Lecture Notes

Aspects of Symmetry in Unconventional Superconductors

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Unconventional Superconductors

Many novel superconductors show properties different from standard superconductors (overview); Aim of this lecture:

- discuss structure of Cooper pairs from a symmetry point of view - key symmetries: time reversal and inversion symmetry
- learn the techniques of the phenomenological approach: generalized Ginzburg-Landau theories - broken symmetries and order parameters
- discuss phenomena due to symmetry breaking: example broken time reversal symmetry
- analyze consequences of lack of key symmetries

Some literature:

- V.P. Mineev and K.V. Samokhin, *Introduction to Unconventional Superconductivity*, Gordon and Breach Science Publisher (1999).
- M. Sigrist, *Introduction to Unconventional Superconductivity*, AIP Conf. Proc. 789, 165 (2005).
- M. Sigrist, *Introduction to unconventional superconductivity in non-centrosymmetric metals*, AIP Conf. Proc. 1162, 55 (2009).

1. General form of Cooper pairing and BCS theory

BCS theory of superconductivity describes an instability of a normal metal state,
normal metal ground state:

$$|\Psi_0\rangle = \prod_{\boldsymbol{k}}^{|\boldsymbol{k}|\leq k_F} \hat{c}^\dagger_{\boldsymbol{k}\uparrow}\hat{c}^\dagger_{-\boldsymbol{k}\downarrow}|0\rangle \tag{1}$$

note the states created by $\hat{c}^\dagger_{\boldsymbol{k}\uparrow}$ and $\hat{c}^\dagger_{-\boldsymbol{k}\downarrow}$, $|\boldsymbol{k}\uparrow\rangle$ and $|\boldsymbol{k}\uparrow\rangle$ are degenerate

$$\epsilon_{\boldsymbol{k}\uparrow} = \epsilon_{-\boldsymbol{k}\downarrow} = \epsilon_{\boldsymbol{k}} \qquad \text{single-electron energy} \tag{2}$$

guaranteed by time reversal symmetry (time reversal operator $\hat{K}$):

$$|\boldsymbol{k}\uparrow\rangle \overset{\hat{K}}{\longleftrightarrow} |-\boldsymbol{k}\downarrow\rangle \tag{3}$$

BCS ground state:

$$|\Psi_{BCS}\rangle = \prod_{\boldsymbol{k}} \left[u_{\boldsymbol{k}} + v_{\boldsymbol{k}} \hat{c}^\dagger_{\boldsymbol{k}\uparrow} \hat{c}^\dagger_{-\boldsymbol{k}\downarrow} \right] |0\rangle \tag{4}$$

coherent state of electron pairs of opposite momenta

$$b_{\boldsymbol{k}} = \langle \Psi_{BCS} | \hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} | \Psi_{BCS} \rangle = u^*_{\boldsymbol{k}} v_{\boldsymbol{k}} \tag{5}$$

non-vanishing for $|\boldsymbol{k}|$ very close to k_F: BCS state affects mainly Fermi surface. electron number not fixed (grand canonical viewpoint - coherent state like BEC)

1.1. Cooper problem - generalized

Cooper instability through interaction between two electrons added to normal state $|\Psi_0\rangle$ of free electrons ($\epsilon_{\boldsymbol{k}} = \hbar^2 \boldsymbol{k}^2 / 2m$)

2 electron states $|\boldsymbol{k}_1 s_1\rangle$ and $|\boldsymbol{k}_2 s_2\rangle$, assume $\boldsymbol{k}_1 + \boldsymbol{k}_2$ and $|\boldsymbol{k}_1|, |\boldsymbol{k}_2| > k_F$ (restricted by Pauli exclusion principle)

Schrödinger equation for 2 interacting electrons

$$\left\{ -\frac{\hbar^2}{2m} \left(\boldsymbol{\nabla}^2_{r_1} + \boldsymbol{\nabla}^2_{r_2} \right) + V(\boldsymbol{r}_1 - \boldsymbol{r}_2) \right\} \psi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2) = E \, \psi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2) \tag{6}$$

$V(\boldsymbol{r}_1 - \boldsymbol{r}_2)$: 2 -particle interaction;

change to center of mass and relative coordinates: $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2)$ and $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$

$$\psi(\boldsymbol{r}_1, s_1; \boldsymbol{r}_2, s_2) = \phi_{s_1 s_2}(\boldsymbol{r}) e^{i\boldsymbol{q}\cdot\boldsymbol{R}} = \phi_{s_1 s_2}(\boldsymbol{r}) \qquad \text{since} \quad \boldsymbol{q} = \boldsymbol{k}_1 + \boldsymbol{k}_2 = 0 \tag{7}$$

Symmetry aspect:

Pauli exclusion principle → antisymmetric wave function: $\phi_{s_1 s_2}(\boldsymbol{r}) = -\phi_{s_2 s_1}(-\boldsymbol{r})$

$$\phi_{s_1 s_2}(\boldsymbol{r}) = \phi(\boldsymbol{r}) \chi_{s_1 s_2} = \begin{cases} \phi(\boldsymbol{r}) = \phi(-\boldsymbol{r}), \ \chi_{s_1 s_2} = -\chi_{s_2 s_1} & \textbf{even} \text{ parity, spin } \textbf{singlet} \\ \\ \phi(\boldsymbol{r}) = -\phi(-\boldsymbol{r}), \ \chi_{s_1 s_2} = \chi_{s_2 s_1} & \textbf{odd} \text{ parity, spin } \textbf{triplet} \end{cases} \tag{8}$$

with $\phi(\boldsymbol{r})$ orbital and $\chi_{s_1 s_2}$ spin part of wave function[1]

$$\Rightarrow \quad -\frac{\hbar^2}{m} \boldsymbol{\nabla}^2 \phi(\boldsymbol{r}) + V(\boldsymbol{r}) \phi(\boldsymbol{r}) = E \, \phi(\boldsymbol{r}) \tag{10}$$

turn to Fourier (momentum) space:

$$g_{\boldsymbol{k}} = \int d^3 r \; e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \phi(\boldsymbol{r}) \; , \quad V_{\boldsymbol{q}} = \int d^3 r \; e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} V(\boldsymbol{r}) \tag{11}$$

[1] Spin part of wave function:

$$\begin{array}{llll} \text{spin singlet} & S=0: & \chi_{s_1 s_2} = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) & \chi_{s_1 s_2} = -\chi_{s_2 s_1} \\ \text{spin triplet} & S=1: & \chi_{s_1 s_2} = |\uparrow\uparrow\rangle, \ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \ |\downarrow\downarrow\rangle & \chi_{s_1 s_2} = \chi_{s_2 s_1} \end{array} \tag{9}$$

$$\Rightarrow \quad \frac{\hbar^2 \boldsymbol{k}^2}{m} g_{\boldsymbol{k}} + \frac{1}{\Omega} \sum_{\boldsymbol{k}'} V_{\boldsymbol{k}-\boldsymbol{k}'} g_{\boldsymbol{k}'} = E \, g_{\boldsymbol{k}} \tag{12}$$

with $\Omega = L^3$ volume $\boldsymbol{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$ ($n_{x,y,z}$: integers)

Symmetry aspect: assume full spherical rotation symmetry, symmetry group $O(3)$ expansion in spherical harmonics $|lm\rangle$

$$\begin{aligned} V_{\boldsymbol{k}-\boldsymbol{k}'} &= \textstyle\sum_{l=0}^{\infty} V_l(k,k') \sum_{m=-l}^{+l} Y_{lm}(\hat{\boldsymbol{k}}) Y^*_{lm}(\hat{\boldsymbol{k}}') \\ g_{\boldsymbol{k}} &= \textstyle\sum_{l=0}^{\infty} \sum_{m=-l}^{+l} g_{lm}(k) Y_{lm}(\hat{\boldsymbol{k}}) \end{aligned} \tag{13}$$

with $k = |\boldsymbol{k}|$ and $\hat{\boldsymbol{k}} = \boldsymbol{k}/k$; [2]

set $\{|lm\rangle| - l \leq m \leq +l\}$ is $(2l+1)$-dimensional basis of the irreducible representation of $O(3)$ labelled by l

define $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \epsilon_F = \frac{\hbar^2 k^2}{2m} - \epsilon_F$, $\Delta E = E - \epsilon_F$ and rewrite $V_l(k,k') \to V_l(\xi_{\boldsymbol{k}}, \xi_{\boldsymbol{k}'})$ and $g_{lm}(k) \to g_{lm}(\xi_{\boldsymbol{k}})$

$$\frac{1}{\Omega} \sum_{\boldsymbol{k}} \to \int \frac{d^3k}{(2\pi)^3} \to \int d\xi \; N(\xi) \frac{d\Omega_{\boldsymbol{k}}}{4\pi} \tag{15}$$

with density of states

$$N(\xi) = \frac{1}{\Omega} \sum_{\boldsymbol{k}} \delta(\xi - \xi_{\boldsymbol{k}}) \tag{16}$$

