

Unconventional superconductivity — a general view, d-wave pairing etc. ①

§ Definition: (real space picture)

The Cooper pairing structure can be classified by its symmetry property.

Let us consider a strong coupling limit such that Cooper pairs can be viewed as diatom molecule whose real space wavefunctions can be written as

$$\psi_{\alpha_1 \alpha_2}(\vec{r}_1, \vec{r}_2) = \Phi(\vec{R}) \phi(\vec{r}_1 - \vec{r}_2) \chi_{\alpha_1 \alpha_2}$$

where $\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$ is the center of mass coordinate, $\vec{r} = \vec{r}_1 - \vec{r}_2$ is the relative coordinate, $\chi_{\alpha_1 \alpha_2}$ is the spin-wave function. For simplicity, we assume

$\Phi(\vec{R}) = \text{constant}$, i.e. momentum zero pairing. In isotropic system, we can expand $\phi(\vec{r}_1 - \vec{r}_2)$ in terms of angular momentum basis. If no spin-orbit

coupling, $\chi_{\alpha_1 \alpha_2}$ can be classified as $\chi_s = \frac{|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}$ (spin singlet)

and $\chi_{t, S_z=1,0,-1} = \begin{cases} |\uparrow_1\rangle|\uparrow_2\rangle, \\ \frac{|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}, \\ |\downarrow_1\rangle|\downarrow_2\rangle \end{cases}$ (spin triplet).

Considering the fermionic statistics, $\psi_{\alpha_1 \alpha_2}(\vec{r}_1, \vec{r}_2) = -\psi_{\alpha_2 \alpha_1}(\vec{r}_2, \vec{r}_1)$, we have

$$\psi_{\alpha_1 \alpha_2}(\vec{r}_1, \vec{r}_2) = \begin{cases} R_n(r) Y_{lm}(\vec{r}) \chi_s & (\text{for } l = \text{even}) \\ R_n(r) Y_{lm}(\vec{r}) \chi_{t, 0, \pm 1} & (\text{for } l = \text{odd}). \end{cases}$$

$R_n(r)$ is the radial wavefunction, and n is the radial quantum number.

classification: according to symmetry.

① conventional pairing: s-wave, spin singlet, $R_{n=0}(r)$ positive definite. — Hg, Al, Pb, etc

② unconventional pairing: all other pairing symmetries except the s-wave.

example: d-wave high T_c cuprates, singlet (Nobel prize)

p-wave ^3He -A and B phases, spin triplet (Nobel prizes)
 Sr_2RuO_4 (?) almost

f-wave ? UPt_3

They may be nodal or nodeless, may be topologically trivial or not.

③ Extended s-wave: pairing wavefunction does not change sign as varying angular variables, but changes sign along radial direction.

(e.g. Iron-based superconductors, but not fully settled yet!)

* Unconventional pairing can save Coulomb repulsion energy since $\phi(\vec{r}=0) = 0$. The probability of two electrons coincide at the same point vanishes!

§ Weak coupling (momentum space picture) — gap equation

we first consider the unconventional pairing in the singlet channel.

The simplest and most celebrated example is the high T_c cuprates, whose physics mainly occurs in the 2D CuO plane. The lattice structure is square, and the rotation symmetry is only 4-fold.

Background:

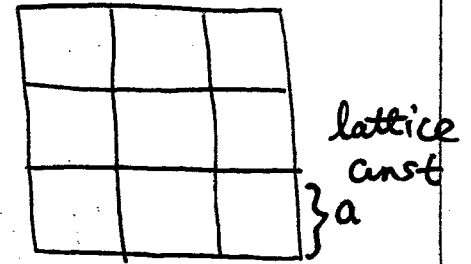
The kinetic energy: tight-binding model

$$H_0 = -t \sum_{\langle i,j \rangle} C_{i\sigma}^{\dagger} C_{j\sigma} + \text{h.c.}$$

plug in Fourier component

$$C_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \vec{r}_i} C_{\mathbf{k}}$$

N is the number of lattice sites



$$\Rightarrow H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} C_{\mathbf{k}\sigma}^{\dagger} C_{\mathbf{k}\sigma} \quad \text{with} \quad \epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$$

Ex: ① please derive the H_0 in momentum space.

② prove that at half filling, i.e. $\langle n \rangle = \langle C_{i\sigma}^{\dagger} C_{i\sigma} \rangle = 1$.

The chemical potential $\mu = 0$, and the Fermi surface has the shape of a diamond, i.e.

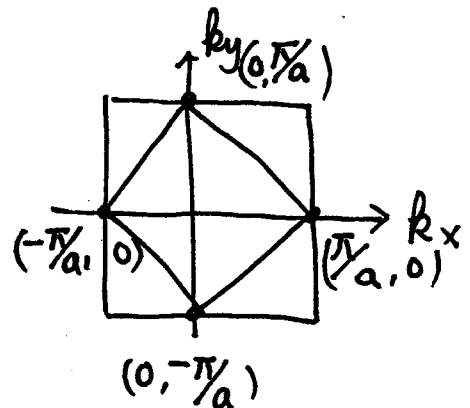
$$\cos k_x + \cos k_y = 0$$

③ please also plot Fermi surfaces

for negative values of μ ,

say $|\mu/t| = 0.05, 0.1, \text{etc.}$

This corresponds to the situation of doping.



Due to the strong onsite Coulomb interaction, we consider the pairing on NN bonds. (The mechanism for the gluing force remains unknown).

$$H_{int} = -\frac{V}{2} \sum_{\delta = \pm \hat{x}, \pm \hat{y}} (C_{i+\delta\downarrow}^\dagger C_{i\uparrow}^\dagger - C_{i+\delta\uparrow}^\dagger C_{i\downarrow}^\dagger) (C_{i\uparrow} C_{i+\delta\downarrow} - C_{i\downarrow} C_{i+\delta\uparrow})$$

— phenomenological interaction leading to d-wave pairing

perform Fourier transformation, and keep the pairing term

$$H_{pair} = -\frac{V}{2N} \sum_{\mathbf{k}, \mathbf{k}'} \sum_{\vec{\delta}} e^{i\mathbf{k}' \cdot \vec{\delta}} e^{-i\mathbf{k} \cdot \vec{\delta}} \left[\begin{array}{c} C_{-\mathbf{k}'\downarrow}^\dagger C_{\mathbf{k}'\uparrow}^\dagger \\ - C_{-\mathbf{k}'\uparrow}^\dagger C_{\mathbf{k}'\downarrow}^\dagger \end{array} \right] \left[\begin{array}{c} C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} \\ - C_{\mathbf{k}\downarrow} C_{-\mathbf{k}\uparrow} \end{array} \right]$$

$$= -\frac{V}{2N} \sum_{\mathbf{k}, \mathbf{k}'} 4 (\cos k'_x \cos k_y + \cos k'_y \cos k_x) C_{-\mathbf{k}'\downarrow}^\dagger C_{\mathbf{k}'\uparrow}^\dagger C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow}$$

$$= -\frac{V}{N} \sum_{\mathbf{k}, \mathbf{k}'} \left\{ (\cos k'_x + \cos k'_y) C_{-\mathbf{k}'\downarrow}^\dagger C_{\mathbf{k}'\uparrow}^\dagger (\cos k_x + \cos k_y) C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} \right. \\ \left. + (\cos k'_x - \cos k'_y) C_{-\mathbf{k}'\downarrow}^\dagger C_{\mathbf{k}'\uparrow}^\dagger (\cos k_x - \cos k_y) C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} \right\}$$

Define $\Delta_s = \frac{V}{N} \sum_{\mathbf{k}} C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} (\cos k_x + \cos k_y)$

$$\Delta_d = \frac{V}{N} \sum_{\mathbf{k}} C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} (\cos k_x - \cos k_y)$$

$$\frac{1}{N} H_{MF} = -\frac{V}{2N} \sum_{\mathbf{k}} \Delta_s^* (\cos k_x + \cos k_y) C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} + h.c$$

$$- \frac{V}{N} \sum_{\mathbf{k}} \Delta_d^* (\cos k_x - \cos k_y) C_{\mathbf{k}\uparrow} C_{-\mathbf{k}\downarrow} + h.c$$

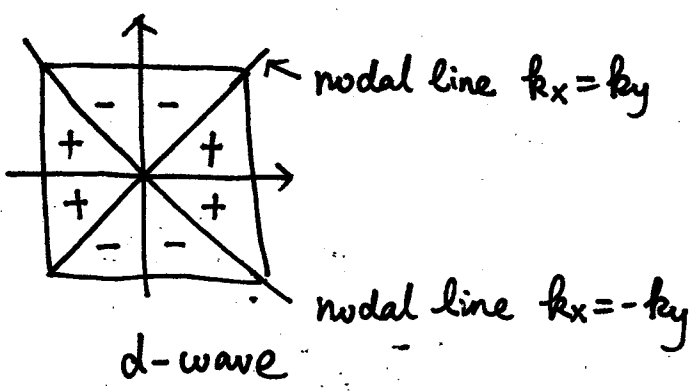
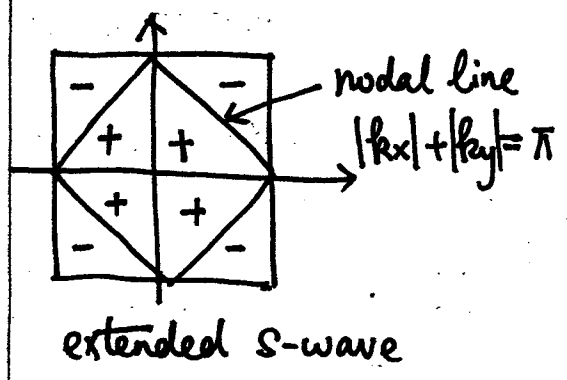
$$+ \frac{1}{V} (\Delta_s^* \Delta_s + \Delta_d^* \Delta_d)$$

We have chosen the interaction $V(k, k') = V_0 (\cos k'_x \cos k_x + \sin k'_y \sin k_y)$.

This interaction can give rise to two possible singlet pairing symmetries:

the extended s-wave: gap function $\Delta_s(\cos k_x + \cos k_y)$

d-wave: gap function $\Delta_d(\cos k_x - \cos k_y)$.



rotational invariant

but changes sign acrossing

$|k_x| + |k_y| = \pi$.

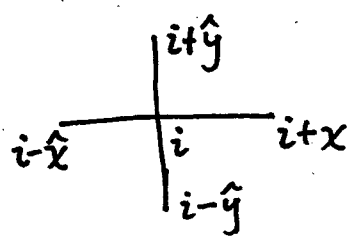
rotate 90°

$\Delta_d \rightarrow -\Delta_d$

Ex: please perform Fourier transformation back to real space.

① Δ_s corresponds to the real space pattern

$\Delta(i, i+x) = \Delta(i, i-x) = \Delta(i, i+\hat{y}) = \Delta(i, i-\hat{y})$



② Δ_d corresponds to the pattern

$\Delta(i, i+x) = \Delta(i, i-x) = -\Delta(i, i+\hat{y}) = -\Delta(i, i-\hat{y})$

where $\Delta(i, i+\delta) = V \langle C_{i\uparrow} C_{i+\delta\downarrow} - C_{i\downarrow} C_{i+\delta\uparrow} \rangle$.

The extended s-wave and d-wave compete, and the d-wave pairing wins. The reason is that the nodal lines of Δ_s coincide with the Fermi surface at half-filling (For high T_c cuprates, the filling is very close to half-filling), thus the gap function is suppressed on Fermi surface. Now let us only keep the d-wave channel.

$$\frac{H}{N} = \frac{1}{N} \sum_{\mathbf{k}} \begin{pmatrix} C_{\mathbf{k}\uparrow}^+ & C_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & \Delta_d (c_{\mathbf{k}_x} - c_{\mathbf{k}_y}) \\ \Delta_d^* (c_{\mathbf{k}_x} - c_{\mathbf{k}_y}) & -(\epsilon_{\mathbf{k}} - \mu) \end{pmatrix} \begin{pmatrix} C_{\mathbf{k}\uparrow} \\ C_{-\mathbf{k}\downarrow}^+ \end{pmatrix}$$

$$+ \frac{1}{N} \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) + \frac{1}{V} \Delta_d^* \Delta_d$$

Introducing Bogoliubov transformation, and assume Δ_d is real

$$\begin{pmatrix} C_{\mathbf{k}\uparrow} \\ C_{-\mathbf{k}\downarrow}^+ \end{pmatrix} = \begin{pmatrix} \cos \theta_{\mathbf{k}} & -\sin \theta_{\mathbf{k}} \\ \sin \theta_{\mathbf{k}} & \cos \theta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \beta_{-\mathbf{k}\downarrow}^+ \end{pmatrix}$$

we have

$$\rightarrow \begin{pmatrix} \alpha_{\mathbf{k}\uparrow}^+ & \beta_{-\mathbf{k}\downarrow}^+ \end{pmatrix} \underbrace{\begin{pmatrix} \cos \theta_{\mathbf{k}} & \sin \theta_{\mathbf{k}} \\ -\sin \theta_{\mathbf{k}} & \cos \theta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} & \Delta(k) \\ \Delta(k) & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \cos \theta_{\mathbf{k}} & -\sin \theta_{\mathbf{k}} \\ \sin \theta_{\mathbf{k}} & \cos \theta_{\mathbf{k}} \end{pmatrix}}_{\Downarrow} \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \beta_{-\mathbf{k}\downarrow}^+ \end{pmatrix}$$

$$= \begin{bmatrix} \xi_{\mathbf{k}} \cos 2\theta_{\mathbf{k}} + \Delta(k) \sin 2\theta_{\mathbf{k}}, & -\xi_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} + \Delta(k) \cos 2\theta_{\mathbf{k}} \\ -\xi_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} + \Delta(k) \cos 2\theta_{\mathbf{k}}, & -\xi_{\mathbf{k}} \cos 2\theta_{\mathbf{k}} - \Delta(k) \sin 2\theta_{\mathbf{k}} \end{bmatrix}$$

$$(\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu, \quad \Delta(k) = \Delta_d (c_{\mathbf{k}_x} - c_{\mathbf{k}_y}))$$

