Aspects of Unconventional Superconductivity

Ref: Sigrist and Ueda, Rev. Mod. Phys. 63, 239

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Plan

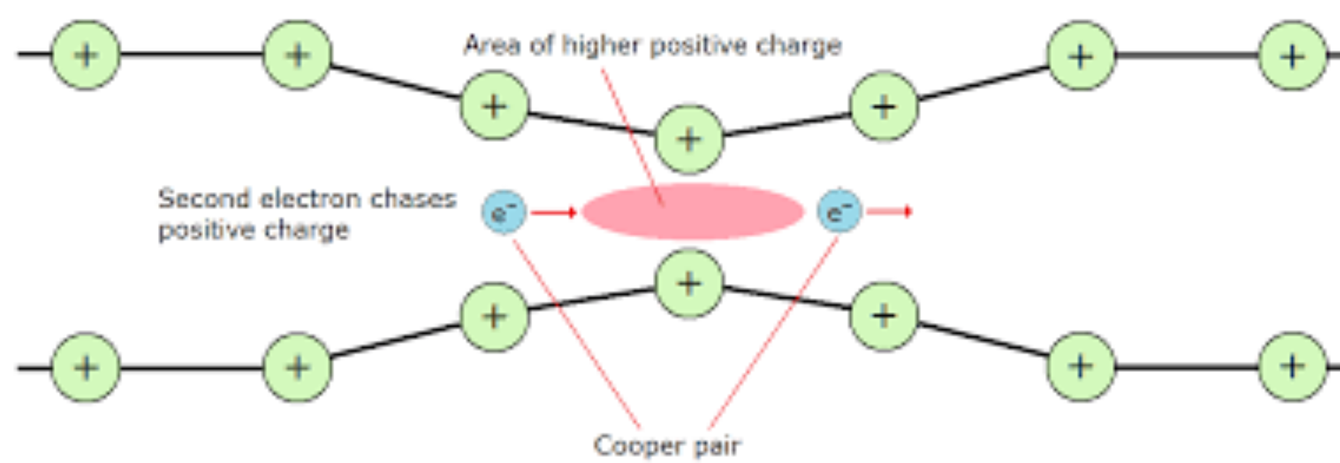
- Introduction
- Generalised BCS and some example gap functions
- Properties of observables

Superconductivity

- Phase of matter.
- Well explained by BCS theory.
- Phonon "induced" attraction between electrons → form Cooper pairs.
- $H = KE + Attractive\ part$
- Ground state:

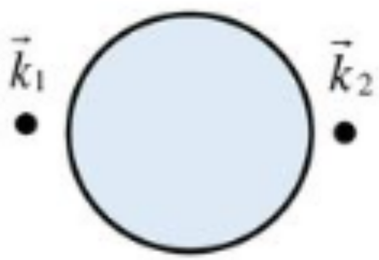
$$|\Psi_{BCS}\rangle = \prod_{\boldsymbol{k}} \left[u_{\boldsymbol{k}} + v_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} \right] |0\rangle$$

$$E = \sqrt{\xi_k^2 + \Delta^2}$$



Cooper problem

- Add two electrons interacting with each other over a fermi sea.



- 2 electron states: $|\vec{k}_1 s_1\rangle$ and $|\vec{k}_2 s_2\rangle$, with $|k_1|, |k_2| > k_F$
- Normal state: $\Delta E > 2E_F$, but SC gives $\Delta E < 2E_F$ (normal state unstable)

- Specialise: $\vec{k}_1 + \vec{k}_2 = 0 \rightarrow \Psi(r_1, s_1; r_2, s_2) = \phi(r_1 - r_2) \cdot \chi_{s_1 s_2} = \phi(r) \cdot \chi$