Schrödinger equation decouples in different channels l (angular momentum):

$$(2\xi - \Delta E) g_{lm} + \int d\xi' \; N(\xi') V_l(\xi, \xi') g_{lm}(\xi') = 0 \tag{17}$$

for practical reasons: $N(\xi) \approx N(0)$ and

$$V_l(\xi, \xi') = \begin{cases} \nu_l & -\epsilon_c \leq \xi, \xi' \leq \epsilon_c \\ 0 & \text{otherwise} \end{cases} \tag{18}$$

with $\epsilon_c \ll \epsilon_F$;

solving the equation, searching for bound state of 2 electrons, ie. $\Delta E < 0$:

$$g_{lm}(\xi) = \frac{-N(0)\nu_l}{2\xi - \Delta E} \int_0^{\epsilon_c} d\xi' \; g_{lm}(\xi') = \frac{-N(0)\nu_l}{2\xi - \Delta E} I_{lm} \qquad \text{for} 0 \leq \xi \leq \epsilon_c \tag{19}$$

for $\nu_l < 0$:

$$I_{lm} = -I_{lm} N(0) \nu_l \int_0^{\epsilon_c} \frac{d\xi'}{2\xi' - \Delta E} = -I_{lm} \frac{N(0)\nu_l}{2} \ln\left(\frac{\Delta E - 2\epsilon_c}{\Delta E}\right) \tag{20}$$

$$\Rightarrow \quad \Delta E = -2\epsilon_c e^{2/N(0)\nu_l} \tag{21}$$

[2]Spherical harmonics: orthogonality relation

$$\int \frac{d\Omega_{\boldsymbol{k}}}{4\pi} Y^*_{lm}(\hat{\boldsymbol{k}}) Y_{l'm'}(\hat{\boldsymbol{k}}) = \delta_{ll'} \delta_{mm'} \tag{14}$$

if $\Delta E \ll \epsilon_c$ (note: ϵ_c functions as a somewhat arbitrary cutoff for the integral);

bound state with energy $E < 2\epsilon_F \Rightarrow$ instability: lowest bound state for strongest "attractive" channel l ($\nu_l < \nu_{l'}$ for $l \neq l'$).

Symmetry aspect:

bound state parity distinguished by l: $(-1)^l \quad \Rightarrow \quad \begin{cases} l = 0, 2, 4, \ldots & \text{even parity, spin singlet} \\ l = 1, 3, 5, \ldots & \text{odd parity, spin triplet} \end{cases}$.

Examples:

electron-phonon interaction:

$$V_{\boldsymbol{k}-\boldsymbol{k}'} = \begin{cases} \nu_0(\xi, \xi') < 0 & -\epsilon_D \leq \xi, \xi' \leq \epsilon_D \\ 0 & \text{otherwise} \end{cases} \tag{22}$$

interaction without angular dependence (contact interaction): pairing channel $l = 0, S = 0$ **"s-wave"** (complete symmetric in orbital and spin space

simple anisotropic "repulsive" interaction: $V_{\boldsymbol{k}-\boldsymbol{k}'} = V(\xi, \xi')(\hat{\boldsymbol{k}} - \hat{\boldsymbol{k}}')^2$

$$V(\xi, \xi') = \begin{cases} \nu > 0 & -\epsilon_c \leq \xi, \xi' \leq \epsilon_c \\ 0 & \text{otherwise} \end{cases} \tag{23}$$

but

$$\nu(\hat{\boldsymbol{k}} - \hat{\boldsymbol{k}}')^2 = 2\nu[1 - \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}'] = \underbrace{8\pi\nu}_{=\nu_0 > 0} Y_{00}(\hat{\boldsymbol{k}}) Y_{00}^*(\hat{\boldsymbol{k}}') \underbrace{-\frac{8\pi}{3}\nu}_{=\nu_1 < 0} \sum_{m=-1}^{+1} Y_{1m}(\hat{\boldsymbol{k}}) Y_{1m}^*(\hat{\boldsymbol{k}}') \tag{24}$$

no bound state in $l = 0, S = 0$ (repulsive) channel; bound state in (attractive) $l = 1, S_1$ channel: odd parity spin triplet **"p-wave"**.

1.2. Generalized BCS theory

we introduce a general form of a BCS Hamiltonian:

$$\mathcal{H}_{BCS} = \sum_{\boldsymbol{k},s} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}s} c_{\boldsymbol{k}s} + \frac{1}{2} \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\boldsymbol{k},\boldsymbol{k}';s_1s_2s_3s_4} c^\dagger_{\boldsymbol{k}s_1} c^\dagger_{-\boldsymbol{k}s_2} c_{-\boldsymbol{k}'s_3} c_{\boldsymbol{k}'s_4} \tag{25}$$

we restrict to the BCS scattering channel

$$V_{\boldsymbol{k},\boldsymbol{k}';s_1s_2s_3s_4} = \langle -\boldsymbol{k}, s_1; \boldsymbol{k}, s_2 | \widehat{V} | -\boldsymbol{k}', s_3; \boldsymbol{k}', s_4 \rangle \,. \tag{26}$$

and the Pauli exclusion principle requires

$$V_{\boldsymbol{k},\boldsymbol{k}';s_1s_2s_3s_4} = -V_{-\boldsymbol{k},\boldsymbol{k}';s_2s_1s_3s_4} = -V_{\boldsymbol{k},-\boldsymbol{k}';s_1s_2s_4s_3} = V_{-\boldsymbol{k},-\boldsymbol{k}';s_2s_1s_4s_3} \,. \tag{27}$$

instability discussed by decoupling through generalized mean field like $b_{\boldsymbol{k}}$ in Eq.5:

$$c_{-\boldsymbol{k}'s} c_{\boldsymbol{k}'s'} = b_{\boldsymbol{k},ss'} + (c_{-\boldsymbol{k}'s} c_{\boldsymbol{k}'s'} - b_{\boldsymbol{k},ss'}) \qquad \text{with} \qquad b_{\boldsymbol{k},ss'} = \langle c_{-\boldsymbol{k}'s} c_{\boldsymbol{k}'s'} \rangle \tag{28}$$

inserting leads to mean field Hamiltonian

$$\mathcal{H}_{mf} = \frac{1}{2}\sum_{\boldsymbol{k},s} \xi_{\boldsymbol{k}} (c^\dagger_{\boldsymbol{k}s} c_{\boldsymbol{k}s} - c_{-\boldsymbol{k}s} c^\dagger_{-\boldsymbol{k}s}) - \frac{1}{2}\sum_{\boldsymbol{k},s_1,s_2} \left[\Delta_{\boldsymbol{k},s_1 s_2} c^\dagger_{\boldsymbol{k}s_1} c^\dagger_{-\boldsymbol{k}s_2} + \Delta^*_{\boldsymbol{k},s_1 s_2} c_{\boldsymbol{k}s_1} c_{-\boldsymbol{k}s_2} \right] + K \ , \quad (29)$$

where

$$K = -\frac{1}{2}\sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\boldsymbol{k},\boldsymbol{k}';s_1 s_2 s_3 s_4} \langle c^\dagger_{\boldsymbol{k}s_1} c^\dagger_{-\boldsymbol{k}s_2} \rangle \langle c_{-\boldsymbol{k}' s_3} c_{\boldsymbol{k}' s_4} \rangle + \frac{1}{2}\sum_{\boldsymbol{k},s} \xi_{\boldsymbol{k}}. \quad (30)$$

and the self-consistency equations

$$\Delta_{\boldsymbol{k},ss'} = -\sum_{\boldsymbol{k}',s_3 s_4} V_{\boldsymbol{k},\boldsymbol{k}';ss' s_3 s_4} b_{\boldsymbol{k},s_3 s_4} \quad \text{and} \quad \Delta^*_{\boldsymbol{k},ss'} = -\sum_{\boldsymbol{k}' s_1 s_2} V_{\boldsymbol{k}',\boldsymbol{k};s_1 s_2 s' s} b^*_{\boldsymbol{k},s_2 s_1} \ . \quad (31)$$

