(11)

4.9. Attractive interactions, pairing

- Lots of credit: Gora Shlyapnikov "Ultracold quantum Gases, Part-II Degenerate Fermi gases" → e.g. www.t-qc.ru/education/lecture-courses/uqg

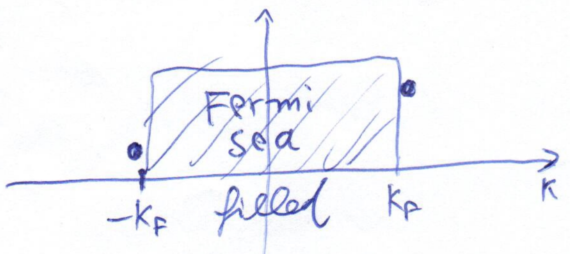
- On first sight our previous discussion should be equally valid for weak attractive interactions ($U_0 < 0$ in Eq. (4.24))

- However another phenomenon precludes this, by making a filled Fermi-sea up to E_F a bad starting point: Superfluid pairing.

4.9.1. Two-body Cooper-pairing

- The same pairing phenomenon gives rise to superconductivity in condensed matter systems (2.3.1. example D, electron gas & 4.4.), we will discuss that case (reason @ end of section)

Assume a degenerate Fermi system at $T=0$ ⇒ all momentum states filled up to k_F, these particles don't interact but Pauli-block all states up to $|k| = k_F$. (see section 2.2.4)



Now we add two interacting particles on top of Fermi sea

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\nabla^2_{x_1} + \nabla^2_{x_2}\right) + V(\underbrace{\vec{x}_1 - \vec{x}_2}_{\equiv \vec{r}}) \qquad (4.30)$$

We make Ansatz

$$\varphi_0(\vec{x}_1, \vec{x}_2) = \sum_{k} \frac{g_k}{\sqrt{\mathcal{V}}} \underbrace{\cos(\vec{k}(\vec{x}_1 - \vec{x}_2))}_{\text{symmetric}} \underbrace{\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]/\sqrt{2}}_{\text{anti-symmetric}} \qquad (4.31)$$

for the wavefunction of relative motion.
(c.m. co-ordinate, ignored here)

sertion into relative-motion Schrödinger eqn:

$$\sum_k \underbrace{\frac{\hbar^2 k^2}{m}}_{\equiv 2\varepsilon_k} g_k \cos(\vec{k}(\vec{x}_1-\vec{x}_2)) + V(x_1-x_2)\sum_k g_k \cos(k(x_1-x_2)) = E\sum_k g_k \cos(k(x_1-x_2)) \qquad (4.32)$$

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

- Write $\cos(kr) = \frac{1}{2}(e^{ikr}+e^{-ikr})$, then both sides $\frac{1}{\sqrt{\mathcal{V}}}\int dr\, e^{-ik'r}\dots$

$$2\varepsilon_{k'}\underbrace{\frac{g_{k'}+g_{-k'}}{2}}_{=g_{k'} \text{ assume symmetric}} - E g_{k'} = -\frac{1}{\mathcal{V}}\int d^3r\, e^{-ik'r}\, V(r)\sum_k \frac{g_k}{2}\left(e^{ikr}+e^{-ikr}\right) \qquad (4.33)$$

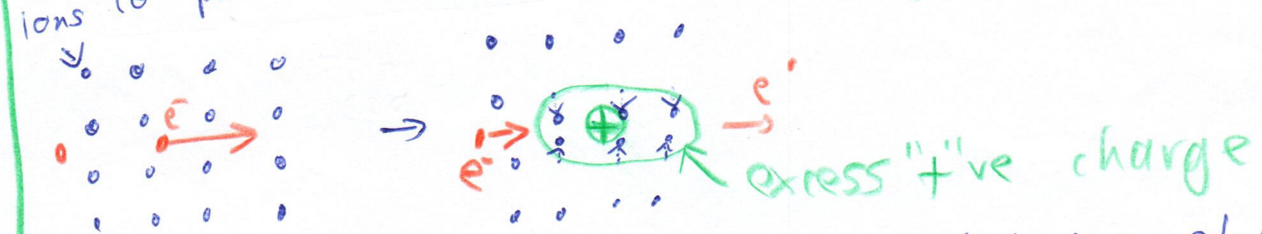
$\Rightarrow$

We define $V_{k'k} = \frac{1}{\mathcal{V}}\int d^3r\, e^{-ik'r}\, V(r)\, e^{ikr}$

$$g_{k'}(2\varepsilon_{k'} - E) = -\frac{1}{2}\sum_k \left(V_{k'k}\, g_k + V_{k'(-k)}\, g_k\right) \qquad (4.34)$$

