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

§ 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 $\Phi(\vec{R})$ = constant, i.e. momentum zero pairing. In isotropic system, we can expane $\phi(\vec{r}_1 - \vec{r}_2)$ 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
$$\chi_{t,\, S_z = 1,0,-1} = \begin{cases} |\uparrow\rangle_1 |\uparrow_2\rangle, \\ \frac{|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}, \\ |\downarrow\rangle_1 |\downarrow_2\rangle \end{cases} \quad \text{(spin triplet)}.$$

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

$$\psi_{\alpha_1\alpha_2}(\vec{r}_1, \vec{r}_2) = \begin{cases} R_n(r)\, Y_{lm}(\vec{r})\, \chi_s & (\text{for } l = \text{even}) \\ R_n(r)\, Y_{lm}(\vec{r})\, \chi_{t,\,0,\pm1} & (\text{for } l = \text{odd}). \end{cases}$$

* $R_n(r)$ 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: paring wavefunction does not change sign as varying angular variables, but changes sign along radial direction.

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

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

§ Weak coupling (momentum space picture) — gap equation

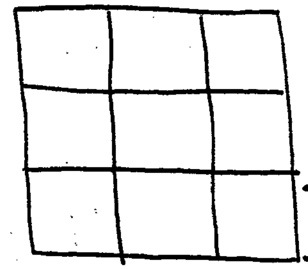
cnt.

we first consider the unconventional pairing in the singlet channel.

- The simplest and most celebrate 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.

$\boxed{\text{Background:}}$

The kinetic energy : tight-binding model



$$H_0 = -t \sum_{\langle ij \rangle} C^{+}_{i\sigma} C_{j\sigma} + h.c.$$

plug in Fourier component

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

N is the number of lattice sites

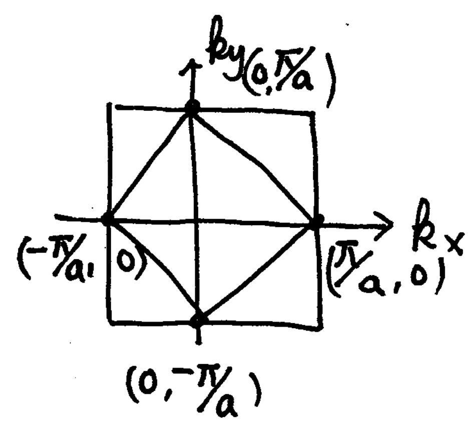
$$\Rightarrow H_0 = \sum_k \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} \quad \text{with } \varepsilon_k = -2t(\cos k_x + \cos k_y) - \mu$$

Ex: ① please derive the H_0 in momentum space.

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

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

$$\boxed{\cos k_x + \cos k_y = 0}$$



③ please also plot Fermi surfaces for negative values of μ,

say $|\mu/t| = 0.05, 0.1$, 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).

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

— phenomenological interaction leading to d-wave pairing

perform Fourier transformation, and keep the pairing term

$$H_{pair} = -\frac{V}{2N}\sum_{k',k}\sum_{\vec{\delta}} e^{i\vec{k}'\cdot\vec{\delta}} \cdot e^{-i\vec{k}\cdot\vec{\delta}} \left[C^\dagger_{-k'\downarrow} C^\dagger_{k'\uparrow} - C^\dagger_{-k'\uparrow} C^\dagger_{k'\downarrow}\right]\left[C_{k\uparrow} C_{-k\downarrow} - C_{k\downarrow} C_{-k\uparrow}\right]$$

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

$$= -\frac{V}{N}\sum_{k'k}\Big\{(\cos k'_x + \cos k'_y)\, C^\dagger_{-k'\downarrow} C^\dagger_{k'\uparrow}\, (\cos k_x + \cos k_y)\, C_{k\uparrow} C_{-k\downarrow}$$

$$+ (\cos k'_x - \cos k'_y)\, C^\dagger_{-k'\downarrow} C^\dagger_{k'\uparrow}\, (\cos k_x - \cos k_y)\, C_{k\uparrow} C_{-k\downarrow}\Big\}$$

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

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

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

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

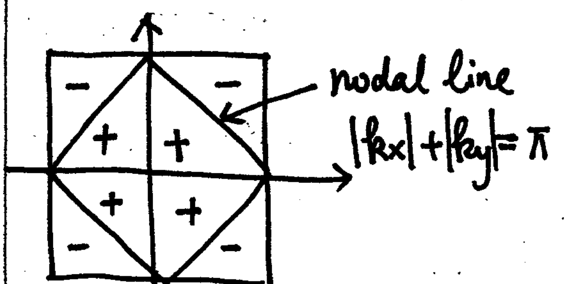
$$+ \frac{1}{V}\left(\Delta_s^* \Delta_s + \Delta_d^* \Delta_d\right)$$

We have chosen the interaction $V(kk') = V_0(\cos k_x' \cos k_x + \cos k_y' \cos k_y)$.