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

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

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

- Symmetry Aspect: If we assume that V has full spherical rotational symmetry, then $V_{\vec{k},\vec{k}'}$ can be expanded in spherical harmonics as

$$V_{\boldsymbol{k}-\boldsymbol{k}'} = \sum_{l=0}^{\infty} V_l(k,k') \sum_{m=-l}^{+l} Y_{lm}(\hat{\boldsymbol{k}}) Y_{lm}^*(\hat{\boldsymbol{k}}')$$

$$g_{\boldsymbol{k}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} g_{lm}(k) Y_{lm}(\hat{\boldsymbol{k}})$$

- Doing this expansion decouples the Schrödinger eqn for different channels l:

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

$$\Delta E = E - 2\epsilon_F$$

- Solving for bound state of electrons i.e. $\Delta E < 0$ we get

$$V_l(\xi,\xi') = \begin{cases} \nu_l & -\epsilon_c \leq \xi, \xi' \leq \epsilon_c \\ 0 & \text{otherwise} \end{cases} \implies \Delta E = -2\epsilon_c e^{2/N(0)\nu_l}$$

$\therefore$ lowest bound state is attained for strongest "attractive" channel

- Parity: $(-1)^l$, l= 0,2,4,…. (Even parity) and $l = 1,3,5...$ (odd parity)

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"**.

- Definition: "Conventional superconductor $\Longrightarrow$ pairing in l=0 channel. Unconventional are all other states with $l > 0$."

Generalised BCS theory

$$\boxed{\mathscr{H} = \sum_{\vec{k},s} \xi_{\vec{k}} c^\dagger_{\vec{k}s} c_{\vec{k}s} + \frac{1}{2} \sum_{\vec{k},\vec{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\vec{k},\vec{k}';s_1s_2s_3s_4} c^\dagger_{\vec{k}s_1} c^\dagger_{-\vec{k}s_2} c_{-\vec{k}'s_3} c_{\vec{k}'s_4}}$$

- $$V_{\vec{k},\vec{k}';s_1s_2s_3s_4} = \langle -\vec{k}, s_1; \vec{k}, s_2 | \widehat{V} | -\vec{k}', s_3; \vec{k}', s_4 \rangle$$
- COM at rest, attractive only in a thin shell ($-\epsilon_c < \xi_k, \xi_{k'} < \epsilon_c$).

$$b_{\vec{k},ss'} = \langle c_{-\vec{k}s} c_{\vec{k}s'} \rangle \qquad \mathscr{H}' = \sum_{\vec{k},s} \xi_{\vec{k}} c^\dagger_{\vec{k}s} c_{\vec{k}s} - \frac{1}{2} \sum_{\vec{k},s_1,s_2} \left[\Delta_{\vec{k},s_1s_2} c^\dagger_{\vec{k}s_1} c^\dagger_{-\vec{k}s_2} + \Delta^*_{\vec{k},s_1s_2} c_{\vec{k}s_1} c_{-\vec{k}s_2} \right]$$

- Gap function now a 2×2 matrix in spin space:

$$\Delta_{\vec{k},ss'} = - \sum_{\vec{k}',s_3s_4} V_{\vec{k},\vec{k}';ss's_3s_4} b_{\vec{k},s_3s_4} \qquad \widehat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k},\uparrow\uparrow} & \Delta_{\vec{k},\uparrow\downarrow} \\ \Delta_{\vec{k},\downarrow\uparrow} & \Delta_{\vec{k},\downarrow\downarrow} \end{pmatrix}$$

- $\hat{b}_{\vec{k}}$ → wave-function of the Cooper pairs. Separate into orbital and spin parts

$$b_{\vec{k},s_1s_2} = \phi(\vec{k})\chi_{s_1s_2}$$

$$\text{Even Parity:} \quad \phi(\vec{k}) = \phi(-\vec{k}) \quad \Leftrightarrow \quad \chi_{s_1s_2} = \tfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \qquad \text{spin singlet}$$

$$\text{Odd Parity:} \quad \phi(\vec{k}) = -\phi(-\vec{k}) \quad \Leftrightarrow \quad \chi_{s_1s_2} = \begin{cases} |\uparrow\uparrow\rangle \\ \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{cases} \qquad \text{spin triplet}$$

