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle_{\mathbf{k}} \quad (\text{the other two terms vanish}) \\ &= -uv \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} + uv \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle_{\mathbf{k}} \\ &= -uv \hat{c}_{\mathbf{k}\uparrow}^\dagger (1 - \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}) |0\rangle_{\mathbf{k}} + uv \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle_{\mathbf{k}} \\ &= -uv \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle_{\mathbf{k}} + uv \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle_{\mathbf{k}} = 0. \end{aligned}$$

Therefore $\hat{\alpha}_k|\phi_k\rangle = \hat{\beta}_k|\phi_k\rangle = 0$. Since the full BCS state is the product over independent $(\mathbf{k}, -\mathbf{k})$ sectors, it follows that $\hat{\alpha}_k|\Psi_{\text{BCS}}\rangle = \hat{\beta}_k|\Psi_{\text{BCS}}\rangle = 0$ for all \mathbf{k} .

Part II: derive $|\phi_{\mathbf{k}}\rangle = (u + v \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle_{\mathbf{k}}$ from the quasiparticle constraints.

Impose the two-mode quasiparticle-vacuum constraints for a general $(\mathbf{k}, -\mathbf{k})$ sector state $|G_{\mathbf{k}}\rangle$:

$$(u \hat{c}_{\mathbf{k}\uparrow} - v \hat{c}_{-\mathbf{k}\downarrow}^\dagger)|G_{\mathbf{k}}\rangle = 0, \quad (u \hat{c}_{-\mathbf{k}\downarrow} + v \hat{c}_{\mathbf{k}\uparrow}^\dagger)|G_{\mathbf{k}}\rangle = 0, \quad (23)$$

with real u, v .

Step 1: expand in the fermionic occupation basis. Since each mode has occupation 0 or 1, the most general state is

$$|G_{\mathbf{k}}\rangle = A |0\rangle + B |\uparrow\rangle + C |\downarrow\rangle + D |\text{pair}\rangle,$$

where $|\uparrow\rangle = \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle$, $|\downarrow\rangle = \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle$, $|\text{pair}\rangle = \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle$.

Step 2: convert operator constraints into algebraic equations. Using the elementary actions

$$\hat{c}_{\mathbf{k}\uparrow}|\uparrow\rangle = |0\rangle, \quad \hat{c}_{\mathbf{k}\uparrow}|\text{pair}\rangle = |\downarrow\rangle, \quad \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle = |\downarrow\rangle, \quad \hat{c}_{-\mathbf{k}\downarrow}^\dagger |\uparrow\rangle = -|\text{pair}\rangle,$$

the first constraint in Eq. (23) gives

$$uB|0\rangle + (uD - vA)|\downarrow\rangle + vB|\text{pair}\rangle = 0 \implies B = 0, \quad uD = vA.$$

Similarly, using

$$\hat{c}_{-\mathbf{k}\downarrow}|\downarrow\rangle = |0\rangle, \quad \hat{c}_{-\mathbf{k}\downarrow}|\text{pair}\rangle = -|\uparrow\rangle, \quad \hat{c}_{\mathbf{k}\uparrow}^\dagger|0\rangle = |\uparrow\rangle, \quad \hat{c}_{\mathbf{k}\uparrow}^\dagger|\downarrow\rangle = |\text{pair}\rangle,$$

the second constraint gives

$$uC|0\rangle + (vA - uD)|\uparrow\rangle + vC|\text{pair}\rangle = 0 \implies C = 0, \quad vA = uD,$$

which is consistent with $uD = vA$.

Step 3: only empty and paired components survive. Thus $B = C = 0$ and $D = (v/u)A$. Up to normalization,

$$|G_{\mathbf{k}}\rangle = A\left(|0\rangle + \frac{v}{u}|\text{pair}\rangle\right) = A\left(1 + \frac{v}{u}\hat{c}_{\mathbf{k}\uparrow}^\dagger\hat{c}_{-\mathbf{k}\downarrow}^\dagger\right)|0\rangle.$$

Choosing $A = u$ (and imposing $u^2 + v^2 = 1$ for normalization) yields

$$|G_{\mathbf{k}}\rangle = (u + v\hat{c}_{\mathbf{k}\uparrow}^\dagger\hat{c}_{-\mathbf{k}\downarrow}^\dagger)|0\rangle,$$

and taking the product over independent $(\mathbf{k}, -\mathbf{k})$ sectors reproduces the standard BCS product form.

(ii) Momentum distribution and anomalous average.

The momentum distribution is

$$n_{\mathbf{k}\sigma} \equiv \langle \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} \rangle = v_{\mathbf{k}'}^2 \quad (24)$$

and the pairing (anomalous) expectation value is

$$\langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle = u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta}{2E_{\mathbf{k}}}. \quad (25)$$

Explicitly evaluating $n_{\mathbf{k}\sigma}$ and $\langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle$

Reduce to a single $(\mathbf{k}, -\mathbf{k})$ sector. Fix \mathbf{k} . Define the pair creation operator

$$\hat{b}_{\mathbf{k}}^\dagger \equiv \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger, \quad (\hat{b}_{\mathbf{k}}^\dagger)^2 = 0.$$

The $(\mathbf{k}, -\mathbf{k})$ sector has basis

$$|0\rangle_{\mathbf{k}}, \quad |\uparrow\rangle_{\mathbf{k}} \equiv \hat{c}_{\mathbf{k}\uparrow}^\dagger|0\rangle_{\mathbf{k}}, \quad |\downarrow\rangle_{\mathbf{k}} \equiv \hat{c}_{-\mathbf{k}\downarrow}^\dagger|0\rangle_{\mathbf{k}}, \quad |\text{pair}\rangle_{\mathbf{k}} \equiv \hat{b}_{\mathbf{k}}^\dagger|0\rangle_{\mathbf{k}}.$$

In $|\Psi_{\text{BCS}}\rangle$, the \mathbf{k} -sector state is

$$|\phi_{\mathbf{k}}\rangle = u_{\mathbf{k}}|0\rangle_{\mathbf{k}} + v_{\mathbf{k}}|\text{pair}\rangle_{\mathbf{k}}, \quad \langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}} \rangle = u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1.$$

Compute $n_{\mathbf{k}\uparrow}$.

Use $\hat{n}_{\mathbf{k}\uparrow} \equiv \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow}$. One has $\hat{n}_{\mathbf{k}\uparrow}|0\rangle_{\mathbf{k}} = 0$ and $\hat{n}_{\mathbf{k}\uparrow}|\text{pair}\rangle_{\mathbf{k}} = |\text{pair}\rangle_{\mathbf{k}}$, hence

$$n_{\mathbf{k}\uparrow} = \langle \phi_{\mathbf{k}} | \hat{n}_{\mathbf{k}\uparrow} | \phi_{\mathbf{k}} \rangle = |v_{\mathbf{k}}|^2.$$

Similarly $n_{-\mathbf{k}\downarrow} = v_{\mathbf{k}}^2$. This yields Eq. (24).

Compute the anomalous average.

Note that

$$\hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} |\text{pair}\rangle_{\mathbf{k}} = \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}} = |0\rangle_{\mathbf{k}}, \quad \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} |0\rangle_{\mathbf{k}} = 0,$$

so

$$\langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle = \langle \phi_{\mathbf{k}} | \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} | \phi_{\mathbf{k}} \rangle = u_{\mathbf{k}} v_{\mathbf{k}}.$$

Show $u_{\mathbf{k}} v_{\mathbf{k}} = \Delta / (2E_{\mathbf{k}})$.