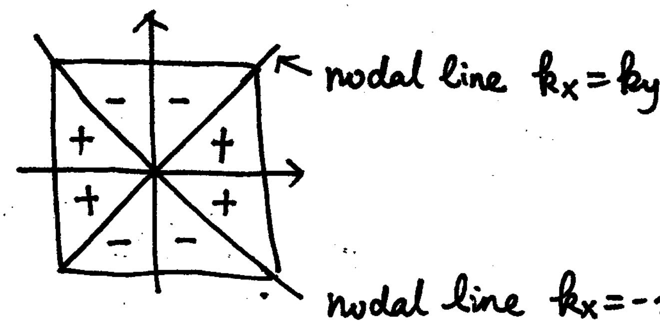
This interaction can give rise to two possible singlet pairing symmetries:

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

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



extended s-wave



d-wave

rotational invariant
but changes sign acrossing
$|k_x| + |k_y| = \pi$.

rotate 90°
$\Delta d \to -\Delta d$

Ex: please perform Fourier transformation back to real space.

① Δ_s corresponds to the real space pattern

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

$i+\hat{y}$, $i-\hat{x}$, i, $i+x$, $i-\hat{y}$

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 nodallines of Δ_s coincide with the Fermi surface at half-filling (For high Tc 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 channal.

$$\frac{H}{N} = \frac{1}{N}\sum_k \begin{pmatrix} c_{k\uparrow}^+ & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_k-\mu & \Delta_d(\cos k_x-\cos k_y) \\ \Delta_d^*(\cos k_x - \cos k_y) & -(\varepsilon_k-\mu) \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^+ \end{pmatrix}$$

$$+ \frac{1}{N}\sum_k(\varepsilon_k-\mu) + \frac{1}{V}\Delta_d^*\Delta_d$$

Introducing Bogoliubov transformation, and assum Δ_d is real

$$\begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^+ \end{pmatrix} = \begin{pmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k \end{pmatrix} \begin{pmatrix} \alpha_{k\uparrow} \\ \beta_{-k\downarrow}^+ \end{pmatrix}$$

we have

$$\rightarrow (\alpha_{k\uparrow}^+ \ \beta_{-k\downarrow}) \underbrace{\begin{pmatrix} \cos\theta_k & \sin\theta_k \\ -\sin\theta_k & \cos\theta_k \end{pmatrix} \begin{pmatrix} \xi_k & \Delta(k) \\ \Delta(k) & -\xi_k \end{pmatrix} \begin{pmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k \end{pmatrix}} \begin{pmatrix} \alpha_{k\uparrow} \\ \beta_{-k\downarrow}^+ \end{pmatrix}$$

$$\Downarrow$$

$$= \begin{bmatrix} \xi_k\cos 2\theta_k + \Delta(k)\sin 2\theta_k, & -\xi_k \sin 2\theta_k + \Delta(k)\cos 2\theta_k \\ -\xi_k\sin 2\theta_k + \Delta(k)\cos 2\theta_k, & -\xi_k\cos 2\theta_k - \Delta(k)\sin 2\theta_k \end{bmatrix}$$

$$(\xi_k = \varepsilon_k - \mu, \quad \Delta(k) = \Delta_d(\cos k_x - \cos k_y)\,]$$