Electrons in crystal

- Effective weakly attractive interaction due to phonon-exchange



- $\ominus$ve charge of electrons causes distortion of $\oplus$vely charged ion lattice with a lot of delay. Resulting excess charge can attract another electron
- Dominant over $e^- - e^-$ Coulomb repulsion at large distances since the latter is screened
- QM treatment: energy cutoff for these interactions at Debye frequency: $\hbar\omega_D$ (see below) (Momentum cutoff $\equiv \Delta k$)

thus take (attractive; for simplicity; Debye cut-off)

$$V_{kk'} = \begin{cases} -|V| & k_F < |k|,|k'| < k_F + \Delta K \\ 0 & \end{cases} \quad (4.35)$$

Hence $V_{k'k} = V_{k'(-k)}$

Our solution to Schrödinger-eqn (4.34) then becomes

$$g_{k'} = \frac{+|V| \sum_{k=k_F}^{k_F+\Delta K} g_K}{(2\varepsilon_{k'} - E)} \quad (4.36)$$

both sides $\sum_{k'}$, $\sum_k g_K$ cancel

then

$$\frac{1}{|V|} = \sum_{k=k_F}^{k_F+\Delta K} \frac{1}{(2\varepsilon_K - E)}$$

Convert to integral (see e.g. page 54)

$$\frac{1}{|V|} = (4\pi) \int_{k_F}^{k_F+\Delta K} dK \frac{K^2}{(2\varepsilon_K - E)} D \quad (4.37)$$

Change integration variable to energy $dK = \frac{m}{\hbar^2 k} d\varepsilon$

$$\frac{1}{|V|} = \left(\frac{4\pi m L^3}{\hbar^2 \pi^2}\right) \int_{\varepsilon_F}^{\varepsilon_F+\hbar\omega_D} \frac{k}{(2\varepsilon - E)} d\varepsilon \quad (4.38)$$

$k \approx k_F$ due to $\hbar\omega_D \ll \varepsilon_F$

We arrive at

$$\frac{1}{|V|} = N \int_{\varepsilon_F}^{\varepsilon_F+\hbar\omega_D} \frac{d\varepsilon}{(2\varepsilon - E)} = \frac{N}{2} \log\left(\frac{2E_F - E + 2\hbar\omega_D}{2E_F - E}\right) \quad (4.39)$$

with $N = \frac{4\pi m L^3 k_F}{\hbar^2 \pi^2}$

For $N \cdot |V| \ll 1$ (weak coupling approximation), we find

a Cooper pair energy (size ≫ interparticle distance in medium)

$$E_{pair} = E = 2E_F - 2\hbar\omega_D e^{-\frac{2}{N \cdot |V|}} \quad (4.40)$$

↘ Why P.T. fails

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 repulsive case, non-interacting scenario is not a good starting point for PT here)

- For repulsive interactions $E > 2E_F$ (no problem)
- Without blocked Fermi sea (let $\int_0^{\hbar\omega_D} d\epsilon$ in (4.39)) we get $E > 0$ (no bound state).
- Without Debye cutoff: (4.39) is <u>UV divergent</u> → need <u>regularisation / renormalisation</u> (see (3.52))

The last point is why we did the calculation for solid-state rather than cold atom Fermion gases: Fermi-gas does not have natural cutoff, so calculation needs renormalisation. But cooper-pairs form there for the same reason. For atoms one finds (O.O.M.)

$$E_{pair} = 2E_F - 2E_F \exp\left[-\frac{\pi}{2k_F|a_s|}\right] \quad (4.41)$$

roughly
- (4.38) keep k, $\hbar\omega_D \to E_F$
- $|V| = \frac{4\pi\hbar^2|a_s|}{m}$ degenerate

4.9.2. BCS - Theory

- Previous section: attractively interaction Fermi-gas unstable to <u>pair formation</u>.
- Tight Pairs (Molecules) would be <u>Bosons</u>, they could condense. What happens here?
- have to also include all vs. all interactions, not just among a single pair as in 4.9!
- Many-body theory due to <u>B</u>ardeen-<u>C</u>ooper-<u>S</u>chrieffer, also explains <u>superconductivity</u>

As in section 3.3.2, we want to build the statements above into a useful <u>Ansatz</u> for the many-body wavefunction. Unlike there, we want to now describe the <u>condensation of pairs</u>.

First quantized we could write

Anti-symmetrisation operation

$$\Psi(\vec{x}) = \sum_P (-1)^P \varphi_0(x_1, x_2)\,\varphi_0(x_3, x_4) \ldots \varphi(x_{N-1}, x_N) \quad (4.42)$$

P: permutation operator

We could write (4.42) more elegantly as

$$\hat{C}^+|0\rangle$$

with $\hat{C}^+ = \int d^3\vec{x} \int d^3\vec{y}\ \varphi_0(\vec{x},\vec{y})\,\hat{\Psi}^+_\uparrow(\vec{x})\,\hat{\Psi}^+_\downarrow(y)$ (4.43)

the ~~pairin~~ <u>Cooper-pair creation operator</u>

We can then state that these pairs condense [tight pairs => Bosons here? Not quite!]

in a <u>coherent state of pairs</u>

$$|\Psi_{BCS}\rangle = \mathcal{N} e^{\gamma \hat{C}^+}|0\rangle \quad (4.44)$$

- $\mathcal{N}$ Normalisation factor, $\gamma \leftrightarrow \alpha$ c.f. (2.34)