$\Delta_{\boldsymbol{k},ss'}$ or $b_{\boldsymbol{k},ss'}$ characterize BCS state

Bogolyubov quasiparticle spectrum: matrix formulation

$$\mathcal{H}_{mf} = \sum_{\boldsymbol{k}} \mathbf{C}^\dagger_{\boldsymbol{k}} \widehat{\mathcal{E}}_{\boldsymbol{k}} \mathbf{C}_{\boldsymbol{k}} + K \ , \quad (32)$$

with

$$\mathbf{C}_{\boldsymbol{k}} = \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c_{\boldsymbol{k}\downarrow} \\ c^\dagger_{-\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} \ , \qquad \widehat{\mathcal{E}}_{\boldsymbol{k}} = \frac{1}{2}\begin{pmatrix} \xi_{\boldsymbol{k}}\widehat{\sigma}_0 & \widehat{\Delta}_{\boldsymbol{k}} \\ \widehat{\Delta}^\dagger_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}}\widehat{\sigma}_0 \end{pmatrix} \quad \text{and} \quad \widehat{\Delta}_{\boldsymbol{k}} = \begin{pmatrix} \Delta_{\boldsymbol{k},\uparrow\uparrow} & \Delta_{\boldsymbol{k},\uparrow\downarrow} \\ \Delta_{\boldsymbol{k},\downarrow\uparrow} & \Delta_{\boldsymbol{k},\downarrow\downarrow} \end{pmatrix} . \quad (33)$$

to be diagonalized into

$$\mathcal{H} = \sum_{\boldsymbol{k}} \mathbf{A}^\dagger_{\boldsymbol{k}} \widehat{E}_{\boldsymbol{k}} \mathbf{A}_{\boldsymbol{k}} + K \quad (34)$$

where

$$\mathbf{A}_{\boldsymbol{k}} = \begin{pmatrix} a_{\boldsymbol{k}\uparrow} \\ a_{\boldsymbol{k}\downarrow} \\ a^\dagger_{-\boldsymbol{k}\uparrow} \\ a^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} \quad \text{and} \quad \widehat{E}_{\boldsymbol{k}} = \begin{pmatrix} E_{\boldsymbol{k}}\widehat{\sigma}_0 & 0 \\ 0 & -E_{\boldsymbol{k}}\widehat{\sigma}_0 \end{pmatrix} \quad (35)$$

Bogolyubov transformation with unitary matrix

$$\widehat{U}_{\boldsymbol{k}} = \begin{pmatrix} \widehat{u}_{\boldsymbol{k}} & \widehat{v}_{\boldsymbol{k}} \\ \widehat{v}^*_{-\boldsymbol{k}} & \widehat{u}^*_{-\boldsymbol{k}} \end{pmatrix} \quad \Rightarrow \quad \mathbf{C}_{\boldsymbol{k}} = \widehat{U}_{\boldsymbol{k}} \mathbf{A}_{\boldsymbol{k}} \quad \text{and} \quad \widehat{E}_{\boldsymbol{k}} = \widehat{U}^\dagger_{\boldsymbol{k}} \widehat{\mathcal{E}}_{\boldsymbol{k}} \widehat{U}_{\boldsymbol{k}} \quad (36)$$

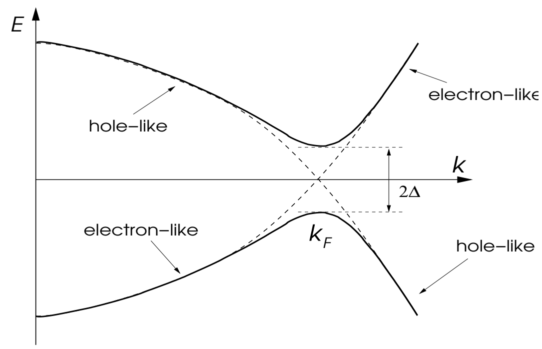
and $\widehat{U}_{\boldsymbol{k}} \widehat{U}^\dagger_{\boldsymbol{k}} = \widehat{U}^\dagger_{\boldsymbol{k}} \widehat{U}_{\boldsymbol{k}} = \widehat{1}$. with

$$\widehat{u}_{\boldsymbol{k}} = \frac{(E_{\boldsymbol{k}} + \xi_{\boldsymbol{k}})\widehat{\sigma}_0}{\sqrt{2E_{\boldsymbol{k}}(E_{\boldsymbol{k}} + \xi_{\boldsymbol{k}})}} \quad \text{and} \quad \widehat{v}_{\boldsymbol{k}} = \frac{-\widehat{\Delta}_{\boldsymbol{k}}}{\sqrt{2E_{\boldsymbol{k}}(E_{\boldsymbol{k}} + \xi_{\boldsymbol{k}})}} \quad (37)$$

and the quasiparticle energy

$$E_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2} \quad \text{with} \quad |\Delta_{\boldsymbol{k}}|^2 = \frac{1}{2}\mathrm{tr}\left(\widehat{\Delta}^\dagger_{\boldsymbol{k}} \widehat{\Delta}_{\boldsymbol{k}}\right) \ . \quad (38)$$

Quasiparticle spectrum with excitation gap (electron-hole hybridization at the Fermi energy):



Self-consistence equation (gap equation):

$$\Delta_{\boldsymbol{k},s_1s_2} = -\sum_{\boldsymbol{k}',s_3s_4} V_{\boldsymbol{k},\boldsymbol{k}';s_1s_2s_3s_4} \frac{\Delta_{\boldsymbol{k}',s_4s_3}}{2E_{\boldsymbol{k}}} \tanh\left(\frac{E_{\boldsymbol{k}}}{2k_BT}\right) \tag{39}$$

and BCS coherent ground state:

$$|\Psi_{BCS}\rangle = \prod_{\boldsymbol{k},s,s'} \left\{ u_{\boldsymbol{k},ss'} + v_{\boldsymbol{k},ss'} \hat{c}^\dagger_{\boldsymbol{k}s} \hat{c}^\dagger_{-\boldsymbol{k}s'} \right\} |0\rangle \tag{40}$$

gap matrix parametrization:

structure of the mean field: $b_{\boldsymbol{k},ss'} = \phi(\boldsymbol{k})\chi_{ss'} \quad \Rightarrow$

$$\phi(\boldsymbol{k}) = \begin{cases} +\phi(-\boldsymbol{k}) & \text{even parity, spin singlet} \\ \\ -\phi(-\boldsymbol{k}) & \text{odd parity, spin triplet} \end{cases} \tag{41}$$

Pauli exclusion principle: $\widehat{\Delta}_{\boldsymbol{k}} = -\widehat{\Delta}^T_{-\boldsymbol{k}}$ for both even and odd parity

even parity - spin singlet:

$$\widehat{\Delta}_{\boldsymbol{k}} = \begin{pmatrix} \Delta_{\boldsymbol{k},\uparrow\uparrow} & \Delta_{\boldsymbol{k},\uparrow\downarrow} \\ \Delta_{\boldsymbol{k},\downarrow\uparrow} & \Delta_{\boldsymbol{k},\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 0 & \psi(\boldsymbol{k}) \\ -\psi(\boldsymbol{k}) & 0 \end{pmatrix} = i\hat{\sigma}_y \psi(\boldsymbol{k}) \ . \tag{42}$$

with even scalar gap function, $\psi(\boldsymbol{k}) = \psi(-\boldsymbol{k})$,

odd parity - spin triplet:

$$\widehat{\Delta}_{\boldsymbol{k}} = \begin{pmatrix} \Delta_{\boldsymbol{k},\uparrow\uparrow} & \Delta_{\boldsymbol{k},\uparrow\downarrow} \\ \Delta_{\boldsymbol{k},\downarrow\uparrow} & \Delta_{\boldsymbol{k},\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} -d_x(\boldsymbol{k}) + id_y(\boldsymbol{k}) & d_z(\boldsymbol{k}) \\ d_z(\boldsymbol{k}) & d_x(\boldsymbol{k}) + id_y(\boldsymbol{k}) \end{pmatrix} = i \left(\boldsymbol{d}(\boldsymbol{k}) \cdot \hat{\boldsymbol{\sigma}} \right) \hat{\sigma}_y \ , \tag{43}$$

with odd vector gap function, $\boldsymbol{d}(\boldsymbol{k}) = -\boldsymbol{d}(-\boldsymbol{k})$
Note: spin configuration $\boldsymbol{d} \perp \boldsymbol{S}$ because

$$d_x(|\downarrow\downarrow\rangle - |\uparrow\uparrow\rangle) - id_y((|\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle) + d_z(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \tag{44}$$

excitation gap:

we use $|\Delta_{\boldsymbol{k}}|^2 = \frac{1}{2} tr \left\{ \widehat{\Delta}_{\boldsymbol{k}} \widehat{\Delta}_{\boldsymbol{k}}^\dagger \right\}$:

$$\begin{aligned} \widehat{\Delta}_{\boldsymbol{k}} \widehat{\Delta}_{\boldsymbol{k}}^\dagger &= |\psi(\boldsymbol{k})|^2 \hat{\sigma}_0 && \Rightarrow \quad |\Delta_{\boldsymbol{k}}|^2 = |\psi(\boldsymbol{k})|^2 \quad \text{even parity - spin singlet} \\ \widehat{\Delta}_{\boldsymbol{k}} \widehat{\Delta}_{\boldsymbol{k}}^\dagger &= |\boldsymbol{d}(\boldsymbol{k})|^2 \hat{\sigma}_0 + i(\boldsymbol{d}(\boldsymbol{k}) \times \boldsymbol{d}(\boldsymbol{k})^*) \cdot \hat{\boldsymbol{\sigma}} && \Rightarrow \quad |\Delta_{\boldsymbol{k}}|^2 = |\boldsymbol{d}(\boldsymbol{k})|^2 \quad \text{odd parity spin triplet} \end{aligned} \tag{45}$$

note for "unitary states": $\boldsymbol{d}(\boldsymbol{k}) \times \boldsymbol{d}(\boldsymbol{k})^* = 0$.

