Week 11

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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These notes are provided for the students of the class above only. There is no warranty for correctness, please contact me if you spot a mistake.

4.10 Attractive interactions, pairing

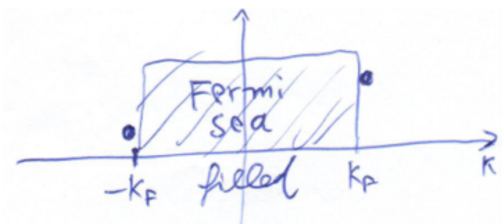
Lots of credit: Gora Shlyapnikov "Ultracold quantum gases, Degenerate Fermi gases". Part-II (internet).

- On first sight our previous discussion should be equally valid for weak attractive interactions ($U_0 < 0$ in Eq. (4.33)).
- However, another phenomenon precludes this, by making a filled Fermi-sea up to E_F, a bad starting point: Superfluid pairing.

4.10.1 Two-body Cooper-pairing

- The same pairing phenomenon gives rise to superconductivity in condensed matter systems (example D in section 2.3.1, free electron gas), we will discuss the condensed matter case here, not the cold-atom case, for a reason given at end of this section.

Assume a degenerate Fermi system at $T = 0 \implies$ all momentum states filled up to k_F. We assume for simplicity that these particles don't interact, but importantly Pauli-block all states up to $|k| = k_F$. (see section 2.2.2):



Now we add two interacting particles on top of this Fermi-sea, with Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla^2_{\mathbf{x}_1} + \nabla^2_{\mathbf{x}_2}) + V(\underbrace{\mathbf{x}_1 - \mathbf{x}_2}_{\equiv \mathbf{r}}). \tag{4.41}$$

We make the Ansatz

$$\psi_0(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2\pi}^3}\int d^3\mathbf{k}\frac{g_\mathbf{k}}{\sqrt{\mathcal{V}}}\underbrace{\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2))}_{\text{symmetric}}\frac{1}{\sqrt{2}}[\underbrace{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}_{\text{anti-symmetric}}] \tag{4.42}$$

for the complete wavefunction including relative motion and spin, but ignoring the irrelevant center-of-mass co-ordinate. Note that the Ansatz has the correct symmetry for Fermions.

Insertion into relative-motion Schrödinger equation following from (4.41):

$$\int d^3\mathbf{k}\underbrace{\frac{\hbar^2\mathbf{k}^2}{m}}_{\equiv 2\epsilon_\mathbf{k}} g_\mathbf{k}\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2))+V(\mathbf{x}_1-\mathbf{x}_2)\int d^3\mathbf{k}\;\; g_\mathbf{k}\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)) = E\int d^3\mathbf{k}\;\; g_\mathbf{k}\cos(\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)). \tag{4.43}$$

($\hat{H}$ is spin independent)

- Write $\cos(\mathbf{kr}) = \frac{1}{2}(e^{i\mathbf{kr}} + e^{-i\mathbf{kr}})$, then apply on both sides $\frac{1}{\sqrt{2\pi}^3}\int d^3\mathbf{r}\, e^{-i\mathbf{k}'\mathbf{r}}$... and use that $\int d^3\mathbf{r}\, e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}} = (2\pi)^3\delta(\mathbf{k}'-\mathbf{k})$:

$$2\epsilon_{\mathbf{k}'}\underbrace{\frac{(g_{\mathbf{k}'}+g_{-\mathbf{k}'})}{2}}_{\substack{= g_{\mathbf{k}'}\text{ assume}\\ \text{symmetric}}} - Eg_{\mathbf{k}'} = -\frac{1}{(2\pi)^3}\int d^3\mathbf{k}\int d^3\mathbf{r}\, e^{-i\mathbf{k}'\mathbf{r}}V(\mathbf{r})\frac{g_\mathbf{k}}{2}(e^{i\mathbf{kr}} + e^{-i\mathbf{kr}}). \tag{4.44}$$

We define:

$$V_{\mathbf{k}'\mathbf{k}} = \frac{1}{(2\pi)^3}\int d^3\mathbf{r}\, e^{-i\mathbf{k}'\mathbf{r}}V(\mathbf{r})\, e^{i\mathbf{kr}}$$

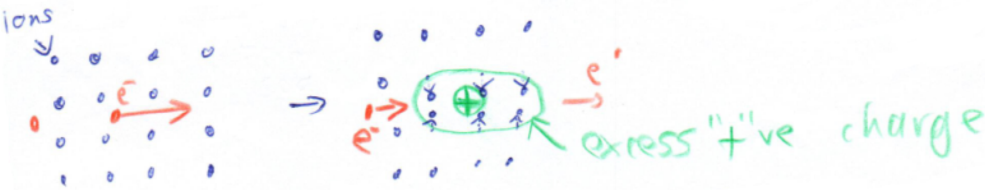
and then can write (4.44) as

$$\Longrightarrow\; g_{\mathbf{k}'}(2\epsilon_{\mathbf{k}'} - E) = -\frac{1}{2}\int d^3\mathbf{k}\;\; (V_{\mathbf{k}'\mathbf{k}}\, g_\mathbf{k} + V_{\mathbf{k}'(-\mathbf{k})}\, g_\mathbf{k}). \tag{4.45}$$

Before proceeding, let us now ask how or why our two Fermions on top of the Fermi sea would interact, for the specific case of electron in a solid crystal.

Electrons in crystal:

- Surprisingly these effectively experience a weakly attractive interaction due to phonon-exchange.



- Negative charge of electron causes distortion of positively charged ion lattice with a lot of delay, due to inertia of the ions. The resulting local excess charge after the ions have finally moved, can attract another electron, see sketch.

- This effect can even be dominant over the direct $e^- - e^-$ Coulomb repulsion for large distances between the electrons, since the direct Coulomb interaction is heavily screened by the crystal ions.

- A QM treatment of the phonon mediated interactions in the figure, gives an energy cutoff for these interactions at the Debye frequency $\hbar\omega_D$, or equivalently a momentum cutoff $\equiv \Delta k$.