For BEC we had assumed a non-zero <u>mean-field</u>, now we can assume a <u>non-zero pairing-field</u>: (also "order parameter")

$$0 \neq \Delta(\vec{x}) = U_0 \langle \hat{\Psi}_\uparrow(\vec{x})\,\hat{\Psi}_\downarrow(\vec{x}_0)\rangle \quad (4.45)$$

(follows from exercise)

From these initial considerations, we will now approximately diagonalize the interacting Hamiltonian (4.23) with $U_0 < 0$, assuming <u>equal numbers of $\uparrow,\downarrow$ Fermions</u> in a <u>homogeneous</u> system

We "simplify" the interaction term as

$$U_0\,\hat{\Psi}^+_\uparrow(\vec{x})\hat{\Psi}^+_\downarrow(\vec{x})\,\hat{\Psi}_\downarrow(\vec{x})\hat{\Psi}_\uparrow(\vec{x}) \approx$$

$$\frac{U_0}{2}\Big\{\langle\hat{\Psi}^+_\uparrow(\vec{x})\hat{\Psi}^+_\downarrow(\vec{x})\rangle\,\hat{\Psi}_\downarrow(\vec{x})\hat{\Psi}_\uparrow(\vec{x}) + \langle\hat{\Psi}_\downarrow(x)\hat{\Psi}_\uparrow(x)\rangle\,\hat{\Psi}^+_\uparrow(\vec{x})\hat{\Psi}^+_\downarrow(\vec{x})$$

$$+\langle\hat{\Psi}^+_\uparrow(\vec{x})\hat{\Psi}_\uparrow(\vec{x})\rangle\,\hat{\Psi}^+_\downarrow(\vec{x})\hat{\Psi}_\downarrow(\vec{x}) + \langle\hat{\Psi}^+_\downarrow(\vec{x})\hat{\Psi}_\downarrow(\vec{x})\rangle\,\hat{\Psi}^+_\uparrow(\vec{x})\hat{\Psi}_\uparrow(\vec{x})$$

$$-\left(\langle\hat{\Psi}^+_\uparrow\Psi_\downarrow\rangle\,\hat{\Psi}^+_\downarrow\Psi_\uparrow + \langle\hat{\Psi}^+_\downarrow\hat{\Psi}_\uparrow\rangle\,\hat{\Psi}^+_\uparrow\Psi_\downarrow\right)\Big\}$$

(needs modification!)

- This is motivated again by Wick's theorem (3.47)
- Wick's theorem get's $\ominus$es when Fermions are involved

(→ Modify ... for Fermions ... fixe)

We further define:

Hartree fields $\quad U_\uparrow(\vec{x}) \stackrel{U_0}{=} \langle \hat{\varphi}^\dagger_\uparrow(\vec{x}) \hat{\varphi}_\uparrow(\vec{x}) \rangle \quad$ same for $\downarrow$

Fock fields $\quad F_\uparrow(\vec{x}) = U_0 \langle \hat{\varphi}^\dagger_\uparrow(\vec{x}) \hat{\varphi}_\downarrow(\vec{x}) \rangle \quad$ same for $\uparrow \leftrightarrow \downarrow$ $\quad (4.46)$

PROOF → exercise

- In the paired state (4.44) $F_{\uparrow,\downarrow} = 0$
- In the homogeneous system $\Delta(\vec{x}) = \Delta$, $U_\uparrow(\vec{x}) = U_\downarrow(\vec{x}) = U$, $\Delta \in \mathbb{R}$

Finally we have:

$$U_0 \hat{\varphi}^\dagger_\uparrow(\vec{x}) \hat{\varphi}^\dagger_\downarrow(\vec{x}) \hat{\varphi}_\downarrow(\vec{x}) \hat{\varphi}_\uparrow(\vec{x}) \simeq$$

$$\Delta^* \hat{\varphi}_\downarrow(\vec{x}) \hat{\varphi}_\uparrow(\vec{x}) + \Delta \hat{\varphi}^\dagger_\uparrow(\vec{x}) \hat{\varphi}^\dagger_\downarrow(\vec{x}) + U\left(\hat{\varphi}^\dagger_\uparrow(\vec{x}) \hat{\varphi}_\uparrow(\vec{x}) + \hat{\varphi}^\dagger_\downarrow(\vec{x}) \hat{\varphi}_\downarrow(\vec{x})\right)$$

$\frac{1}{2}$

Finally we re-assemble the Hamiltonian (4.23) and augment it to a grand-canonical one $\hat{K} = \hat{H} - \mu \hat{N}$:

$$\hat{K} = \sum_{\sigma=\uparrow,\downarrow} \int d^3x \, \hat{\varphi}^\dagger_\sigma(\vec{x}) \left[-\frac{\hbar^2 \nabla^2}{2m} + U - \mu \right] \hat{\varphi}_\sigma(\vec{x}) \qquad (3.49)$$

$$+ \int d^3x \left[\Delta^* \hat{\varphi}_\downarrow(\vec{x}) \hat{\varphi}_\uparrow(\vec{x}) + \Delta \hat{\varphi}^\dagger_\uparrow(\vec{x}) \hat{\varphi}^\dagger_\downarrow(\vec{x}) \right]$$