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

$$\widehat{\Delta}_{\vec{k}} = \begin{pmatrix} -d_x(\vec{k}) + id_y(\vec{k}) & d_z(\vec{k}) \\ d_z(\vec{k}) & d_x(\vec{k}) + id_y(\vec{k}) \end{pmatrix} = i\left(\vec{d}(\vec{k}) \cdot \hat{\vec{\sigma}}\right)\hat{\sigma}_y \quad \vec{d}(\vec{k}) = -\vec{d}(-\vec{k})$$

- The low energy excitations are given by

$$E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + |\Delta_{\vec{k}}|^2} \qquad |\Delta_{\vec{k}}|^2 = \frac{1}{2}\mathrm{tr}\left(\widehat{\Delta}_{\vec{k}}^\dagger \widehat{\Delta}_{\vec{k}}\right)$$

$$\widehat{\Delta}_{\vec{k}}\widehat{\Delta}_{\vec{k}}^\dagger = |\psi(\vec{k})|^2\hat{\sigma}_0 \qquad \text{spin singlet}$$

$$\widehat{\Delta}_{\vec{k}}\widehat{\Delta}_{\vec{k}}^\dagger = |\vec{d}|^2\hat{\sigma}_0 + i(\vec{d}\times\vec{d}^*)\cdot\hat{\vec{\sigma}} \quad \text{spin triplet .}$$

- Triplet pairing with non-zero $\overrightarrow{q}(\overrightarrow{k}) = i(\overrightarrow{d}^*(\overrightarrow{k}) \times \overrightarrow{d}(\overrightarrow{k}))\cdot\overrightarrow{\sigma}$ are called non-unitary states, related to pairing with intrinsic spin polarization. For such states, there can exist two different gaps:

$$|\Delta_{\vec{k}\pm}|^2 = |\vec{d}(\vec{k})|^2 \pm |\vec{d}^*(\vec{k}) \times \vec{d}(\vec{k})|$$

Examples of Gap functions

- Isotropic Pairing: conventional (l=0) or s-wave spin singlet

$$\psi(\vec{k}) = \Delta_0 \longrightarrow |\Delta_{\vec{k}}| = |\Delta_0|$$

unconventional: spin triplet "BW state" (e.g. ^3He B-phase)

$$\vec{d}(\vec{k}) = \frac{\Delta_0}{k_F}(\hat{x}k_x + \hat{y}k_y + \hat{z}k_z) = \frac{\Delta_0}{k_F}\begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}$$

$$|\Delta_{\vec{k}}|^2 = \frac{1}{2}\mathrm{tr}(\widehat{\Delta}^\dagger_{\vec{k}}\widehat{\Delta}_{\vec{k}}) = |\vec{d}(\vec{k})|^2 = |\Delta_0|^2\frac{|\vec{k}|^2}{k_F^2} = |\Delta_0|^2$$