We thus take an attractive interaction for $V_{\mathbf{k}'\mathbf{k}}$ and assume it to be constant below the cutoff for simplicity:

$$V_{\mathbf{k}'\mathbf{k}} = \begin{cases} -|V| & ;\ k_F < |\mathbf{k}|, |\mathbf{k}'| < k_F + \Delta k \leftarrow \text{Debye cutoff} \\ 0 & ;\ \text{otherwise} \end{cases} \tag{4.46}$$

Hence $V_{\mathbf{k}'\mathbf{k}} = V_{\mathbf{k}'(-\mathbf{k})}$. Setting $V_{\mathbf{k}'\mathbf{k}} = 0$ for $|\mathbf{k}|, |\mathbf{k}'| < k_F$ incorporates the fact that due to the filled Fermi sea in the background, electrons cannot get scattered to these momenta through any interaction [5].

Our Schrödinger equation (Eq. (4.45)) can then be written as

$$g_{\mathbf{k}'} = \frac{+|V|}{(2\epsilon_{\mathbf{k}'} - E)} \int d^3\mathbf{k}\Big|_{\mathbf{k}:k_F<|\mathbf{k}|<k_F+\Delta k} g_{\mathbf{k}} \tag{4.47}$$

Next we perform the integral $\int d^3\mathbf{k}$ on both sides and cancel terms $\int d^3\mathbf{k} g_{\mathbf{k}}$, to reach

$$\frac{1}{|V|} = \int d^3\mathbf{k}\Big|_{\mathbf{k}:k_F<|\mathbf{k}|<k_F+\Delta k} \frac{1}{(2\epsilon_{\mathbf{k}} - E)}.$$

We convert the integral to spherical polar coordinates and reach

$$\frac{1}{|V|} = (4\pi) \int_{k_F}^{k_F+\Delta k} dk \frac{k^2}{(2\epsilon_k - E)}. \tag{4.48}$$

[5] Note, that we can interpret $\mathbf{k}$ as indicating both$^{(*)}$, the relative momentum of the pair $\mathbf{p}_{rel} = \hbar\mathbf{k}$, or the momentum of one of the members of the pair, e.g. $\mathbf{p}_1 = \hbar\mathbf{k}$ (the other member has momentum $\mathbf{p}_2 = -\mathbf{p}_1$ in that case. The constraints written above on possible values of $\mathbf{k}$ arise from the latter view.

$^{(*)}$ *[This slightly confusing fact is due to the need to have CM momentum $\mathbf{k}_{CM} \approx 0$ and the relative momentum being defined as $\mathbf{p}_{rel} = (\mathbf{p}_1 - \mathbf{p}_2)/2$. See some texts on QM of the two-body problem. One way to justify this, is that we want $[\hat{\mathbf{r}}, \hat{\mathbf{p}}_{rel}] = i\hbar$, where $\hat{\mathbf{r}} = \hat{\mathbf{x}}_1 + \hat{\mathbf{x}}_2$]*

Change integration variable to energy $dk = m/\hbar^2 k\, d\epsilon$

$$\frac{1}{|V|} = \left(\frac{4\pi m}{\hbar^2}\right) \int_{\epsilon_F}^{\epsilon_F+\hbar\omega_D} d\epsilon \frac{\overbrace{k}^{\approx k_F \text{ due to } \hbar\omega_D \ll \epsilon_F}}{(2\epsilon - E)}. \tag{4.49}$$

We finally arrive at

$$\frac{1}{|V|} = \mathcal{N} \int_{\epsilon_F}^{\epsilon_F+\hbar\omega_D} \frac{d\epsilon}{(2\epsilon - E)} = \frac{\mathcal{N}}{2} \log\left(\frac{2E_F - E + 2\hbar\omega_D}{2E_F - E}\right), \tag{4.50}$$

where we have used the shortcut notation $\mathcal{N} = 4\pi m k_F/\hbar^2$. For $\mathcal{N}|V| \ll 1$ (weak coupling approximation), we can solve this for E and then obtain the

Cooper pair energy:

$$E_{\text{pair}} = E = 2E_F - 2\hbar\omega_D \exp\left[-\frac{2}{\mathcal{N}|V|}\right]. \tag{4.51}$$

(size $\gg$ inter-particle distance in medium)

Comments:

- $E < 2E_F$ for arbitrarily weak interactions. This signals an instability of the Fermi-sea towards bound states (Cooper pairs) (relative to E_F). (Unlike the repulsion case, non-interacting scenario is not a good starting point here.)
- A cooper pair is a bound state of Fermions above the Fermi sea, bound together by very weak attractive, phonon-mediated interactions.
- In the discussion in this section, we only concluded that the Cooper pair is a bound-state since the pairing gives a negative energy shift to the energy of two unpaired Fermions on the Fermi surface. This view is further corroborated when evaluating the coefficients $g_{\mathbf{k}}$ to first write the wave function of a Cooper pair first in Fourier space, and then in position space. One finds a wavefunction for relative motion $\psi_0(\mathbf{x}, \mathbf{y})\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, with symmetric $\psi_0(\mathbf{x}, \mathbf{y})$, that goes to zero for large $|\mathbf{x} - \mathbf{y}|$, hence is a bound state. See [A. Kadin, Journal of Superconductivity and Novel Magnetism, "*Spatial Structure of the Cooper Pair*" (2007)] for a discussion of the spatial Cooper pair wave function.
- For repulsive interactions $E > 2E_F$ (no problem).
- Without blocked Fermi-sea (let $\int_0^{\hbar\omega_D} d\epsilon$ in Eq. (4.50)), we get $E > 0$ (no bound states).
- The size (orbital radius)(of a Cooper pair is typically much larger than the inter-particle distance in medium.
- Without Debye cutoff: Eq. (4.50) is UV divergent $\rightarrow$ need regularisation/renormalisation, see section 3.5.2.

The last point is the reason why we did the calculation for a solid-state setup rather cold atom Fermion gases: In the Fermi-gas there is no natural cutoff, so the calculation would need renormalisation, which we want to avoid here. But Cooper-pairs form in cold atomic Fermi gases for the same reason as in an electron gas. One finds a

Cooper pair energy in an atomic Fermi gas that is a spin-mixture of $\uparrow$ and $\downarrow$:

$$E_{\text{pair}} = E = 2E_F - 2E_F \exp\left[-\frac{\pi}{2k_F|a_s|}\right]. \tag{4.52}$$

This sets the right order of magnitude.

- Roughly, to reach this keep variable k in Eq. (4.49), change cutoff from $\hbar\omega_D$ to $\to E_F$ and use $|V| = 4\pi\hbar^2|a_s|/m$.