In the homogeneous case, it is again simpler to work in the momentum basis. As we did for Eq. (4.24), we reach the

BCS / pairing Hamiltonian: $\qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m} + U - \mu \qquad (4.47)$

$$(\hat{K}) = \hat{H}_{BCS} = \sum_{\vec{k}, \sigma=\uparrow,\downarrow} \varepsilon_k \hat{a}^\dagger_{\sigma,k} \hat{a}_{\sigma k} + \Delta \sum_k \left(\hat{a}_{\downarrow k} \hat{a}_{\uparrow -k} + \hat{a}^\dagger_{\uparrow(-k)} \hat{a}^\dagger_{\downarrow k} \right)$$

- In section (3.4), we had kept only Bose-gas excitations up to order $\hat{a}^2$, and then diagonalized the Hamiltonian using the Bogoliubov transformation (e.g. 3.47 b)
- This works generically for Hamiltonians up to quadratic in $\hat{a}$, $\hat{a}^\dagger$, thus also here, for (4.47)

($u_k = u_{-k}$ from parity invariance)

$$\hat{K} = \sum_k \xi_k \Big[\big(\overbrace{u_k \hat{\alpha}^+_{\uparrow k} - v_k \hat{\alpha}_{\downarrow(-k)}}^{\hat{a}^+_{\uparrow k}}\big)\big(\overbrace{u_k \hat{\alpha}_{\uparrow k} - v_k \hat{\alpha}^+_{\downarrow(-k)}}^{\hat{a}_{\uparrow k}}\big)$$

$$+ \big(\overbrace{u_k \hat{\alpha}^+_{\downarrow k} + v_k \hat{\alpha}_{\uparrow(-k)}}^{\hat{a}^+_{\downarrow k}}\big)\big(\overbrace{u_k \hat{\alpha}_{\downarrow k} + v_k \hat{\alpha}^+_{\uparrow(-k)}}^{\hat{a}_{\downarrow k}}\big)\Big]$$

$$+ \Delta \Big[\big(\overbrace{u_k \hat{\alpha}_{\downarrow k} + v_k \hat{\alpha}^+_{\uparrow(-k)}}^{\hat{a}_{\downarrow k}}\big)\big(\overbrace{u_{-k} \hat{\alpha}_{\uparrow(-k)} - v_{(-k)} \hat{\alpha}^+_{\downarrow k}}^{\hat{a}_{\uparrow(-k)}}\big)$$

$$+ \big(\overbrace{u_k \hat{\alpha}^+_{\uparrow(-k)} - v_k \hat{\alpha}_{\downarrow(k)}}^{\hat{a}^+_{\uparrow(-k)}}\big)\big(\overbrace{u_k \hat{\alpha}^+_{\downarrow k} + v_k \hat{\alpha}_{\uparrow(-k)}}^{\hat{a}^+_{\downarrow(+k)}}\big)\Big]$$

*(-1) anti-commu. *(-1)

$$= \sum_k \xi_k \Big[u_k^2 \hat{\alpha}^+_{\uparrow k} \hat{\alpha}_{\uparrow k} - u_k v_k \hat{\alpha}^+_{\uparrow k} \hat{\alpha}^+_{\downarrow(-k)} - u_k v_k \hat{\alpha}_{\downarrow(-k)} \hat{\alpha}_{\uparrow k} + v_k^2 \hat{\alpha}_{\downarrow(-k)} \hat{\alpha}^+_{(-k)}$$

$$+ u_k^2 \hat{\alpha}^+_{\downarrow k} \hat{\alpha}_{\downarrow k} + u_k v_k \hat{\alpha}^+_{\downarrow k} \hat{\alpha}^+_{\uparrow(-k)} + u_k v_k \hat{\alpha}_{\uparrow(-k)} \hat{\alpha}_{\downarrow k} + v_k^2 \hat{\alpha}_{\uparrow(-k)} \hat{\alpha}^+_{\uparrow(-k)} \Big]$$

$$+ \Delta \Big[u_k^2 \hat{\alpha}_{\downarrow k} \hat{\alpha}_{\uparrow(-k)} - u_k v_k \hat{\alpha}_{\downarrow k} \hat{\alpha}^+_{\downarrow k} + u_k v_k \hat{\alpha}^+_{\uparrow(-k)} \hat{\alpha}_{\uparrow(-k)} - v_k^2 \hat{\alpha}^+_{\uparrow(-k)} \hat{\alpha}^+_{\downarrow k}$$

$$+ u_k^2 \hat{\alpha}^+_{\uparrow(-k)} \hat{\alpha}^+_{\downarrow(k)} + u_k v_k \hat{\alpha}^+_{\uparrow(-k)} \hat{\alpha}_{\uparrow(-k)} - u_k v_k \hat{\alpha}_{\downarrow k} \hat{\alpha}^+_{\downarrow k} - v_k^2 \hat{\alpha}_{\downarrow k} \hat{\alpha}_{\uparrow(-k)} \Big]$$