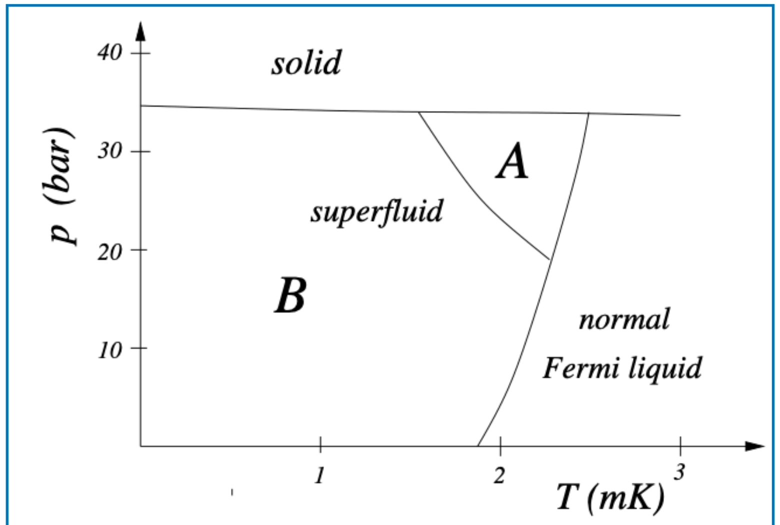


FIGURE 7. Phase diagram of ^{3}He.

- Anisotropic spin-singlet: l=2 or "d-wave" pairing (e.g. HTSC)

$$\psi(\vec{k}) = \frac{\Delta_0}{k_F}(k_x^2 - k_y^2) \longrightarrow$$ Line nodes for $(k_x, k_y) \parallel (\pm 1, \pm 1)$