From $u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 = \frac{1}{4} (1 - \xi_{\mathbf{k}}^2 / E_{\mathbf{k}}^2)$,

$$u_{\mathbf{k}} v_{\mathbf{k}} = \frac{1}{2} \sqrt{1 - \frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}} = \frac{1}{2} \frac{\sqrt{E_{\mathbf{k}}^2 - \xi_{\mathbf{k}}^2}}{E_{\mathbf{k}}} = \frac{1}{2} \frac{|\Delta|}{E_{\mathbf{k}}} = \frac{\Delta}{2E_{\mathbf{k}}},$$

where in the last step we used $\Delta > 0$ by convention.

(iii) Gap equation and what it determines. The mean-field order parameter is defined by

$$\Delta = -\frac{g}{V} \sum_{\mathbf{k}} \langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle. \quad (26)$$

Using Eq. (25) gives

$$\Delta = -\frac{g}{V} \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}}.$$

For a paired solution with $\Delta \neq 0$, divide both sides by Δ to obtain

$$-\frac{1}{g} = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}}. \quad (27)$$

For a contact interaction this sum is UV divergent; eliminate g in favor of the scattering length a_s (via the standard renormalization relation) to obtain the finite, physical gap equation

$$-\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \sum_{\mathbf{k}} \left(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}} \right). \quad (28)$$

Variational derivation: $\partial E_{\text{BCS}} / \partial \Delta = 0$ reproduces the gap equation

The gap equation can also be obtained by minimizing the BCS mean-field ground-state energy with respect to Δ . After Bogoliubov diagonalization one may write the mean-field energy (up to Δ -independent constants) as

$$E_{\text{BCS}}(\Delta) = \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) + \frac{V}{g} \Delta^2, \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}. \quad (29)$$

Taking the derivative and using $\frac{\partial E_{\mathbf{k}}}{\partial \Delta} = \frac{\Delta}{E_{\mathbf{k}}}$, we find

$$\frac{\partial E_{\text{BCS}}}{\partial \Delta} = - \sum_{\mathbf{k}} \frac{\Delta}{E_{\mathbf{k}}} + \frac{2V}{g} \Delta. \quad (30)$$

Requiring stationarity for a paired solution $\Delta \neq 0$, $\frac{\partial E_{\text{BCS}}}{\partial \Delta} = 0$, and dividing by Δ gives

$$-\frac{1}{g} = \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}}, \quad (31)$$

which is exactly Eq. (27).

As before, for a contact interaction the momentum sum in Eq. (31) is UV divergent, and the bare coupling g must be eliminated in favor of the physical scattering length a_s via

$$-\frac{1}{g} = -\frac{m}{4\pi\hbar^2 a_s} + \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}}, \quad (32)$$

which turns Eq. (31) into the renormalized, finite gap equation

$$-\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \sum_{\mathbf{k}} \left(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}} \right), \quad (33)$$

identical to Eq. (28).

What Eq. (28) solves for. Equation (28) is the self-consistency condition that determines the pairing gap Δ (and, together with the number equation, also fixes μ) for a given interaction strength a_s and density. At $T = 0$, the number equation is

$$n = \frac{1}{V} \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma} = \frac{2}{V} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 = \frac{1}{V} \sum_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right),$$

so (28) and this equation are solved simultaneously for (Δ, μ) .

(iv) Excitation spectrum and excitation wavefunctions. Single-quasiparticle excitations are $\hat{\alpha}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle$ and $\hat{\beta}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle$, both with energy $E_{\mathbf{k}}$. A two-quasiparticle excitation $\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle$ has energy $2E_{\mathbf{k}}$. The minimum of $E_{\mathbf{k}}$ occurs at the Fermi surface $\xi_{\mathbf{k}} = 0$, where $E_{\mathbf{k}} = \Delta$, giving a gapped spectrum.

Explicit action of $\hat{\alpha}_{\mathbf{k}}^\dagger, \hat{\beta}_{\mathbf{k}}^\dagger$, and $\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}^\dagger$ on $|\Psi_{\text{BCS}}\rangle$

Separate the \mathbf{k} -sector. Write

$$|\Psi_{\text{BCS}}\rangle = (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger) \prod_{\mathbf{p} \neq \mathbf{k}} (u_{\mathbf{p}} + v_{\mathbf{p}} \hat{b}_{\mathbf{p}}^\dagger) |0\rangle \equiv |\phi_{\mathbf{k}}\rangle \otimes |\Phi_{\neq \mathbf{k}}\rangle,$$

where $|\phi_{\mathbf{k}}\rangle = u_{\mathbf{k}} |0\rangle_{\mathbf{k}} + v_{\mathbf{k}} |\text{pair}\rangle_{\mathbf{k}}$ and $|\Phi_{\neq \mathbf{k}}\rangle \equiv \prod_{\mathbf{p} \neq \mathbf{k}} (u_{\mathbf{p}} + v_{\mathbf{p}} \hat{b}_{\mathbf{p}}^\dagger) |0\rangle$.

Compute $\hat{\alpha}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle$. Using $\hat{\alpha}_{\mathbf{k}}^\dagger = u_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger - v_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}^\dagger$, and $\hat{c}_{-\mathbf{k}\downarrow} |\text{pair}\rangle_{\mathbf{k}} = -|\uparrow\rangle_{\mathbf{k}}$,

$$\hat{\alpha}_{\mathbf{k}}^\dagger |\phi_{\mathbf{k}}\rangle = u_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger (u_{\mathbf{k}} |0\rangle_{\mathbf{k}} + v_{\mathbf{k}} |\text{pair}\rangle_{\mathbf{k}}) - v_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}^\dagger (u_{\mathbf{k}} |0\rangle_{\mathbf{k}} + v_{\mathbf{k}} |\text{pair}\rangle_{\mathbf{k}}) = (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) |\uparrow\rangle_{\mathbf{k}} = |\uparrow\rangle_{\mathbf{k}}.$$

Therefore

$$\hat{\alpha}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle = \hat{c}_{\mathbf{k}\uparrow}^\dagger \prod_{\mathbf{p} \neq \mathbf{k}} (u_{\mathbf{p}} + v_{\mathbf{p}} \hat{c}_{\mathbf{p}\uparrow}^\dagger \hat{c}_{-\mathbf{p}\downarrow}^\dagger) |0\rangle. \quad (34)$$

Compute $\hat{\beta}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle$. Similarly, with $\hat{\beta}_{\mathbf{k}}^\dagger = v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow} + u_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}^\dagger$ and $\hat{c}_{\mathbf{k}\uparrow} |\text{pair}\rangle_{\mathbf{k}} = |\downarrow\rangle_{\mathbf{k}}$,

$$\hat{\beta}_{\mathbf{k}}^\dagger |\phi_{\mathbf{k}}\rangle = (v_{\mathbf{k}}^2 + u_{\mathbf{k}}^2) |\downarrow\rangle_{\mathbf{k}} = |\downarrow\rangle_{\mathbf{k}},$$

so

$$\hat{\beta}_{\mathbf{k}}^\dagger |\Psi_{\text{BCS}}\rangle = \hat{c}_{-\mathbf{k}\downarrow}^\dagger \prod_{\mathbf{p} \neq \mathbf{k}} (u_{\mathbf{p}} + v_{\mathbf{p}} \hat{c}_{\mathbf{p}\uparrow}^\dagger \hat{c}_{-\mathbf{p}\downarrow}^\dagger) |0\rangle. \quad (35)$$

Compute the two-quasiparticle excitation. Acting once more,

$$\hat{\alpha}_k^\dagger \hat{\beta}_k^\dagger |\phi_k\rangle = \hat{\alpha}_k^\dagger |\downarrow\rangle_k = u_k |\text{pair}\rangle_k - v_k |0\rangle_k = (-v_k + u_k \hat{b}_k^\dagger) |0\rangle_k,$$

hence

$$\hat{\alpha}_k^\dagger \hat{\beta}_k^\dagger |\Psi_{\text{BCS}}\rangle = (-v_k + u_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger) \prod_{p \neq k} (u_p + v_p \hat{c}_{p\uparrow}^\dagger \hat{c}_{-p\downarrow}^\dagger) |0\rangle. \quad (36)$$

2.5 Physical Meaning of Δ

■ $\Delta \rightarrow 0$ Limit.