$$\sum_k \xi_k \hat{\alpha}^+_{(-k)} \hat{\alpha}_{(-k)} = \sum_k \xi_k \hat{\alpha}^+_k \hat{\alpha}_k$$

$$= \sum_k \Big[\xi_k (u_k^2 - v_k^2) + 2\Delta u_k v_k \Big] \big(\hat{\alpha}^+_{\uparrow k} \hat{\alpha}_{\uparrow k} + \hat{\alpha}^+_{\downarrow k} \hat{\alpha}_{\downarrow k} \big) \quad \underbrace{+ 2\xi_k v_k^2 - 2\Delta u_k v_k}_{\text{from commutators}}$$

$$+ \Big[2\xi_k u_k v_k - (u_k^2 - v_k^2)\Delta \Big] \big(\hat{\alpha}^+_{\downarrow k} \hat{\alpha}^+_{\uparrow(-k)} + \hat{\alpha}_{\uparrow(-k)} \hat{\alpha}_{\downarrow k} \big)$$

Bogoliubov-transformation (BCS-system)

$$\hat{\alpha}_{\uparrow k} = u_k \hat{a}_{\uparrow k} + v_k \hat{a}^{+}_{\downarrow(-k)}$$
$$\hat{\alpha}_{\downarrow k} = u_k \hat{a}_{\downarrow k} - v_k \hat{a}^{+}_{\uparrow(-k)} \qquad (4.48)$$

Comparison to BEC: in chapter 3 we were more ambitious and did Bogoliubov trafo for in-homogeneous system. For homogeneous case, Eq. (3.47 b) gives:

$$\hat{\alpha}_k = u_k \hat{a}_k + v_k \hat{a}_k^{+} \qquad \text{(quite similar)}$$

$\uparrow$ use $\hat{\Psi}(\vec{x}) = \int d^3k \, \frac{\hat{a}_k}{\sqrt{2\pi}^3} \varphi_k(\vec{x})$ & δ-fct..

Quasi-particle operators (4.48) should satisfy Fermi commutation relations:

$$\{\hat{\alpha}_{\sigma k}, \hat{\alpha}^{+}_{\sigma' k'}\} \underset{\text{excercise}}{=} (u_k^2 + v_k^2)\, \delta_{kk'} \delta_{\sigma\sigma'}$$

We thus have to require Normalisation $u_k^2 + v_k^2 = 1$.
Using the latter, we can derive the

inverse Bogoliubov transformation (4.49)

$$\hat{a}_{\uparrow k} = u_k \hat{\alpha}_{\uparrow k} - v_k \hat{\alpha}^{+}_{\downarrow(-k)}$$
$$\hat{a}_{\downarrow k} = u_k \hat{\alpha}_{\downarrow k} + v_k \hat{\alpha}^{+}_{\uparrow(-k)} \qquad \text{(Proof, exercise)}$$

Inserting (4.49) into (4.47) gives

$$\hat{K} = \sum_k \Big\{ \underbrace{\left[(\varphi_k u_k + \Delta v_k) u_k - (\varphi_k v_k - \Delta u_k) v_k\right]}_{(A)} \left(\hat{\alpha}^{+}_{\uparrow k} \hat{\alpha}_{\uparrow k} + \hat{\alpha}^{+}_{\downarrow k} \hat{\alpha}_{\downarrow k}\right)$$
$$+ \underbrace{\left[(\Delta v_k + \varphi_k u_k) v_k - (\Delta u_k - \varphi_k v_k) u_k\right]}_{(B)} \left(\hat{\alpha}^{+}_{\downarrow k} \hat{\alpha}^{+}_{\uparrow(-k)} + \hat{\alpha}^{+}_{\uparrow(-k)} \hat{\alpha}_{\downarrow k}\right)$$
$$+ 2\varphi_k v_k^2 - 2\Delta u_k v_k \Big\}$$

(steps see p. 78b)

By demanding Bogoliubov de Gennes equations ... (BCS, Fermions)

$$\varphi_k u_k + \Delta v_k = \varepsilon_k u_k$$
$$-\varphi_k v_k + \Delta u_k = \varepsilon_k v_k \qquad (4.50)$$

... We diagonalize the Hamiltonian into

$$\hat{K} = E_0 + \sum_{k,s} \varepsilon_k \hat{\alpha}^+_{k,s} \hat{a}_{k,s} \quad (4.51)$$

$$E_0 = \sum_k 2(\varphi_k v_k^2 - \Delta u_k v_k)$$

↳ Non-interacting quasi-particle form again.