4.10.2 Many Cooper pairs

- In the previous section we saw that an attractively interacting degenerate Fermi-gas is unstable to pair formation, but we dealt with a single pair. What happens for many?
- Tight pairs (molecules) would be Bosons, they could condense. What does that cause? But these pairs are not that tightly bound....
- Also: Now we also want to include all versus all interactions, not just among a single pair as in section 4.10.

As we did in section 3.3.2 for a BEC, we want to build the statements above into a useful mathematical Ansatz for the many-body wave function. Unlike there, we would want to now describe the condensation of pairs.

In first quantization, we could write

$$\psi(\mathbf{x}) = \hat{\mathcal{P}}_F \left[\psi_0(x_1, x_2)\psi_0(x_3, x_4)...\psi_0(x_{N-1}, x_N)\right], \tag{4.53}$$

where ψ_0 is the pairing wave function we had found in section 4.10.1. Here, $\hat{\mathcal{P}}_F$ is the anti-symmetrisation operator introduced in Eq. (2.1).

We could write Eq. (4.53) more elegantly as

$$\hat{c}^{\dagger^N}|0\rangle$$

for N Cooper pairs, with

$$\hat{c}^\dagger = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x}, \mathbf{y})\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{y}), \tag{4.54}$$

the Cooper-pair creation operator.[6]

Using the operator (4.54), we could write a Cooper pair condensate as a

Coherent state of pairs

$$|\psi_{\mathrm{BCS}}\rangle = \mathcal{N} e^{\gamma \hat{c}^\dagger} |\, 0 \,\rangle \tag{4.55}$$

where, $\mathcal{N}$ is normalisation factor, and γ the complex number characterising the coherent state (c.f. α in (2.42)).

- If $\hat{c}^\dagger$ was a bosonic operator, this would be analogous to our earlier treatments of BEC. But in general, we can neither clearly associate commutation, nor anti-commutation relations with $\hat{c}^\dagger$.
- We need some more powerful theory....

4.10.3 BCS-Theory

Let us consider the BCS Many-body theory of Fermion pairing due to Bardeen-Cooper-Schrieffer, which also explains superconductivity. Instead of attempting to deal with Cooper pairs, this starts out with the following trick Where for a BEC, we had assumed a non-zero mean-field, now we can assume a

non-zero pairing-field: (also "**Order parameter**")

$$0 \neq \Delta(\mathbf{x}) = U_0 \langle \hat{\Psi}_\uparrow(\mathbf{x}) \hat{\Psi}_\downarrow(\mathbf{x}) \rangle \tag{4.56}$$

- It shall turn out only after we did the ensuing calculation, that this assumption is in fact related to Cooper pairing.
- Clearly (4.56) involves an assumption on the many-body quantum state. All states that we find in the following, have to be checked for consistency with (4.56) in the end.
- For the moment just take (4.56) as a mathematical assumption, and let's see where it leads us....

[6] To see that this name makes sense, write $\hat{c}^\dagger |\, 0 \,\rangle$ and apply the field operators to the vacuum to reach a Fermionic Fock state $|\, \mathbf{y} \downarrow, \mathbf{z} \uparrow \rangle$ expressed using the position basis. Then write the position-space representation: $\langle\, \mathbf{x}'\mathbf{y}' \,| \hat{c}^\dagger |\, 0 \,\rangle$. Using $\langle\, \mathbf{x} \,|\, \mathbf{x}' \,\rangle = \delta(\mathbf{x} - \mathbf{x}')$, you should find the result discussed at the end of section 4.10.1.

From these initial considerations, we will now approximately diagonalize the interacting Hamiltonian (4.30) with $U_0 < 0$, assuming equal numbers of $\uparrow, \downarrow$ Fermions in a homogeneous system.

We "simplify" the interaction term as

$$U_0 \hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) \approx \frac{1}{2}\Big\{\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\rangle\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \langle\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x}) + \langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle\psi^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x}) \tag{4.57}$$

$$+ \langle\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle\psi^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) - \Big(\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle\psi^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \langle\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle\psi^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\Big)\Big\}. \tag{4.58}$$

Comments:

- This is motivated again by Wick's theorem (3.86), use Fermionic signs as discussed earlier.
- Wick's theorem gets some minus signs when Fermions are involved.
- The red factor of 1/2 is required to make the assumption consistent with Wick's theorem. I am confused as it is not there in some of the literature.

We further define:

Hartree fields	$\mathcal{U}_\uparrow(\mathbf{x}) = U_0\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x})\rangle$	(same for $\downarrow$)	(4.59)
Fock fields	$\mathcal{F}_\uparrow(\mathbf{x}) = U_0\langle\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle$	(same for $\uparrow\leftrightarrow\downarrow$)	(4.60)

- In the paired state (Eq. (4.55)), $\mathcal{F}_{\uparrow,\downarrow} = 0$ (Proof $\rightarrow$ Assignment 6).
- In a homogeneous system, $\Delta(\mathbf{x}) = \Delta$ ($\Delta \in \mathbb{R}$), $\mathcal{U}_\uparrow(\mathbf{x}) = \mathcal{U}_\downarrow(\mathbf{x}) = U$ can be constant. Note: $U \neq U_0$, but includes it.

From (4.58) we now have:

$$U_0 \hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) \approx \Delta^*\hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \Delta\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{x}) + U\big(\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \hat{\Psi}^\dagger_\downarrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\big).$$

Finally, we re-assemble the Hamiltonian (4.30) and augment it to a grand-canonical one $\hat{K} = \hat{H} - \mu\hat{N}$:

$$\hat{K} = \sum_{s=\uparrow,\downarrow} \int d^3\mathbf{x}\, \hat{\Psi}_s^\dagger(\mathbf{x}) \Big[-\frac{\hbar^2\nabla^2}{2m} + U - \mu \Big] \hat{\Psi}_s(\mathbf{x})$$
$$+ \int d^3\mathbf{x} \Big[\Delta^* \hat{\Psi}_\downarrow(\mathbf{x})\hat{\Psi}_\uparrow(\mathbf{x}) + \Delta\, \hat{\Psi}_\uparrow^\dagger(\mathbf{x})\hat{\Psi}_\downarrow^\dagger(\mathbf{x}) \Big].$$

In the homogeneous case, it is again simpler to work in the momentum basis. As we did for (4.33), we reach the