Set $\tan 2\theta_{\mathbf{k}} = \frac{\Delta(k)}{\xi_{\mathbf{k}}}$ $\cos 2\theta_{\mathbf{k}} = \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}$, $\sin 2\theta_{\mathbf{k}} = \frac{\Delta(k)}{E_{\mathbf{k}}}$

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

$$\Rightarrow \frac{H}{N} = \frac{1}{N} \sum_{\mathbf{k}} E_{\mathbf{k}} \cdot \left[(\alpha_{\mathbf{k}\uparrow}^{\dagger} \alpha_{\mathbf{k}\uparrow} - 1/2) + (\beta_{\mathbf{k}\downarrow}^{\dagger} \beta_{\mathbf{k}\downarrow} - 1/2) \right]$$

$$+ \frac{1}{N} \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) + \frac{1}{V} |\Delta_d|^2,$$

$$\cos^2 \theta_{\mathbf{k}} = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right), \quad \sin^2 \theta_{\mathbf{k}} = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right).$$

§ Self-consistency.

$$\frac{F}{N} = \frac{1}{N} \sum_{\mathbf{k}} -\frac{2}{\beta} \ln \left(e^{\frac{\beta}{2} E_{\mathbf{k}}} + e^{-\frac{\beta}{2} E_{\mathbf{k}}} \right) + \frac{1}{N} \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) + \frac{\Delta_d^2}{V}$$

$$= -\frac{2}{\beta} \int_{\text{FBZ}} \frac{d^2 k}{(2\pi)^2} \ln 2 \cosh \frac{\beta}{2} E_{\mathbf{k}} + \frac{\Delta_d^2}{V} + \text{const}$$

$$\frac{\partial F}{\partial \Delta_d} = -\frac{2}{\beta} \int_{\text{FBZ}} \frac{d^2 k}{(2\pi)^2} \frac{\sinh \frac{\beta}{2} E_{\mathbf{k}}}{\cosh \frac{\beta}{2} E_{\mathbf{k}}} \cdot \frac{\beta}{2} \frac{\Delta_d (\cos k_x - \cos k_y)^2}{E_{\mathbf{k}}} + \frac{2\Delta_d}{V} = 0$$

$$\Rightarrow \Delta_d = V \int_{\text{FBZ}} \frac{d^2 k}{(2\pi)^2} \frac{\Delta_d (\cos k_x - \cos k_y)^2}{2 E_{\mathbf{k}}} \tanh \frac{\beta}{2} E_{\mathbf{k}} \quad \leftarrow \text{Gap equation "d-wave"}$$

$$n = -\frac{1}{N} \frac{\partial F}{\partial \mu} \Rightarrow \frac{1}{N} \frac{\partial F}{\partial \mu} = -\frac{2}{\beta} \int_{\text{FBZ}} \frac{d^2 k}{(2\pi)^2} \tanh \frac{\beta}{2} E_{\mathbf{k}} \cdot \frac{\beta}{2} \frac{-\xi_{\mathbf{k}}}{E_{\mathbf{k}}} - 1 = -n$$

$$\Rightarrow 1 - n = \int_{\text{FBZ}} \frac{d^2 k}{(2\pi)^2} \tanh \frac{\beta}{2} E_{\mathbf{k}} \cdot \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \quad \leftarrow \text{particle number}$$

Gap equation: Gf. the general form of gap equation:

$$\Delta(\mathbf{k}) = \int_{\text{FBZ}} \frac{d^2 k'}{(2\pi)^d} V(\mathbf{k}, \mathbf{k}') \frac{\Delta(\mathbf{k}')}{2\sqrt{\xi^2 + \Delta^2(\mathbf{k}')}} \tanh \frac{\beta}{2} \sqrt{\xi^2 + \Delta^2(\mathbf{k}')}$$

plug in $\Delta(\mathbf{k}) = \Delta_d (\cos k_x - \cos k_y)$, $V(\mathbf{k}, \mathbf{k}') = V (\cos k_x - \cos k_y) (\cos k'_x - \cos k'_y)$.

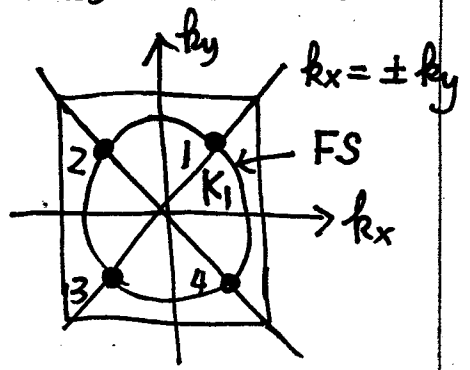
we will get the d-wave gap equation.

⊗ Dirac spectra (nodal quasi-particle)

$$\pm E_k = \pm \sqrt{\xi_k^2 + \Delta^2(k)} : \xi_k = 0 \text{ (Fermi surface)}$$

$$\Delta(k) = 0 \text{ gap nodal line}$$

Zeros of E_k : crossing points of gap nodal lines and Fermi surface. There are nodal points.

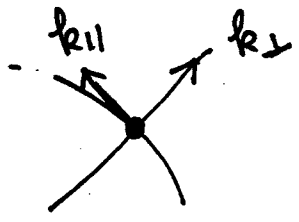


"d"-wave superconductivity is NOT fully gapped, but gapless. The nodal quasi-particles dominates over the low energy thermodynamic properties!

Let us linearize the d-wave Hamiltonian around one of the nodes,

Say, node 1.

$$\left\{ \begin{aligned} \xi_k &= \hbar v_F \delta k_{\perp} \\ \Delta(k) &= \Delta_d \delta k_{\parallel} \end{aligned} \right.$$



where $\delta k_{\perp} = \frac{\delta k_x + \delta k_y}{\sqrt{2}}$ and $\delta k_{\parallel} = \frac{-\delta k_x + \delta k_y}{\sqrt{2}}$ and $\delta \vec{k} = \vec{k} - \vec{K}_1$

$$H(k) = \begin{pmatrix} \xi_k & \Delta(k) \\ \Delta(k) & -\xi_k \end{pmatrix} = \hbar v_F \delta k_{\perp} \tau_z + \Delta_d \delta k_{\parallel} \tau_x$$

Thermodynamics of nodal superconductors (singlet) ① 2D-d-wave

In this lecture, we will study new features associated with the nodal quasi-particles of the d-wave superconductors. The d-wave gap equation can be solved analytically in the continuum approximation:

① Assume $\xi_{\mathbf{k}}$ is isotropic, i.e. independent of the azimuthal angle $\varphi_{\mathbf{k}}$

$\int \frac{d^2k}{(2\pi)^2} \rightarrow \int \frac{d\varphi}{2\pi} \int_{-\omega_0}^{\omega_0} d\xi \rho_0(\xi)$, where $\rho_0(\xi)$ is the density of states. If $\rho_0(\xi)$ does not have singularity, it can be replaced by N_F , i.e. the DOS right at Fermi surface. ω_0 is the cut off, which plays the role of Debye frequency in conventional SC. In high T_c , the origin of ω_0 is still in debate, most probably, it arises from antiferromagnetic fluctuations.

② We replace the lattice version of the angular form factor $\cos k_x - \cos k_y$ by $\cos 2\varphi_{\mathbf{k}}$, which has the same $d_{x^2-y^2}$ symmetry. An issue is the normalization, which can be absorbed in the definition of Δ_d and V . Say, $\cos k_x - \cos k_y \sim C \cdot \cos 2\varphi_{\mathbf{k}}$

$$\Rightarrow \int_0^{2\pi} \frac{d\varphi}{2\pi} \int_0^{\omega_0} d\xi \frac{C^2 \cos^2 2\varphi_{\mathbf{k}}}{\sqrt{\xi^2 + \Delta_d^2 C^2 \cos^2 2\varphi_{\mathbf{k}}}} \tanh \frac{\beta}{2} \sqrt{\xi^2 + \Delta_d^2 C^2 \cos^2 2\varphi_{\mathbf{k}}} = \frac{1}{N_F V}$$

We can define $\frac{1}{VC^2} \rightarrow \frac{1}{V}$ and $\Delta_d^2 C^2 \rightarrow \Delta_d^2$, we have

$$\int_0^{2\pi} \frac{d\varphi}{2\pi} \int_0^{\omega_0} d\xi \frac{\cos^2 2\varphi}{\sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}} \tanh \frac{\beta}{2} \sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi} = \frac{1}{N_F V}$$

* Solve T_c

we have around T_c , $\Rightarrow \int_0^{\frac{\omega_0}{2k_B T_c}} dx \frac{\tanh x}{x} = \frac{2}{N_F V}$

($x = \frac{\beta_c \xi}{2}$, the ^{"2"} factor on RHS comes from $\int \frac{d\varphi}{2\pi} \delta\varphi^2 = \frac{1}{2}$).

Integral by part \Rightarrow LHS = $\ln \frac{\omega_0}{2k_B T_c} \tanh \frac{\omega_0}{2k_B T_c} - \int_0^{\frac{\omega_0}{2k_B T_c}} dx \ln x \operatorname{sech}^2 x$

define $C_0 = \frac{1}{2} \exp \left[- \int_0^{\infty} dx \frac{\ln x}{\cosh^2 x} \right]$

= 1.134

$\Rightarrow k_B T_c \approx C_0 \omega_0 e^{-\frac{2}{N_F V}}$

we can set $\frac{\omega_0}{2k_B T_c} \rightarrow \infty$ converge!

Because ω_0, V are difficult to know, this equation does not tell much useful information!

* Solve gap value at $T=0$,

$\beta \rightarrow \infty$, $\tanh \frac{\beta}{2} E \rightarrow 1$, we have

$\int_0^{2\pi} \frac{d\varphi}{2\pi} \int_0^{\omega_0} d\xi \frac{\cos^2 \varphi}{\sqrt{\xi^2 + \Delta_d^2 \cos^2 \varphi}} = \frac{1}{N_F V}$

$\int dx \frac{1}{\sqrt{x^2 + a^2}} = \ln(x + \sqrt{x^2 + a^2}) + C$

$\Rightarrow \int_0^{\omega_0} d\xi \frac{1}{\sqrt{\xi^2 + \Delta_d^2 \cos^2 \varphi}} = \ln(\xi + \sqrt{\xi^2 + \Delta_d^2 \cos^2 \varphi}) \Big|_0^{\omega_0} = \ln \frac{\omega_0 + \sqrt{\omega_0^2 + \Delta_d^2 \cos^2 \varphi}}{\Delta_d |\cos 2\varphi|}$

$\Rightarrow \int_0^{2\pi} d\varphi \cos^2 \varphi \ln \frac{\omega_0 + \sqrt{\omega_0^2 + \Delta_d^2 \cos^2 \varphi}}{\Delta_d |\cos 2\varphi|} = \frac{\pi}{N_F V}$

consider the case of $\omega_0 \gg \Delta_d$; we can approximate the integral as

$$\int_0^{\pi} d\varphi \cos^2 2\varphi \ln \frac{2\omega_0}{\Delta_d |\cos 2\varphi|} \simeq \frac{\pi}{N_F V}$$

$$\Rightarrow \frac{\pi}{2} \ln \frac{2\omega_0}{\Delta_d} = \frac{\pi}{N_F V} + \int_0^{\pi} d\varphi \cos^2 2\varphi \ln |\cos 2\varphi|$$

$\leftarrow 2 \int_0^{\pi/2} d\varphi \cos^2 \varphi \ln \cos \varphi$

$$\Rightarrow \frac{2\omega_0}{\Delta_d} = \frac{2}{N_F V} + \frac{4}{\pi} \int_0^{\pi/2} d\varphi \cos^2 \varphi \ln \cos \varphi$$

$$\Rightarrow \boxed{\Delta_d = C_1 \omega_0 e^{-\frac{2}{N_F V}}}, \text{ where } C_1 = 2 \cdot \exp\left[-\frac{4}{\pi} \int_0^{\pi/2} d\varphi \cos^2 \varphi \ln \cos \varphi\right]$$

$\simeq 2.426$

We arrive the relation between gap and T_c .

$$\boxed{\frac{2\Delta_d}{k_B T_c} \simeq 4.28}$$

which is slightly higher than the s-wave value 3.53.