- (A) → $\varepsilon_k(u_k^2 + v_k^2) = \varepsilon_k$
- (B) → $\varepsilon_k(u_k v_k - u_k v_k) = 0$

- Comments, see p. 80 b

To find out more about excitations, we have to solve (4.50). In matrix form

$$\begin{bmatrix} \varphi_k & \Delta \\ \Delta & -\varphi_k \end{bmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \varepsilon \begin{pmatrix} u_k \\ v_k \end{pmatrix},$$

proceeds as for (3.49), using also $u_k^2 + v_k^2 = 1$. Solutions are:

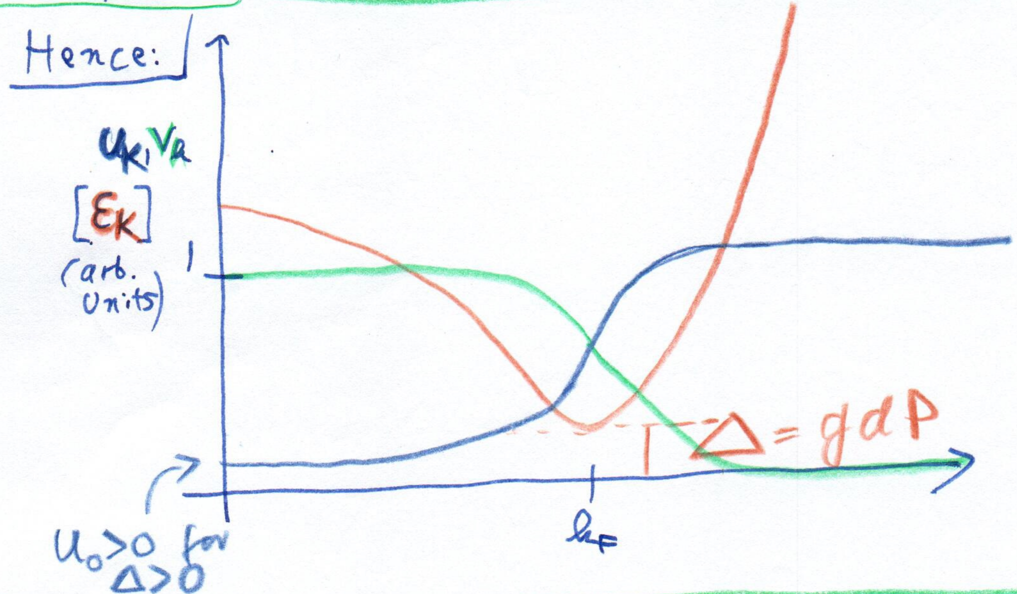
$$u_k^2 = \frac{1}{2}\left(1 + \frac{\varphi_k}{\varepsilon_k}\right), \quad v_k^2 = \frac{1}{2}\left(1 - \frac{\varphi_k}{\varepsilon_k}\right), \quad \varepsilon_k = \sqrt{\varphi_k^2 + \Delta^2} \quad (4.52)$$

for particle amplitude u_k, hole amplitude v_k and dispersion relation ε_k

- Recall $\varphi_k = \frac{\hbar^2 k^2}{2m} + U - \mu = \frac{\hbar^2 k^2}{2m} - \tilde{\mu}$ (see Eq. (4.47)) (absorb $U - \mu$)

- $\tilde{\mu}$ is the Fermi-energy at $T=0$

Hence:



- Behaviour of u, v logical from particle/hole interpretation

- Crucial feature of dispersion relation is the energy gap $\varepsilon_{min} = \Delta$. Thus if $\Delta > 0$, ε_k never is zero.

Discussion of diagonalized Hamiltonian (4.51)

GROUND STATE

Already from (4.51) we can understand the system better:

- As was the case for Bose-gas, the ground state of the system is one with <u>no quasiparticles</u> (c.f. (3.47))

- Definition for this <u>quasi-particle vacuum</u>

$$\hat{\alpha}_{sk}|\Psi_0\rangle = 0 \qquad (4.51\,b)$$

(compare $\hat{a}_{sk}|0\rangle = 0$ for <u>bare vacuum</u>)

- We can easily write one such state

$$|\Psi_0\rangle = \prod_{k',s'} \hat{\alpha}_{s'k'}|0\rangle \qquad (4.51\,c)$$

This works since $\hat{\alpha}_{sk}^2 = 0$ (from $\{\hat{\alpha}_{sk}, \hat{\alpha}_{s'k'}\} = 0$)

- We can use (4.48) to obtain

BCS-state:

$$|\Psi_{BCS}\rangle = |\Psi_0\rangle = \prod_{k} \left(u_k + v_k\, \hat{a}^+_{\vec{k}\uparrow}\, \hat{a}^+_{(-\vec{k})\downarrow}\right)|0\rangle \qquad (4.51\,d)$$

~~of fermions exist in a "superposition of~~ • each possible pair can be either occupied (v) or unoccupied (u)

GROUNDSTATE-ENERGY

We can already verify that the pairing assumption $\Delta \neq 0$ has <u>lowered the energy</u> compared to the un-paired Fermi sea.

$$\langle\Psi_{BCS}|\hat{K}|\Psi_{BCS}\rangle - \langle FS|\hat{K}|FS\rangle =$$

$$\underbrace{\sum_k \left(2\varphi_k v_k^2 - 2\Delta u_k v_k\right)}_{E_0,\ \text{see } (4.51)} - \sum_k^{|k|<k_F} (2\,\varphi_k)$$