When $\Delta \rightarrow 0$, $E_k \rightarrow |\xi_k|$. From Eq. (17),

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right) \rightarrow \begin{cases} 1, & \xi_k < 0, \\ 0, & \xi_k > 0, \end{cases} \quad u_k^2 = \frac{1}{2} \left(1 + \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right) \rightarrow \begin{cases} 0, & \xi_k < 0, \\ 1, & \xi_k > 0. \end{cases} \quad (37)$$

Thus $n_{k\sigma} = v_k^2$ becomes a sharp step at $\xi_k = 0$ (i.e. $|\mathbf{k}| = k_F$), recovering the filled Fermi sea.

Using the fermionic Bogoliubov transformation (Eq. (18) in your notation),

$$\hat{\alpha}_k = u_k \hat{c}_{k\uparrow} - v_k \hat{c}_{-k\downarrow}^\dagger, \quad \hat{\beta}_k = u_k \hat{c}_{-k\downarrow} + v_k \hat{c}_{k\uparrow}^\dagger,$$

the limiting forms follow from Eq. (37):

$$\hat{\alpha}_k^\dagger \rightarrow \begin{cases} -\hat{c}_{-k\downarrow}, & \xi_k < 0, \\ \hat{c}_{k\uparrow}^\dagger, & \xi_k > 0, \end{cases} \quad \hat{\beta}_k^\dagger \rightarrow \begin{cases} \hat{c}_{-k\downarrow}^\dagger, & \xi_k < 0, \\ \hat{c}_{k\uparrow}, & \xi_k > 0. \end{cases}$$

Accordingly, the operators $\hat{\alpha}_k^\dagger$ and $\hat{\beta}_k^\dagger$ always *create* Bogoliubov quasiparticle excitations with positive energy E_k . For $\xi_k > 0$, these excitations correspond to creating particle states above the Fermi sea, while for $\xi_k < 0$, they correspond to creating hole excitations, i.e. removing particles from filled states below the Fermi surface.

In this sense the quasiparticle vacuum condition reduces to the statement that all $\xi_k < 0$ states are occupied and all $\xi_k > 0$ states are empty, i.e. the free Fermi sea.

■ Finite Δ Case: Deviation from a Fermi liquid.

For $\Delta > 0$, $n_{k\sigma} = v_k^2$ is a smooth function of \mathbf{k} with no discontinuity at $\xi_k = 0$. This violates the defining quasiparticle-discontinuity criterion of a Fermi liquid, reflecting that the BCS state is an ordered phase with a gap.

Why far from the Fermi surface the state looks like a Fermi Liquid. If $|\xi_k| \gg \Delta$, expand

$$E_k = |\xi_k| \sqrt{1 + \frac{\Delta^2}{\xi_k^2}} \approx |\xi_k| + \frac{\Delta^2}{2|\xi_k|}, \quad \frac{\xi_k}{E_k} = \text{sgn}(\xi_k) \left(1 - \frac{\Delta^2}{2\xi_k^2} + O\left(\frac{\Delta^4}{\xi_k^4}\right) \right).$$

Therefore

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{E_k} \right) \approx \begin{cases} 1 - \frac{\Delta^2}{4\xi_k^2}, & \xi_k < 0, \\ \frac{\Delta^2}{4\xi_k^2}, & \xi_k > 0, \end{cases} \quad u_k^2 \approx \begin{cases} \frac{\Delta^2}{4\xi_k^2}, & \xi_k < 0, \\ 1 - \frac{\Delta^2}{4\xi_k^2}, & \xi_k > 0. \end{cases} \quad (38)$$

Hence away from $\xi_{\mathbf{k}} = 0$ the coherence factors approach the free-fermion values with *algebraically* small corrections $O(\Delta^2/\xi_{\mathbf{k}}^2)$, and the BCS reconstruction is confined to an energy window $\sim \Delta$ around the Fermi surface.⁴

The many-body wavefunction is reconstructed mainly near the Fermi Surface.

The difference between the paired state and the free Fermi sea is appreciable only in the window $|\xi_{\mathbf{k}}| \lesssim \Delta$; thus BCS pairing reconstructs the many-body state primarily near the Fermi surface.

2.6 Momentum-space pairing as a Two-Level problem

Why focusing on the $q = 0$ sector captures BCS pairing.

Pick a point \mathbf{k}_0 on the Fermi surface. Time-reversal symmetry places $-\mathbf{k}_0$ on the Fermi surface as well. For $q \neq 0$, it is generically impossible to have both $\mathbf{k}_0 + \mathbf{q}/2$ and $-\mathbf{k}_0 + \mathbf{q}/2$ simultaneously on the Fermi surface; BCS pairing relies on the special degeneracy of \mathbf{k} and $-\mathbf{k}$ at the Fermi surface, motivating the $q = 0$ focus.

Comment on FFLO (Fulde–Ferrell–Larkin–Ovchinnikov) states

If the Fermi surface geometry allows a nonzero \mathbf{q} such that $\mathbf{k} + \mathbf{q}/2$ and $-\mathbf{k} + \mathbf{q}/2$ can both lie on the Fermi surface for many \mathbf{k} , pairing with $\mathbf{q} \neq 0$ becomes possible. The resulting paired state breaks translational symmetry and is referred to as an FFLO state. This is outside the standard uniform BCS ansatz.

Four basis states in a fixed $(\mathbf{k}, -\mathbf{k})$ sector.

To make the physical picture explicit, fix a momentum pair $(\mathbf{k}, -\mathbf{k})$ and introduce the four-dimensional sector basis

$$|0\rangle_{\mathbf{k}}, \quad |\uparrow\rangle_{\mathbf{k}} \equiv \hat{c}_{\mathbf{k}\uparrow}^\dagger |0\rangle_{\mathbf{k}}, \quad |\downarrow\rangle_{\mathbf{k}} \equiv \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}}, \quad |\text{pair}\rangle_{\mathbf{k}} \equiv \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |0\rangle_{\mathbf{k}}.$$

In BCS mean-field theory the Hamiltonian is

$$\hat{H}_{\text{BCS}} = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger - \Delta \sum_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} - \frac{V\Delta^2}{g}, \quad (39)$$

where $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$. The pairing term only mixes the $|0\rangle_{\mathbf{k}}$ and $|\text{pair}\rangle_{\mathbf{k}}$ states, while the singly occupied states $|\uparrow\rangle_{\mathbf{k}}$ and $|\downarrow\rangle_{\mathbf{k}}$ remain uncoupled.

Level splitting at the Fermi surface: an explicit two-level problem.