Set $\tan 2\theta_k = \dfrac{\Delta(k)}{\xi_k}$ $\quad \cos 2\theta_k = \dfrac{\xi_k}{E_k}$, $\sin 2\theta_k = \dfrac{\Delta_k}{E_k}$

with $E_k = \sqrt{\xi_k^2 + \Delta^2(k)}$

$$\Rightarrow \frac{H}{N} = \frac{1}{N}\sum_k E_k \left[(\alpha^+_{k\uparrow}\alpha_{k\uparrow} - 1/2) + (\beta^+_{-k\downarrow}\beta_{-k\downarrow} - 1/2) \right]$$

$$+ \frac{1}{N}\sum_k (\varepsilon_k - \mu) + \frac{1}{V}|\Delta_d|^2 ,$$

$$\cos^2\theta_k = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right), \quad \sin^2\theta_k = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right).$$

§ Self-consistency

$$\frac{F}{N} = \frac{1}{N}\sum_k -\frac{2}{\beta}\ln\left(e^{\frac{\beta}{2}E_k} + e^{-\frac{\beta}{2}E_k}\right) + \frac{1}{N}\sum_k (\varepsilon_k - \mu) + \frac{\Delta_d^2}{V}$$

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

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

$$\Rightarrow \boxed{\Delta_d = V\int_{FBZ}\frac{d^2k}{(2\pi)^2}\frac{\Delta_d(\cos k_x - \cos k_y)^2}{2E_k}\tanh\frac{\beta}{2}E_k .}$$ ← Gap equation "d-wave".

$$n = -\frac{1}{N}\frac{\partial F}{\partial \mu} \Rightarrow \frac{1}{N}\frac{\partial F}{\partial \mu} = -\frac{2}{\beta}\int_{FBZ}\frac{d^2k}{(2\pi)^2}\tanh\frac{\beta}{2}E_k\cdot\frac{\beta}{2}\,\frac{-\xi_k}{E_k} - 1 = -n$$

$$\Rightarrow \boxed{1 - n = \int_{FBZ}\frac{d^2k}{(2\pi)^2}\tanh\frac{\beta}{2}E_k\cdot\frac{\xi_k}{E_k}}$$ ← particle number

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

$$\boxed{\Delta(k) = \int\frac{d^dk'}{(2\pi)^d} V(k,k')\frac{\Delta(k')}{2\sqrt{\xi^2 + \Delta^2(k')}}\tanh\frac{\beta}{2}\sqrt{\xi^2 + \Delta^2(k')}}$$

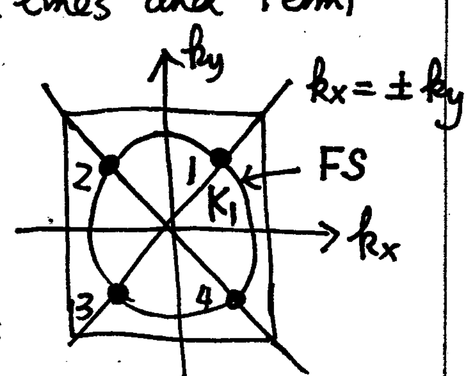
plug in $\Delta(k) = \Delta_d(\cos k_x - \cos k_y)$, $V(k,k') = V(\cos k_x - \cos k_y)(\cos k_x' - \cos k_y')$.

we will get the d-wave gap equation.

(*) Dirac spectra (nodal quasi-particle)

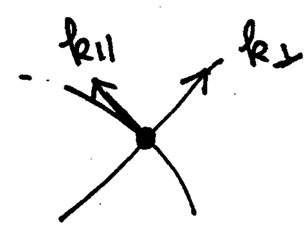
$$\pm E_k = \pm\sqrt{\xi_k^2 + \Delta^2(k)} \quad : \quad \xi_k = 0 \ \text{(Fermi surface)}$$
$$\Delta(k) = 0 \ \text{gap nodal line}$$

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.



$$\begin{cases} \xi_k = \hbar v_F \delta k_\perp \\ \Delta(k) = \Delta_d \delta k_\parallel a \end{cases}$$

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

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

Thermodynamics of nodal superconductors (singlet)

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. Assum ξ_k is isotropic, i.e. independent of the azimuthal angle φ_k

$$\int \frac{d^2k}{(2\pi)^2} \longrightarrow \int \frac{d\varphi}{2\pi} \int_{-\omega_0}^{\omega_0} d\xi \; \rho_0(\xi),$$ where $\rho_0(\xi)$ is the density of states. If $\rho_0(\xi)$ doesnot have sigularity, it can be replace 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 antiferro-magnetic fluctuations.