(2: spin $\uparrow\downarrow$; $\varphi_k = \frac{\hbar^2 k^2}{2m} - \tilde{\mu} = \frac{\hbar^2}{2m}(k^2 - k_F^2)$: energy relative to Fermi sea)

$$= \sum_k \Big\{ 2 v_k \underbrace{(\varphi_k v_k - \Delta u_k)}_{= -E_k u_k \text{ Eq. (4.50)}} - \sum_k^{|\vec{k}|<k_F} (2\varphi_k) \Big\}$$

$$\overset{?}{>} \sum_k^{|\vec{k}|<k_F} \Big\{ -2 \underbrace{\sqrt{\varphi_k^2 + \Delta^2}}_{E_k} v_k^2 - (2\varphi_k) \Big\} \overset{(4.52)}{=} \sum_k \underbrace{\big(\underbrace{-\varphi_k}_{>0} - \sqrt{\Delta^2 + \varphi_k^2} \big)}_{<0}$$

*Reason: See Fig page 80: $v_k^2 \to 0$ for $|\vec{k}| > k_F$

- Overall we lower the energy for a nonzero gap Δ.

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* We can now actually see that the BCS state we got IS the pair-coherent state we guessed in (4.44)

By going to Fourier-space, we can rewrite pair operator

$$\hat{C}^+ = \int d^3x \int d^3y \, \varphi_0(x-y) \, \hat{\varphi}^+_\uparrow(x) \, \hat{\varphi}^+_\downarrow(y) \qquad \text{(see 4.43)}$$

as

$$\hat{C}^+ = \sum_k \varphi_k \, \hat{a}^+_{k\uparrow} \hat{a}^+_{(-k)\downarrow} \qquad (4.51e)$$

(Proof see page 80d) Then Campbell Baker Hausdorff formula and $[\hat{a}^+_k \hat{a}^+_{(-k)}, \hat{a}^+_{k'} \hat{a}^+_{(-k')}] = 0$ [see p. 80d]

$$\mathcal{N} e^{\gamma \hat{C}^+} = \mathcal{N} e^{\sum_k \gamma \varphi_k \hat{a}^+_{k\uparrow} \hat{a}^+_{(-k)\downarrow}} = \mathcal{N} \prod_k e^{\gamma \varphi_k \hat{a}^+_{k\uparrow} \hat{a}^+_{(-k)\downarrow}}$$

$$\overset{\text{Fermions}}{=} \mathcal{N} \prod_k (1 + \gamma \varphi_k \hat{a}^+_{k\uparrow} \hat{a}^+_{(-k)\downarrow})$$

With moving $\mathcal{N}$ into the product we reach the form BCS state as coherent pair state

$$|\Psi_{BCS}\rangle = \mathcal{N} e^{\gamma \hat{C}^+} |0\rangle = \prod_k (u_k + v_k \hat{a}^+_{k\uparrow} \hat{a}^+_{(-k)\downarrow}) |0\rangle \qquad (4.51f)$$

$$\hat{C}^+ = \int d^3x \int d^3y \; \varphi_0(x-y)\, \hat{\psi}_\uparrow^+(x)\, \hat{\psi}_\downarrow^+(y)$$

Use $\hat{\psi}_\uparrow(x) = \sum_k \frac{1}{\sqrt{2\pi}^3} \hat{a}_{\uparrow,k} \frac{e^{ikx}}{\sqrt{V}}$ (see p. 70)

$$= \frac{1}{V} \sum_{k,k'} \frac{1}{\sqrt{2\pi}^3} \int d^3x \int d^3y \; \varphi_0(x-y)\, e^{-ikx} e^{-ik'y}\, \hat{a}^+_{\uparrow,k}\, a^+_{\downarrow,k'}$$

Change to relative & C.M. co-ordinates $\vec{r} = \vec{x} - \vec{y}$, $\vec{R} = \frac{\vec{x}+\vec{y}}{2}$

$$= \frac{1}{V} \sum_{k,k'} \frac{\int d^3r \int d^3R}{(2\pi)^3} \varphi_0(\vec{r})\, e^{-ik(\vec{R}-\frac{\vec{r}}{2})}\, e^{-ik'(\vec{R}+\frac{\vec{r}}{2})}\, \hat{a}^+_{\uparrow k}\, \hat{a}^+_{\downarrow k'}$$

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

$$= \sum_k \varphi_k\, \hat{a}^+_{\uparrow k}\, \hat{a}^+_{\downarrow(-k)} \quad \text{with } \varphi_k = \frac{\tilde{\varphi}_0(-k)\sqrt{2\pi}^3}{V}$$

$$\left[\hat{a}^+_{\uparrow k}\, \hat{a}^+_{\downarrow k},\; \hat{a}^+_{\uparrow k'}\, \hat{a}^+_{\downarrow k'}\right] = \hat{a}^+_{\uparrow k}\, \hat{a}^+_{\downarrow k}\, \hat{a}^+_{\uparrow k'}\, \hat{a}^+_{\downarrow k'} - \hat{a}^+_{\uparrow k'}\, \hat{a}^+_{\downarrow k'}\, \hat{a}^+_{\uparrow k}\, \hat{a}^+_{\downarrow k}$$

$* (-1)^4$ use anti-commutators

$$= 0$$

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 4.9.2.).