We consider $\mathbf{k} = \mathbf{k}_0$ at the Fermi surface, *i.e.* $|\mathbf{k}_0| = k_F$ and $\xi_{\mathbf{k}_0} = 0$. The kinetic energies of $|0\rangle_{\mathbf{k}_0}$ and $|\text{pair}\rangle_{\mathbf{k}_0}$ are degenerate (measured relative to μ), so we may restrict \hat{H}_{BCS} to the two-dimensional subspace $\text{span}\{|0\rangle_{\mathbf{k}_0}, |\text{pair}\rangle_{\mathbf{k}_0}\}$. In the ordered basis $\{|0\rangle_{\mathbf{k}_0}, |\text{pair}\rangle_{\mathbf{k}_0}\}$, the \mathbf{k}_0 -sector Hamiltonian reads

$$\hat{H}_{\text{BCS}}^{(\mathbf{k}_0)} = \begin{pmatrix} 0 & -\Delta \\ -\Delta & 0 \end{pmatrix},$$

whose eigenstates and eigenvalues are

$$|\psi_-\rangle_{\mathbf{k}_0} = \frac{1}{\sqrt{2}} (|0\rangle_{\mathbf{k}_0} + |\text{pair}\rangle_{\mathbf{k}_0}), \quad E_- = -\Delta,$$

⁴In weak-coupling BCS theory with a short-range attraction, the self-consistent solution is typically $\Delta \ll E_F$ and is often *exponentially small* in the dimensionless coupling (e.g. $\Delta/E_F \sim e^{-\pi/(2k_F|a_s|)}$ for $k_F a_s \rightarrow 0^-$).

$$|\psi_+\rangle_{\mathbf{k}_0} = \frac{1}{\sqrt{2}}(|0\rangle_{\mathbf{k}_0} - |\text{pair}\rangle_{\mathbf{k}_0}), \quad E_+ = +\Delta.$$

Thus the pairing term produces a splitting of size 2Δ : the BCS-like superposition $|\psi_-\rangle_{\mathbf{k}_0}$ lowers the energy by Δ , while the orthogonal superposition $|\psi_+\rangle_{\mathbf{k}_0}$ is raised by Δ .

Identifying the excitations at $\xi_{\mathbf{k}_0} = 0$. The singly occupied states $|\uparrow\rangle_{\mathbf{k}_0}$ and $|\downarrow\rangle_{\mathbf{k}_0}$ are not mixed by the pairing term in Eq. (39), and at $\xi_{\mathbf{k}_0} = 0$ their energies stay at 0 in this sector. Therefore, relative to the paired ground state energy $E_- = -\Delta$, they represent one-quasiparticle excitations with excitation energy Δ . Meanwhile the excited superposition $|\psi_+\rangle_{\mathbf{k}_0}$ lies at $+\Delta$, i.e. its excitation energy above the paired ground state is $E_+ - E_- = 2\Delta$; this matches the two-quasiparticle excitation energy at the Fermi surface.

Away from the Fermi surface

When $\xi_{\mathbf{k}} \neq 0$, the two states $|0\rangle_{\mathbf{k}}$ and $|\text{pair}\rangle_{\mathbf{k}}$ are no longer degenerate, because the kinetic term in Eq. (39) contributes an energy bias $2\xi_{\mathbf{k}}$ between them. Restricting the BCS Hamiltonian to the $\{|0\rangle_{\mathbf{k}}, |\text{pair}\rangle_{\mathbf{k}}\}$ subspace, one obtains the effective 2×2 Hamiltonian

$$H_{\mathbf{k}} = \begin{pmatrix} 0 & -\Delta \\ -\Delta & 2\xi_{\mathbf{k}} \end{pmatrix}, \quad (40)$$

up to an irrelevant constant shift.

Diagonalizing Eq. (40) yields the quasiparticle energies $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$ and the corresponding ground-state eigenvector

$$|\phi_{\mathbf{k}}\rangle = u_{\mathbf{k}}|0\rangle_{\mathbf{k}} + v_{\mathbf{k}}|\text{pair}\rangle_{\mathbf{k}}, \quad u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right). \quad (41)$$

The limiting behavior of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ follows directly from Eq. (41). For momenta far *below* the Fermi surface, $\xi_{\mathbf{k}} \ll -\Delta$, one has $E_{\mathbf{k}} \simeq |\xi_{\mathbf{k}}|$ and

$$u_{\mathbf{k}}^2 \simeq \frac{1}{2}\left(1 - \frac{|\xi_{\mathbf{k}}|}{|\xi_{\mathbf{k}}|}\right) = 0, \quad v_{\mathbf{k}}^2 \simeq 1, \quad (42)$$

so the ground state approaches $|\phi_{\mathbf{k}}\rangle \simeq |\text{pair}\rangle_{\mathbf{k}}$, corresponding to an almost certainly occupied pair of states $(\mathbf{k}, -\mathbf{k})$. Physically, in this regime the kinetic energy strongly favors filling both states, and the pairing term only weakly perturbs this configuration.

Conversely, for momenta far *above* the Fermi surface, $\xi_{\mathbf{k}} \gg \Delta$, one again has $E_{\mathbf{k}} \simeq \xi_{\mathbf{k}}$, leading to

$$u_{\mathbf{k}}^2 \simeq 1, \quad v_{\mathbf{k}}^2 \simeq 0, \quad (43)$$

and the ground state approaches $|\phi_{\mathbf{k}}\rangle \simeq |0\rangle_{\mathbf{k}}$, indicating that the corresponding momentum states are essentially empty.

This shows again that far away from the Fermi surface the state behaves like a Fermi Liquid.

Only within an energy window $|\xi_{\mathbf{k}}| \lesssim \Delta$ around the Fermi surface does the pairing term compete effectively with the kinetic energy, resulting in a coherent superposition of empty and doubly occupied configurations. In this sense, the coherence factors $u_{\mathbf{k}}, v_{\mathbf{k}}$ interpolate smoothly between the “empty” and “paired” limits as a function of $\xi_{\mathbf{k}}/\Delta$.

Momentum-space pairing vs real-space “closeness”. Momentum-space pairing means that the $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ pair is either both occupied or both empty; singly occupied configurations are excluded because they cannot participate in the scattering processes that gain interaction

energy. This differs from an intuitive real-space picture of two particles “coming close” to gain attraction. In the weak-coupling BCS regime the Cooper-pair size (coherence length scale)

$$\xi_{\text{pair}} \sim \frac{\hbar v_F}{\pi \Delta}$$

is typically much larger than k_F^{-1} , i.e., the pair is spatially extended.

3 Tan Framework: Contact and Universal Short-Distance Physics

The Tan framework refers to a set of universal relations governing quantum many-body systems with short-range (zero-range) interactions. Its central statement is that all short-distance and high-momentum properties of such systems are controlled by a single state variable, the *contact* C . The contact quantifies the strength of opposite-spin correlations at vanishing separation and is independent of whether the system is in equilibrium or of the underlying quantum statistics.

Physically, the contact characterizes how frequently two particles approach each other within a distance much shorter than any other microscopic length scale. As a consequence, the same contact appears in seemingly different observables, such as the universal high-momentum tail $n_k \sim C/k^4$ and properly renormalized local density correlations. In the following, we use the BCS mean-field theory as a concrete example to illustrate how this universal short-distance physics is encoded in the pairing amplitude and how the contact emerges naturally from the local structure of the many-body state.

3.1 Universal $1/k^4$ tail from short-distance behavior

Short-distance boundary condition and UV universality. For a three-dimensional zero-range interaction, the opposite-spin two-body wavefunction obeys the Bethe–Peierls boundary condition: when the relative distance $r = |\mathbf{r}_\uparrow - \mathbf{r}_\downarrow| \rightarrow 0$,

$$\psi(\mathbf{r}) \sim A \left(\frac{1}{r} - \frac{1}{a_s} \right),$$

with A depending on the many-body state. The Fourier transform of a $1/r$ singularity behaves as $1/k^2$, implying $n_k \sim |\psi(\mathbf{k})|^2 \sim 1/k^4$ at large momentum.