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

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

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

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

* Solve T_c

we have around T_c, $\underbrace{}_{\Delta=0}$ $\Rightarrow$ $$\int_0^{\frac{\omega_0}{2k_BT_c}} dx \frac{\tanh x}{x} = \frac{2}{N_F V}$$

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

Integral by part $\Rightarrow$ LHS= $$\ln\frac{\omega_0}{2k_BT_c}\tanh\frac{\omega_0}{2k_BT_c} - \int_0^{\frac{\omega_0}{2k_BT_c}} dx \ln x \,\mathrm{sech}^2 x$$

we can set $\frac{\omega_0}{2k_BT_c} \to \infty$ converge!

define $$C_0 = \frac{1}{2}\exp\left[-\int_0^\infty dx \frac{\ln x}{\cosh^2 x}\right] = 1.134$$

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

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

* Solve gap value at $T=0$,

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

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

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

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

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

Consider the case of $\omega_0 \gg \Delta_d$, we can approximate the integral as

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

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

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

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

$$\Rightarrow \boxed{\Delta_d = C_1 \omega_0 e^{-\frac{2}{N_F V}}}, \quad \text{where } C_1 = 2\cdot\exp\left[-\frac{4}{\pi}\int_0^{\pi/2} d\varphi \cos^2\varphi \ln\cos\varphi\right] \simeq 2.426$$

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

$$\rho(\omega) = \frac{2}{Vol}\sum_k \left(u_k^2 \delta(\omega - E_k) + v_k^2 \delta(\omega + E_k)\right)$$

$$= 2\int \frac{d^2k}{(2\pi)^2} \frac{1}{2}\left[\left(1 + \frac{\xi_k}{E_k}\right)\delta(\omega - E_k) + \left(1 - \frac{\xi_k}{E_k}\right)\delta(\omega + E_k)\right]$$

$$= \int \frac{d\varphi}{2\pi}\int d\xi \frac{N_F}{2}\left[\left(1+\frac{\xi}{E}\right)\delta(\omega - E) + \left(1 - \frac{\xi}{E}\right)\delta(\omega + E)\right]$$

← odd function

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

$$= \int \frac{d\varphi}{2\pi}\int_0 d\xi \frac{N_F}{2}\delta\left(\omega - \sqrt{\xi^2 + \Delta_d^2\cos^2 2\varphi}\right)$$

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

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

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

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

$$= N_F \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 2\varphi}} \, \theta(\omega > |\Delta \cos 2\varphi|)$$

$$= N_F \, \frac{1}{2} \int^{4\pi} \frac{d\varphi'}{2\pi} \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 \varphi'}} \, \theta(\omega > |\Delta \cos 2\varphi|) = \frac{2N_F}{\pi} \int_0^{\pi/2} d\varphi' \frac{\omega}{\sqrt{\omega^2 - \Delta^2 \cos^2 \varphi'}} \, \theta(\cdots)$$

① if $\omega > \Delta \Rightarrow$ $\rho(\omega) = \dfrac{2N_F}{\pi} \displaystyle\int_0^{\pi/2} d\varphi' \frac{1}{\sqrt{1 - (\Delta/\omega)^2 \cos^2 \varphi'}} = \frac{2N_F}{\pi} \int_0^{\pi/2} d\varphi' \frac{1}{\sqrt{1 - \left(\frac{\Delta}{\omega}\right)^2 \sin^2 \varphi'}}$

This is the complete Elliptic integral of 1st kind.

as $\boxed{\begin{array}{ll} \Delta/\omega \to 1, \text{ we have} & \rho(\omega) \simeq \frac{N_F}{\pi} \ln \frac{8}{1 - \Delta/\omega} \\ \Delta/\omega \to \infty & \rho(\omega) = N_F \end{array}}$