BCS/pairing Hamiltonian:

$$\hat{K} = \hat{H}_{\text{BCS}} = \sum_{\mathbf{k},s=\uparrow,\downarrow} \xi_\mathbf{k} \hat{a}_{\sigma\mathbf{k}}^\dagger \hat{a}_{\sigma\mathbf{k}} + \Delta \sum_\mathbf{k} \left(\hat{a}_{\downarrow\mathbf{k}} \hat{a}_{\uparrow(-\mathbf{k})} + \hat{a}_{\uparrow(-\mathbf{k})}^\dagger \hat{a}_{\downarrow\mathbf{k}}^\dagger \right) \tag{4.61}$$

where,

$$\xi_\mathbf{k} = \frac{\hbar^2 k^2}{2m} + U - \mu.$$

- In section 3.4, we had kept only Bose-gas excitations up to order $\hat{\chi}^2$, and then diagonalized the Hamiltonian using the Bogoliubov transformation (e.g. Eq. (3.66)).
- This trick works generically for Hamiltonians up to quadratic in $\hat{a}$, $\hat{a}^\dagger$, thus also here, for Eq. (4.61) . Here we define the

Bogoliubov-transformation (BCS-system)

$$\hat{\alpha}_{\uparrow\mathbf{k}} = u_\mathbf{k} \hat{a}_{\uparrow\mathbf{k}} - v_\mathbf{k} \hat{a}_{\downarrow(-\mathbf{k})}^\dagger$$
$$\hat{\alpha}_{\downarrow\mathbf{k}} = u_\mathbf{k} \hat{a}_{\downarrow\mathbf{k}} + v_\mathbf{k} \hat{a}_{\uparrow(-\mathbf{k})}^\dagger \tag{4.62}$$

Comparison to BEC: In Chapter-3, we were more ambitious and did the Bogoliubov transformation directly for an inhomogeneous system. For the homogeneous case, Eq. (3.66) gives:

$$\hat{\alpha}_\mathbf{k} = u_\mathbf{k} \hat{a}_\mathbf{k} + v_\mathbf{k} \hat{a}_\mathbf{k}^\dagger, \tag{4.63}$$

which is quite similar to (4.62). To reach this, use $\hat{\Psi}(\mathbf{x}) = \int d^3\mathbf{k} \frac{\hat{a}_\mathbf{k}}{\sqrt{2\pi}^3} \varphi_\mathbf{k}(\mathbf{x})$ and the definition of a δ function.

The quasi-particle operators (Eq. (4.62)) should satisfy Fermi commutation relations:

$$\left\{ \hat{\alpha}_{s\mathbf{k}}, \hat{\alpha}_{s'\mathbf{k}'}^\dagger \right\} \stackrel{\text{exercise}}{=} (u_\mathbf{k}^2 + v_\mathbf{k}^2) \delta_{\mathbf{k}\mathbf{k}'} \delta_{ss'}.$$

We thus have to require the normalisation $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$.

Using the latter, we can derive the

inverse Bogoliubov transformation (Proof → exercise, signs might be wrong)

$$\hat{a}_{\uparrow\mathbf{k}} = u_{\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}$$
$$\hat{a}_{\downarrow\mathbf{k}} = u_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}. \tag{4.64}$$

Inserting Eq. (4.62) into Eq. (4.61) gives

$$\begin{aligned}\hat{K} = \sum_{\mathbf{k}} \Big\{ &\Big[\Big(\xi_{\mathbf{k}} u_{\mathbf{k}} + \Delta v_{\mathbf{k}}\Big) u_{\mathbf{k}} - \Big(\xi_{\mathbf{k}} v_{\mathbf{k}} - \Delta u_{\mathbf{k}}\Big) v_{\mathbf{k}}\Big]\Big(\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} + \hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\Big) \\ &+ \Big[\Big(\Delta v_{\mathbf{k}} + \xi_{\mathbf{k}} u_{\mathbf{k}}\Big) v_{\mathbf{k}} - \Big(\Delta u_{\mathbf{k}} - \xi_{\mathbf{k}} v_{\mathbf{k}}\Big) u_{\mathbf{k}}\Big]\Big(\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})} + \hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}}\Big) \\ &+ 2\xi_{\mathbf{k}} v_{\mathbf{k}}^2 - 2\Delta u_{\mathbf{k}} v_{\mathbf{k}} \Big\} \qquad \text{(steps see p.786)}\end{aligned}$$

Detailed steps: Note: ($u_{\mathbf{k}} = u_{-\mathbf{k}}$, $v_{\mathbf{k}} = v_{-\mathbf{k}}$ from parity invariance).

$$\begin{aligned}\hat{K} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \Big[&\overbrace{\Big(u_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}_{\downarrow(-\mathbf{k})}\Big)}^{\hat{a}^\dagger_{\uparrow\mathbf{k}}}\overbrace{\Big(u_{\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} - v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}\Big)}^{\hat{a}_{\uparrow\mathbf{k}}} + \overbrace{\Big(u_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\Big)}^{\hat{a}^\dagger_{\downarrow\mathbf{k}}}\overbrace{\Big(u_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\Big)}^{\hat{a}_{\downarrow\mathbf{k}}}\Big] \\ + \Delta\Big[&\underbrace{\Big(u_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\Big)}_{\hat{a}_{\downarrow\mathbf{k}}}\underbrace{\Big(u_{-\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})} - v_{-\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\Big)}_{\hat{a}_{\uparrow(-\mathbf{k})}} + \underbrace{\Big(u_{-\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} - v_{-\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\Big)}_{\hat{a}^\dagger_{\uparrow(-\mathbf{k})}}\underbrace{\Big(u_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} + v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\Big)}_{\hat{a}^\dagger_{\downarrow\mathbf{k}}}\Big] \\ = \sum_{\mathbf{k}} \xi_{\mathbf{k}}\Big[&u_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\downarrow(-\mathbf{k})}\hat{\alpha}_{\uparrow\mathbf{k}} + v_{\mathbf{k}}^2\hat{\alpha}_{\downarrow(-\mathbf{k})}\hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})} \\ &+ u_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}} + v_{\mathbf{k}}^2\hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\Big] \\ + \Delta\Big[&u_{\mathbf{k}}^2\hat{\alpha}_{\downarrow\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}} - v_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}} \\ &+ u_{\mathbf{k}}^2\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} + u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\uparrow(-\mathbf{k})} - u_{\mathbf{k}}v_{\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\downarrow\mathbf{k}} - v_{\mathbf{k}}^2\hat{\alpha}_{\downarrow\mathbf{k}}\hat{\alpha}_{\uparrow(-\mathbf{k})}\Big] \\ &\left(\text{Use } \sum_{\mathbf{k}} \xi_{\mathbf{k}}\hat{\alpha}^\dagger_{(-\mathbf{k})}\hat{\alpha}_{(-\mathbf{k})} = \sum_{\mathbf{k}} \xi_{\mathbf{k}}\hat{\alpha}^\dagger_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}, \text{ since } \xi_{\mathbf{k}} = \xi_{-\mathbf{k}}\right) \\ = \sum_{\mathbf{k}} \Big[&\xi_{\mathbf{k}}(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) + 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}\Big]\big(\hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\hat{\alpha}_{\uparrow\mathbf{k}} + \hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}_{\downarrow\mathbf{k}}\big) + \underbrace{2\xi_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}}_{\text{from commutators}} \\ + \Big[&2\xi_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} - (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2)\Delta\Big]\big(\hat{\alpha}^\dagger_{\downarrow\mathbf{k}}\hat{\alpha}^\dagger_{\uparrow(-\mathbf{k})} + \hat{\alpha}_{\uparrow(-\mathbf{k})}\hat{\alpha}_{\downarrow\mathbf{k}}\big)\end{aligned}$$