§ DOS in d-wave superconductor

$$\begin{aligned} \rho(\omega) &= \frac{2}{\text{Vol}} \sum_{\mathbf{k}} \left(u_{\mathbf{k}}^2 \delta(\omega - E_{\mathbf{k}}) + v_{\mathbf{k}}^2 \delta(\omega + E_{\mathbf{k}}) \right) \\ &= 2 \int \frac{d^2 k}{(2\pi)^2} \frac{1}{2} \left[\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \delta(\omega - E_{\mathbf{k}}) + \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \delta(\omega + E_{\mathbf{k}}) \right] \\ &= \int \frac{d\varphi}{2\pi} \int d\xi \frac{N_F}{2} \left[\left(1 + \frac{\xi}{E}\right) \delta(\omega - E) + \left(1 - \frac{\xi}{E}\right) \delta(\omega + E) \right] \end{aligned}$$

\leftarrow odd function

consider $\omega > 0 \Rightarrow \rho(\omega) = \int \frac{d\varphi}{2\pi} \int d\xi N_F \left(1 + \frac{\xi}{E}\right) \delta(\omega - E)$

$$= \int \frac{d\varphi}{2\pi} \int d\xi \frac{N_F}{2} \delta\left(\omega - \sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}\right)$$

The solution of $\omega^2 = \xi^2 + \Delta_d^2 \cos^2 2\varphi \Rightarrow \xi = \pm \sqrt{\omega^2 - \Delta_d^2 \cos^2 2\varphi}$

$$\Rightarrow \delta(\omega - E) = \frac{\delta(\xi - \sqrt{\omega^2 - \Delta_d^2 \cos^2 2\varphi}) + \delta(\xi + \sqrt{\omega^2 - \Delta_d^2 \cos^2 2\varphi})}{|\xi| \sqrt{\xi^2 + \Delta_d^2 \cos^2 2\varphi}}$$

$$\delta(\omega - E) = \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}} \left[\delta(\xi - \sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}) + \delta(\xi + \sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}) \right]$$

$$\begin{aligned} P(\omega) &= \frac{N_F}{2} \int \frac{d\varphi}{2\pi} \int d\xi \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}} \left[\delta(\xi - \sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}) + \delta(\xi + \sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}) \right] \\ &= N_F \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}} \Theta(\omega > |\Delta \cos 2\varphi|) \\ &= N_F \frac{1}{2} \int \frac{d\varphi'}{2\pi} \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 \varphi'}} \Theta(\omega > |\Delta \cos \varphi'|) = \frac{2N_F}{\pi} \int_0^{\pi/2} \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 \varphi'}} \Theta(\dots) \end{aligned}$$

① if $\omega > \Delta \Rightarrow P(\omega) = \frac{2N_F}{\pi} \int_0^{\pi/2} \frac{1}{\sqrt{1 - (\Delta/\omega)^2 \cos^2 \varphi'}} = \frac{2N_F}{\pi} \int_0^{\pi/2} \frac{1}{\sqrt{1 - (\Delta/\omega)^2 \sin^2 \varphi'}}$

This is the complete Elliptic integral of 1st kind.

as $\Delta/\omega \rightarrow 1$, we have $P(\omega) \simeq \frac{N_F}{\pi} \ln \frac{\delta}{1 - \Delta/\omega}$
 as $\Delta/\omega \rightarrow \infty$ $P(\omega) = N_F$

② if $\omega < \Delta$ define $\cos \phi = \frac{\Delta}{\omega} \cos \varphi' \Rightarrow \sin \phi d\phi = \frac{\Delta}{\omega} \sin \varphi' d\varphi'$

$$P(\omega) = \frac{2N_F}{\pi} \int_0^{\pi/2} \left(\frac{\Delta}{\omega} \right)^{-1} \frac{\sin \phi}{\sin \varphi'} d\phi \cdot \frac{1}{\sqrt{1 - \cos^2 \phi}}$$

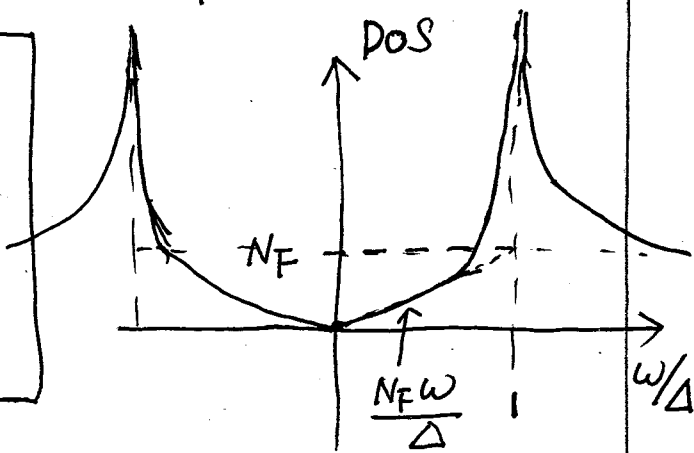
$$\frac{\omega}{\Delta} \frac{2N_F}{\pi} \int_0^{\pi/2} \frac{d\phi}{\sin \varphi'} \leftarrow \sin \varphi' = \sqrt{1 - \cos^2 \varphi'} = \sqrt{1 - \left(\frac{\omega}{\Delta}\right)^2 \cos^2 \varphi'}$$

$$= \frac{\omega}{\Delta} \frac{2N_F}{\pi} \int_0^{\pi/2} d\phi \frac{1}{\sqrt{1 - (\frac{\omega}{\Delta})^2 \cos^2 \varphi'}} = \frac{\omega}{\Delta} \frac{2N_F}{\pi} \int_0^{\pi/2} \frac{1}{\sqrt{1 - (\frac{\omega}{\Delta})^2 \sin^2 \varphi'}}$$

as $\omega \rightarrow \Delta$

$$P(\omega) \rightarrow \frac{N_F \omega}{\pi \Delta} \ln \frac{\delta}{1 - \omega/\Delta}$$

as $\omega \rightarrow 0$ $P(\omega) \rightarrow \frac{N_F \omega}{\Delta}$



§ Specific heat

The free energy density $\frac{F(T)}{\text{Vol}} = -k_B T \ln Z$

← $\text{Vol} = N a^d$
 a : lattice constant

$$\frac{F(T)}{\text{Vol}} = -k_B T \frac{1}{\text{Vol}} \sum_{\mathbf{k}} 2 \ln \left(e^{-\frac{1}{2} \beta E_{\mathbf{k}}} + e^{\frac{1}{2} \beta E_{\mathbf{k}}} \right) + \frac{\Delta_d^2}{V}$$

$$= -k_B T \int_{\text{FBZ}} \frac{d^d k}{(2\pi)^d} 2 \ln 2 \cosh \frac{\beta}{2} E_{\mathbf{k}} + \frac{\Delta_d^2}{V}$$

$$\frac{S}{\text{Vol}} = -\frac{\partial F}{\partial T} = k_B \int_{\text{FBZ}} \frac{d^d k}{(2\pi)^d} 2 \ln 2 \cosh \frac{\beta}{2} E_{\mathbf{k}} + k_B T \int_{\text{FBZ}} \frac{d^d k}{(2\pi)^d} 2 \tanh \frac{\beta}{2} E_{\mathbf{k}} \frac{\partial}{\partial T} \left(\frac{\beta E_{\mathbf{k}}}{2} \right) - 2 \frac{\Delta_d}{V} \frac{\partial \Delta_d}{\partial T}$$

gap Eq: $\frac{\Delta_d}{V} = \int_{\text{FBZ}} \frac{d^d k}{(2\pi)^d} \frac{\Delta_d (\cos k_x - \cos k_y)^2}{2 E_{\mathbf{k}}} \tanh \frac{\beta}{2} E_{\mathbf{k}}$

$$\frac{\partial}{\partial T} \left(\frac{\beta}{2} E_{\mathbf{k}} \right) = \frac{-1}{2 k_B T^2} E_{\mathbf{k}} + \frac{\beta}{2} \frac{\Delta_d (\cos k_x - \cos k_y)^2}{E_{\mathbf{k}}} \frac{\partial \Delta_d}{\partial T}$$

$$\Rightarrow \frac{S}{\text{Vol}} = 2 k_B \int_{\text{FBZ}} \frac{d^d k}{(2\pi)^d} \ln \left(2 \cosh \frac{\beta}{2} E_{\mathbf{k}} \right) - 2 k_B \int_{\text{FBZ}} \frac{d^d k}{(2\pi)^d} \tanh \frac{\beta}{2} E_{\mathbf{k}} \frac{\beta E_{\mathbf{k}}}{2} \quad (\text{other term cancels})$$

Ex: check $\frac{S}{\text{Vol}}$ can also be written as

$$\frac{S}{\text{Vol}} = -2 k_B \sum_{\mathbf{k}} \left[(1 - f_{\mathbf{k}}) \ln (1 - f_{\mathbf{k}}) + f_{\mathbf{k}} \ln f_{\mathbf{k}} \right]$$

with $f_{\mathbf{k}} = \frac{1}{e^{\beta E_{\mathbf{k}}} + 1}$. Check it's consistent with the above Eq.

$$\begin{aligned} C = T \frac{\partial S}{\partial T} &= -\beta \frac{\partial S}{\partial \beta} = 2 \beta k_B \frac{1}{\text{Vol}} \sum_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}}{\partial \beta} \ln \frac{f_{\mathbf{k}}}{1 - f_{\mathbf{k}}} = -2 \beta^2 k_B \frac{1}{\text{Vol}} \sum_{\mathbf{k}} E_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}}{\partial \beta} \\ &= -2 \beta^2 k_B \frac{1}{\text{Vol}} \sum_{\mathbf{k}} E_{\mathbf{k}} \frac{df_{\mathbf{k}}}{d(\beta E_{\mathbf{k}})} \left(\frac{d(\beta E_{\mathbf{k}})}{d\beta} \right) \leftarrow \frac{d(\beta E_{\mathbf{k}})}{d\beta} = E_{\mathbf{k}} + \beta \frac{dE_{\mathbf{k}}}{d\beta} \\ &= 2 \beta k_B \frac{1}{\text{Vol}} \sum_{\mathbf{k}} \left(-\frac{\partial f_{\mathbf{k}}}{\partial E_{\mathbf{k}}} \right) \left(E_{\mathbf{k}}^2 + \frac{1}{2} \beta \frac{dE_{\mathbf{k}}^2}{d\beta} \right) \end{aligned}$$

$$\frac{C}{Vol} = 2k_B \int \frac{dk}{(2\pi)^2} \frac{e^{\beta E_k}}{(e^{\beta E_k} + 1)^2} \left(\frac{E_k^2}{k_B^2 T^2} - \frac{1}{2} \frac{dE_k^2}{k_B^2 T dT} \right)$$

① Next we consider low T limit.

Now we use continuum approx: $E_k^2 = \xi^2 + \Delta_d^2 \cos^2 2\varphi_k$

$$\frac{E_k^2}{k_B^2 T^2} = \frac{\xi^2 + \Delta_d^2(T) \cos^2 2\varphi_k}{k_B^2 T^2}$$

$$\frac{E_k dE_k}{k_B^2 T dT} = \frac{\Delta_d(T)}{k_B T} \frac{d\Delta_d(T)}{k_B dT} \cos^2 2\varphi_k = \frac{\Delta_d^2(T)}{(k_B T)^2} \cos^2 2\varphi_k \left(\frac{k_B T}{\Delta_d(T)} \right)^3$$

because at $T \ll \Delta(T)$, $\frac{d\Delta(T)}{k_B dT} \approx \frac{k_B T^2}{\Delta_d^2(T)}$ (for d-wave),

we can neglect the contribution from the second term.

$$\Rightarrow \text{at } T \ll \Delta, \quad \frac{C}{k_B} = \frac{1}{k_B^2 T^2} N_F \int \frac{d\varphi}{2\pi} \int d\xi \frac{e^{\beta E}}{(e^{\beta E} + 1)^2} E^2$$

$$= \frac{N_F}{4 k_B^2 T^2} \int \frac{d\varphi}{2\pi} \int_{-\infty}^{+\infty} d\xi \frac{E^2}{\cosh^2(E/2T)}$$

The factor $\cosh^2 E/2T$ suppresses the contribution except from the nodal region:

$$|\xi| > |\Delta| |\cos 2\varphi|. \Rightarrow \Delta\varphi \sim |\varphi - \pi/4| \ll \frac{|\xi|}{2|\Delta|}$$

consider there're four nodes,

$$\frac{C}{k_B} = \frac{N_F}{k_B^2 T^2} \int_{-\infty}^{+\infty} d\xi \frac{\xi^2}{\cosh^2(\xi/2T)} \int_{-\frac{|\xi|}{2|\Delta|}}^{\frac{|\xi|}{2|\Delta|}} d\varphi + o(e^{-4/T})$$

$$\approx \frac{N_F}{k_B^2 T^2} \frac{1}{\Delta} \int_{-\infty}^{+\infty} d\xi \frac{|\xi|^3}{\cosh^2 \xi/2T k_B} \quad \text{defin } \chi = \frac{\xi}{2T k_B}$$

$$\frac{C}{k_B} \approx \frac{2^5 N_F k_B^2 T^2}{\Delta} \int_0^{+\infty} d\chi \frac{\chi^3}{\cosh^2 \chi} \approx \text{const.} \frac{N_F (k_B T)^2}{\Delta}$$

(7)

The low temperature specific heat in 2D nodal SC

$$\frac{C}{k_B} \simeq \text{const.} \frac{N_F (k_B T)^2}{\Delta_d}, \quad \text{which is}$$

Consistent with the low energy DOS $\simeq N_F \frac{\omega}{\Delta_d}$

Paramagnetic susceptibility / Knight shift

Consider the pairing sector $k \uparrow$ and $-k \downarrow$. The Hilbert space is 4-dimensional: $| \uparrow \downarrow \rangle$, $\alpha_{k \uparrow}^\dagger | \uparrow \downarrow \rangle$, $\beta_{-k \downarrow}^\dagger | \uparrow \downarrow \rangle$, $\alpha_{k \uparrow}^\dagger \beta_{-k \downarrow}^\dagger | \uparrow \downarrow \rangle$.