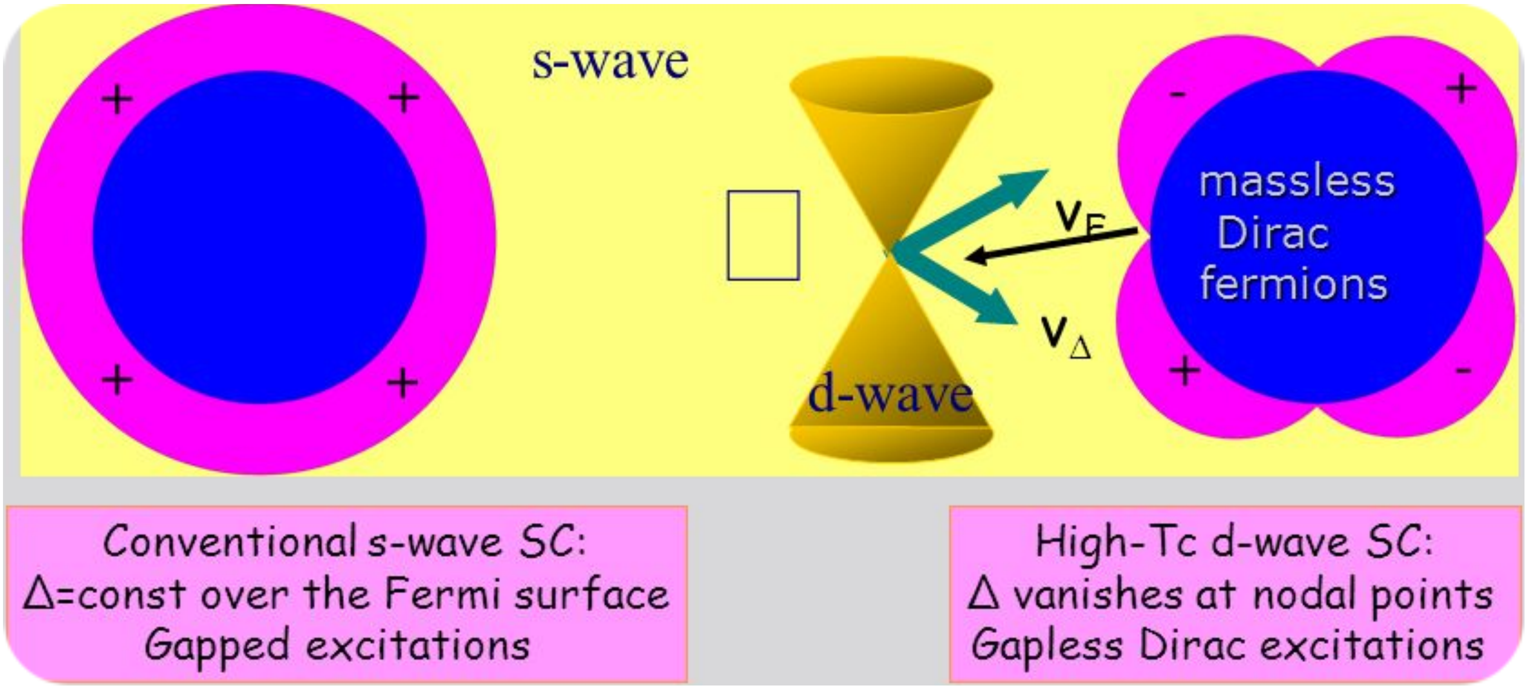
D-wave on a square lattice

- Order parameter for d-wave SC on a square lattice is given by

$$\Delta(k_x, k_y) = \Delta_0(cos(k_x a) - cos(k_y a))$$

- KE : $t_k = -t(cos(k_x a) + cos(k_y a))$

Hot spots: $\vec{k} = (\pm 1, \pm 1)\frac{\pi}{2a}$



Linearising H_{BdG} around hot spots yields

$$\hat{H}_{++} = \begin{pmatrix} ta(k_x + k_y) & \Delta_0 a(k_x - k_y) \\ \Delta_0 a(k_x - k_y) & -ta(k_x + k_y) \end{pmatrix}$$

$$\downarrow$$

$$\boxed{\hat{H}_{++} \to k_1\sigma_1 + k_2\sigma_2}$$

Gapless Dirac excitations !

- Anisotropic spin-triplet: $l = 1$ or "p-wave" states (e.g. ^3He A-phase and Sr_2RuO_4)

$$\vec{d}(\vec{k}) = \frac{\Delta_0}{k_F}\hat{z}(k_x \pm ik_y) \qquad |\Delta_{\vec{k}}|^2 = |\Delta_0|^2 \frac{k_x^2 + k_y^2}{k_F^2}$$

has point nodes for $\overrightarrow{k} \| (0,0,1)$.

- Non-Unitary state: e.g. A_1-phase of ^3He

$$\vec{d}(\vec{k}) = \frac{\Delta_0}{k_F}(\hat{x} - i\hat{y})k_z \qquad \Rightarrow \qquad \widehat{\Delta}_{\vec{k}} = \begin{pmatrix} -k_z & 0 \\ 0 & 0 \end{pmatrix}$$

pairs in only $|\uparrow\uparrow\rangle$ state i.e. leaves half of all electrons unpaired. Hard to stabilise due to reduced condensation energy.

Properties

- USCs, with anisotropic gap function, can harbour quasi-particles with "sub-gap" energies.

$$N(E) = N_0 \begin{cases} 0 & |E| < \Delta_m \\ \dfrac{E}{\sqrt{E^2 - |\Delta_m|^2}} & \Delta_m \leq |E| \end{cases}$$