New parametrization:
rewrite interaction to separate even and odd parity:

$$V_{\boldsymbol{k},\boldsymbol{k}';s_1 s_2 s_3 s_4} = J^0_{\boldsymbol{k},\boldsymbol{k}'} \hat{\sigma}^0_{s_1 s_4} \hat{\sigma}^0_{s_2 s_3} + J_{\boldsymbol{k},\boldsymbol{k}'} \hat{\boldsymbol{\sigma}}_{s_1 s_4} \cdot \hat{\boldsymbol{\sigma}}_{s_2 s_3} \ , \tag{46}$$

leads to gap equations for even parity,

$$\psi(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \underbrace{(J^0_{\boldsymbol{k},\boldsymbol{k}'} - 3J_{\boldsymbol{k},\boldsymbol{k}'})}_{= v^s_{\boldsymbol{k},\boldsymbol{k}'}} \frac{\psi(\boldsymbol{k}')}{2E_{\boldsymbol{k}'}} \tanh\left(\frac{E_{\boldsymbol{k}'}}{2k_B T}\right) \tag{47}$$

for odd parity,

$$\boldsymbol{d}(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} \underbrace{(J^0_{\boldsymbol{k},\boldsymbol{k}'} + J_{\boldsymbol{k},\boldsymbol{k}'})}_{= v^t_{\boldsymbol{k},\boldsymbol{k}'}} \frac{\boldsymbol{d}(\boldsymbol{k}')}{2E_{\boldsymbol{k}'}} \tanh\left(\frac{E_{\boldsymbol{k}'}}{2k_B T}\right) \tag{48}$$

where

$$v^{s,t}_{\boldsymbol{k},\boldsymbol{k}'} = \sum_l{}' \nu^{s,t}_l(\xi_{\boldsymbol{k}}, \xi_{\boldsymbol{k}'}) \sum_{m=-l}^{+l} Y_{lm}(\hat{\boldsymbol{k}}) Y^*_{lm}(\hat{\boldsymbol{k}}') \tag{49}$$

note sum over l restricts to given parity $(-1)^l$ and $\nu^{s,t}_l(\xi, \xi')$ with the usual restrictions

linearized gap equation: $T \to T_{c-}$, $\widehat{\Delta}_{\boldsymbol{k}} \to 0$ and $E_{\boldsymbol{k}} = |\xi_{\boldsymbol{k}}|$,
case: even parity

$$\begin{aligned} \psi(\boldsymbol{k}) &= -\sum_{\boldsymbol{k}'} \nu^s_{\boldsymbol{k},\boldsymbol{k}'} \frac{\psi(\boldsymbol{k}')}{2\xi_{\boldsymbol{k}'}} \tanh\left(\frac{\xi_{\boldsymbol{k}'}}{2k_B T}\right) \\ &= -N(0) \langle \nu^s_{\boldsymbol{k},\boldsymbol{k}'} \psi(\boldsymbol{k}') \rangle_{\boldsymbol{k}',FS} \underbrace{\int_0^{\epsilon_c} d\xi \frac{1}{\xi} \tanh\left(\frac{\xi}{2k_B T}\right)}_{= \ln(1.14\epsilon_c / k_B T)} \end{aligned} \tag{50}$$

eigenvalue equation (λ: dimensionless eigenvalue defining T_c)

$$-\lambda \psi(\boldsymbol{k}) = -N(0) \langle \nu^s_{\boldsymbol{k},\boldsymbol{k}'} \psi(\boldsymbol{k}') \rangle_{\boldsymbol{k}',FS} \quad \text{with} \quad k_B T_c = 1.14 \epsilon_c e^{-1/\lambda} \tag{51}$$

analogous for odd parity

$$-\lambda \boldsymbol{d}(\boldsymbol{k}) = -N(0) \langle v^t_{\boldsymbol{k},\boldsymbol{k}'} \boldsymbol{d}(\boldsymbol{k}') \rangle_{\boldsymbol{k}',FS} \tag{52}$$

where $\langle \cdots \rangle_{\boldsymbol{k},FS}$ angular average on Fermi surface largest eigenvalue determines highest $T_c \rightarrow$ superconducting instability

Symmetry operations:

symmetries of the normal state:

- **orbital rotation** $O(3)$: $\hat{g}|\boldsymbol{k},s\rangle = |R_g\boldsymbol{k},s\rangle$ with R_g; rotation matrix of element $\hat{g} \in O(3)$
- **spin rotation** $SU(2)$: $\hat{g}|\boldsymbol{k},s\rangle = \sum_{s'} D(g)_{ss'}|\boldsymbol{k},s'\rangle$; $\hat{D}(g) = \exp[i\hat{\boldsymbol{S}}\cdot\boldsymbol{\theta}_g]$ with $\hat{g} \in SU(2)$
- **time reversal** $\hat{K}$: $\hat{K}|\boldsymbol{k},s\rangle = \sum_{s'}(-i\sigma_y)_{ss'}|-\boldsymbol{k},s'\rangle$; $\hat{K} = -i\hat{\sigma}_y\hat{C}$ with $\hat{C}$ complex conjugation ($\hat{K} \in \mathcal{K} = \{\hat{E},\hat{K}\}$.
- **inversion** $\hat{I}$: $\hat{I}|\boldsymbol{k},s\rangle = |-\boldsymbol{k},s\rangle$ with $\hat{I} \in \mathcal{I} = \{\hat{E},\hat{I}\}$
- **gauge** $U(1)$: $\hat{\Phi}|\boldsymbol{k},s\rangle = e^{i\phi/2}|\boldsymbol{k},s\rangle$ with $\hat{\Phi} \in U(1)$

Symmetry operations on gap function:

- **Fermion exchange**: $\hat{\Delta}_{\boldsymbol{k}} = -\hat{\Delta}^T_{-\boldsymbol{k}}$
- **orbital rotation**: $\hat{g}\hat{\Delta}_{\boldsymbol{k}} = \Delta_{R_g\boldsymbol{k}}$
- **spin rotation**: $\hat{g}\hat{\Delta}_{\boldsymbol{k}} = \hat{D}(g)^\dagger\hat{\Delta}_{\boldsymbol{k}}\hat{D}(g)$
- **time reversal**: $\hat{K}\hat{\Delta}_{\boldsymbol{k}} = \hat{\sigma}_y\hat{\Delta}^*_{\boldsymbol{k}}\hat{\sigma}_y$
- **inversion**: $\hat{I}\hat{\Delta}_{\boldsymbol{k}} = \hat{\Delta}_{-\boldsymbol{k}}$
- **gauge**: $\hat{\Phi}\Delta_{\boldsymbol{k}} = e^{i\phi}\hat{\Delta}_{\boldsymbol{k}}$

transferred to the gap functions $\psi(\boldsymbol{k})$ and $\boldsymbol{d}(\boldsymbol{k})$:

	even parity	odd parity
Fermion exchange	$\psi(\boldsymbol{k}) = \psi(-\boldsymbol{k})$	$\boldsymbol{d}(\boldsymbol{k}) = -\boldsymbol{d}(-\boldsymbol{k})$
Orbital rotation	$\hat{g}\psi(\boldsymbol{k}) = \psi(R_g\boldsymbol{k})$	$\hat{g}\boldsymbol{d}(\boldsymbol{k}) = \boldsymbol{d}(R_g\boldsymbol{k})$
Spin rotation	$\hat{g}\psi(\boldsymbol{k}) = \psi(\boldsymbol{k})$	$\hat{g}\boldsymbol{d}(\boldsymbol{k}) = R_g\boldsymbol{d}(\boldsymbol{k})$
Time-reversal	$\widehat{K}\psi(\boldsymbol{k}) = \psi^*(-\boldsymbol{k})$	$\widehat{K}\boldsymbol{d}(\boldsymbol{k}) = -\boldsymbol{d}^*(-\boldsymbol{k})$
Inversion	$\hat{I}\psi(\boldsymbol{k}) = \psi(-\boldsymbol{k})$	$\hat{I}\boldsymbol{d}(\boldsymbol{k}) = \boldsymbol{d}(-\boldsymbol{k})$
$U(1)$-gauge	$\widehat{\Phi}\psi(\boldsymbol{k}) = e^{i\phi}\psi(\boldsymbol{k})$	$\widehat{\Phi}\boldsymbol{d}(\boldsymbol{k}) = e^{i\phi}\boldsymbol{d}(\boldsymbol{k})$

Conventional pairing state: most symmetric pairing state $l = 0, S = 0 \quad \Rightarrow \quad \psi(\boldsymbol{k}) = \psi_0$

Unconventional pairing state: $l \neq 0, S = 0, 1$

Examples of unconventional pairing states:

cuprate high-temperature superconductors: quasi-two-dimensional $\psi(\boldsymbol{k}) = \Delta_0(k_x^2 - k_y^2)$ with $l = 2, S = 0$ **"d-wave"**;
excitation gap with line nodes: $|\Delta_{\boldsymbol{k}}| = |\Delta_0||k_x^2 - k_y^2|$.