The partition function $1 + e^{-\beta E_k} + e^{-\beta E_k} + e^{-2\beta E_k} = (1 + e^{-\beta E_k})^2$

if adding external field, $E_{\alpha_{k \uparrow}} = E_k - \mu_B H$

$$E_{\beta_{-k \downarrow}} = E_k + \mu_B H$$

$$\Rightarrow M = \mu_B \sum_k \frac{e^{-\beta(E_k - \mu_B H)}}{(1 + e^{-\beta E_k})^2} - \frac{e^{-\beta(E_k + \mu_B H)}}{(1 + e^{-\beta E_k})^2}$$

we neglect the dependence on H in the denominator at the linear order of H

$$\Rightarrow \chi = \frac{\partial M}{\partial H} = \mu_B^2 \sum_k \frac{e^{-\beta E_k}}{(1 + e^{-\beta E_k})^2} (2\beta)$$

$$\Rightarrow \frac{\chi}{\text{Vol}} = \beta \mu_B^2 N_F \int d\mathcal{E} \int \frac{d\varphi}{2\pi} \frac{1}{(e^{-\beta \mathcal{E}/2} + e^{\beta \mathcal{E}/2})^2}$$

$$\frac{2 \sum_k}{\text{Vol}} \rightarrow N_F \int d\mathcal{E} \int \frac{d\varphi}{2\pi}$$

Define Yoshida function $Y(\varphi, T) = \frac{\beta}{4} \int_{-\infty}^{+\infty} \frac{d\mathcal{E}}{(\cosh \frac{\mathcal{E}(\varphi)}{2T})^2}$

$$\Rightarrow \frac{\chi}{\text{Vol}} = \mu_B^2 N_F \int \frac{d\varphi}{2\pi} Y(\varphi, T)$$

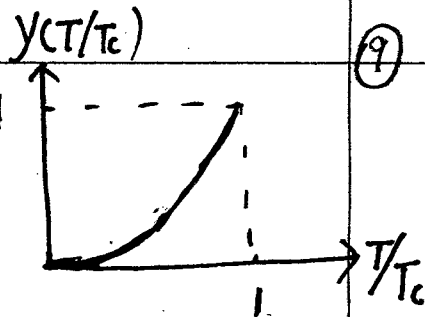
For the s-wave case, $\frac{\chi}{\chi_n} = \frac{\beta}{4} \int_{-\infty}^{+\infty} \frac{d\mathcal{E}}{[\cosh(\frac{\mathcal{E}^2 + \Delta^2}{2T})^{1/2}]^2} = \frac{\beta}{2} \int_0^{+\infty} d\mathcal{E} \operatorname{sech}^2 \frac{\beta \mathcal{E}}{2}$

$$= Y(T) \leftarrow \text{isotropic case}$$

at $T = T_c$, $Y(1) = \int_0^{+\infty} \text{sech}^2 x dx = 1$

$T \ll \Delta$, $Y(T/\Delta)$ is suppressed exponentially.

$$\sim e^{-\Delta/T}$$



Now let us consider the d-wave case:

$$\frac{\chi}{\chi_n} = \int_0^{+\infty} d\xi \frac{\beta}{2} \frac{1}{\cosh^2\left(\frac{\xi}{2T}\right)} \int_{-\frac{\xi}{2\Delta}}^{\frac{\xi}{2\Delta}} d\varphi$$

← the low T contribution
+ $O(e^{-\Delta/T})$ from $\xi > \Delta \cos 2\varphi$

$$\approx \int_0^{+\infty} d\xi \frac{1}{2k_B T} \frac{\xi}{\Delta} \frac{1}{\cosh^2\left(\frac{\xi}{2k_B T}\right)}$$

$$\Rightarrow |\varphi| \ll \frac{\xi}{2\Delta}$$

define $\chi = \frac{\xi}{2k_B T}$

$$\Rightarrow \frac{\chi}{\chi_n} \sim \frac{2k_B T}{\Delta} \int_0^{+\infty} dx \frac{\chi}{\cosh^2(x)} \approx \text{const.} \frac{k_B T}{\Delta}$$

This is also consistent with the low T Dos $\sim N_F \frac{\omega}{\Delta}$.

χ can be measured through NMR knight shift. The NMR

frequency of nuclear in solids is different from that

in vacuum: $B_{\text{eff}} = B_{\text{ex}} + B_{\text{mol}}$; and $B_{\text{mol}} \propto M = B_{\text{ex}} \chi$.

From the frequency shift (Knight shift), we can infer the magnetic susceptibility of the environment, i.e. electronic structure.

Phase-sensitive measurement — d-wave symmetry ①

The thermodynamic anomalies of the d-wave superconductors only detect the linear density of states of nodal quasi-particles. They are not phase sensitive — we need smoking gun evidence for sign-change of gap functions. Below we will see this from Josephson tunneling junction.

According to linear-response theory, the tunneling currents between SCs (see Dan's notes)

$$A = \sum_{kq\sigma} T_{kq} C_{L,k\sigma}^\dagger C_{Rq\sigma}, \rightarrow A(t) = \sum_{kq\sigma} T_{kq} C_{L,k\sigma}^\dagger(t) C_{Rq\sigma}(t).$$

$$K_0 = H_0 - \mu_L N_L - \mu_R N_R, \text{ and } eU = \mu_L - \mu_R$$

$$\rightarrow C_{\alpha,k\sigma}(t) = e^{-ik_0 t} C_{\alpha,k\sigma} e^{ik_0 t}, \quad \alpha = R, L.$$

The tunneling currents $I(t) = I_Q(t) + I_J(t)$

$$I_Q(t) = -\frac{2e}{\hbar^2} \text{Im} \int_{-\infty}^{+\infty} dt' e^{ieU(t-t')} X_{\text{ret}}(t-t') \leftarrow \text{normal current}$$

$$I_J(t) = \frac{2e}{\hbar^2} \text{Im} \int_{-\infty}^{+\infty} dt' e^{-ieU(t+t')} Y_{\text{ret}}(t-t') \leftarrow \text{Josephson tunneling}$$

retarded Green's function

$$X_{\text{ret}}(t-t') = -i\theta(t-t') \langle [A(t), A^\dagger(t')] \rangle_0$$

$$Y_{\text{ret}}(t-t') = -i\theta(t-t') \langle [A^\dagger(t), A^\dagger(t')] \rangle_0 \leftarrow \text{tunneling } L \rightarrow R.$$

⇒ The Josephson channel

$$I_J(t) = \frac{2e}{\hbar^2} \text{Im} [e^{-2ieUt} Y_{\text{ret}}(\Omega = eU)]$$

where $Y_{ret}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} y_{ret}(t)$

$$Y_{ret}(\omega) = e^{i(\phi_R + \phi_L)} \sum_{kq} T_{kq} T_{-k-q} \frac{\Delta_L(k)}{E_L(k)} \cdot \frac{\Delta_R(q)}{E_R(q)}$$

$$\left[\frac{1}{\hbar\omega + E_L(k) + E_R(q) + i\eta} - \frac{1}{\hbar\omega - E_L(k) - E_R(q) + i\eta} \right]$$

* Check dimension $[I] = \frac{e}{\hbar^2} \cdot [time] \cdot [energy]^2 = \frac{e}{\hbar} e [Volt] = \frac{e^2}{\hbar} [Voltage]$

correct: $\frac{e^2}{\hbar}$ is the unit of conductance.

Assuming T_{kq} 's are momentum independent \Rightarrow

$$Y_{ret}(\omega) = \frac{\hbar^2 G_{IV}}{2\pi e^2} e^{i(\phi_R - \phi_L)} \int_0^{+\infty} dS_L \int_0^{+\infty} dS_R \int \frac{d\phi_L}{2\pi} \int \frac{d\phi_R}{2\pi}$$

$$\left\{ \frac{\Delta_L(S_L, \phi_L)}{E_L} \frac{\Delta_R(S_R, \phi_R)}{E_R} \right\} \left[\frac{1}{\hbar\omega + E_L + E_R + i\eta} - \frac{1}{\hbar\omega - E_L - E_R + i\eta} \right]$$

The new property of unconventional SC is the appearance of angular dependence of

$$\int \frac{d\phi_L}{2\pi} \int \frac{d\phi_R}{2\pi} \Delta_L(S_L, \phi_L) \Delta_R(S_R, \phi_R)$$

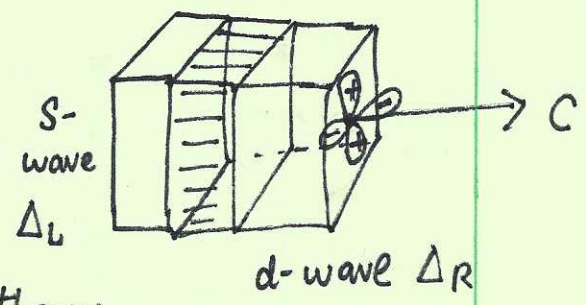
(if in 3d system $\int \frac{d\phi_{L,R}}{2\pi} \rightarrow \int \frac{d\Omega_{L,R}}{4\pi}$)

we can neglect angular dependence in E_L and E_R , because their dependence

is $|\Delta_L|^2$ and $|\Delta_R|^2$.

① Tunneling between s-wave and d-wave SC along the c-axis

$$\int \frac{d\phi_R}{2\pi} \Delta_R^* (\delta_R \cdot \phi_R) = 0!$$



No Josephson tunneling. This result is exact up to second order perturbation theory.

Q: Effective Ginzburg-Landau equation: Can we write down a coupling at the quadratic order? YBCO is a different story: it's s+d

$\Delta F = -J(\Delta_s^* \Delta_d + c.c.)$ No! this term is not invariant under rotation 90° around c-axis.

but s and d-wave part do can couple at quartic order as

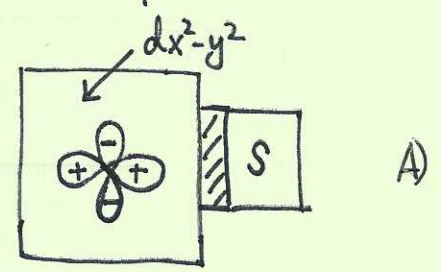
$$\Delta F = J(\Delta_d^* \Delta_s)^2 + c.c.$$

$$\rightarrow I \propto \sin[2(\phi_R - \phi_L + eU t)]$$

high order Josephson effect, two-pair tunneling.

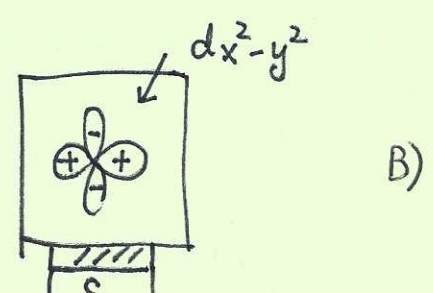
② how over, if the junction is set in the ab-plane

due to geometry, we cannot neglect the momentum dependence of $T_{k,q}$.

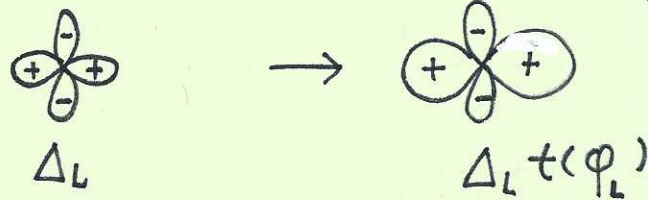


For example, the tunneling matrix elements for $k \parallel$ surface

and $k \perp$ surface are different.



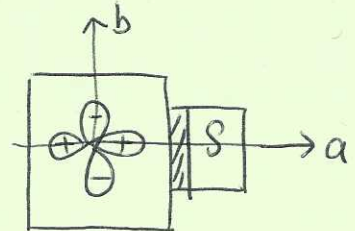
For example, in A) we expect that the tunneling for $\vec{k} \parallel \hat{x}$ is the much stronger than $\vec{k} \parallel \hat{y}$. Thus the d-wave gap function is not averaged evenly, i.e. $\int \frac{d\varphi_L}{2\pi} \Delta_L(\varphi_L) t(\varphi_L) \neq 0$.



effect from tunneling matrix element.

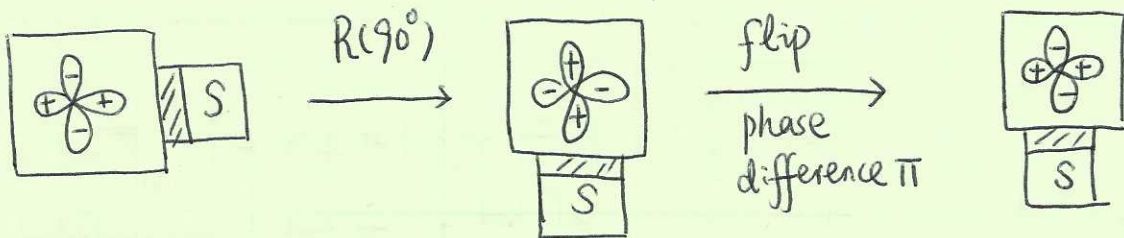
We do have coupling at quadratic level as

$$\Delta F_x = -J (\Delta_{s_1}^* \Delta_d + c.c.)$$



(There's no symmetry about this set-up which can change the sign of the d-wave part!)