Isotropic

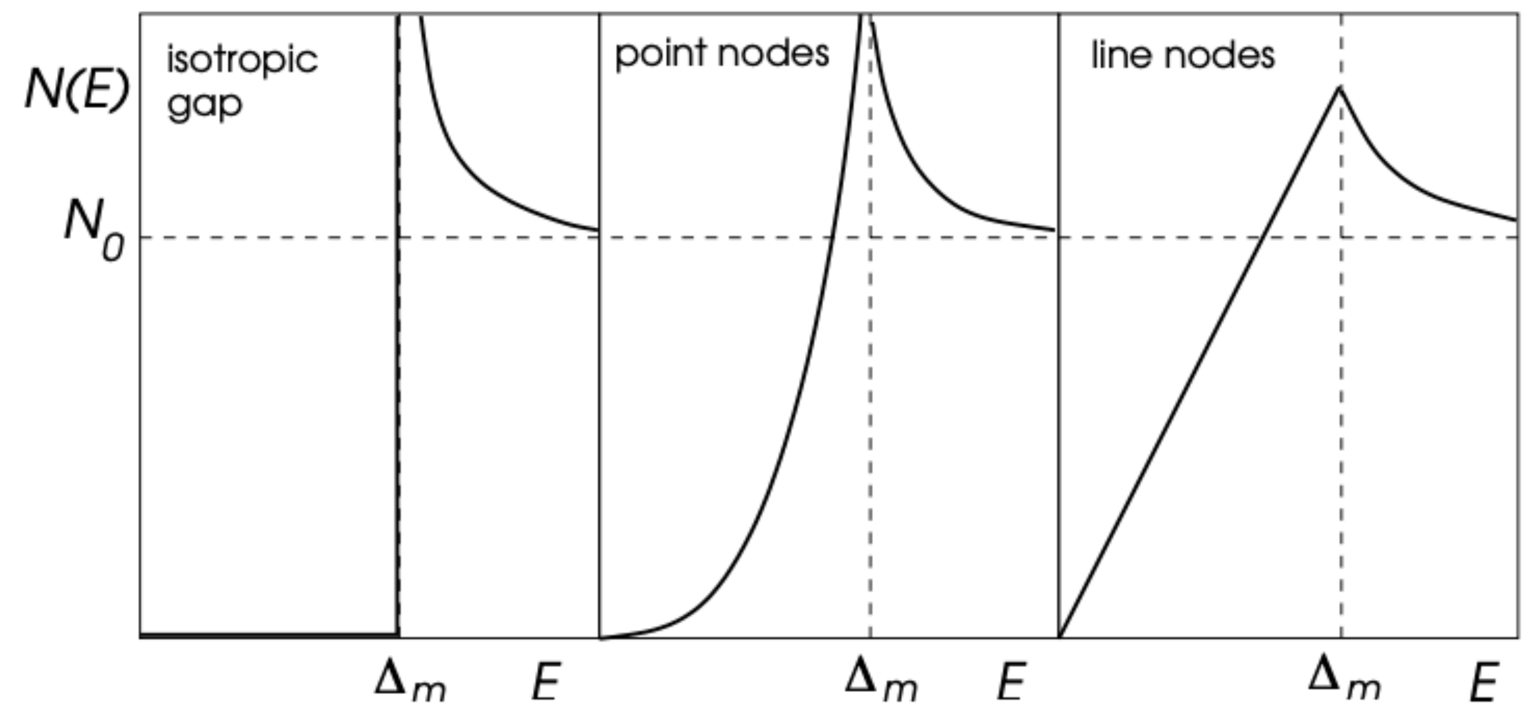


FIGURE 8. Quasiparticle density of states $N(E)$ for the isotropic gap, the gap with point nodes and line nodes.

$$N(E) = N_0 \frac{E}{\Delta_m} \begin{cases} \dfrac{\pi}{2} & |E| < \Delta_m \\ \arcsin\left(\dfrac{\Delta_m}{E}\right) & \Delta_m \leq |E| \end{cases}$$

Line Nodes

$$N(E) = N_0 \frac{E}{\Delta_m} \ln \left| \frac{1 + \frac{E}{\Delta_m}}{1 - \frac{E}{\Delta_m}} \right|$$

$N(E) \propto E^2$ for $E \to 0$

Point Nodes

- Node topology → changes DOS.

- At low temp, gap gets saturated. So only QP DOS dominates thermodynamics. E.g. Specific heat

$$C(T) \sim N_0 k_B \left(\frac{\Delta_m}{k_B T}\right)^2 \sqrt{2\pi k_B T \Delta_m} e^{-\Delta_m/k_B T}$$

thermally activated behaviour (gapped system).

- However, for nodal SCs, power law in DOS translates to power law in T dependence. For $N(E) \to E^n, \; E \to 0$

$$C(T) = \int dE\, N(E)\, \frac{E^2}{k_B T^2} \frac{1}{4\cosh^2(E/2k_B T)} \propto \int dE\, E^n\, \frac{E^2}{k_B T^2} \frac{1}{4\cosh^2(E/2k_B T)} \propto T^{n+1}$$

- More generally, quantities like C_v, κ and λ show power law T dependence.