By demanding the

Bololiubov de Gennes equations (BCS, Fermions)

$$\xi_{\mathbf{k}} u_{\mathbf{k}} + \Delta v_{\mathbf{k}} = \epsilon_{\mathbf{k}} u_{\mathbf{k}}$$
$$-\xi_{\mathbf{k}} v_{\mathbf{k}} + \Delta u_{\mathbf{k}} = \epsilon_{\mathbf{k}} v_{\mathbf{k}}. \tag{4.65}$$

We diagonalize the Hamiltonian into

$$\hat{K} = E_0 + \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k},s} \hat{\alpha}_{\mathbf{k},s} \tag{4.66}$$

where, $E_0 = \sum_{\mathbf{k}} 2(\xi_{\mathbf{k}} v_{\mathbf{k}}^2 - \Delta u_{\mathbf{k}} v_{\mathbf{k}})$.

- This again has the form of non-interacting quasi-particles.

To find out more about the excitations of the system, we have to solve Eq. (4.65). In matrix form

$$\begin{pmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \epsilon_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}. \tag{4.67}$$

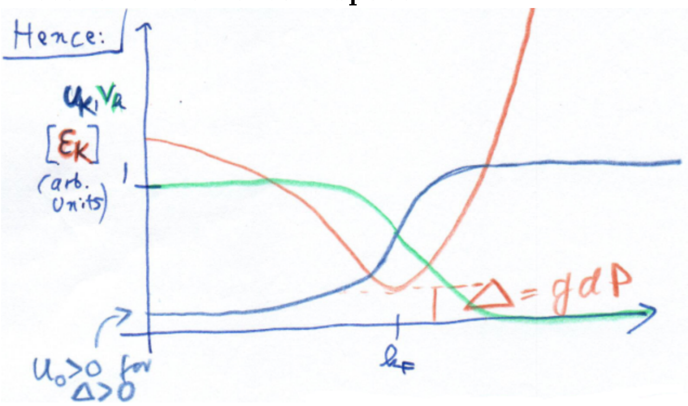
Using also $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$, we proceed as for (3.68). The solutions are:

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right), v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right), \epsilon_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} \tag{4.68}$$

for particle amplitude $u_{\mathbf{k}}$, hole amplitude $v_{\mathbf{k}}$ and dispersion relation, quasiparticle-energy $\epsilon_{\mathbf{k}}$.

- Recall $\xi_{\mathbf{k}} = \hbar^2 \mathbf{k}^2/2m + U - \mu = \hbar^2 \mathbf{k}^2/2m - \tilde{\mu}$ (see Eq. (4.61)), using $\tilde{\mu} = \mu - U$.
- $\tilde{\mu}$ is the Fermi-energy at $T = 0$.

Picture in momentum space:



- k_f comes in via $\mu = E_F$.
- Behavior of u, v logical from particle/hole excitation interpretation (look at $\alpha^\dagger$). Above the Fermi energy, there are no holes to make.
- Crucial feature of dispersion relation is the energy gap $\epsilon_{\min} = \Delta$. Thus, if $\Delta > 0$, ϵ_k is never zero.

Discussion of diagonalized Hamiltonian (4.66):

Ground state:

Already from (Eq. (4.66)), we can understand the system better:

- As was the case for Bose-gas, the ground state of the system is one with no quasi-particles (c.f. Eq. (3.63)). We call this state the quasi-particle vacuum $|\psi_0\rangle$, and define it via

$$\hat{\alpha}_{s\mathbf{k}}|\psi_0\rangle = 0. \tag{4.69}$$

(compare $\hat{\alpha}_{s\mathbf{k}}|\,0\,\rangle = 0$ for the bare vacuum)

- We can easily write one such state explicitly, namely

$$|\psi_0\rangle = \prod_{\mathbf{k}'s'} \hat{\alpha}_{\mathbf{k}'s'}|\,0\,\rangle \tag{4.70}$$

Reason: This works since $\hat{\alpha}^2_{s\mathbf{k}} = 0$ (from $\{\hat{\alpha}_{s\mathbf{k}}, \hat{\alpha}_{s\mathbf{k}}\} = 0$).

We can then use Eq. (4.62) to explicitly obtain the

BCS state:

$$|\psi_{\text{BCS}}\rangle = |\psi_0\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}\uparrow}\hat{a}^\dagger_{(-\mathbf{k})\downarrow})|\,0\,\rangle. \tag{4.71}$$

- To see this, start by first evaluating $\hat{\alpha}_{\downarrow(-\mathbf{k})}\hat{\alpha}_{\uparrow(\mathbf{k})}|\,0\,\rangle = \cdots = v_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}\uparrow}\hat{a}^\dagger_{(-\mathbf{k})\downarrow})|\,0\,\rangle$. Then do the same for all other $\mathbf{k}'$. Finally a factor $\prod_{\mathbf{k}} v_{\mathbf{k}}$ is taken care of by normalising the state.
- Each possible pair can be either occupied (v) or unoccupied (u).