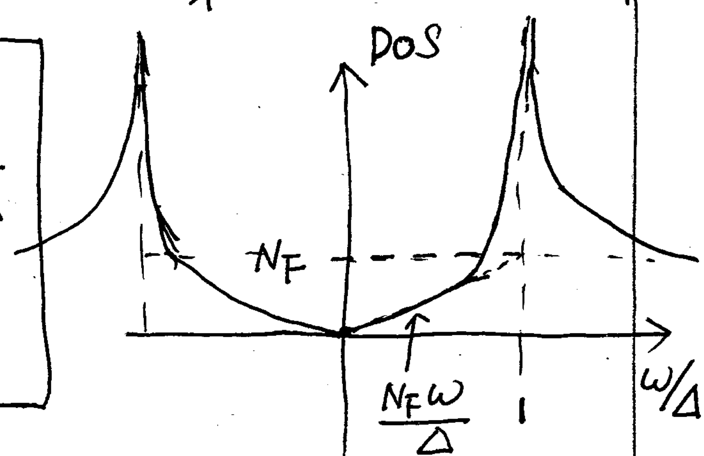
② if $\omega < \Delta$ define $\cos\phi = \dfrac{\Delta}{\omega} \cos\varphi' \Rightarrow \sin\phi \, d\phi = \dfrac{\Delta}{\omega} \sin\varphi' \, d\varphi'$

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

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

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

$$\boxed{\begin{array}{l} \text{as } \omega \to \Delta \\ \qquad \rho(\omega) \to \dfrac{N_F \omega}{\pi \Delta} \ln \dfrac{8}{1 - \omega/\Delta} \\ \text{as } \omega \to 0 \quad \rho(\omega) \to \dfrac{N_F \omega}{\Delta} \end{array}}$$



§ Specific heat

$\leftarrow$ $Vol = Na^2$

a: lattice constant

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

$$\frac{F(T)}{Vol} = -k_B T \frac{1}{Vol} \sum_k 2 \ln \left(e^{-\frac{1}{2}\beta E_k} + e^{\frac{1}{2}\beta E_k} \right) + \frac{\Delta_d^2}{V}$$

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

$$\frac{S}{Vol} = -\frac{\partial F}{Vol\, \partial T} = k_B \int \frac{d^2k}{(2\pi)^2} \, 2\ln 2\cosh \frac{\beta}{2} E_k + k_B T \int \frac{d^2k}{(2\pi)^2} \, 2 \tanh \frac{\beta}{2} E_k \frac{\partial}{\partial T} \left(\frac{\beta E_k}{2} \right)$$

$$- \frac{2\Delta_d}{V} \frac{\partial \Delta_d}{\partial T}$$

gap Eq: $\frac{\Delta_d}{V} = \int \frac{d^2k}{(2\pi)^2} \, \Delta_d \frac{(\cos k_x - \cos k_y)^2}{2E_k} \tanh \frac{\beta}{2} E_k$

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

$$\Rightarrow \frac{S}{Vol} = 2k_B \int \frac{d^2k}{(2\pi)^2} \ln\left(2\cosh \frac{\beta}{2} E_k\right) - 2k_B \int \frac{d^2k}{(2\pi)^2} \tanh \frac{\beta}{2} E_k \frac{\beta E_k}{2}$$

(other term cancels)

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

$$\frac{S}{Vol} = -2k_B \sum_k \left[(1-f_k) \ln (1-f_k) + f_k \ln f_k \right]$$

with $f_k = \frac{1}{e^{\beta E_k}+1}$. Check it's consistent with the above Eq.

$$\frac{C}{Vol} = T\frac{\partial S}{\partial T} = -\beta \frac{\partial S}{\partial \beta} = 2\beta k_B \frac{1}{Vol} \sum_k \frac{\partial f_k}{\partial \beta} \ln \frac{f_k}{1-f_k} = -2\beta^2 k_B \frac{1}{Vol} \sum_k E_k \frac{\partial f_k}{\partial \beta}$$

$$= -2\beta^2 k_B \frac{1}{Vol} \sum_k E_k \frac{df_k}{d(\beta E_k)} \left(\frac{d(\beta E_k)}{d\beta} \right) \leftarrow \frac{d\beta E_k}{d\beta} = E_k + \beta \frac{dE_k}{d\beta}$$

$$= 2\beta k_B \frac{1}{Vol} \sum_k \left(-\frac{\partial f_k}{\partial E_k} \right) \left(E_k^2 + \frac{1}{2} \beta \frac{d E_k^2}{d\beta} \right)$$

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

① Next we consider low T limit.
Now we use continuum approx: $E_k^2 = \xi^2 + \Delta_d^2 \cos^2 2\varphi_k$

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

$$\frac{E_K dE_K}{k_B^2 TdT} = \frac{\Delta_d(T)}{k_B T} \frac{d\Delta_d(T)}{k_B dT} \cos^2 2\varphi_K = \frac{\Delta^2(T)}{(k_B T)^2} \cos^2 2\varphi_K \left(\frac{k_B T}{\Delta_d(T)}\right)^3$$

because at $T << \Delta(T)$, $\frac{d\Delta(T)}{k_B dT} \simeq \frac{k_B^2 T^2}{\Delta_d^2(T)}$ (for d-wave),
we can neglect the contribution from the second term.