^{3}*He B-phase :* $\boldsymbol{d}(\boldsymbol{k}) = \Delta_0 \boldsymbol{k}$ with $l = 1, S = 1$ **"p-wave"**;
excitation gap without nodes (isotropic): $|\Delta_{\boldsymbol{k}}| = |\Delta_0||\boldsymbol{k}|$.

^{3}*He A-phase :* $\boldsymbol{d}(\boldsymbol{k}) = \Delta_0 \boldsymbol{k} \hat{z}(k_x \pm i k_y)$ **"p-wave"** (2-fold degenerate);
excitation gap point nodes: $|\Delta_{\boldsymbol{k}}| = |\Delta_0||k_x \pm i k_y|$.

gap nodes influence low-temperature thermodynamic properties, e.g. specific heat

$$C(T) \propto \begin{cases} T^{-3/2} e^{-\Delta/k_B T} & \text{nodeless} \\ T^3 & \text{point nodes} \\ T^2 & \text{line nodes} \end{cases} \tag{53}$$

power laws versus thermally activated behavior, also observable in other quantities relying on a thermal average over low-energy states (London penetration depth, NMR-T_1^{-1}, ultrasound absorption, ...)

2. Generalized Ginzburg-Landau theory of superconductivity

Ginzburg-Landau theory for 2^{nd}-order phase transitions based on concept of spontaneous symmetry breaking
key quantity: **order parameter** which grows continuously from zero crossing the transition temperature into the order phase

2.1. Conventional Ginzburg-Landau theory

order parameter: gap function $\hat{\Delta}_{\boldsymbol{k}}$ or pair mean field $b_{,ss'}$
free energy expansion in order parameter $\eta = \eta(\boldsymbol{r}, T)$ for $T \approx T_c$:

$$F[\eta, \boldsymbol{A}; T] = \int_\Omega d^3r \left[a(T)|\eta|^2 + b(T)|\eta|^4 + K(T)|\boldsymbol{\Pi}\eta|^2 + \frac{1}{8\pi}(\boldsymbol{\nabla} \times \boldsymbol{A})^2 \right] , \tag{54}$$

with $\boldsymbol{\Pi} = \frac{\hbar}{i}\boldsymbol{\nabla} + \frac{2e}{c}\boldsymbol{A}$ and $a(T) \approx a'(T - T_c)$, $b(T) \approx b(T_c) = b > 0$ and $K(T) = K(T_c) = K > 0$; $\boldsymbol{A}$ is vector potential and $\boldsymbol{\nabla} \times \boldsymbol{A} - \boldsymbol{B}$ is magnetic field.

variational minimization of F with respect to η and $\boldsymbol{A} \Rightarrow$ Ginzburg-Landau equations

$$\begin{aligned} & a\eta + 2b\eta|\eta|^2 - K\boldsymbol{\Pi}^* \cdot \boldsymbol{\Pi}\eta = 0 \\ & \underbrace{\frac{2e}{c} K \left\{ \eta^* \boldsymbol{\Pi}\eta + \eta \boldsymbol{\Pi}^* \eta^* \right\}}_{= \boldsymbol{j}/c} - \frac{1}{4\pi} \boldsymbol{\nabla} \times \underbrace{(\boldsymbol{\nabla} \times \boldsymbol{A})}_{= \boldsymbol{B}} = 0 \end{aligned} \tag{55}$$

1. equation: uniform case for phase transition

$$0 = a(T)\eta + 2b\eta|\eta|^2 \qquad \Rightarrow \qquad |\eta|^2 = \begin{cases} 0 & T > T_c \\ -\dfrac{a(T)}{2b} & T \leq T_c \end{cases} \tag{56}$$

2. equation: London equation

$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{B}) = -\frac{4\pi}{c}\frac{8e^2}{c} K|\eta|^2 \boldsymbol{B} \qquad \Rightarrow \qquad \boldsymbol{\nabla}^2 \boldsymbol{B} = \frac{1}{\lambda_L^2}\boldsymbol{B} \,, \tag{57}$$

with

$$\lambda_L^{-2} = \frac{32\pi e^2}{c^2} K|\eta|^2 = \frac{4\pi e^2 n_s}{mc^2} \tag{58}$$

n_s density of superfluid electrons

describes the phenomenology of the superconducting phase: phase transition and Meissner-Ochsenfeld effect (screening of magnetic fields)

construction of free energy functional

$F[\eta, \boldsymbol{A}]$ is a scalar under all symmetries of the normal state: $\mathcal{G} = O(3) \times SU(2) \times \mathcal{K} \times \mathcal{I} \times U(1)$

order parameter: η is a scalar under $O(3)$ and $SU(2)$ because of pairing in fully symmetric channel $l = 0, S = 0$

$$\begin{aligned} &\text{time reversal :} \quad \widehat{K}\eta = \eta^* \\ &U(1) \text{ gauge :} \quad \widehat{\Phi}\eta = \eta e^{i\phi} \end{aligned} \tag{59}$$

gradient and vector potential: $\mathbf{\Pi}$ invariant under $SU(2)$

$$\begin{aligned} &\text{orbital rotation:} \quad \hat{g}\mathbf{\Pi} = R_g \mathbf{\Pi} \\ &\text{time reversal :} \quad \widehat{K}\mathbf{\Pi} = -\mathbf{\Pi}^* = \frac{\hbar}{i}\boldsymbol{\nabla} - \frac{2e}{c}\boldsymbol{A} \\ &\text{inversion:} \quad \widehat{I}\mathbf{\Pi} = -\mathbf{\Pi} \\ &U(1) \text{ gauge :} \quad \widehat{\Phi}\mathbf{\Pi} = \mathbf{\Pi} + \frac{e}{c}\boldsymbol{\nabla}\phi \end{aligned} \tag{60}$$

scalar combinations: $\eta^*\eta$, $(\eta^*\eta)^2$ and $(\mathbf{\Pi}\eta)^* \cdot (\mathbf{\Pi}\eta)^*$ as well as $(\boldsymbol{\nabla} \times \boldsymbol{A})^2$

broken symmetry at phase transition: $U(1)$ with $\mathcal{G}' = O(3) \times SU(2) \times \mathcal{K} \times \mathcal{I}$

2.2. Ginzburg-Landau theory for unconventional pairing

linearized gap equation:

$$\begin{aligned} -\lambda\psi(\boldsymbol{k}) &= -N(0)\langle v^s_{\boldsymbol{k},\boldsymbol{k}'}\psi(\boldsymbol{k}')\rangle_{\boldsymbol{k}',FS} \\ -\lambda\boldsymbol{d}(\boldsymbol{k}) &= -N(0)\langle v^t_{\boldsymbol{k},\boldsymbol{k}'}\boldsymbol{d}(\boldsymbol{k}')\rangle_{\boldsymbol{k}',FS} \end{aligned} \tag{61}$$

generally degenerate solutions for eigenvalues λ: largest $\lambda \quad \Rightarrow \quad$ highest T_c

degenerate solution form the basis of an irreducible representation of the normal state symmetry group, e.g. for $O(3)$ states classified according to angular momentum l with degeneracy $2l+1$ (dimension of representation)
assume even parity spin singlet Cooper pairs with $l \neq 0$: scalar gap function $\psi(\boldsymbol{k}) = \sum_m \eta_m(\boldsymbol{r})\psi_m(\boldsymbol{k})$ where $\{\psi_m(\boldsymbol{k})\}$ are basis function of the irreducible representation D^l and η_m is the order parameter
generalized scalar free energy involves invariant terms of η_m, η_m^* and $\boldsymbol{\Pi}$

example $O(3) \times \mathcal{I} \to D_{4h}$**:** discrete rotation symmetry
D_{4h} tetragonal point group (16 elements = 8 rotations + 8 rotations × inversion)
moreover we assume spin-orbit coupling: orbital and spin part rotate simultaneously
irrelevant for even parity spin singlet Cooper pairing

odd-parity spin-triplet states:

$$\begin{aligned} \text{rotation:} \quad & \hat{g}\boldsymbol{d}(\boldsymbol{k}) = R_g \boldsymbol{d}(R_g \boldsymbol{k}) \\ \text{inversion:} \quad & \hat{I}\boldsymbol{d}(\boldsymbol{k}) = \boldsymbol{d}(-\boldsymbol{k}) = -\boldsymbol{d}(\boldsymbol{k}) \end{aligned} \tag{62}$$

basis functions for the irreducible representations of D_{4h}:

Γ	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	I	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	basis function	used names
A_{1g}	1	1	1	1	1	1	1	1	1	1	$\psi = 1$	s-wave
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	$\psi = k_x k_y (k_x^2 - k_y^2)$	g-wave
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	$\psi = k_x^2 - k_y^2$	$d_{x^2-y^2}$-wave
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1	$\psi = k_x k_y$	d_{xy}-wave
E_g	2	0	-2	0	0	2	0	-2	0	0	$\psi = \{k_x k_z, k_y k_z\}$	d-wave
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1	$\boldsymbol{d} = \hat{x}k_x + \hat{y}k_y$	p-wave
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	$\boldsymbol{d} = \hat{x}k_y - \hat{y}k_x$	p-wave
B_{1u}	1	-1	1	1	-1	-1	1	- 1	- 1	1	$\boldsymbol{d} = \hat{x}k_x - \hat{y}k_y$	p-wave
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	- 1	$\boldsymbol{d} = \hat{x}k_y + \hat{y}k_x$	p-wave
E_u	2	0	-2	0	0	-2	0	2	0	0	$\boldsymbol{d} = \{\hat{z}k_x, \hat{z}k_y\}$	p-wave

there are 4 non-degenerate and 1 2-fold degenerate order parameter for each even and odd parity case
for the *one-dimensional representations* the free energy functional looks identical to the case of conventional order parameters

two-dimensional representation:

$$\psi(\boldsymbol{k}) = \eta_x k_x k_z + \eta_y k_y k_z \qquad \text{or} \qquad \boldsymbol{d}(\boldsymbol{k}) = \eta_x \hat{z} k_x + \eta_y \hat{z} k_y \tag{63}$$

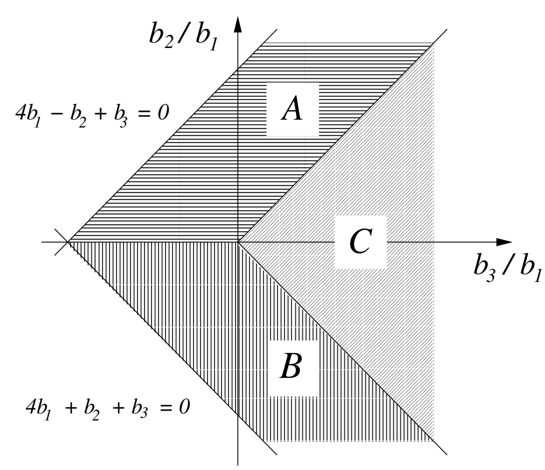
with the scalar free energy of the order parameter $\boldsymbol{\eta} = (\eta_x, \eta_y)$ and vector potential $\boldsymbol{A}$:

$$F[\boldsymbol{\eta},\boldsymbol{A};T] = \int d^3r \Big[a(T)|\boldsymbol{\eta}|^2 + b_1|\boldsymbol{\eta}|^4 + \frac{b_2}{2}\{\eta_x^{*2}\eta_y^2 + \eta_x^2\eta_y^{*2}\} + b_3|\eta_x|^2|\eta_y|^2$$
$$+K_1\{|\Pi_x\eta_x|^2 + |\Pi_y\eta_y|^2\} + K_2\{|\Pi_x\eta_y|^2 + |\Pi_y\eta_x|^2\}$$
$$+K_3\{(\Pi_x\eta_x)^*(\Pi_y\eta_y) + c.c.\} + K_4\{(\Pi_x\eta_y)^*(\Pi_y\eta_x) + c.c.\} \tag{64}$$
$$+K_5\{|\Pi_z\eta_x|^2 + |\Pi_z\eta_y|^2\} + \frac{1}{8\pi}(\boldsymbol{\nabla}\times\boldsymbol{A})^2\Big]$$

where $a(T) = a'(T-T_c)$, $b_1 > 0$, $4b_1 - |b_2| + b_3 > 0$ and $K_{1,\dots,5} > 0$.

uniform superconducting phase: 3 phases possible for symmetry reasons (table of basis functions)

Phase	$\psi(\boldsymbol{k})$	$\boldsymbol{d}(\boldsymbol{k})$	broken	symmetry
A	$k_z(k_x \pm ik_y)$	$\hat{z}(k_x \pm ik_y)$	$U(1), \mathcal{K}$	broken time reversal symmetry
B	$k_z(k_x \pm k_y)$	$\hat{z}(k_x \pm k_y)$	$U(1), D_{4h} \to D_{2h}$	broken rotation symmetry
C	k_zk_x, k_zk_y	$\hat{z}k_x, \hat{z}k_y$	$U(1), D_{4h} \to D_{2h}$	broken rotation symmetry



Which phase is most stable from a microscopic view point ? Consider $T = 0$ condensation energy (weak coupling),

$$
\begin{aligned}
E_{cond} &= \langle \mathcal{H}' \rangle_\Delta - \langle \mathcal{H}' \rangle_{\Delta=0} = \frac{1}{2} \sum_{\boldsymbol{k},s} (\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}}) + \frac{1}{2} \sum_{\boldsymbol{k},s_1,s_2} \frac{\Delta^*_{\boldsymbol{k},s_1 s_2} \Delta_{\boldsymbol{k},s_2 s_1}}{2E_{\boldsymbol{k}}} \\
&= 2N(0) \int_0^{\epsilon_c} d\xi \; (\xi - \langle \sqrt{\xi^2 + |\Delta_{\boldsymbol{k}}|^2} \rangle_{\boldsymbol{k},FS}) + \left\langle |\Delta_{\boldsymbol{k}}|^2 \int_0^{\epsilon_c} d\xi \; \frac{1}{\sqrt{\xi^2 + |\Delta_{\boldsymbol{k}}|^2}} \right\rangle_{\boldsymbol{k},FS} \\
&\approx -\frac{N(0)}{2} \langle |\Delta_{\boldsymbol{k}}|^2 \rangle_{\boldsymbol{k},FS}
\end{aligned} \tag{65}
$$

Gap structure important for stability: simple discussion assuming spherical Fermi surface: determine $\langle |\Delta_{\boldsymbol{k}}|^2 \rangle_{\boldsymbol{k},FS}$

Phase	$\langle \lvert\psi(\boldsymbol{k})\rvert^2 \rangle_{\boldsymbol{k},FS}$	$\langle \lvert\boldsymbol{d}(\boldsymbol{k})^2 \rangle_{\boldsymbol{k},FS}$
A	2/15	2/3
B	1/15	1/3
C	1/15	1/3

result: for even and odd parity the A-phase is most stable as it has least nodes.

Broken symmetries and physical properties

Normal state Symmetry including spin-orbit coupling: $\mathcal{G} = D_{4h} \times \mathcal{K} \times U(1)$

Broken U(1)-gauge symmetry yields London equation (Meissner-Ochsenfeld effect) and flux quantization

Impact of further broken symmetries:

"Nematic phase" through broken crystal rotation symmetry as in phase B and C: $\mathcal{G}' = D_{2h} \times \mathcal{K}$

$$
\boldsymbol{\eta} = \begin{cases} (1,1),\ (1,-1) & B\text{-phase} \\ (1,0),\ (0,1) & C\text{-phase} \end{cases} \tag{66}
$$

coupling to lattice strain $\epsilon_{\mu\nu}$: invariant terms in free energy

$$
F_{\epsilon-\boldsymbol{\eta}} = \int d^3r \left[\{ \gamma_1 (\epsilon_{xx} + \epsilon_{yy}) + \gamma_1' \epsilon_{zz} \} |\boldsymbol{\eta}|^2 + \gamma_2 (\epsilon_{xx} - \epsilon_{yy})(|\eta_x|^2 - |\eta_y|^2) + \gamma_3 \epsilon_{xy} (\eta_x^* \eta_y + \eta_x \eta_y^*) \right] \tag{67}
$$

with γ_i real coefficients. This free energy has to be supplemented by the elastic energy: $F_{el} = \int d^3r \sum_{\mu_1,\ldots,\mu_4} \frac{1}{2} C_{\mu_1 \cdots \mu_4} \epsilon_{\mu_1\mu_2} \epsilon_{\mu_3\mu_4}$.

- B-phase couples to the strain ϵ_{xy} $\Rightarrow$ uniaxial distorting along [110] or [1$\bar{1}$0]
- C-phase couples to the strain $\epsilon_{xx} - \epsilon_{yy}$ $\Rightarrow$ uniaxial distorting along [100] or [010]
- A-phase does not coupling to anisotropic strain $\Rightarrow$ not nematic

Single domain phase through cooling under application of uniaxial stress to sample.