Symmetries and Phenomenology

- Apart from microscopics, unconventional SCs can also be treated by constructing a phenomenological Ginzburg - Landau functional.

- Strength: can be formulated w/o full knowledge of microscopics, based on symmetry considerations.

$$\text{time reversal}: \quad \widehat{K}\eta = \eta^*$$

$$U(1)\text{ gauge}: \quad \widehat{\Phi}\eta = \eta e^{i\phi}$$

$$F[\eta, \vec{A}; T] = \int_\Omega d^3r \left[a(T)|\eta|^2 + b(T)|\eta|^4 + K(T)|\vec{\Pi}\eta|^2 \cdot \right.$$

$$G = K \times U(1)$$

- Additional symmetries can be spontaneously broken too (rotational symmetry breaking "nematic" pairing for e.g.).

Summary

- BCS supports large class of gap functions.
- Pairing can be singlet, triplet, spin-polarised, rotational symmetry breaking etc etc.
- Node topology can produce non-trivial effects on thermodynamics observables, often even changing the nature of low energy excitations.

Thank you for your patience!

Review Slides

- Symmetry Aspect: If we assume that V has full spherical rotational symmetry, then $V_{\vec{k},\vec{k}'}$ can be expanded in spherical harmonics as

$$V_{\boldsymbol{k}-\boldsymbol{k}'} = \sum_{l=0}^{\infty} V_l(k,k') \sum_{m=-l}^{+l} Y_{lm}(\hat{\boldsymbol{k}}) Y^*_{lm}(\hat{\boldsymbol{k}}')$$

- Why? $V_{k,k'} = \langle k | V | k' \rangle$, which must be still be invariant under simultaneous rotation of $\vec{k}$ and $\vec{k}'$, and thus can be written in terms of $\hat{k} \cdot \hat{k}'$ as

$$V_{\boldsymbol{k}k'} = \sum_{k} V_l(k,k')\ P_l(\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}')\ = \sum_{l=0}^{\infty} V_l(k,k') \sum_{m=-l}^{+l} Y_{lm}(\hat{\boldsymbol{k}}) Y^*_{lm}(\hat{\boldsymbol{k}}')$$