BCS example: explicit large- k asymptotics $n_k \sim 1/k^4$

For the BCS state, $n_\mathbf{k} = v_\mathbf{k}^2$ with Eq. (17). At large k , $\epsilon_\mathbf{k} \gg \mu, \Delta$, hence $\xi_\mathbf{k} \approx \epsilon_\mathbf{k}$ and

$$E_\mathbf{k} = \sqrt{\xi_\mathbf{k}^2 + \Delta^2} \approx \xi_\mathbf{k} \left(1 + \frac{\Delta^2}{2\xi_\mathbf{k}^2} \right).$$

Then

$$v_\mathbf{k}^2 = \frac{1}{2} \left(1 - \frac{\xi_\mathbf{k}}{E_\mathbf{k}} \right) \approx \frac{1}{2} \left(1 - \frac{1}{1 + \frac{\Delta^2}{2\xi_\mathbf{k}^2}} \right) \approx \frac{\Delta^2}{4\xi_\mathbf{k}^2} \approx \frac{\Delta^2}{4\epsilon_\mathbf{k}^2} = \frac{m^2 \Delta^2}{\hbar^4 k^4}.$$

Thus $n_k \rightarrow m^2 \Delta^2 / (\hbar^4 k^4)$ at sufficiently large k .

3.2 Definition of Contact

Contact as the coefficient of the $1/k^4$ tail. Define the *Contact* C by the large- k asymptotic of the momentum distribution:

$$C = \lim_{k \rightarrow \infty} k^4 n_k. \quad (44)$$

For the BCS state, using the result above,

$$C = \frac{m^2 \Delta^2}{\hbar^4}. \quad (45)$$

Physical meaning. C quantifies short-distance opposite-spin correlations and controls UV tails of many observables. It is a state variable characterizing the intensity of short-range pairing correlations, independent of whether the system is in equilibrium, and independent of quantum statistics in the general Tan framework.

3.3 Energy–Contact relation

Adiabatic relation. For a three-dimensional system with zero-range interaction in equilibrium, one has the universal identity

$$\frac{dE}{d(a_s^{-1})} = -\frac{\hbar^2 V}{4\pi m} C. \quad (46)$$

Derivation sketch in BCS mean field and why it is universal

Start from the mean-field ground state energy $E_{\text{BCS}}(\Delta, g)$ in Eq. (29). Differentiate with respect to a_s^{-1} :

$$\frac{dE}{d(a_s^{-1})} = \frac{\partial E}{\partial \Delta} \frac{\partial \Delta}{\partial (a_s^{-1})} + \frac{\partial E}{\partial (g^{-1})} \frac{\partial (g^{-1})}{\partial (a_s^{-1})}.$$

By self-consistency (gap equation), $\partial E / \partial \Delta = 0$. Moreover $\partial E / \partial (g^{-1}) = -V\Delta^2$ from Eq. (29), and Eq. (2) implies

$$\frac{\partial (g^{-1})}{\partial (a_s^{-1})} = \frac{m}{4\pi\hbar^2}.$$

Hence

$$\frac{dE}{d(a_s^{-1})} = -\frac{mV}{4\pi\hbar^2} \Delta^2 = -\frac{\hbar^2 V}{4\pi m} \left(\frac{m^2 \Delta^2}{\hbar^4} \right) = -\frac{\hbar^2 V}{4\pi m} C,$$

using $C = m^2 \Delta^2 / \hbar^4$ in Eq. (45). The final identity Eq. (46) holds beyond BCS: it is a Tan relation valid for general equilibrium states with zero-range interactions.

3.4 Contact and local density correlations

Consider the local density–density correlator

$$\langle \hat{n}_\uparrow(\mathbf{r}) \hat{n}_\downarrow(\mathbf{r}) \rangle, \quad \hat{n}_\sigma(\mathbf{r}) = \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_\sigma(\mathbf{r}).$$

Because the two density operators are evaluated at the same spatial point, this correlator probes the $r \rightarrow 0$ behavior of opposite-spin two-body correlations. For zero-range (contact) interactions, the short-distance structure of the many-body wave function is universal, and the same UV physics controls both this local correlator and the high-momentum tail $n_\mathbf{k} \sim C/k^4$.

BCS evaluation via Wick factorization: background term and pairing term

Writing the operator product explicitly,

$$\hat{n}_\uparrow(\mathbf{r})\hat{n}_\downarrow(\mathbf{r}) = \hat{\psi}_\uparrow^\dagger(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow^\dagger(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r}),$$

and evaluating it in the BCS mean-field state (which is Gaussian), Wick's theorem applies. Only two distinct contractions survive:

$$\langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle = \langle \hat{\psi}_\uparrow^\dagger \hat{\psi}_\uparrow \rangle \langle \hat{\psi}_\downarrow^\dagger \hat{\psi}_\downarrow \rangle + |\langle \hat{\psi}_\downarrow \hat{\psi}_\uparrow \rangle|^2. \quad (47)$$

The first term, $\langle n_\uparrow \rangle \langle n_\downarrow \rangle$, is a smooth “background” contribution describing uncorrelated occupation of opposite-spin particles. It is insensitive to short-distance physics. The second term originates from the anomalous contraction $\langle \hat{\psi}_\downarrow \hat{\psi}_\uparrow \rangle$ and represents genuine short-range pairing correlations.

Using translational invariance,

$$\langle \hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r}) \rangle = \frac{1}{V} \sum_{\mathbf{k}} \langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle = \frac{1}{V} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}},$$

we find

$$|\langle \hat{\psi}_\downarrow \hat{\psi}_\uparrow \rangle|^2 = \frac{1}{V^2} \left(\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \right)^2.$$

For a contact interaction, the sum $\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \sim \sum_{\mathbf{k}} \Delta/(2E_{\mathbf{k}})$ is linearly UV divergent. This divergence is not physical by itself, but is precisely compensated by the UV dependence of the bare coupling constant. Multiplying by g^2 and using the self-consistency condition $\Delta = -\frac{g}{V} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}$, one obtains the finite identity

$$g^2 |\langle \hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r}) \rangle|^2 = \Delta^2. \quad (48)$$

Why the background term does not contribute at order g^2 . The background contribution $\langle n_\uparrow \rangle \langle n_\downarrow \rangle$ is UV finite, since the momentum distribution decays as $n_{\mathbf{k}} \sim 1/k^4$. At fixed scattering length a_s , the renormalized contact coupling scales as $g(\Lambda) \sim \Lambda^{-1}$ with UV cutoff Λ . Consequently, $g^2(\Lambda) \langle n_\uparrow \rangle \langle n_\downarrow \rangle \rightarrow 0$ as $\Lambda \rightarrow \infty$. Thus, in the properly renormalized product $g^2 \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle$, only the pairing term survives.

Contact-local-correlation relation. Combining Eq. (45) with Eq. (48), we arrive at

$$\frac{\hbar^4}{m^2} C = g^2 \langle \hat{n}_\uparrow(\mathbf{r})\hat{n}_\downarrow(\mathbf{r}) \rangle, \quad (49)$$

which expresses the Tan contact equivalently in terms of a properly renormalized local density correlation.

Two equivalent UV diagnostics. The same short-distance physics manifests itself either as a universal high-momentum tail $n_{\mathbf{k}} \sim C/k^4$ or as a finite local correlator $g^2 \langle n_\uparrow n_\downarrow \rangle \propto C$. Both provide equivalent diagnostics of the contact.