Ground state energy:

We can now verify that the pairing assumption $\Delta \neq 0$ has lowered the energy compared to the unpaired Fermi-sea.

$$\langle\psi_{\mathrm{BCS}}|\hat{K}|\psi_{\mathrm{BCS}}\rangle - \langle FS|\hat{K}|FS\rangle = \sum_{\mathbf{k}} \big(\underbrace{2\xi_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\Delta u_{\mathbf{k}}v_{\mathbf{k}}}_{E_0,\text{ see (4.66)}}\big) - \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} \underbrace{2}_{\substack{\text{spin}\\ \uparrow\downarrow}} \underbrace{\xi_{\mathbf{k}}}_{\substack{\text{energy relative}\\ \text{to Fermi-sea}}}$$

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

$$= \sum_{\mathbf{k}} \{2v_{\mathbf{k}}\underbrace{(\xi_{\mathbf{k}}v_{\mathbf{k}} - \Delta u_{\mathbf{k}})}_{\substack{= -\epsilon_{\mathbf{k}}v_{\mathbf{k}}\\ Eq.\ (4.65)}}\} - \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} 2\xi_{\mathbf{k}} \overset{*}{=} \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} \{-2\epsilon_{\mathbf{k}}v_{\mathbf{k}}^2 - 2\xi_{\mathbf{k}}\}$$

$$\overset{\text{Eq. (4.68)}}{=\!=} \sum_{\mathbf{k}}^{|\mathbf{k}|<k_F} (-\epsilon_{\mathbf{k}}\left(1 - \frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right) - 2\xi_{\mathbf{k}}) = \sum_{\mathbf{k}} \underbrace{(\underbrace{-\xi_{\mathbf{k}}}_{>0} - \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2})}_{<0}$$

(*): The reason we can restrict the first sum also to $|\mathbf{k}| < k_F$ is that $v_{\mathbf{k}}^2 \to 0$ for $|k| > k_F$, see figure on page 98

- Overall we lower the total energy of the system only for a non-zero gap Δ.

We can now finally actually see that the BCS state we got is the pair-coherent state we guessed in Eq. (4.55). By going to Fourier-space, we can rewrite the pair operator

$$\hat{c}^\dagger = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y})\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{y}) \qquad \text{(see Eq. (4.54))}$$

as

$$\hat{c}^\dagger = \sum_{\mathbf{k}} \varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}. \tag{4.72}$$

(see details A below). Then, using Campbell Baker Hausdorff formula (see assignment 2) and $[\hat{a}^\dagger_{\mathbf{k}}\hat{a}^\dagger_{(-\mathbf{k})}, \hat{a}^\dagger_{\mathbf{k}'}\hat{a}^\dagger_{(-\mathbf{k}')}] = 0$ (see details A&B below)

$$\mathcal{N}e^{\gamma\hat{c}^\dagger} = \mathcal{N}e^{\sum_{\mathbf{k}}\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}} \overset{(*)}{=\!=} \mathcal{N}\prod_{\mathbf{k}} e^{\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}}$$
$$\overset{\text{Fermions}}{=\!=} \mathcal{N}\prod_{\mathbf{k}}\left(1+\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right).$$

With moving $\mathcal{N}$ into the product (detail C below), we reach the the form

BCS state as coherent pair state

$$|\psi_{\text{BCS}}\rangle = e^{\gamma\hat{c}^\dagger}|\,0\,\rangle = \prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right)|\,0\,\rangle \tag{4.73}$$

Proof details
A:

$$\hat{c}^\dagger = \int d^3\mathbf{x}\int d^3\mathbf{y}\,\varphi_0(\mathbf{x},\mathbf{y})\hat{\Psi}^\dagger_\uparrow(\mathbf{x})\hat{\Psi}^\dagger_\downarrow(\mathbf{y})$$
$$\left(\text{Use } \hat{\Psi}_\uparrow(\mathbf{x}) = \sum_{\mathbf{k}}\frac{1}{\sqrt[3]{2\pi}}\hat{a}_{\uparrow\mathbf{k}}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{\mathcal{V}}}\right)$$
$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}'}\frac{1}{(2\pi)^3}\int d^3\mathbf{x}\int d^3\mathbf{y}\varphi_0(\mathbf{x}-\mathbf{y})e^{-i\mathbf{k}\cdot\mathbf{x}}e^{-i\mathbf{k}'\cdot\mathbf{y}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}'}$$

change to relative and C.M. co-ordinates $\mathbf{r} = \mathbf{x}-\mathbf{y},\ \mathbf{R} = (\mathbf{x}+\mathbf{y})/2$

$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}'}\frac{1}{(2\pi)^3}\int d^3\mathbf{r}\int d^3\mathbf{R}\varphi_0(\mathbf{r})e^{-i\mathbf{k}\cdot(\mathbf{R}-\frac{\mathbf{r}}{2})}e^{-i\mathbf{k}'\cdot(\mathbf{R}+\frac{\mathbf{r}}{2})}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}'}$$
$$= \frac{1}{\mathcal{V}}\sum_{\mathbf{k},\mathbf{k}'}\underbrace{\left(\frac{\int d^3\mathbf{r}}{\sqrt[3]{2\pi}}\varphi_0(\mathbf{r})e^{-i(\frac{\mathbf{k}'-\mathbf{k}}{2})\cdot\mathbf{r}}\right)}_{F.T.\ \tilde{\varphi}_0\left(\frac{\mathbf{k}'-\mathbf{k}}{2}\right)}\underbrace{\left(\frac{\int d^3\mathbf{R}}{\sqrt[3]{2\pi}}e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{R}}\right)}_{=\sqrt[3]{2\pi}\delta(\mathbf{k}+\mathbf{k}')}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}'}$$
$$= \sum_{\mathbf{k}}\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\ \text{ with } \varphi_{\mathbf{k}} = \frac{\sqrt[3]{2\pi}\tilde{\varphi}_0(-\mathbf{k})}{\mathcal{V}}.$$

B:

$$\left[\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}}, \hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow\mathbf{k}'}\right] = \hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow\mathbf{k}'} - \hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow\mathbf{k}'}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow\mathbf{k}} \overset{\text{use anti-}}{\underset{\text{commutators}}{=\!=}} 0$$