"Magnetic phase" through broken time reversal symmetric as in A-phase: $\mathcal{G}' = D_{4h}$
define Cooper pair angular moment:

$$\boldsymbol{L} = i\hbar \langle \psi(\boldsymbol{k})^* (\boldsymbol{k} \times \boldsymbol{\nabla}_k) \psi(\boldsymbol{k}) \rangle_{\boldsymbol{k},FS} \tag{68}$$

and analog for odd parity state
with $\psi(\boldsymbol{k}) = \eta_x k_z k_x + \eta_y k_z k_y$

$$\boldsymbol{L} = i\hbar \hat{z} \left\{ \eta_x^* \eta_y \langle k_z^2 k_x^2 \rangle_{\boldsymbol{k},FS} - \eta_y^* \eta_x \langle k_z^2 k_y^2 \rangle_{\boldsymbol{k},FS} \right\} \propto i\hbar (\eta_x^* \eta_y - \eta_y^* \eta_x) \hat{z} \tag{69}$$

Categories of time reversal symmetry breaking phases (G.E. Volovik and L.P. Gor'kov):
"Ferromagnetic" phase: $\boldsymbol{L} \neq 0$ example: A-phase (see above)
"Antiferromagnetic" phase: $\boldsymbol{L} = 0$ example: $s + id_{x^2-y^2}$-wave state $\psi(\boldsymbol{k}) = \eta_s + i\eta_d (k_x^2 - k_y^2)$

$$\boldsymbol{L} = i\hbar \begin{pmatrix} \langle (\eta_s^* - i\eta_d (k_x^2 - k_y^2)) 2i\eta_d k_y k_z \rangle_{\boldsymbol{k},FS} \\ \langle (\eta_s^* - i\eta_d (k_x^2 - k_y^2)) 2i\eta_d k_z k_x \rangle_{\boldsymbol{k},FS} \\ -\langle (\eta_s^* - i\eta_d (k_x^2 - k_y^2)) 2i\eta_d k_x k_y \rangle_{\boldsymbol{k},FS} \end{pmatrix} = 0 \tag{70}$$

from a group theoretical point of view: components of $\boldsymbol{L}$ are basis functions of irreducible representations of point group
example D_{4h}: $\{L_x, L_y\} \to E_g$ and $L_z \to A_{2g}$

- order parameter of A-phase: $\boldsymbol{\eta} = \{\eta_x, \eta_y\} \to E_g$: $E_g \otimes E_g = A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g}$; the decomposition of this Kronecker product contains A_{2g} which is connected with L_z; thus the L_z-component can be finite.
- order parameter of $s + id$-wave phase: $\boldsymbol{\eta} = \{\eta_s, \eta_d\} \to A_{1g} \oplus B_{1g}$: $(A_{1g} \oplus B_{1g}) \otimes (A_{1g} \oplus B_{1g}) = 2A_{1g} \oplus 2B_{1g}$; the decomposition of this Kronecker product does not contain any representation connected with $\boldsymbol{L}$; thus $\boldsymbol{L}$ cannot be constructed for the order parameter and vanishes.

topological view point:

- ferromagnetic $\longleftrightarrow$ chiral $\Rightarrow$ phase has chiral subgap edge states (spontaneous edge currents)

- antiferromagnetic $\longleftrightarrow$ not chiral $\Rightarrow$ edge subgap states exist and give rise to spontaneous currents, but not connected with topological bulk properties.

Conserved charge (G.E. Volovik):
assume full rotation symmetry around z-axis (cylindrical instead of tetragonal symmetry)

$$\left.\begin{array}{ll} U(1) \text{ gauge} & \hat{\Phi}\psi(\boldsymbol{k}) = e^{i\phi}\psi(\boldsymbol{k}) \\ \text{rotation around } z\text{-axis} & \hat{\Theta}\psi(\boldsymbol{k}) = e^{i\theta}\psi(\boldsymbol{k}) \end{array}\right\} \Rightarrow \quad \hat{\Phi}\hat{\Theta}^{-1} = \hat{E} \quad \text{for } \phi = \theta \tag{71}$$

thus there is a conserved charge: $\hat{Q} = \hat{L}_z - \hat{N}/2$: changes of angular momentum and charge are coupled

removing a Cooper pair ($N \to N-2$) changes the angular momentum of the system by $\pm\hbar\hat{z}$: spatial fluctuations in Cooper pair density induces local angular momentum density or orbital magnetic flux

$\Rightarrow$ "anomalous electro-magnetism" $\Rightarrow$ spontaneous edge currents and current patterns around defects $\Rightarrow$ polar Kerr effect (theory still incomplete)

Spontaneous edge currents: Ginzburg-Landau description of the time reversal symmetry breaking phase

consider planar edge with normal vector $\boldsymbol{n} = (100)$ ($x \geq 0$ superconductor and $x < 0$ vacuum)

boundary conditions for the order parameter (scattering at the edge is pair breaking), simplified as matching condition for mirror operation on order parameter at planar edge ($x < 0$ virtual)

$$(\eta_x, \eta_y) \quad \longleftrightarrow \quad (-\eta_x, \eta_y) \qquad \Rightarrow \qquad \begin{cases} \eta_x(x) = -\eta_x(-x) \\ \eta_y(x) = \eta_y(-x) \end{cases} \tag{72}$$

Ginzburg-Landau equation give simplified solution:

$$\eta_x(x) = \eta_0 \tanh(x/\xi) \qquad \text{and} \qquad \eta_y(x) = i\eta_0 \qquad \text{with} \quad \eta_0^2 = \frac{a'(T-T_c)}{4b_1 - b_2 + b_3} \tag{73}$$

supercurrent density: $\boldsymbol{j} = -c\partial F/\partial \boldsymbol{A}$,

$$\begin{aligned} j_x &= 8\pi e \left[K_1 \eta_x^* \Pi_x \eta_x + K_2 \eta_y^* \Pi_x \eta_y + K_3 \eta_x^* \Pi_y \eta_y + K_4 \eta_y^* \Pi_y \eta_x + c.c.\right] \\ j_y &= 8\pi e \left[K_1 \eta_y^* \Pi_y \eta_y + K_2 \eta_x^* \Pi_y \eta_x + K_3 \eta_y^* \Pi_x \eta_x + K_4 \eta_x^* \Pi_x \eta_y + c.c.\right] \\ j_z &= 8\pi e K_5 \{\eta_x^* \Pi_z \eta_x + \eta_y^* \Pi_z \eta_y + c.c.\} \, . \end{aligned} \tag{74}$$

with $A_x = A_z = 0$ we find $j_x(x) = 0 \quad \Rightarrow \quad$ no current flows through the edge

$$j_y(x) = 16\pi e K_3 \eta_y \frac{\hbar}{i}\frac{\partial \eta_x}{\partial x} + \frac{c}{4\pi\lambda^2} A_y = \underbrace{\frac{16\pi e\hbar}{\xi} \frac{\eta_0^2}{\cosh^2(x/\xi)}}_{= j_y^{(0)}(x)} + \frac{c}{4\pi\lambda^2} A_y \, . \tag{75}$$

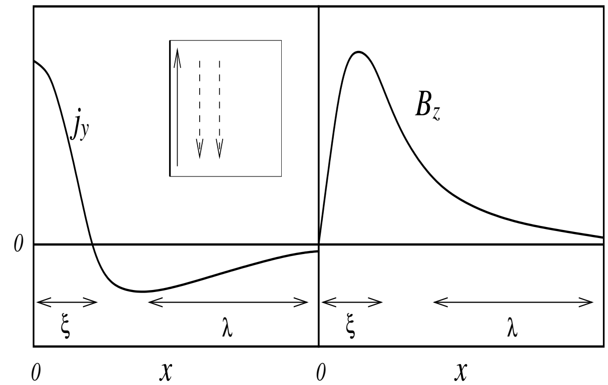
which enters the London equation

$$\frac{\partial^2 A_y}{\partial x^2} - \frac{1}{\lambda^2} A_y = \frac{4\pi}{c} j_y^{(0)}(x) \tag{76}$$

where $j_y^{(0)}$ spontaneous current parallel to the edge on a width $\xi = \sqrt{-K_1/a(T)}$; there is a Meissner screening current which compensates $j_y^{(0)}$ such that the magnetic flux induced is located close to the surface only and penetrates over the London penetration depth λ,

$$\frac{1}{\lambda^2} = \frac{32\pi^2 e^2}{c^2}(K_1 + K_2)|\eta_0|^2 \tag{77}$$

observation of spontaneous magnetic fields by zero-field μSR, measures internal magnetic field



spread in sample, enhancement of magnetism in superconducting phase: Sr_2RuO_4, $PrOs_4Sb_{12}$, (U,Th)Be_{13}, SrPtAs, Re_6Zr, ...
no direct observation of edge currents so far

Possible realizations:

Sr_2RuO_4: $\boldsymbol{d}(\boldsymbol{k}) = \Delta_0 \hat{z}(k_x \pm i k_y)$

URu_2Si_2: $\psi(\boldsymbol{k}) = \Delta_0 k_z (k_x \pm i k_y)$

3. Role of key symmetry

two key symmetries, time reversal and inversion, to form zero-momentum Cooper pairs of two partners of identical energy (Anderson, 1959, 1984)
search Cooper pair partner for $|\boldsymbol{k}\uparrow\rangle$

$$\begin{array}{llll} \text{time reversal:} & \hat{K}|\boldsymbol{k}\uparrow\rangle = |-\boldsymbol{k}\downarrow\rangle & \Rightarrow \quad |\boldsymbol{k}\uparrow\rangle, |-\boldsymbol{k}\downarrow\rangle & \text{form even-parity spin-singlet pair} \\ \text{inversion:} & \hat{I}|\boldsymbol{k}\uparrow\rangle = |-\boldsymbol{k}\downarrow\rangle & \Rightarrow \quad |\boldsymbol{k}\uparrow\rangle, |-\boldsymbol{k}\downarrow\rangle & \text{form odd-parity spin-triplet pair} \end{array} \tag{78}$$

What happens if one of the two key symmetries is absent?