4 Response to a Zeeman Field

4.1 Zeeman term and spin-dependent chemical potentials

Add a Zeeman term

$$\hat{H}_Z = h \sum_{\mathbf{k}} (\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow} - \hat{c}_{\mathbf{k}\downarrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}) = 2h\hat{S}_z. \quad (50)$$

This is equivalent to shifting the chemical potentials:

$$\mu_\uparrow = \mu - h, \quad \mu_\downarrow = \mu + h.$$

Only the kinetic term changes; the pairing structure remains the same at the mean-field level.

4.2 Shifted quasiparticle spectra and spin susceptibility

Quasiparticle energy.

For each $(\mathbf{k}, -\mathbf{k})$ sector, the mean-field Hamiltonian can still be diagonalized by the same fermionic Bogoliubov transformation, yielding

$$\hat{H}_{\text{MF}}(h) = E_{\text{BCS}} + \sum_{\mathbf{k}} [(E_{\mathbf{k}} + h) \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + (E_{\mathbf{k}} - h) \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}],$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$ and E is the ground-state energy constant (29).

Why $\hat{\alpha}^\dagger$ and $\hat{\beta}^\dagger$ create opposite-spin excitations

Use the standard Bogoliubov modes (real $u_{\mathbf{k}}, v_{\mathbf{k}}$)

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

Then, within the $(\mathbf{k}, -\mathbf{k})$ sector, the BCS vacuum satisfies $\hat{\alpha}_{\mathbf{k}}|\Psi_{\text{BCS}}\rangle = \hat{\beta}_{\mathbf{k}}|\Psi_{\text{BCS}}\rangle = 0$. A one-quasiparticle excitation $\hat{\alpha}_{\mathbf{k}}^\dagger|\Psi_{\text{BCS}}\rangle$ contains an *unpaired* \uparrow component (from $\hat{c}_{\mathbf{k}\uparrow}^\dagger$) while $\hat{\beta}_{\mathbf{k}}^\dagger|\Psi_{\text{BCS}}\rangle$ contains an unpaired \downarrow component (from $\hat{c}_{-\mathbf{k}\downarrow}^\dagger$); thus they carry opposite $S_z = \pm \frac{1}{2}$.

The ground state $|\Psi_{\text{BCS}}\rangle$ doesn't have polarization and is a spin singlet.^a

Moreover, in the quasiparticle basis the spin operator takes a particularly transparent form. One finds, for each \mathbf{k} ,

$$\hat{n}_{\mathbf{k}\uparrow} - \hat{n}_{\mathbf{k}\downarrow} = \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} - \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}},$$

so that

$$\hat{S}_z = \frac{1}{2} \sum_{\mathbf{k}} (\hat{n}_{\mathbf{k}\uparrow} - \hat{n}_{\mathbf{k}\downarrow}) = \frac{1}{2} \sum_{\mathbf{k}} (\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} - \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}). \quad (51)$$

Consequently the Zeeman coupling $\hat{H}_h = 2h\hat{S}_z$ is *exactly* a difference of quasiparticle number operators, which explains why the spectra shift to $E_{\mathbf{k}} \pm h$.

^aHere "spin singlet" means the many-body state is invariant under global $SU(2)$ spin rotations, i.e. it transforms in the trivial representation. This notion does not require the state to contain only two particles; a macroscopic paired superfluid can still be an $SU(2)$ singlet.

Spin gap \Rightarrow vanishing spin susceptibility at $T = 0$. At $T = 0$, the ground state in the quasiparticle description is obtained by occupying all modes with negative energy. Since $\min_{\mathbf{k}} E_{\mathbf{k}} = \Delta$, for $0 < h < \Delta$ both branches satisfy $E_{\mathbf{k}} \pm h > 0$ for all \mathbf{k} . Therefore no quasiparticles

are occupied in the ground state, i.e. it remains the same quasiparticle vacuum as at $h = 0$. Using Eq. (51), this immediately implies

$$M \equiv \langle \hat{S}_z \rangle = \frac{1}{2} \sum_{\mathbf{k}} (\langle \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} \rangle - \langle \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rangle) = 0, \quad (0 < h < \Delta).$$

Hence the zero-temperature spin susceptibility vanishes:

$$\chi_s \equiv \left. \frac{\partial M}{\partial h} \right|_{h \rightarrow 0} = 0.$$

4.3 Normal state, Chandrasekhar–Clogston limit, and first-order transition

Normal state gains energy from polarization. Consider the normal state with $\Delta = 0$. Then fermions near the Fermi surface can be polarized immediately by a Zeeman field; the \uparrow and \downarrow Fermi surfaces split, and the normal-state energy decreases with increasing h .

Energy competition and critical field. At $h = 0$, the paired BCS state has lower energy than the normal state. As h increases, there exists a critical field h_c where their energies cross; for $h > h_c$ the normal state is energetically favored. In weak coupling, one finds

$$h_c = \frac{\Delta}{\sqrt{2}},$$

typically smaller than Δ . The transition is first order: the spin polarization jumps from zero to a finite value at $h = h_c$, and then increases with h .

Chandrasekhar–Clogston limit. The critical field h_c at which the unpolarized paired state gives way to a polarized normal state is known as the Chandrasekhar–Clogston limit.

4.4 Cold-atom realization and spatial phase separation in a trap

In ultracold-atom experiments there is typically *no real* Zeeman field applied to the neutral atoms in the condensed-matter sense. Instead, one engineers an *effective* Zeeman field by preparing the two hyperfine “spin” components with unequal populations, $N_\uparrow \neq N_\downarrow$, which in the grand-canonical description corresponds to different chemical potentials $\mu_\uparrow \neq \mu_\downarrow$. It is therefore convenient to parameterize

$$\bar{\mu} \equiv \frac{\mu_\uparrow + \mu_\downarrow}{2}, \quad h \equiv \frac{\mu_\uparrow - \mu_\downarrow}{2},$$

so that h plays the role of a Zeeman coupling $2h\hat{S}_z$ in the mean-field Hamiltonian.

Under the local density approximation (LDA), the trap enters as a slowly varying external potential $V(r)$ that shifts the local chemical potentials in the same way for both components:

$$\mu_\sigma(r) = \mu_\sigma^0 - V(r), \tag{52}$$

where μ_σ^0 are the global (central) chemical potentials fixed by the prepared atom numbers N_σ . Consequently the *imbalance* is spatially constant,

$$h(r) = \frac{\mu_\uparrow(r) - \mu_\downarrow(r)}{2} = \frac{\mu_\uparrow^0 - \mu_\downarrow^0}{2} \equiv h, \tag{53}$$

while the *average* chemical potential decreases with radius,

$$\bar{\mu}(r) = \frac{\mu_\uparrow(r) + \mu_\downarrow(r)}{2} = \frac{\mu_\uparrow^0 + \mu_\downarrow^0}{2} - V(r). \quad (54)$$

Thus, in a trapped cloud one realizes a situation where the effective Zeeman parameter h is fixed by the imposed particle-number imbalance, whereas $\bar{\mu}(r)$ (hence the local density scale and the local gap Δ) varies with r through the trap potential.

Why a critical radius appears. As r increases, $\bar{\mu}(r)$ decreases, the local Fermi energy decreases, and the local gap $\Delta(r)$ decreases accordingly. Therefore $h/\Delta(r)$ increases with r , and there exists a critical radius R_c where the Chandrasekhar–Clogston criterion is reached. This produces a shell structure:

- **Region I** ($r < R_c$). unpolarized paired superfluid with $n_\uparrow = n_\downarrow$ and zero polarization;
- **Region II** ($r > R_c$). partially polarized normal region with increasing polarization;
- **Region III.** fully polarized outer region where the minority component vanishes.