C: Determine $\mathcal{N}$ for which $|\,\psi_{pair}\,\rangle \equiv \mathcal{N}\prod_{\mathbf{k}}\left(1+\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right)$ is normalized $\langle\,\psi_{pair}\,|\,\psi_{pair}\,\rangle = 1$. Let us rewrite $|\,0\,\rangle = |\,0_{\mathbf{k}\uparrow}, 0_{\mathbf{k}\downarrow}, 0_{-\mathbf{k}\uparrow}, 0_{-\mathbf{k}\downarrow}\,\rangle \otimes |\,0_{\text{other }\mathbf{k}}\,\rangle$, where we have singled out the Fock space occupations for the forward and backward direction of a specific $\mathbf{k}$, with all possible spins. Since $\hat{a}_{\pm\mathbf{k}'}$ for any other $\mathbf{k}' \neq \mathbf{k}$ do not affect this sub-space, we can calculate normalisation separately in each of these segments. Then

$$\langle\,\psi_{pair}\,|\,\psi_{pair}\,\rangle = \mathcal{N}^2 \prod_{\mathbf{k},\mathbf{k}'} \langle\,0\,|\left(1+\gamma^*\varphi^*_{\mathbf{k}}\hat{a}_{\downarrow(-\mathbf{k})}\hat{a}_{\uparrow\mathbf{k}}\right)\left(1+\gamma\varphi_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}}\hat{a}^\dagger_{\downarrow(-\mathbf{k})}\right)|\,0\,\rangle$$

$$= \mathcal{N}^2 \prod_{\mathbf{k},\mathbf{k}'(halfspace)} \langle\,0\,|\left(1+\gamma^*\varphi^*_{\mathbf{k}}\hat{a}_{\downarrow(-\mathbf{k})}\hat{a}_{\uparrow\mathbf{k}}\right)\left(1+\gamma^*\varphi^*_{-\mathbf{k}}\hat{a}_{\downarrow(\mathbf{k})}\hat{a}_{\uparrow(-\mathbf{k})}\right)$$

$$\times\left(1+\gamma\varphi'_{\mathbf{k}}\hat{a}^\dagger_{\uparrow\mathbf{k}'}\hat{a}^\dagger_{\downarrow(-\mathbf{k}')}\right)\left(1+\gamma\varphi_{-\mathbf{k}'}\hat{a}^\dagger_{\uparrow(-\mathbf{k}')}\hat{a}^\dagger_{\downarrow\mathbf{k}'}\right)|\,0\,\rangle \tag{4.74}$$

In the second equality we have split the products over $\mathbf{k}$ such that the symbol only contains half of space (say with positive k_x) and the pieces in the other half are made explicit by writing a part with $\mathbf{k}\to(-\mathbf{k})$. We can now collect the combination in which operators may act so that rhs and lhs are not orthogonal in the end. You shall find

$$\langle\,\psi_{pair}\,|\,\psi_{pair}\,\rangle = \mathcal{N}^2 \prod_{\mathbf{k},\mathbf{k}'(halfspace)} \left(1+|\gamma|^2|\varphi_{\mathbf{k}}|^2\right)\left(1+|\gamma|^2|\varphi'_{\mathbf{k}}|^2\right) = \mathcal{N}^2\left(\prod_{\mathbf{k}(halfspace)}\left(1+|\gamma|^2|\varphi_{\mathbf{k}}|^2\right)\right)^2$$

$$\stackrel{\varphi_{\mathbf{k}}=\varphi_{-\mathbf{k}}}{=} \mathcal{N}^2\prod_{\mathbf{k}}\left(1+|\gamma|^2|\varphi_{\mathbf{k}}|^2\right) \tag{4.75}$$

We now see that a way to normalize the state is the choice $\mathcal{N}=\prod_{\mathbf{k}}\frac{1}{\sqrt{1+|\gamma|^2|\varphi_{\mathbf{k}}|^2}}$. Inserting this into $|\,\psi_{pair}\,\rangle$ and distributing each factor for $\mathbf{k}$ from $\mathcal{N}$ onto the main expression gives the form (4.73) if we call $u_{\mathbf{k}}=1/\sqrt{1+|\gamma|^2|\varphi_{\mathbf{k}}|^2}$ and $v_{\mathbf{k}}=\gamma\varphi_{\mathbf{k}}/\sqrt{1+|\gamma|^2|\varphi_{\mathbf{k}}|^2}$.

4.10.4 Self consistency of BCS-Theory

Before we move to the consequences of the gap, let us calculate it. (Recall, we just assumed $\langle\hat{\Psi}\hat{\Psi}\rangle=\Delta$ at the onset of section 4.10.3.)

Recall that the BCS calculation started with an input non-vanishing pairing field $\Delta=U_0\langle\hat{\Psi}_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle$. Now we have actually found the quantum ground state with which to evaluate the right hand side, namely (4.71). That state depends on u, v and these in turn depend on Δ through (4.65). We now have to check that the theory is self consistent, which means we can correctly get Δ out, when we evaluate $U_0\langle\hat{\Psi}_\uparrow(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle$.

Starting state (**): We assume $\langle\ \rangle$ pertains to a Fock-state (or thermal mixture of those) with $N_{\mathbf{k}}$ Bogoliubov excitations in mode k. For all $N_{\mathbf{k}}=0$, this includes the BCS ground state (4.71).

Let us evaluate the pairing field. Since we are in a homogenous system $\Delta(\mathbf{x})$ does not depend on $\mathbf{x}$ and is equal to its mean value over space $\Delta=\int d^3\mathbf{x}\,\Delta(\mathbf{x})/\mathcal{V}$, where $\mathcal{V}$ is some quantisation volume.