Of course, $\langle\hat\Psi\hat\Psi\rangle$ depends on u, v and the quantum state, where we have used Δ to get u, v. So now we have to make the theory self-consistent ($\Delta \Leftrightarrow u, v$)

Evaluation of pairing field

(to be justified later) (& assignment 4)

$$\Delta = U_0 \langle \hat\Psi_\uparrow(\vec{x})\, \hat\Psi_\downarrow(\vec{x}) \rangle = \frac{U_0}{\mathcal{V}} \sum_{k} \langle \hat a_{\downarrow(-k)}\, \hat a_{\uparrow(k)} \rangle$$

$$\underset{\text{Eq. 4.49}}{=} \frac{U_0}{\mathcal{V}} \sum_k \left\langle \left(u_k \hat\alpha_{\downarrow(-k)} + v_k \hat\alpha^\dagger_{\uparrow k}\right)\left(u_k \hat\alpha_{\uparrow k} - v_k \hat\alpha^\dagger_{\downarrow(-k)}\right)\right\rangle$$

We assume $\langle\,\rangle$ is a Fock state with N_k Bogoliubov excitations in mode k. (or thermal mixture of those)

$$\underset{\text{as usual}}{=} -\frac{U_0}{\mathcal{V}} \sum_k u_k v_k \left(1 - 2N_k\right) \qquad N_k = \frac{1}{\exp(E_k/k_B T) + 1}$$

We have $u_k v_k = \Delta / 2E_k$ from Eq. (4.52), hence we reach the gap-equation (consistency condition)

$$\left(\begin{matrix}\text{here we}\\ \text{needed}\\ U_0 < 0\end{matrix}\right) |U_0| \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{\tanh\left(\frac{E_k}{2k_B T}\right)}{2E_{\vec{k}}} = 1 \qquad (4.53)$$

At zero temperature:

$$|U_0| \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{2\sqrt{\Delta_0^2 + \xi_k^2}} = 1 \qquad (4.54)$$

Main contribution from $|\vec{k}| \approx k_F$ (denominator smallest (see p. 80)) and there:

$$|\xi_k| = \hbar v_F \left| |\vec{k}| - k_F \right| \ll E_F \qquad (4.55)$$

(↑ Taylor-expand ξ_k to $\mathcal{O}(1)$ around k_F)

$$\Rightarrow |U_0|(4\pi) \int_0^{\mathcal{K}_{E\text{-cutoff}}} dk \frac{k^2}{2\sqrt{\Delta_0^2 + (\hbar v_F)^2 (k - k_F)^2}} \underset{\text{integration}}{\overset{\text{nasty}}{=}} \lambda \ln\left(\frac{E_{cut}}{\Delta_0}\right) \overset{!}{=} 1$$

$$\lambda = \frac{2 k_F |a_s|}{\pi} \qquad (4.56)$$

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

<u>zero-temperature gap:</u>

$$\Delta_0 = E_F \exp\left(-\frac{\pi}{2 k_F |a_s|}\right) \ll E_F \qquad (4.57)$$

- Comparison with (4.41) now gives a neat ~~expla~~ interpretation: Since $\Delta_0 = \left|\frac{E_{pair} - 2E_F}{2}\right|$, i.e. half the ~~bram~~ binding energy of a Cooper pair:

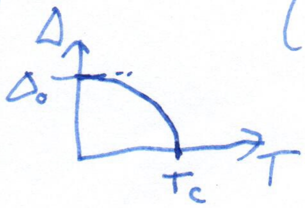
Excitations become gapped, since in order to make one, I would have to <u>break a pair</u>.

We can also evaluate Δ from (4.53) for $T>0$ and find <u>finite-temperature gap</u> ~~and~~

$$\Delta = 3.06\, T_c \left(1 - T/T_c\right)^{1/2} \qquad (4.58)$$

and <u>critical temperature</u>

$$T_c \approx 0.57\, \Delta_0 \ll T_F$$



4.9.3. Fermionic superfluidity and superconductivity

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

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

$$v_{crit} = \min_{\vec{k}} \left(\frac{\epsilon_{\vec{k}}}{\hbar \vec{k}}\right)$$

We see from Eq. (4.52) [and plot below], that

<u>Fermion critical velocity for superfluidity:</u>

$$v_{crit} = 0 \text{ if } \Delta = 0, \text{ but } v_{crit} = \frac{\Delta}{\hbar k_F} \qquad (4.59)$$

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

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

This is used as an experimental signature of Fermionic superfluidity.

4.10 Outlook

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

The effect is not there at all in a few body (e.g. 2) picture.