Imaging and inverse Abel transform. Absorption imaging typically measures a column-integrated density along the imaging axis, which smears sharp features such as a first-order jump in polarization. To resolve the jump, experiments reconstruct the three-dimensional density profile from column densities using the inverse Abel transform.

A Explicit evaluation of $f(E/E_F)$ in the vacuum and Cooper problems

General setup and dimensionless variables. Throughout this appendix we focus on the bound-state (or Cooper-bound) solutions with $E < 0$. We use

$$E_F = \frac{\hbar^2 k_F^2}{2m}, \quad x \equiv \frac{E}{E_F},$$

and convert momentum sums to integrals via

$$\frac{1}{V} \sum_{\mathbf{k}} \rightarrow \int \frac{d^3 k}{(2\pi)^3} = \frac{1}{2\pi^2} \int_0^\infty dk k^2.$$

A.1 Vacuum equation: closed form of $f_{\text{vac}}(x)$ and its behavior

Start from the renormalized vacuum equation. We begin with

$$\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \sum_{\mathbf{k}} \left(\frac{1}{E - 2\epsilon_{\mathbf{k}}} + \frac{1}{2\epsilon_{\mathbf{k}}} \right), \quad 2\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{m}. \quad (55)$$

For $E < 0$, define $\kappa > 0$ by

$$E = -\frac{\hbar^2 \kappa^2}{m}. \quad (56)$$

Then

$$\frac{1}{E - 2\epsilon_{\mathbf{k}}} = -\frac{m}{\hbar^2} \frac{1}{k^2 + \kappa^2}, \quad \frac{1}{2\epsilon_{\mathbf{k}}} = \frac{m}{\hbar^2} \frac{1}{k^2}.$$

Hence Eq. (55) becomes

$$\frac{1}{4\pi a_s} = \int \frac{d^3 k}{(2\pi)^3} \left(\frac{1}{k^2} - \frac{1}{k^2 + \kappa^2} \right). \quad (57)$$

Evaluate the convergent integral. Using spherical symmetry,

$$\int \frac{d^3k}{(2\pi)^3} \left(\frac{1}{k^2} - \frac{1}{k^2 + \kappa^2} \right) = \frac{1}{2\pi^2} \int_0^\infty dk \left(1 - \frac{k^2}{k^2 + \kappa^2} \right) = \frac{1}{2\pi^2} \int_0^\infty dk \frac{\kappa^2}{k^2 + \kappa^2}.$$

The last integral is elementary:

$$\int_0^\infty dk \frac{\kappa^2}{k^2 + \kappa^2} = \kappa \left[\arctan \left(\frac{k}{\kappa} \right) \right]_0^\infty = \frac{\pi}{2} \kappa,$$

so Eq. (57) gives

$$\frac{1}{4\pi a_s} = \frac{\kappa}{4\pi} \implies \kappa = \frac{1}{a_s}. \quad (58)$$

Dimensionless form $\frac{1}{k_F a_s} = f_{\text{vac}}(x)$. From Eq. (56),

$$x = \frac{E}{E_F} = \frac{-\hbar^2 \kappa^2 / m}{\hbar^2 k_F^2 / (2m)} = -2 \frac{\kappa^2}{k_F^2}, \quad \Rightarrow \quad \frac{\kappa}{k_F} = \sqrt{-\frac{x}{2}}.$$

Using $\kappa = 1/a_s$ from Eq. (58), we obtain

$$\frac{1}{k_F a_s} = f_{\text{vac}}(x), \quad f_{\text{vac}}(x) = \sqrt{-\frac{x}{2}} \quad (x < 0). \quad (59)$$

Vacuum behavior of f_{vac} . For bound-state energies $x < 0$, $f_{\text{vac}}(x) > 0$ and

$$\lim_{x \rightarrow 0^-} f_{\text{vac}}(x) = 0.$$

Therefore the vacuum equation admits an $E < 0$ solution only if $1/(k_F a_s) > 0$, i.e. $a_s > 0$.

A.2 Cooper equation: closed form of $f_{\text{FS}}(x)$ and the $E \rightarrow 0^-$ divergence

Start from the renormalized Cooper equation. Now consider

$$\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{V} \left[\sum_{|\mathbf{k}| > k_F} \frac{1}{E - 2(\epsilon_{\mathbf{k}} - \mu)} + \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}} \right], \quad (60)$$

and take $\mu = E_F = \hbar^2 k_F^2 / (2m)$, so that

$$2(\epsilon_{\mathbf{k}} - \mu) = \frac{\hbar^2}{m} (k^2 - k_F^2).$$

Introduce

$$\alpha \equiv \frac{mE}{\hbar^2} = \frac{x}{2} k_F^2, \quad s^2 \equiv k_F^2 + \alpha = k_F^2 \left(1 + \frac{x}{2} \right),$$

so that

$$\frac{1}{E - 2(\epsilon_{\mathbf{k}} - \mu)} = \frac{m}{\hbar^2} \frac{1}{k_F^2 + \alpha - k^2} = -\frac{m}{\hbar^2} \frac{1}{k^2 - s^2}.$$

Splitting the second sum into $k > k_F$ and $k < k_F$, Eq. (60) becomes

$$\frac{1}{4\pi a_s} = \int_{k > k_F} \frac{d^3k}{(2\pi)^3} \left(\frac{1}{k^2} - \frac{1}{k^2 - s^2} \right) + \int_{k < k_F} \frac{d^3k}{(2\pi)^3} \frac{1}{k^2}. \quad (61)$$

Each term is UV finite, and the first term contains the Fermi-surface singular structure.

Evaluate the $k < k_F$ piece.

$$\int_{k < k_F} \frac{d^3k}{(2\pi)^3} \frac{1}{k^2} = \frac{1}{2\pi^2} \int_0^{k_F} dk = \frac{k_F}{2\pi^2}.$$

Evaluate the $k > k_F$ piece (case $s \in \mathbb{R}$, i.e. $-2 < x < 0$). Assume $-2 < x < 0$ so that $0 < s < k_F$. Then

$$\begin{aligned} \int_{k > k_F} \frac{d^3k}{(2\pi)^3} \left(\frac{1}{k^2} - \frac{1}{k^2 - s^2} \right) &= \frac{1}{2\pi^2} \int_{k_F}^{\infty} dk k^2 \left(\frac{1}{k^2} - \frac{1}{k^2 - s^2} \right) \\ &= \frac{1}{2\pi^2} \int_{k_F}^{\infty} dk \left(1 - \frac{k^2}{k^2 - s^2} \right) = -\frac{s^2}{2\pi^2} \int_{k_F}^{\infty} dk \frac{1}{k^2 - s^2}. \end{aligned} \quad (62)$$

Using

$$\int dk \frac{1}{k^2 - s^2} = \frac{1}{2s} \ln \left| \frac{k-s}{k+s} \right|,$$

and noting $\lim_{k \rightarrow \infty} \ln \left(\frac{k-s}{k+s} \right) = 0$, Eq. (62) gives

$$\int_{k > k_F} \frac{d^3k}{(2\pi)^3} \left(\frac{1}{k^2} - \frac{1}{k^2 - s^2} \right) = \frac{s}{4\pi^2} \ln \left(\frac{k_F - s}{k_F + s} \right).$$

Assemble and rewrite as $\frac{1}{k_F a_s} = f_{\text{FS}}(x)$. Plugging the two pieces into Eq. (61),

$$\frac{1}{4\pi a_s} = \frac{k_F}{2\pi^2} + \frac{s}{4\pi^2} \ln \left(\frac{k_F - s}{k_F + s} \right).$$