Implementation in Hamiltonian:

$$\mathcal{H} \quad \longrightarrow \quad \mathcal{H} + \mathcal{H}' = \mathcal{H} + \sum_{\boldsymbol{k}} \sum_{s,s'} \boldsymbol{g}_{\boldsymbol{k}} \cdot \hat{c}^\dagger_{\boldsymbol{k}s} \boldsymbol{\sigma}_{ss'} \hat{c}_{\boldsymbol{k}s'} \tag{79}$$

the term $\mathcal{H}'$ conserves

$$\begin{aligned} &\text{(a) inversion symmetry, if} \qquad && g_{\boldsymbol{k}} = \boldsymbol{g}_{-\boldsymbol{k}} \\ &\text{(b) time reversal symmetry, if} \qquad && g_{\boldsymbol{k}} = -\boldsymbol{g}_{-\boldsymbol{k}} \end{aligned} \tag{80}$$

examples:

case (a): $\boldsymbol{g}_{\boldsymbol{k}} = \mu_B \boldsymbol{H}$ Zeeman field, leads to spin splitting of the Fermi surface (majority / minority spin Fermi sea)

case (b): $\boldsymbol{g}_{\boldsymbol{k}} = \alpha \hat{z} \times \boldsymbol{k}$ Rashba spin-orbit coupling, leads to spin splitting of Fermi surface with $\boldsymbol{k}$ dependent quantization axis

3.1. Ferromagnetic superconductor or superconductor in magnetic Zeeman field

uniform spin polarization leads to *paramagnetic limiting* (Pauli or Clogston-Chandrasekhar limit): breaking of spin singlet Cooper pairs
this is mostly not observable, because the upper critical field H_{c2} of orbital depairing is usually much lower than the limiting field H_p[3]

$$H_{c2}(T=0) = \frac{\Phi_0}{2\pi\xi_0^2} \qquad \text{and} \qquad H_p(T=0) = \frac{H_c(0)}{\sqrt{4\pi\chi_p}} \tag{82}$$

where $H_c(0)$ is the thermodynamic critical field at $T = 0$ and χ_p is the Pauli spin susceptibility.

coupling terms to the free energy expansion due to magnetic field $\boldsymbol{H}$ for order parameters $\psi(\boldsymbol{k}) = \sum_j \eta_j \psi_i(\boldsymbol{k})$ and $\boldsymbol{d}(\boldsymbol{k}) = \sum_{\mu,j} \eta_{\mu j} \hat{\mu} k_j$

2^{nd}-order coupling to $\boldsymbol{H}$ for suppression (paramagnetic limit)

$$F_H^{(2)} = \beta \sum_{\mu,\nu} \sum_j H_\mu H_\nu \left\{ |\eta_j|^2 \delta_{\mu\nu} + \eta_{\mu j}^* \eta_{\nu j} \right\} \propto \boldsymbol{H}^2 \langle |\psi(\boldsymbol{k})|^2 \rangle_{\boldsymbol{k},FS} + \langle |\boldsymbol{H} \cdot \boldsymbol{d}(\boldsymbol{k})|^2 \rangle_{\boldsymbol{k},FS} \tag{83}$$

with $\beta > 0$ (this terms gives correction to spin susceptibility, Yosida)

1^{st}-order coupling to $\boldsymbol{H}$ for the structure of state

$$F_H^{(1)} = i\beta' \sum_{\lambda,\mu,\nu} \epsilon_{\lambda\mu\nu} H_\lambda \eta_{\mu j}^* \eta_{\nu j} \propto i\boldsymbol{H} \cdot \langle \boldsymbol{d}(\boldsymbol{k})^* \times \boldsymbol{d}(\boldsymbol{k}) \rangle_{\boldsymbol{k},FS} \tag{84}$$

[3]Paramagnetic limit: comparison of spin polarization and condensation energy:

$$\frac{H_c(0)}{8\pi} = \frac{\chi_p}{2} H^2 \quad \Rightarrow \quad H_p = \frac{H_c}{\sqrt{4\pi\chi_p}} \tag{81}$$

with $\epsilon_{\lambda\mu\nu}$ completely antisymmetric tensor

Assuming $\boldsymbol{H} \parallel \hat{z}$ we find that spin singlet order parameters generally and spin-triplet order parameters with $\boldsymbol{d} \parallel \boldsymbol{H}$ are suppressed, while spin triplet components with $\boldsymbol{d} \perp \boldsymbol{H}$ is stable yielding $\boldsymbol{H} \cdot (\boldsymbol{d}^* \times \boldsymbol{d}) \neq 0$. This is a *non-unitary* state with

$$\widehat{\Delta}_{\boldsymbol{k}}\widehat{\Delta}_{\boldsymbol{k}}^\dagger = |\boldsymbol{d}(\boldsymbol{k})|^2\hat{\sigma}_0 + i(\boldsymbol{d}(\boldsymbol{k}) \times \boldsymbol{d}(\boldsymbol{k})^*) \cdot \hat{\boldsymbol{\sigma}} \tag{85}$$

which is not equal to $\hat{\sigma}_0$: $|\Delta_{\uparrow\uparrow}| \neq |\Delta_{\downarrow\downarrow}|$ on the two split Fermi surfaces. Note, the A_1-phase of Helium in a magnetic field is non-unitary with $|\Delta_{\uparrow\uparrow}| \neq 0$ and $|\Delta_{\downarrow\downarrow}| = 0$.

3.2. Non-centrosymmetric superconductors

non-centrosymmetric compounds have a crystal lattice lacking an inversion center, this yields spin-orbit coupling e.g. like Rashba spin-orbit coupling
inversion symmetry is important for spin-triplet Cooper pairs:
coupling terms for the spin-orbit coupling term represented by $\boldsymbol{g}_{\boldsymbol{k}} = \sum_{\mu,j} g_{\mu j}\hat{\mu}k_j$

2^{nd}-order coupling to $\boldsymbol{g}_{\boldsymbol{k}}$ for suppression spin-triplet pairing

$$F_g^{(2)} = \beta \sum_{\mu,\nu}\sum_{j,j'} \left\{|g_{\mu j}|^2|\eta_{\nu j'}|^2 - (g_{\mu j}\eta_{\mu j})^*(g_{\nu j'}\eta_{\nu j'})\right\} \propto \langle|\boldsymbol{g}_{\boldsymbol{k}} \times \boldsymbol{d}(\boldsymbol{k})|^2\rangle_{\boldsymbol{k},FS} \tag{86}$$

vskip 0.2 cm 1^{st}-order coupling to $\boldsymbol{g}_{\boldsymbol{k}}$ yields parity-mixing

$$F_g^{(1)} = \beta' \sum_{\mu,j} g_{\mu j}(\eta_{\mu j}^*\eta_s + \eta_{\mu j}\eta_s^*) \propto \langle \boldsymbol{g}_{\boldsymbol{k}} \cdot \boldsymbol{d}(\boldsymbol{k})^*\psi(\boldsymbol{k})\rangle_{\boldsymbol{k},FS} + c.c. \tag{87}$$

where for simplicity we take conventional s-wave pairing for the spin singlet component (different spin singlet states are also possible)
this suggests that $\boldsymbol{d}(\boldsymbol{k})$ and $\boldsymbol{g}_{\boldsymbol{k}}$ have the same symmetry properties and the gap matrix is given by

$$\widehat{\Delta}_{\boldsymbol{k}} = (\psi(\boldsymbol{k}) + \boldsymbol{d}(\boldsymbol{k}) \cdot \hat{\boldsymbol{\sigma}})i\hat{\sigma}^y \quad \Rightarrow \quad \widehat{\Delta}_{\boldsymbol{k}}\widehat{\Delta}_{\boldsymbol{k}}^\dagger = (|\psi|^2 + |\boldsymbol{d}|^2)\hat{\sigma}_0 + \{\psi^*\boldsymbol{d} + \psi\boldsymbol{d}^*\} \cdot \hat{\boldsymbol{\sigma}} \tag{88}$$

which means the mixed-parity state is *non-unitary* with a different gap on the two spin-split Fermi surfaces.