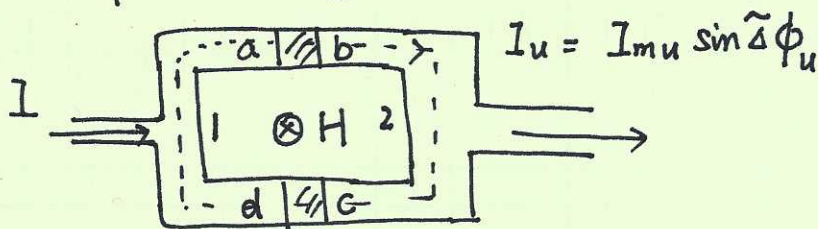
• Nevertheless, we can build up the relation between the coupling configurations of A) and B).



$$\Delta F_y = -J (\Delta_{s_2}^* \Delta_d + c.c.)$$

Digression ①: Coupled two-junction SQUID

①



$$I_d = I_{md} \sin \tilde{\Delta} \phi_d$$

$$I = I_u + I_d = I_{mu} \sin \tilde{\Delta} \phi_u + I_{me} \sin \tilde{\Delta} \phi_d$$

should be gauge invariant phase difference

If $I_{mu} = I_{me} = I_m$, we say that these two junctions are matched.

$$\Rightarrow I = 2I_m \sin \frac{\tilde{\Delta} \phi_u + \tilde{\Delta} \phi_d}{2} \cos \frac{\tilde{\Delta} \phi_u - \tilde{\Delta} \phi_d}{2}$$

$$\oint \nabla \phi \cdot d\ell = (\phi_b - \phi_a) + (\phi_c - \phi_b) + (\phi_d - \phi_c) + (\phi_a - \phi_d) = 2n\pi$$

The phase difference across the up and down junction

gauge invariant phase:

$$\tilde{\Delta} \phi_u = \phi_b - \phi_a - \left(\int_a^b \vec{A} \cdot d\vec{\ell} \right) \frac{2\pi}{\Phi_0}$$

that enters the formula of current.

$$\Rightarrow \phi_b - \phi_a = \tilde{\Delta} \phi_u + \left(\int_a^b \vec{A} \cdot d\vec{\ell} \right) \frac{2\pi}{\Phi_0}$$

$$\phi_d - \phi_c = \tilde{\Delta} \phi_d + \left(\int_c^d \vec{A} \cdot d\vec{\ell} \right) \frac{2\pi}{\Phi_0}$$

(phase across

the junction).

$$\Phi_0 = \frac{hc}{2e} = 2.07 \times 10^{-7} \text{ Gauss} \cdot \text{cm}^2$$

$$\phi_c - \phi_b = \int_b^c \nabla \phi \cdot d\ell = \frac{2\pi}{\Phi_0} \int_b^c \left(\vec{A} + \frac{4\pi}{c} \lambda_L^2 \vec{j} \right) \cdot d\vec{\ell}$$

inside superconductor

$$\phi_a - \phi_d = \int_d^a \nabla \phi \cdot d\ell = \frac{2\pi}{\Phi_0} \int_d^a \left(\vec{A} + \frac{4\pi}{c} \lambda_L^2 \vec{j} \right) \cdot d\vec{\ell}$$

①

$$\text{Add together} \Rightarrow \Delta\phi_u - \Delta\phi_d + \oint \vec{A} \cdot d\vec{l} \left(\frac{2\pi}{\Phi_0} \right) + \frac{2\pi}{\Phi_0} \frac{4\pi\lambda_c^2}{c} \int_{c'} \vec{j} \cdot d\vec{l}$$

$$= 2n\pi$$

$$\Rightarrow \Delta\phi_u - \Delta\phi_d = -\frac{2\pi}{\Phi_0} \oint \vec{A} \cdot d\vec{l} - \frac{2\pi}{\Phi_0} \frac{4\pi\lambda_c^2}{c} \int_{c'} \vec{j} \cdot d\vec{l}$$

← exclude the insulator junction

We can choose the loop deep inside the superconductor, such that $j=0 \Rightarrow$

$$\Delta\phi_u - \Delta\phi_d = -\frac{2\pi}{\Phi_0} \oint \vec{A} \cdot d\vec{l} = -2\pi \frac{\Phi}{\Phi_0}$$

$$\Rightarrow I = 2I_m \sin(\Delta\phi_u + \pi \frac{\Phi}{\Phi_0}) \cos\left(\frac{\pi \Phi}{\Phi_0}\right) \quad \textcircled{1}$$

If the inductance of the loop is considered, the flux Φ consists two part:

$$\Phi = \Phi_{ex} + L I_{cir} \quad \textcircled{2}$$

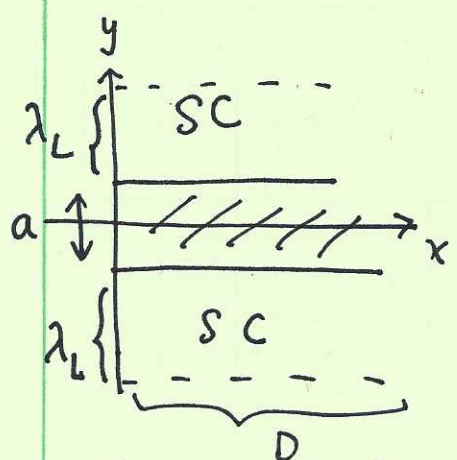
$$\text{and the circulate current } I_{cir} = I_m (\sin \Delta\phi_u - \sin \Delta\phi_d) \quad \textcircled{3}$$

In principle ①, ②, ③ should be solved consistently. If the self-inductance can be neglected, we have

$$I = 2I_m \sin\left(\Delta\phi_u + \pi \frac{\Phi_{ex}}{\Phi_0}\right) \cos\left(\frac{\pi \Phi_{ex}}{\Phi_0}\right),$$

$$\Rightarrow I_{max} = 2I_m \left| \cos \frac{\pi \Phi_{ex}}{\Phi_0} \right|, \quad \text{the maximum supercurrent density oscillate with } \Phi_{ex}/\Phi_0.$$

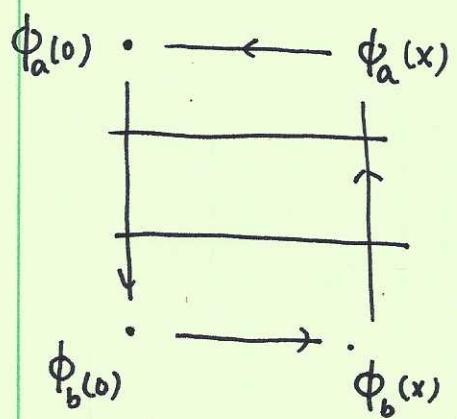
Digression ②: Fraunhofer pattern: a single planar Josephson junction.



$$A_x = 0,$$

$$A_y = \begin{cases} -Bx e^{-(y-a/2)/\lambda_L} & y > a/2 \\ -Bx & a/2 > y > -a/2 \\ -Bx e^{(y+a/2)/\lambda_L} & y < -a/2 \end{cases}$$

the gauge-independent phase difference



$$\Rightarrow \tilde{\Delta}\phi(x) = \tilde{\Delta}\phi(0) - \frac{2e}{\hbar c} \int_{-\infty}^{+\infty} A_y(x) dy$$

$$= \tilde{\Delta}\phi(0) - \frac{2e}{\hbar c} B(a + 2\lambda_L)x$$

$$\left. \begin{matrix} \phi_a(0) & \leftarrow & \phi_a(x) \\ \phi_b(0) & \rightarrow & \phi_b(x) \end{matrix} \right\} \int \nabla\phi d\ell = (\phi_a(x) - \phi_b(x)) + (\phi_a(0) - \phi_b(0)) + (\phi_b(0) - \phi_a(0)) + (\phi_b(x) - \phi_b(0)) = 2n\pi$$

$$\left. \begin{aligned} \tilde{\Delta}\phi_a(x) &= \phi_a(x) - \phi_b(x) - \frac{2\pi}{\Phi_0} \int_{b_x}^{a_x} \vec{A} \cdot d\vec{\ell} \\ \tilde{\Delta}\phi(0) &= \phi_a(0) - \phi_b(0) - \frac{2\pi}{\Phi_0} \int_{b_0}^{a_0} \vec{A} \cdot d\vec{\ell} \\ \Rightarrow \phi_a(0) - \phi_a(x) &= -\frac{2\pi}{\Phi_0} \int_{a_x}^{a_0} \vec{A} \cdot d\vec{\ell} \dots \\ \phi_b(x) - \phi_b(0) &= -\frac{2\pi}{\Phi_0} \int_{b_0}^{b_x} \vec{A} \cdot d\vec{\ell} \end{aligned} \right\}$$

$$\Rightarrow I = \int_0^D j_y(x) dx = j_m \int_0^D dx \sin(\tilde{\Delta} \phi(x))$$

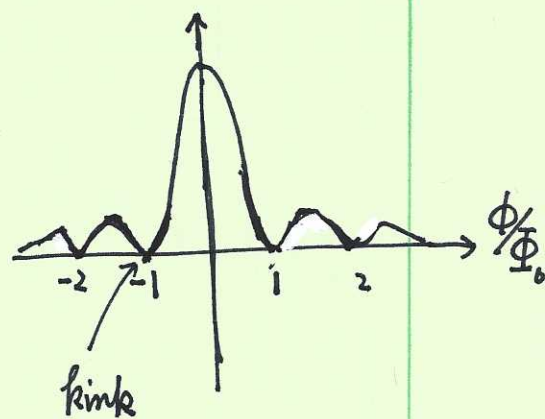
$$= j_m D \int_0^1 dx' \sin(\tilde{\Delta} \phi(0) - \frac{2e}{\hbar c} B D (a + 2\lambda_L) \frac{x'}{D}) \quad \text{define } \phi = B D (a + 2\lambda_L)$$

$$= j_m D \int_0^1 dx' \sin(\tilde{\Delta} \phi(0) - 2\pi \frac{\Phi}{\Phi_0} x')$$

$$= j_m D \frac{1}{2\pi \frac{\Phi}{\Phi_0}} \left(\cos(\tilde{\Delta} \phi(0) - \frac{2\pi}{\Phi_0} \phi) - \cos(\tilde{\Delta} \phi(0)) \right)$$

$$= j_m D \frac{\sin \pi \frac{\Phi}{\Phi_0}}{\pi \frac{\Phi}{\Phi_0}} \cdot \sin\left(\tilde{\Delta} \phi(0) - \frac{\pi \Phi}{\Phi_0}\right)$$

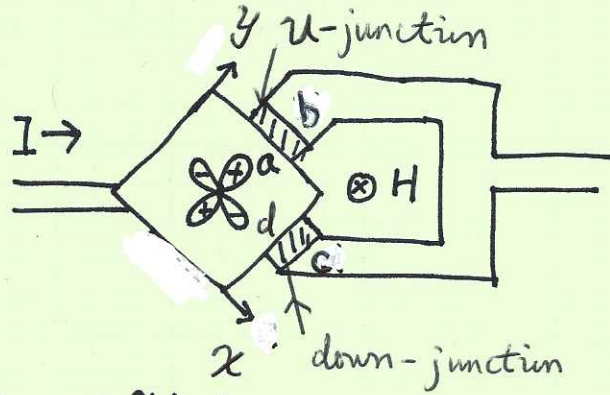
$$\Rightarrow I_{max} = j_m D \left| \frac{\sin \pi \frac{\Phi}{\Phi_0}}{\pi \frac{\Phi}{\Phi_0}} \right|$$



Now let us apply it to the d-wave case

① d-S SQUID:

The two junctions have opposite sign of coupling constants



Constants

$$I = I_u + I_d = I_m (\sin \tilde{\Delta} \phi_u - \sin \tilde{\Delta} \phi_d)$$

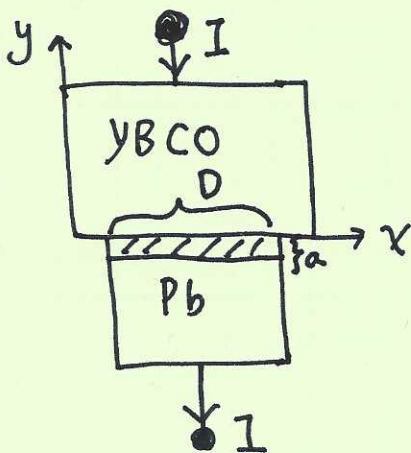
$$= 2I_m \sin \frac{\tilde{\Delta} \phi_u - \tilde{\Delta} \phi_d}{2} \cos \frac{\tilde{\Delta} \phi_u + \tilde{\Delta} \phi_d}{2} = 2I_m \sin \frac{\pi \Phi}{\Phi_0} \cos \left(\Delta \phi_u + \frac{\pi \Phi}{\Phi_0} \right)$$

$$\Rightarrow I_{max} = 2I_m \left| \sin \frac{\pi \Phi}{\Phi_0} \right|$$

The d-S SQUID has maximum current density at $\Phi = \frac{1}{2} \Phi_0$ due to geometric flux π .

② Corner junction

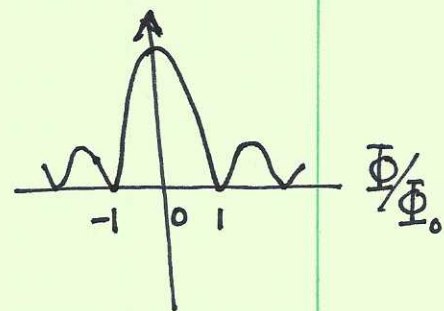
if we make a planar Josephson junction



This planar junction will exhibit the

same Fraunhofer pattern as two s-wave one, i.e

$$I_{max} \propto \left| \frac{\sin \pi \Phi / \Phi_0}{\pi \Phi / \Phi_0} \right|$$



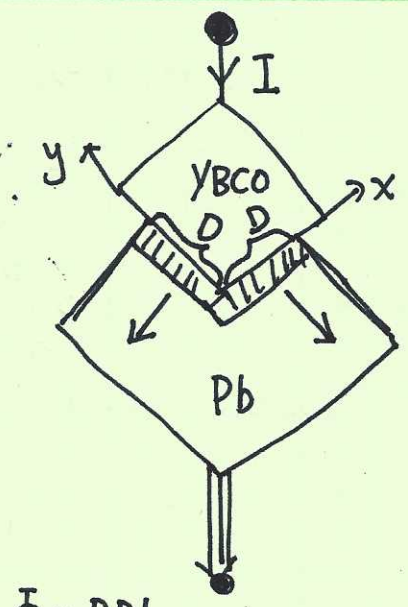
define $L = a + \lambda_{YBCO} + \lambda_{Pb}$

a : is the width of insulating region

L : is effective width of junction

for x -direction junction, its current projection to 45° -direction is

$$\frac{1}{\sqrt{2}} j_m \int_0^L dx' \sin(\tilde{\Delta}\phi(x) - \frac{2\pi\Phi}{\Phi_0} x')$$



When calculate the current to y -direction, we need to change gauge

$$A_y = 0, \quad A_x = B y \quad (\text{c.f. the odd gauge } \begin{matrix} A_x = 0 \\ A_y = -B x \end{matrix})$$