Multiply by 4π and divide by k_F . With $u \equiv s/k_F = \sqrt{1+x/2} \in (0, 1)$, we obtain

$$\frac{1}{k_F a_s} = f_{\text{FS}}(x), \quad f_{\text{FS}}(x) = \frac{2}{\pi} + \frac{u}{\pi} \ln \left(\frac{1-u}{1+u} \right), \quad u = \sqrt{1 + \frac{x}{2}}, \quad (-2 < x < 0). \quad (63)$$

Analytic continuation for $x < -2$ (deep bound side). If $x < -2$, then $1+x/2 < 0$ and $u = iv$ with $v = \sqrt{-1-x/2} > 0$. Using the identity (for $v > 0$)

$$\ln \left(\frac{1-iv}{1+iv} \right) = -2i \arctan v,$$

Eq. (63) continues to

$$f_{\text{FS}}(x) = \frac{2}{\pi} + \frac{2v}{\pi} \arctan v, \quad v = \sqrt{-1 - \frac{x}{2}}, \quad (x < -2). \quad (64)$$

Key behavior of f_{FS} . For $-2 < x < 0$, $u \in (0, 1)$ and $\ln \left(\frac{1-u}{1+u} \right) < 0$. In particular,

$$\lim_{x \rightarrow 0^-} u = 1^-, \quad \ln \left(\frac{1-u}{1+u} \right) \rightarrow -\infty,$$

so

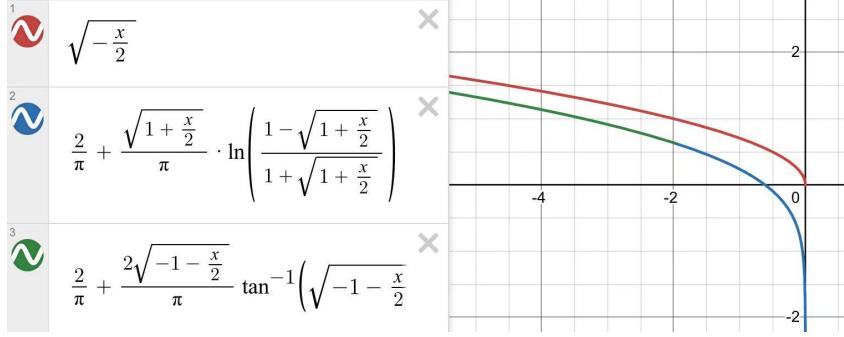
$$\lim_{x \rightarrow 0^-} f_{\text{FS}}(x) = -\infty.$$

Therefore the Cooper equation always has an $E < 0$ solution for any a_s , including $a_s < 0$: the left-hand side $1/(k_F a_s)$ can be any real number, and $f_{\text{FS}}(x)$ sweeps down to $-\infty$ as $E \rightarrow 0^-$.

Connection to the vacuum limit at large binding. From Eq. (64), as $x \rightarrow -\infty$ we have $v \rightarrow \infty$ and $\arctan v \rightarrow \pi/2$, so

$$f_{\text{FS}}(x) = \frac{2}{\pi} + \frac{2v}{\pi} \arctan v \rightarrow \frac{2}{\pi} + v \sim v = \sqrt{-\frac{x}{2}},$$

which matches $f_{\text{vac}}(x) = \sqrt{-x/2}$ in Eq. (59). This reflects that for a very deep bound state the presence of the Fermi sea becomes irrelevant.



B Fermionic Bogoliubov transformation and comparison with bosons

B.1 Motivation: quadratic Hamiltonians and pairing

Why Nambu doubling is unavoidable. Both for bosons and fermions, a generic quadratic Hamiltonian may contain *anomalous* (pairing) terms that mix annihilation and creation operators. Such Hamiltonians cannot be diagonalized by a unitary rotation acting solely within the space of annihilation operators: the pairing terms force us to treat particles and holes on equal footing. This motivates the introduction of an enlarged Nambu space, in which canonical diagonalization becomes possible.

B.2 General quadratic fermion Hamiltonian and BdG form

Structure fixed by fermionic statistics. Consider N fermionic modes collected into

$$\hat{c} = (\hat{c}_1, \dots, \hat{c}_N)^T, \quad \{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}, \quad \{\hat{c}_i, \hat{c}_j\} = 0.$$

Up to an additive constant, the most general quadratic fermion Hamiltonian reads

$$\hat{H} = \hat{c}^\dagger A \hat{c} + \frac{1}{2} (\hat{c}^\dagger B \hat{c}^\dagger + \hat{c} B^\dagger \hat{c}), \quad (65)$$

where $A = A^\dagger$ is Hermitian and $B = -B^\dagger$ is antisymmetric, the latter being enforced by fermionic anticommutation relations.

Introducing the Nambu spinor

$$\hat{\Psi} = \begin{pmatrix} \hat{c} \\ \hat{c}^\dagger \end{pmatrix}, \quad \hat{\Psi}^\dagger = (\hat{c}^\dagger, \hat{c}),$$

the Hamiltonian can be compactly written in Bogoliubov–de Gennes (BdG) form

$$\hat{H} = \frac{1}{2} \hat{\Psi}^\dagger \begin{pmatrix} A & B \\ -B^* & -A^\dagger \end{pmatrix} \hat{\Psi} + \text{const.} \quad (66)$$

B.3 Fermionic Bogoliubov transformation and diagonalization

Canonical transformation in Nambu space. A fermionic Bogoliubov transformation is a linear change of operators

$$\hat{\Gamma} = \begin{pmatrix} \hat{\gamma} \\ \hat{\gamma}^\dagger \end{pmatrix} = W^\dagger \hat{\Psi},$$

such that the new operators $\hat{\gamma}_\alpha$ satisfy canonical anticommutation relations. Writing W in block form,

$$W = \begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix}, \quad \hat{\gamma} = U^\dagger \hat{c} + V^\dagger \hat{c}^\dagger, \quad (67)$$

the fermionic canonical conditions become

$$U^\dagger U + V^\dagger V = \mathbb{I}_N, \quad U^\top V + V^\top U = 0. \quad (68)$$

The first condition ensures proper normalization of quasiparticles, while the second encodes Pauli exclusion and forbids symmetric pairing channels.

With a suitable W , the BdG Hamiltonian can be diagonalized as

$$W^\dagger \mathcal{H}_{\text{BdG}} W = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \quad E_\alpha \geq 0,$$

leading to

$$\hat{H} = E_0 + \sum_{\alpha=1}^N E_\alpha \hat{\gamma}_\alpha^\dagger \hat{\gamma}_\alpha. \quad (69)$$

The ground state is the quasiparticle vacuum and is a Gaussian fermionic state fully characterized by two-point correlators.

B.4 Comparison with bosons: formal similarity and physical difference

Compact versus non-compact canonical groups. For bosons, a formally similar BdG construction exists, but the canonical conditions differ because commutators replace anticommutators. The bosonic Bogoliubov transformation must preserve $[\hat{\beta}_\alpha, \hat{\beta}_\beta^\dagger] = \delta_{\alpha\beta}$, leading to

$$U^\dagger U - V^\dagger V = \mathbb{I}_N, \quad U^\top V - V^\top U = 0.$$

The crucial difference is the sign in front of $V^\dagger V$: fermionic transformations form a compact group, while bosonic ones are symplectic and non-compact. As a result, fermionic BdG Hamiltonians are automatically stable once gapped, whereas bosonic BdG problems require additional positivity conditions to avoid dynamical instabilities.