Then

$$\Delta = U_0 \int d^3\mathbf{x} \langle \hat{\Psi}_\uparrow(\mathbf{x}) \hat{\Psi}_\downarrow(\mathbf{x}) \rangle / \mathcal{V} = \frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \langle \hat{a}_{\uparrow\mathbf{k}} \hat{a}_{\downarrow\mathbf{k}'} \underbrace{\int d^3\mathbf{x} \frac{\exp\left[i(\mathbf{k}+\mathbf{k}')\mathbf{x}\right]}{\mathcal{V}}}_{=\delta_{\mathbf{k},\mathbf{k}'}} \rangle$$

$$= \frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} \langle \hat{a}_{\uparrow\mathbf{k}} \hat{a}_{\downarrow(-\mathbf{k})} \rangle$$

$$\overset{\text{Eq. (4.64)}}{=\!=} \frac{U_0}{\mathcal{V}} \int d^3\mathbf{k} \big\langle \big(u_{\mathbf{k}} \hat{\alpha}_{\downarrow(-\mathbf{k})} + v_{\mathbf{k}} \hat{\alpha}^\dagger_{\uparrow\mathbf{k}}\big)\big(u_{\mathbf{k}} \hat{\alpha}_{\uparrow\mathbf{k}} - v_{\mathbf{k}} \hat{\alpha}^\dagger_{\downarrow(-\mathbf{k})}\big)\big\rangle$$

$$\overset{(**)}{=\!=} -\frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} (1 - 2N_{\mathbf{k}})$$

where,

$$N_{\mathbf{k}} = \frac{1}{\exp(\epsilon_{\mathbf{k}}/k_B T) + 1}.$$

We have $u_{\mathbf{k}} v_{\mathbf{k}} = \Delta/2\epsilon_{\mathbf{k}}$ from Eq. (4.68), hence

$$\Delta = -\frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}} \frac{\Delta}{2\epsilon_{\mathbf{k}}} (1 - 2\frac{1}{\exp(\epsilon_{\mathbf{k}}/k_B T) + 1}). \tag{4.76}$$

We divide both sides by Δ, use $U_0 = -|U_0|$ and reform exp into tanh and turn the sum into an integration to reach

the **gap-equation** (consistency condition)

$$|U_0| \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\tanh(\epsilon_{\mathbf{k}}/2k_B T)}{2\epsilon_{\mathbf{k}}} = 1. \tag{4.77}$$

- Here we really needed $U_0 < 0$, else this would not have a solution. That means that for repulsive interactions, our assumption of pairing $\Delta \neq 0$ could never be consistent.

At zero temperature:

$$|U_0| \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{2\sqrt{\Delta_0^2 + \xi_{\mathbf{k}}^2}} = 1. \tag{4.78}$$

The main contribution to the integral is from $|\mathbf{k}| \approx k_F$ (there the denominator is smallest, *see picture of* Δ *earlier*). Near k_F, we Taylor expand $\xi_{\mathbf{k}}$ to first order:

$$\xi_{\mathbf{k}} \approx \underbrace{\frac{\hbar^2 k_F^2}{2m}}_{E_F} + \underbrace{\frac{\hbar^2}{m} k_F}_{\hbar v_F}(k - k_F) + \mathcal{O}(k - k_F)^2 + U - \underbrace{\mu}_{=E_F}. \tag{4.79}$$

Also assuming small U, we then reach

$$|\xi_{\mathbf{k}}| \approx \hbar v_F(|\mathbf{k}| - k_F) \ll E_F. \tag{4.80}$$

and can find

$$\Longrightarrow |U_0|(4\pi)\int_0^{\overbrace{\kappa}^{\text{cutoff}}} dk \frac{k^2}{2\sqrt{\Delta_0^2+(\hbar v_F)^2(k-k_F)^2}} \underset{\text{integration}}{\overset{\text{nasty}}{=\!=}} \lambda \ln\left(\frac{\epsilon_{cut}}{\Delta_0}\right) \overset{!}{=} 1$$

where, after inserting $U_0 = 4\pi\hbar^2 a_s/m$,

$$\lambda = \frac{2k_F|a_s|}{\pi}. \tag{4.81}$$

We choose an energy-cutoff $\epsilon_{\text{cut}} = E_F = \hbar^2\kappa/2m$, then find

zero-temperature gap:

$$\Delta_0 = E_F \, \exp\left(-\frac{\pi}{2k_F|a_s|}\right) \ll E_F. \tag{4.82}$$

- Comparison with Eq. (4.52) now gives a neat interpretation: Since $\Delta_0 = 1/2|E_{\text{pair}} - 2E_F|$, i.e., half the binding energy of a Cooper pair: Excitations become gapped, since in order to make one, I would have to break a pair.
- Since we have found that $\Delta \neq 0$ in the end, we have in retrospect justified our initial assumption in (4.56). Thus the equation turned out self-consistent (iff, Δ is chosen as (4.82)).

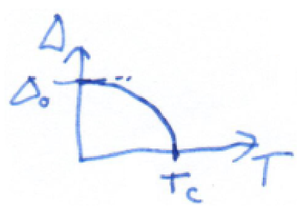
We could also evaluate Δ from Eq. (4.77) for $T > 0$ and would find

finite-temperature gap

$$\Delta = 3.06 T_c \left(1 - \frac{T}{T_c}\right)^{1/2} \tag{4.83}$$

and **critical temperature**

$$T_c \approx 0.57 \Delta_0 \ll T_F. \tag{4.84}$$



4.10.5 Fermionic superfluidity and superconductivity

Now we come to the main consequence of the paired ground-state and gapped excitation spectrum:

Return to our discussion in section 3.4.5 of conditions "when an obstacle with velocity $\mathbf{v}$ can create excitations within the quantum gas". Nothing there was specific to Bosons, so also for Fermions no excitations are possible below an obstacle velocity of

$$v_{\text{crit}} = \min_{\mathbf{k}} \left(\frac{\epsilon_{\mathbf{k}}}{\hbar \mathbf{k}} \right). \tag{4.85}$$

Wee see from Eq. (4.68) (and the plot underneath it), that

Fermion critical velocity for superconductivity

$$v_{\text{crit}} = \frac{\Delta}{\hbar k_F}. \tag{4.86}$$

Superfluidity arises here because we cannot create excitations of our Cooper-pair condensate.

Because the condensate again has a coherent order parameter $\Delta(\mathbf{r}) = \langle \hat{\Psi}_{\uparrow}(\mathbf{r}) \hat{\Psi}_{\downarrow}(\mathbf{r}) \rangle \in \mathbb{C}$, we again have the consequence of quantized-circulation $\implies$ vortices just as in a BEC.

This is used as an experimental signature of Fermionic superfluidity.

4.11 Outlook

- We looked only at $N_{\uparrow} = N_{\downarrow}$ = spin-balanced Fermi gases. New physics for spin-imbalanced $N_{\uparrow} \neq N_{\downarrow}$, or impurities $N_{\uparrow} = 1$, $N_{\downarrow} = N - 1 \rightarrow$ Polarons.
- Fermionic superfluidity and superconductivity are probably one of the most involved and surprising quantum-many-body effects.

  The effect is not there at all in a two-body picture.