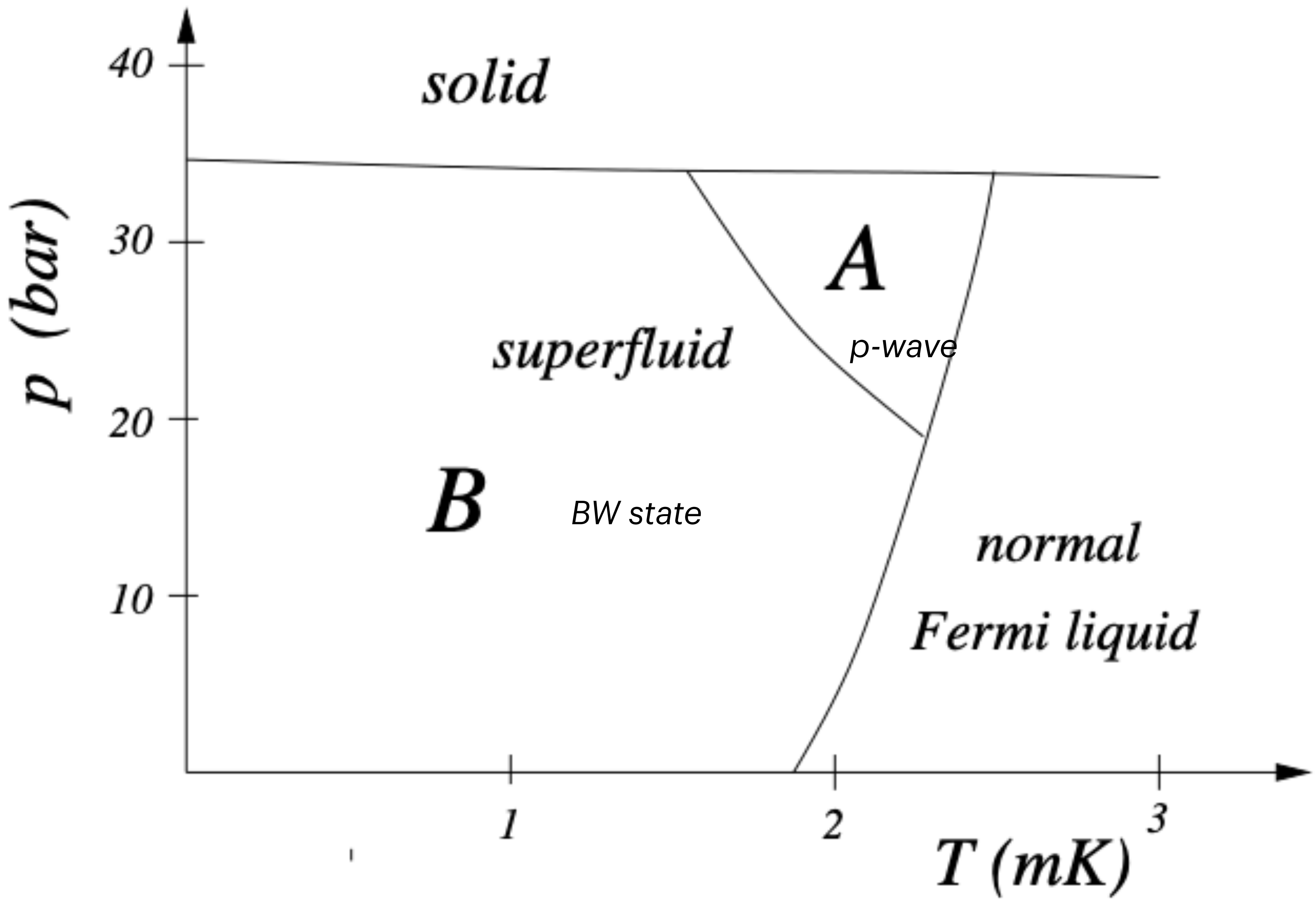
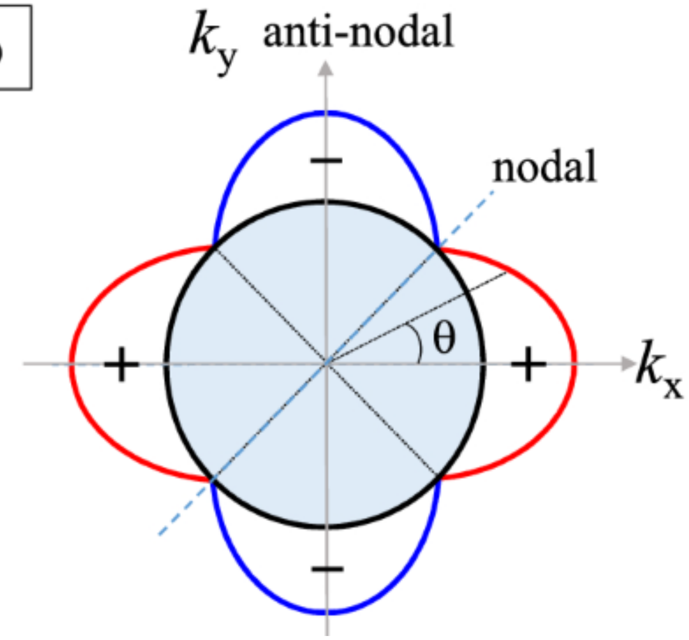


FIGURE 7. Phase diagram of ^{3}He.

2D *d*-wave SC gap



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