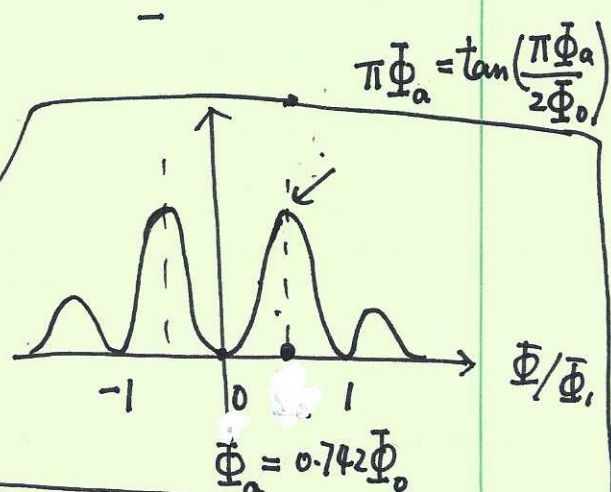
$$\Rightarrow \text{Current along } 45^\circ : -\frac{1}{\sqrt{2}} j_m \int_0^L dy' \sin(\tilde{\Delta}\phi(y) + \frac{2\pi\Phi}{\Phi_0} y')$$

the overall "-" sign comes from the d-wave symmetry

$$\Rightarrow I_{tot} = \frac{j_m D}{\sqrt{2}} \frac{\sin \pi\Phi/\Phi_0}{\pi\Phi/\Phi_0} \left[\sin(\tilde{\Delta}\phi(0) - \frac{\pi\Phi}{\Phi_0}) - \sin(\tilde{\Delta}\phi(0) + \frac{\pi\Phi}{\Phi_0}) \right]$$

$$= \sqrt{2} j_m D \frac{\sin^2 \pi\Phi/\Phi_0}{\pi\Phi/\Phi_0} \cos(\tilde{\Delta}\phi(0))$$

$$\Rightarrow I_{max} = I_0 \frac{\sin^2 \pi\Phi/\Phi_0}{\pi\Phi/\Phi_0}$$

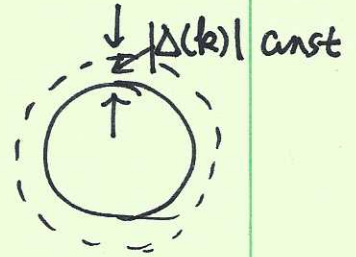


p-wave Cooper pairing and moore

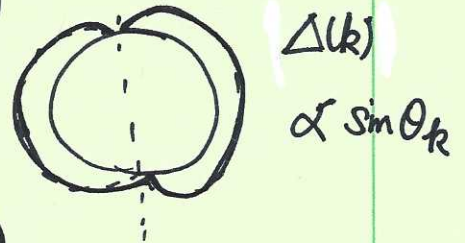
The most celebrated example of the p-wave Cooper pairing is the ^3He . Except that it's charge neutral and thus the EM response is different, they are very similar to paired superconductors. The solid state p-wave system is Sr_2RuO_4 , and ultra-cold dipolar fermions also gives rise to p-wave pairing. P-wave pairing has an enormously rich structure, $L=1, S=1$.

① isotropic - B phase $J = L + S = 0$.

fully gapped, 3D topological pairing



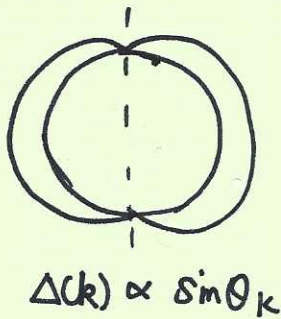
② anisotropic - A phase J is not well-defined,
nodal quasi-particle



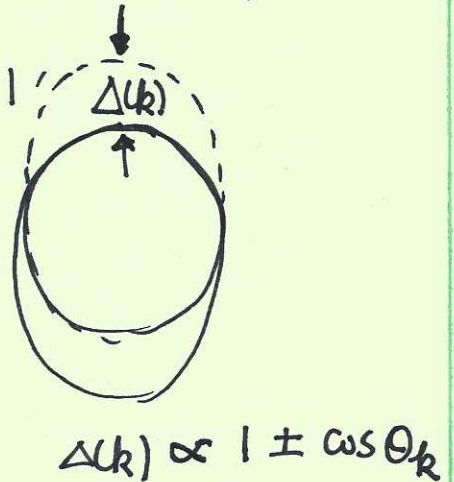
③ J-triplet pairing ($Y\text{Li}$ and C. Wu)

a new pairing pattern $J = L = S = 1$ due to dipolar interaction

$J_z = 0$



$J_z = \pm 1$



We use the continuum model

$$H = \sum_{\mathbf{k}} (\epsilon(\mathbf{k}) - \mu) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{1}{2\text{Vol}} \sum_{\mathbf{k}\mathbf{k}'} V(\mathbf{k}, \mathbf{k}') a_{-\mathbf{k}'\beta}^\dagger a_{\mathbf{k}'\alpha}^\dagger a_{\mathbf{k}\alpha} a_{-\mathbf{k}\beta}$$

and we use a factorizable interaction: $V(\mathbf{k}, \mathbf{k}') = -V_t \vec{k} \cdot \vec{k}'$.

(This pairing interaction mainly arise from ferro-magnetic fluctuation)

define order parameter

$$\Delta_{\sigma\sigma'}^a = - \sum_{\mathbf{k}'} V_t \mathbf{k}' \cdot \langle a_{\mathbf{k}'\sigma} a_{-\mathbf{k}'\sigma'} \rangle$$

$$= \underbrace{\Delta_{\mu\alpha}}_{\text{tensor}} \cdot (\sigma_\mu i \sigma_2)_{\sigma\sigma'}$$

μ - spin channel

α - orbital channel

Thus the p-wave order parameter 3×3 complex matrix, which has 18 real parameters.

We can also define the pairing matrix $\Delta_{\sigma\sigma'}(\mathbf{k}) = \mathbf{k} \cdot \Delta_{\sigma\sigma'}^a$.

$$\Delta_{\sigma\sigma'}(\mathbf{k}) = \Delta_{\mu\alpha} \mathbf{k} \cdot \hat{d}_\mu(\mathbf{k}) (\sigma_\mu i \sigma_2)_{\sigma\sigma'}$$

the tensor $\Delta_{\mu\alpha}$ maps the momentum \vec{k} into

a vector in spin channel — d-vector.

$\Delta(\mathbf{k})$ is a complex number, the spin structure of Cooper pair is described by the d-vector.

The $\hat{d}(\mathbf{k})$ vector is normalized as

$$\hat{d}^*(\mathbf{k}) \cdot \hat{d}(\mathbf{k}) = \sum_{\mu} d_{\mu}^*(\mathbf{k}) d_{\mu}(\mathbf{k}) = 1$$

using d-vector, $\Delta_{00'}(k) = \Delta(k) \begin{pmatrix} -\hat{d}_x(k) + i\hat{d}_y(k), & \hat{d}_z(k) \\ \hat{d}_z(k), & \hat{d}_x(k) + i\hat{d}_y(k) \end{pmatrix}$ ③

★ $\Delta_{00'}(k)$ is a symmetric matrix, (triplet)

in comparison, the singlet channel pairing $\Delta_{00'} = \Delta_s(i\sigma_z)_{00'} = \begin{pmatrix} 0 & \Delta_s \\ -\Delta_s & 0 \end{pmatrix}$ is anti-symmetric.

⊗ physical meaning of d-vector

In many situation, $\hat{d}(k)$ up to an overall phase can be chosen as real, and we attribute the phase to $\Delta(k)$. Nevertheless, the direction of $\hat{d}(k)$ is not well-defined: if we set $\begin{cases} \hat{d}(k) \rightarrow -\hat{d}(k) \\ \Delta(k) \rightarrow e^{i\pi} \Delta(k) \end{cases}$ then $\vec{\Delta}(k)$ and $\Delta_{\mu\nu}(k)$ is invariant!

Thus d-vector is actually a director, not a really vector.

The physical meaning of d-vector: if $\hat{d}(k)$ is real, then $\hat{d}(k)$ is not the spin direction of the Cooper pair. For example, if $\hat{d}(k) = \hat{z}$, it means

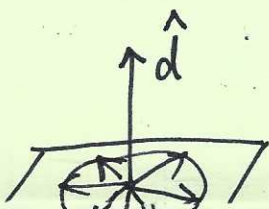
the pairing $\Delta_{00'} = \Delta_z \langle a_{k\uparrow} a_{-k\downarrow} + a_{k\downarrow} a_{-k\uparrow} \rangle$ which's in the

total spin $S=1, S_z=0$. The spin actually fluctuates in the x-y plane

Thus $\hat{d}(k)$ is perpendicular to the spin, or, $\hat{d}(k)$ is the direction

such that $\hat{d} \cdot \vec{S}$ is in the eigenstate with $\hat{d} \cdot \vec{S} = 0$. For such a state

all the spin average value is zero.



However, if \hat{d} is complex, or, $\text{Re } \hat{d} \neq \text{Im } \hat{d}$, then the angular momentum expectation value of Cooper pair is nonzero. Let us consider pairing $a_{k\uparrow}^\dagger a_{-k\uparrow}^\dagger$, which corresponding to $\hat{d} = \frac{1}{\sqrt{2}} (1, i, 0)$, then $S_z = 1$.

$$\hat{d}^* \times \hat{d} = i \Rightarrow \boxed{\vec{S} = -i \hat{d}^* \times \hat{d}}$$

Ex: prove $\boxed{\langle \vec{S}(k) \rangle = -i \hat{d}^* \times \hat{d} |\Delta(k)|^2}$

for a triplet Cooper pair described by $\Delta_{\sigma\sigma'}(k) = \Delta(k) \hat{d}_a(k) (\hat{\sigma}_a)_\sigma$

⊛ Bogoliubov - spectra (mean-field Hamiltonian)

$$\begin{aligned}
 H_{MF} = & \sum_{k\sigma} (\epsilon_k - \mu) a_{k\sigma}^\dagger a_{k\sigma} - \frac{1}{2} \sum_{k\sigma\sigma'} a_{k\sigma}^\dagger a_{-k\sigma'}^\dagger k_a \Delta_{\sigma\sigma'}^a \\
 & - \frac{1}{2} \sum_{k,\sigma\sigma'} a_{-k\sigma'} (\Delta_{\sigma\sigma'}^a k_a)_{\sigma'\sigma} a_{k\sigma} \\
 & + \frac{\text{Vol}}{2Vt} \sum_{\sigma\sigma', a} |\Delta_{\sigma\sigma'}^a|^2
 \end{aligned}$$

using the property $\Delta_{\sigma\sigma'}(-k) = -\Delta_{\sigma'\sigma}(k)$ (please check),

we can simplify $\frac{1}{2} \sum_{k\sigma\sigma'} a_{k\sigma}^+ \Delta_{\sigma\sigma'}(k) a_{-k\sigma'}^+ = \sum'_{k\sigma\sigma'} a_{k\sigma}^+ (\Delta_{\sigma\sigma'}^a \cdot k a) a_{-k\sigma'}^+$

Σ' means only sum over half of the momentum space

$$\Rightarrow H_{MF} = \sum'_{k\sigma} (a_{k\uparrow}^+ \ a_{k\downarrow}^+ \ a_{-k\uparrow} \ a_{-k\downarrow}) H_{\alpha\beta}(k) \begin{pmatrix} a_{k\uparrow} \\ a_{k\downarrow} \\ a_{-k\uparrow}^+ \\ a_{-k\downarrow}^+ \end{pmatrix} + \frac{Vol}{2Vt} \sum_{\sigma\sigma', a} |\Delta_{\sigma'\sigma}^a|^2$$

$$H_{\alpha\beta}(k) = \begin{bmatrix} \mathcal{E}(k) - \mu & \Delta(k)_{\sigma\sigma'} \\ \Delta^+(k) & -(\mathcal{E}(k) - \mu) \end{bmatrix}, \text{ where } \Delta_{\sigma\sigma}(k) = \Delta(k) \cdot \begin{pmatrix} -\hat{d}_x(k) + i\hat{d}_y(k), \hat{d}_z(k) \\ \hat{d}_z(k), \hat{d}_x(k) + i\hat{d}_y(k) \end{pmatrix}.$$

For simplicity, we set $\Delta(k)$ and \hat{d} real. $H_{\alpha\beta}(k)$ can be expressed in terms of P -matrix

$$H_{\alpha\beta}(k) = (\mathcal{E}(k) - \mu) P^1 + \Delta(k) [d_x(k) P^3 + d_y(k) P^4 + d_z(k) P^5]$$

$$P^1 = I \otimes \tau_3, \quad P^2 = \sigma_2 \otimes \tau_1, \quad P^3 = \sigma_3 \otimes \tau_1, \quad P^4 = I \otimes \tau_2, \quad P^5 = -\sigma_1 \otimes \tau_1$$

τ - refers to the particle-hole channel

σ - refers to spin

$$H^2(k) = (\mathcal{E}(k) - \mu)^2 + \Delta^2(k) \Rightarrow \mathcal{E}(k) = \pm \sqrt{(\mathcal{E}(k) - \mu)^2 + \Delta^2(k)}$$

① For the B-phase, the d-vector: $\Delta_{\sigma'\sigma}(k) = \Delta(k) \hat{d}_{\mu}(k) (\sigma_{\mu} i\omega_z)_{\sigma'\sigma}$

and $\Delta(k) \hat{d}_{\mu}(k) = \Delta_{\mu\alpha} k_{\alpha}$. Thus $\Delta_{\mu\alpha}$ maps the momentum space vector \hat{k} to a vector in spin space. If $\Delta_{\mu\alpha}$ is proportional to a

$O(3)$ matrix, i.e., $\Delta_{\mu\alpha} \propto d_{\mu\alpha} \leftarrow O(3) \text{ matrix}$, then it realizes a connection between two triads. In the simplest case $d_{\mu\alpha} \propto \delta_{\mu\alpha}$

i.e. $\hat{d}(k) = \hat{k}$.

$^3\text{He-B}$ is an isotropic phase, i.e.

$$\mathbf{J} = \mathbf{L} + \mathbf{S} = 0.$$

We need to co-rotate spin and momentum together, i.e. spin-orbit coupling (p-p channel)

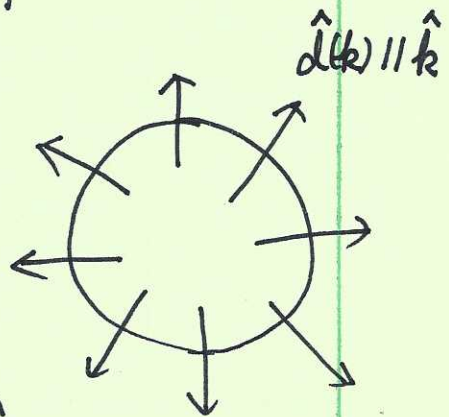
Spontaneously breaking of relative spin-orbit symmetry.

Goldstone mode / manifold $SO_L(3) \otimes SO_S(3) / SO_J(3)$

relative spin-orbit rotation, i.e. the degree of freedom $d_{\mu\alpha}$,

i.e. $\sum_{\mu\alpha} d_{\mu\alpha} \cdot d_{\mu\alpha} = 1$.

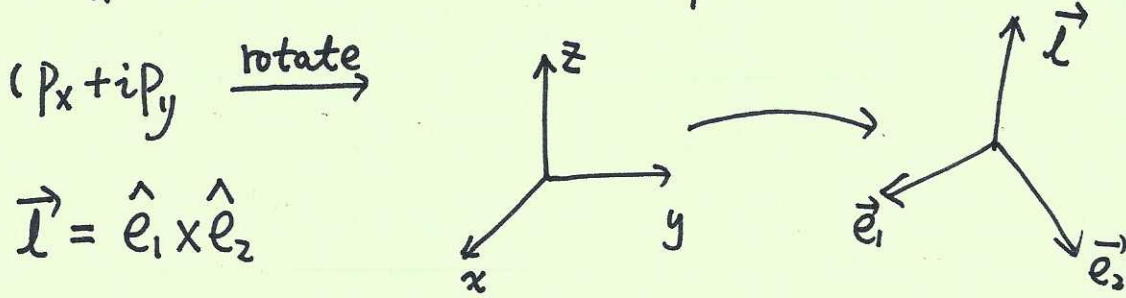
The spectra is fully gapped: $E(k) = \pm \sqrt{(E(k) - \mu)^2 + |\Delta|^2}$.



② The A-phase : $\Delta_{\sigma\sigma'}(\mathbf{k}) = \Delta(\mathbf{k}) \hat{d}_\mu(\mathbf{k}) (\sigma_\mu i\sigma_z)_{\sigma\sigma'}$

$$\Delta(\mathbf{k}) \hat{d}_\mu(\mathbf{k}) = \Delta e^{i\theta} \hat{d}_\mu \{(\hat{e}_1 + i\hat{e}_2) \cdot \hat{\mathbf{k}}\}$$

$\hat{\mathbf{d}}$ -vector is momentum-independent, but $\Delta(\mathbf{k})$ depends on $\hat{\mathbf{k}}$,



direction of orbital angular momentum.

Rotation of the frame \hat{e}_1, \hat{e}_2 around $\vec{\mathbf{l}}$ -vector at angle α , is equivalent to a phase gauge transformation.

$$\hat{e}'_1 + i\hat{e}'_2 = e^{i\alpha} (\hat{e}_1 + i\hat{e}_2)$$

$$\rightarrow \Delta'_\mu(\mathbf{k}) = \Delta_\mu(\mathbf{k}) e^{i\alpha}$$

Now let us set $\hat{e}_1 = \hat{x}, \hat{e}_2 = \hat{y}, \vec{\mathbf{l}} = \hat{z}, \hat{d}_\mu = \hat{z} \Rightarrow$

$$|\Delta(\mathbf{k})|^2 = |\Delta|^2 (\hat{k}_x^2 + \hat{k}_y^2) = |\Delta|^2 \sin^2 \theta_{\mathbf{k}}$$

$$\Rightarrow E(\mathbf{k}) = \pm \sqrt{(E(\mathbf{k}) - \mu)^2 + |\Delta|^2 \sin^2 \theta_{\mathbf{k}}}$$

Dirac fermion at $\theta = 0$, and π .

Green's function (Matsubara)

$$\left[\begin{array}{cc} -T_z \langle a_{\sigma}(k, \tau) a_{\sigma}^{\dagger}(k, 0) \rangle, & -T_z \langle a_{\sigma}(k, \tau) a_{\sigma}(-k, 0) \rangle \\ -T_z \langle a_{\sigma}^{\dagger}(-k, \tau) a_{\sigma}^{\dagger}(k, 0) \rangle, & -T_z \langle a_{\sigma}^{\dagger}(k, \tau) a_{\sigma}(-k, 0) \rangle \end{array} \right]$$

it's Fourier transform $\Rightarrow [i\omega_n - H_{\alpha\beta}(k)]^{-1} = G(k, i\omega_n)$

$$G(k, i\omega_n) = \begin{bmatrix} G_{\sigma\sigma}(k, i\omega_n) & F_{\sigma\sigma}(k, i\omega_n) \\ F_{\sigma\sigma}^{\dagger}(k, i\omega_n) & -G_{\sigma\sigma}(-k, -i\omega_n) \end{bmatrix}$$

$$= \frac{i\omega_n + (\epsilon(k) - \mu) \Gamma' + \Delta(k) (dx P^3 + dy P^4 + dz P^5)}{(i\omega_n)^2 - \overset{2}{E}(k)}$$

Solution for edge modes (P+ip / He-3B).

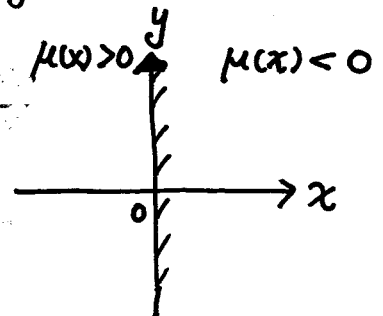
①

① Simplified model

$$\begin{bmatrix} -\mu(x) & \frac{\Delta(-i\partial_x + ik_y)}{k_f} \\ \frac{\Delta(-i\partial_x - ik_y)}{k_f} & \mu(x) \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} e^{ik_y y} = \underbrace{\begin{bmatrix} u_n \\ v_n \end{bmatrix}}_{E_n(k_y)} e^{ik_y y}$$

① $-\mu(x) u_n + \frac{\Delta(-i\partial_x v_n + ik_y v_n)}{k_f} = E_n(k_y) u_n$

② $\frac{\Delta(-i\partial_x u_n - ik_y u_n)}{k_f} + \mu(x) v_n = E_n(k_y) v_n$



We are only interested in the edge states. These states are zero mode along the x-direction. The dispersion purely comes from the plane-wave along y-direction. We should try

$$\begin{cases} \frac{\Delta}{k_f} i k_y v_0 = E_0(k_y) u_0 \\ \frac{\Delta}{k_f} (-i) k_y u_0 = E_0(k_y) v_0 \end{cases} \Rightarrow \begin{cases} u_0 = -i v_0 \\ E_0(k_y) = -\Delta k_y / k_f \end{cases}$$

but actually only one is possible.

or $\begin{cases} u_0 = i v_0 \\ E_0(k_y) = \Delta k_y / k_f \end{cases}$

We need to check the zero mode along the x-direction should be localized at $x=0$.

Set $u_0 = -i v_0 \Rightarrow [-\mu(x) + \frac{\Delta \partial_x}{k_f}] u_n = 0$ from 1st Eq

$[\frac{\Delta \partial_x}{k_f} - \mu(x)] u_n = 0$ from 2nd Eq

\Rightarrow these two Eqs are consistent

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$$\frac{1}{k_f} \partial_x u_0 = \frac{\mu(x)}{\Delta} u_0 \Rightarrow$$

$$u_0(x) \sim e^{-\int_0^{|x|} dx' \frac{k_f}{\Delta} |\mu(x')|} \quad (2)$$

For the current set up, that $\mu(x) < 0$ at $x > 0$, we do have exponential decay solution. The other try that $u_0 = i v_0$ does not work, which gives rise to exponentially divergent solutions.

③ Now let us restore the dispersion $H_0 = f_y(k_y) + f_x(-i\hbar\partial_x) - \mu(x)$

I want to be general!

we have

$$\textcircled{1} - [f_y(k_y) + f_x(-i\hbar\partial_x) - \mu(x)] u_0 + \frac{\Delta}{k_f} (-i\partial_x v_0 + i k_y v_0) = E_0(k_y) u_0$$

$$\textcircled{2} - \frac{\Delta}{k_f} (-i\partial_x u_0 - i k_y u_0) + [-f_y(k_y) - f_x(-i\hbar\partial_x) + \mu(x)] v_0 = E_0(k_y) v_0$$

Still try the solution

$$\begin{cases} \frac{\Delta}{k_f} i k_y v_0 = E_0(k_y) u_0 \\ \frac{\Delta}{k_f} (-i) k_y u_0 = E_0(k_y) v_0 \end{cases} \quad \begin{array}{l} \text{(let's choose} \\ u_0 = -i v_0) \end{array}$$

and the x-direction

$$[f_y(k_y) + f_x(-i\hbar\partial_x) - \mu(x)] u_0 + \frac{\Delta}{k_f} \partial_x u_0 = 0 \quad \text{from } \textcircled{1}$$

$$[\frac{\Delta}{k_f} \partial_x + f_y(k_y) + f_x(-i\hbar\partial_x) - \mu(x)] u_0 = 0 \quad \text{from } \textcircled{2}$$

consistent! \Rightarrow the edge spectra is not affected, which

$E_0(k_y)$ is still determined by the off-diagonal term $E_0(k_y) = -\frac{\Delta k_y}{k_f}$.

but the zero mode Eq along the x-direction \rightarrow

$$\left[f_x(-i\hbar \partial_x) + \frac{\Delta}{k_f} \partial_x \right] \psi_0 = [\mu(x) - f_y(k_y)] \psi_0$$

$$\text{or } \left[\frac{-\hbar^2 \partial_x^2}{2m} + \frac{\Delta}{k_f} \partial_x \right] \psi_0 = \left[\mu(x) - \frac{\hbar^2 k_y^2}{2m} \right] \psi_0$$

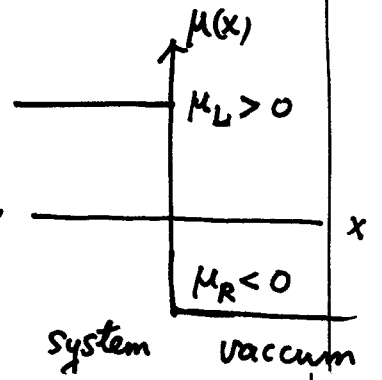
This Eq is more realistic compared with the oversimplified one

$\frac{\Delta}{k_f} \partial_x \psi_0 = \mu(x) \psi_0$. In that case, all the states (k_x, k_y) in the bulk plane wave

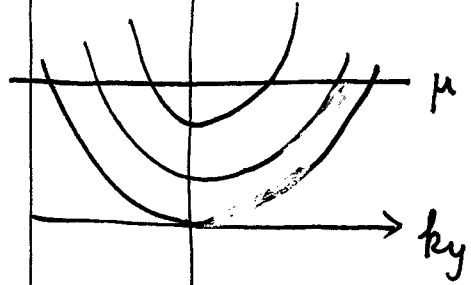
are occupied, i.e. $k_f \rightarrow +\infty$. Now, if for the

value of k_y , such that $\frac{\hbar^2 k_y^2}{2m} > \mu_L$ (see figure),

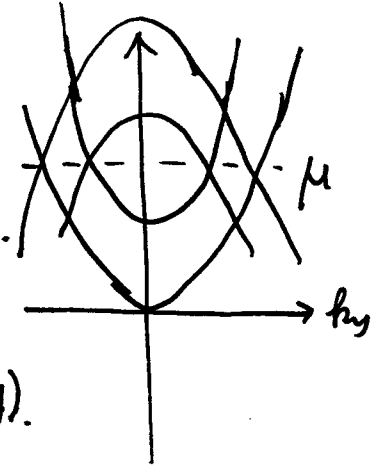
we have no edge states, (because $\mu(x) - \frac{\hbar^2 k_y^2}{2m}$ always negative).



$$E(k_y) = \frac{\hbar^2 k_y^2}{2m} + \frac{\hbar^2 k_x^2}{2m}$$

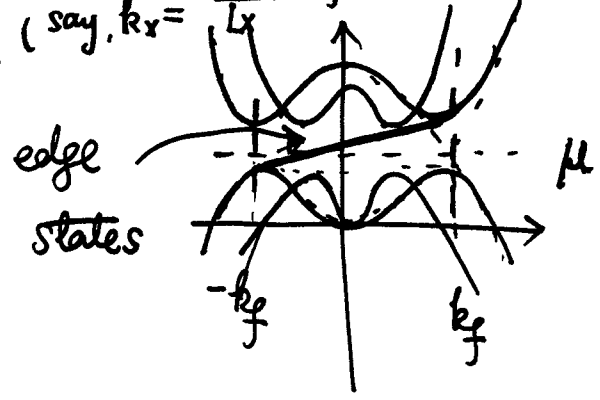


$\Delta = 0$



each parabola is with a different k_x . (say, $k_x = \frac{n\pi}{L_x}$ for open boundary).

$\Delta \neq 0$



estimation of edge state velocity

$$\frac{v}{v_f} = \frac{\Delta}{k_f v_f} \approx \frac{\Delta}{E_f}$$

Surface states of the BW state

$$H = \begin{bmatrix} -\frac{\hbar^2}{2m} \nabla^2 - \mu(x) & \Delta (-i\hbar \vec{\nabla} \cdot \vec{\sigma}) i\sigma_2 \\ \Delta (-i\omega_2 \cdot \vec{\sigma}) (-i\hbar \vec{\nabla}), & \frac{\hbar^2}{2m} \nabla^2 + \mu(x) \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = E \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$$

seek $\begin{bmatrix} \phi_1(z) \\ \phi_2(z) \end{bmatrix} e^{ik_x x + ik_y y}$

$$\Rightarrow \begin{bmatrix} -\frac{\hbar^2}{2m} \nabla^2 - \mu(x) & \Delta (\hbar k_x \sigma_1 + \hbar k_y \sigma_2 - i\hbar \partial_z \sigma_3) i\omega_2 \\ \Delta (-i\omega_2) (\hbar k_x \sigma_1 + \hbar k_y \sigma_2 - i\hbar \partial_z \sigma_3) & \frac{\hbar^2}{2m} \nabla^2 + \mu(x) \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = E(k_x, k_y) \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$$

seek surface state spectra:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - \mu(x) \right] \phi_1 + \Delta (\hbar k_x \sigma_1 + \hbar k_y \sigma_2 - i\hbar \partial_z \sigma_3) \phi_2 = E_0(k_x, k_y) \phi_1$$

$$\Delta (-i\omega_2) (\hbar k_x \sigma_1 + \hbar k_y \sigma_2 - i\hbar \partial_z \sigma_3) \phi_1 + \left(\frac{-\hbar^2 k_{||}^2}{2m} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \mu(x) \right) \phi_2 = E_0(k_x, k_y) \phi_2$$

we want $\Delta \hbar (k_x \sigma_1 + k_y \sigma_2) i\omega_2 \phi_2 = E_0(k_x, k_y) \phi_1$ ①

$\Delta (-i\omega_2) \hbar (k_x \sigma_1 + k_y \sigma_2) \phi_1 = E_0(k_x, k_y) \phi_2$ ②

try $\phi_1 = T \phi_2 \Rightarrow \Delta \hbar (k_x \sigma_1 + k_y \sigma_2) i\omega_2 \phi_2 = E_0(k_x, k_y) T \phi_2$

or $\Delta \hbar \underline{T^{-1} (k_x \sigma_1 + k_y \sigma_2) i\omega_2} \phi_2 = E_0(k_x, k_y) \phi_2$

$\Rightarrow \Delta \hbar \underline{(-i\omega_2) (k_x \sigma_1 + k_y \sigma_2) T} \phi_2 = E_0(k_x, k_y) \phi_2$

we need

$$T^{-1} (k_x \sigma_1 + k_y \sigma_2) i\omega_2 = (-i\omega_2) (k_x \sigma_1 + k_y \sigma_2) T$$

also need to be

$$\Rightarrow T^{-1} i\omega_2 \underbrace{(-k_x \sigma_1 + k_y \sigma_2)} = (-i\omega_2) T \underbrace{T^{-1} (k_x \sigma_1 + k_y \sigma_2) T}_{\text{Hermitian}}$$

we need $-k_x \sigma_1 + k_y \sigma_2 \propto T^{-1} (k_x \sigma_1 + k_y \sigma_2) T$

we can set $T \propto$ either σ_1 , or σ_2 , but not σ_3 .

If we set $T \propto \sigma_2$, we have $T^{-1} (k_x \sigma_1 + k_y \sigma_2) T = (-k_x \sigma_1 + k_y \sigma_2)$

$$\Rightarrow T^{-1} i\omega_2 = (-i\omega_2) T \Rightarrow T = i\omega_2$$

if $T = i\omega_2$, i.e. $\phi_1 = i\omega_2 \phi_2$

$$\left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2 \partial^2}{2m \partial z^2} - \mu(x) \right] i\omega_2 \phi_2 - \Delta (i\hbar \partial_z \sigma_3) i\omega_2 \phi_2 = 0 \quad (1)$$

$$\left[\Delta (-i\sigma_2) (-i\hbar \partial_z \sigma_3) - i\omega_2 \phi_2 + \left[-\frac{\hbar^2 k_{11}^2}{2m} + \frac{\hbar^2 \partial^2}{2m \partial z^2} + \mu(x) \right] \phi_2 \right] = 0 \quad (2)$$

$$(1) \Rightarrow \left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2 \partial^2}{2m \partial z^2} - \mu(x) \right] \phi_2 + \underbrace{i\omega_2 (\sigma_3)}_{\sigma_1} i\omega_2 \hbar \Delta \partial_z \phi_2 = 0$$

This means that ϕ_2 has to satisfy another matrix Eq. This is not

consistent with

$$(-i\omega_2) (k_x \sigma_1 + k_y \sigma_2) (i\omega_2) \phi_2 = E (k_x \hbar y) \phi_2$$

$$\underline{(-k_x \sigma_1 + k_y \sigma_2) \phi_2 = E (k_x \hbar y) \phi_2}$$

In other words, we seek a purely scalar equation for the z -direction. ⁽⁴⁾

The choice of $\phi_1 = i\sigma_2 \phi_2$ doesn't work!

Instead, we choose $\phi_1 = \pm i\sigma_1 \phi_2$ (\pm 's apply to different boundary)

$$\left[+\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} - \mu(x) \right] \phi_1 - \overbrace{\Delta (i\hbar \partial_z \sigma_3) (i\omega_2) (\mp i\sigma_1)}^{\mp \Delta \hbar \partial_z \phi_1} \phi_1 = 0 \quad (1)$$

$$\Delta (-i\omega_2) (-i\hbar \partial_z \sigma_3) \phi_1 + \left[-\frac{\hbar^2 k_{11}^2}{2m} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \mu(x) \right] (\mp i\sigma_1) \phi_1 = 0 \quad (2)$$

$$(2) \Rightarrow \left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} - \mu(x) \right] \phi_1 + \Delta (\mp i\omega_1) (-i\omega_2) (-i\hbar \partial_z \sigma_3) \phi_1 = 0$$

\downarrow
 $\mp \Delta \hbar \partial_z \phi_1$

\Rightarrow consistent

$$\left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} - \mu(x) \right] \phi_1 \mp \Delta \hbar \partial_z \phi_1 = 0$$

$$\boxed{\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \mp \frac{\Delta}{\hbar} \partial_z \right] \phi_1 = \left[\mu(x) - \frac{\hbar^2 k_{11}^2}{2m} \right] \phi_1}$$

which is the same as before

$$\boxed{\phi_1 = \pm i\sigma_1 \phi_2}$$

$$\hbar \Delta (k_x \sigma_1 + k_y \sigma_2) i\sigma_2 (\mp i\sigma_1) \phi_1 = E_0(k_x, k_y) \phi_1$$

$$\boxed{\mp \hbar \Delta (k_x \sigma_2 - k_y \sigma_1) \phi_1 = E_0(k_x, k_y) \phi_1}$$

Now let us solve the normal direction: we use the 2D case.

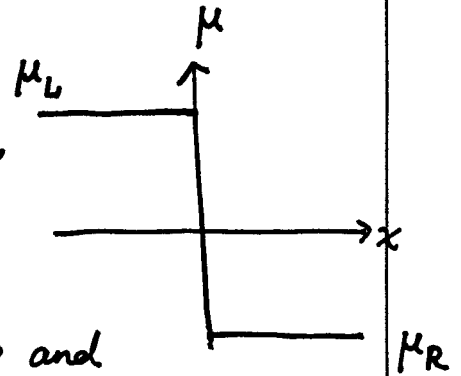
$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{\Delta}{k_f} \frac{\partial}{\partial x} \right] u_0 = \left[\mu_L - \frac{\hbar^2 k_y^2}{2m} \right] u_0 \quad \text{for } x < 0, \text{ where } \mu_L = \frac{\hbar^2 k_F^2}{2m}.$$

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{\Delta}{k_f} \frac{\partial}{\partial x} \right] u_0 = \left[\mu_R - \frac{\hbar^2 k_y^2}{2m} \right] u_0 \quad \text{for } x > 0$$

actually, if both μ_L and $\mu_R > 0$, but $\mu_L \rightarrow \mu_R$,

there may still exist $\mu_L > \frac{\hbar^2 k_y^2}{2m} > \mu_R$, such

that are edge states. This may also be interesting and need check further!



Generally, speaking since 2nd order derivatives are involved, and

μ_L and μ_R steps are finite, we expect non-continuity of $u_0''(x)$,

but $u'(x)$, and $u(x)$ are continuous at the boundary. Imagine that we

set $\mu_R \rightarrow -\infty$, which corresponds to open boundary, i.e. $u_0(x) = 0$ for $x > 0$.

Then $u_0'(x)$ may also be discontinuous, $u_0'(x=0^+) - u_0'(x=0^-)$

but $u_0(x)$ should be continuous,

$$= \int_0^+ u'' \rightarrow \in \underbrace{u''}_{\text{finite}} \text{ may be}$$

i.e. we seek solution

$$u_0(0) = 0, \text{ and } u_0(-\infty) = 0.$$

let us try $u_0 \sim e^{\beta x}$ for $x < 0$, where $\text{Re} \beta > 0$. (we consider the left space, so $\text{Re} \beta > 0$).

β can actually be complex.

$$\Rightarrow \frac{-\hbar^2 \beta^2}{2m} + \frac{\Delta}{k_f} \beta = \mu_L - \frac{\hbar^2 k_y^2}{2m} \Rightarrow \left(\frac{\beta}{k_f} \right)^2 - \frac{\Delta}{E_f} \left(\frac{\beta}{k_f} \right) + \left[1 - \left(\frac{k_y}{k_f} \right)^2 \right] = 0$$

for the usual case that $\frac{\Delta}{E_f} \ll 1$.

① If $k_y/k_f \ll 1$, we have $\left(\frac{\Delta}{E_f} \right)^2 - 4 \left[1 - \left(\frac{k_y}{k_f} \right)^2 \right] < 0$

or for $\left| k_y/k_f \right| < \sqrt{1 - \left(\frac{\Delta}{2E_f} \right)^2}$, the solutions β is a pair of complex variables. \Rightarrow

$$\beta/k_f = \frac{1}{2} \frac{\Delta}{E_f} \pm i \sqrt{\left[1 - \left(\frac{k_y}{k_f} \right)^2 \right] - \left(\frac{\Delta}{2E_f} \right)^2}$$

We seek

$$u_0(x) \sim e^{\frac{k_f \Delta}{2 E_f} x} \cdot \sin \left(\sqrt{\left[1 - \left(\frac{k_y}{k_f} \right)^2 \right] - \left(\frac{\Delta}{2E_f} \right)^2} k_f x \right)$$

in the case of $\frac{k_f \Delta}{2 E_f} \gg \sqrt{\left[1 - \left(\frac{k_y}{k_f} \right)^2 \right] - \left(\frac{\Delta}{2E_f} \right)^2}$, then the oscillation

is cut off by the exponential decay, we can approximate $\sin \# x \sim \# x$

$$u_0(x) \sim x e^{\frac{k_f \Delta}{2 E_f} x} \text{ up to an overall normalization.}$$

② if $\left(\frac{\Delta}{E_f} \right)^2 - 4 \left[1 - \left(\frac{k_y}{k_f} \right)^2 \right] > 0$ and $\left| k_y/k_f \right| \leq 1$, we have 2 real roots positive

$$\frac{\beta_{1,2}}{k_f} = \frac{1}{2} \frac{\Delta}{E_f} \pm \sqrt{\left(\frac{\Delta}{2E_f} \right)^2 - \left[1 - \left(\frac{k_y}{k_f} \right)^2 \right]}$$

or

$$1 \geq \left| k_y/k_f \right| \geq \sqrt{1 - \left(\frac{\Delta}{2E_f} \right)^2}$$

We seek $u_0(x) = e^{\beta_1 x} - e^{\beta_2 x} = e^{\bar{\beta} x} \left(e^{\frac{(\beta_1 - \beta_2)x}{2}} - e^{-\frac{(\beta_1 - \beta_2)x}{2}} \right)$

a) as $\left| \frac{k_y}{k_f} \right| \sim \sqrt{1 - \left(\frac{\Delta}{2E_f} \right)^2}$, $|\beta_1 - \beta_2| \ll \beta_2$.

again in this case, the decay is dominated by $e^{\beta_2 x}$, and

$e^{\frac{(\beta_1 - \beta_2)x}{2}} - e^{-\frac{(\beta_1 - \beta_2)x}{2}} \sim (\beta_1 - \beta_2)x$, $\Rightarrow u_0(x) \sim x e^{\frac{k_f \Delta}{2 E_f} x}$

b) as $\left| \frac{k_y}{k_f} \right| \rightarrow 1$, $\beta_2 \ll \beta_1$, thus the decay becomes

slow

$u_0(x) = e^{\beta_1 x} - e^{\beta_2 x} = e^{\beta_2 x} (1 - e^{(\beta_1 - \beta_2)x})$

$= \begin{cases} \propto x e^{\beta_2 x} \\ \propto e^{\beta_2 x} \end{cases}$

decay length $1/\beta_2 \rightarrow \infty$
and merge to bulk states.

$\sqrt{\left(\frac{\Delta}{2E_f} \right)^2 - \left(1 - \left| \frac{k_y}{k_f} \right| \right)^2} = \left[\left(\frac{\Delta}{2E_f} \right)^2 - 2 \left(1 - \left| \frac{k_y}{k_f} \right| \right) \right]^{1/2} = \frac{\Delta}{2E_f} - \frac{1 - \left| \frac{k_y}{k_f} \right|}{\Delta/2E_f}$

$\beta_2 \sim \frac{k_f - |k_y|}{\Delta/2E_f}$

ⓐ if $k_y > k_f$, two real roots. One positive, one negative.

no way to form a solution $u_0(0) = u_0(-\infty) = 0$. No edge states.

(2) If Δ is so large (unrealistic), such that $\frac{\Delta}{E_f} \geq 2$

Then we for the entire $| > |k_y/k_f| > 0$, we have always

$$\beta_{1,2}/k_f = \frac{1}{2} \frac{\Delta}{E_f} \pm \sqrt{\left(\frac{\Delta}{2E_f}\right)^2 - 1 + \left(\frac{k_y}{k_f}\right)^2}$$

the decay length is determined by $1/\beta_2 k_f$.