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

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

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

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

consider there're four nodes,

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

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

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

The low ~~temperature~~ specific heat in 2D nodal SC

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

consistent with the low energy DOS $\simeq N_F \dfrac{\omega}{\Delta_d}$

Paramagnetic susceptibility / Knight shift

consider the pairing sector $k\uparrow$ and $-k\downarrow$. The Hilbert space is 4-dimensional: $|\Omega\rangle$, $\alpha^\dagger_{k\uparrow}|\Omega\rangle$, $\beta^\dagger_{-k\downarrow}|\Omega\rangle$ $\alpha^\dagger_{k\uparrow}\beta^\dagger_{-k\downarrow}|\Omega\rangle$.

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

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

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

$$\frac{2}{Vol}\sum_k\to N_F\int d\xi\int\frac{d\varphi}{2\pi}$$

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

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

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

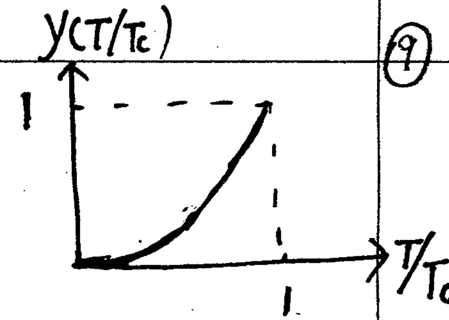
$$=Y(T)$$

isotropic case

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

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

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



Now let us consider the d-wave case:

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

← the low T contribution from $\xi > \Delta \cos 2\varphi$

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

$$\simeq \int_0^{+\infty} d\xi \, \frac{1}{2k_BT} \frac{\xi}{\Delta} \frac{1}{\cosh^2\left(\frac{\xi}{2k_BT}\right)}$$

define $x = \frac{\xi}{2k_BT}$

$$\Rightarrow \boxed{\frac{\chi}{\chi_n} \sim \frac{2k_BT}{\Delta} \int_0^{+\infty} dx \, \frac{x}{\cosh^2(x)} \simeq \text{const.} \frac{k_BT}{\Delta}}$$

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

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

Phase-sensitive measurement — d-wave symmetry

The therodynamic 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)

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

$$K_0 = H_0 - \mu_L N_L - \mu_R N_R, \quad \text{and} \quad e\mathcal{U} = \mu_L - \mu_R$$

$$\rightarrow C_{\alpha,k\sigma}(t) = e^{-iK_0 t}\, C_{\alpha,k\sigma}\, e^{iK_0 t}, \quad \alpha = R, L.$$

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

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

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

retarded Green's function

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

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

⇒ The Josephson channel

$$I_J(t) = \frac{2e}{\hbar^2} \, \mathrm{Im} \left[e^{-2ie\mathcal{U}t} \, Y_{ret}(\Omega = e\mathcal{U}) \right]$$

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

$$y_{ret}(\Omega) = e^{i(\phi_R+\phi_L)} \sum_{kq} T_{kq} \, T_{-k-q} \, \frac{\Delta_L(k)}{E_L(k)} \cdot \frac{\overset{*}{\Delta_R}(q)}{E_R(q)}$$

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

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

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

Aussuming T_{kq}'s are momentum indepedent $\Rightarrow$

$$y_{ret}(\Omega) = \frac{\hbar^2 G_N}{2\pi e^2} \, e^{i(\phi_R - \phi_L)} \int_0^{+\infty} d\xi_L \int_0^{+\infty} d\xi_R \int \frac{d\varphi_L}{2\pi} \int \frac{d\varphi_R}{2\pi}$$

$$\left\{ \frac{\Delta_L(\xi_L, \varphi_L)}{E_L} \, \frac{\overset{*}{\Delta_R}(\xi_R, \varphi_R)}{E_R} \right\} \left[\frac{1}{\hbar\Omega + E_L + E_R + i\eta} - \frac{1}{\hbar\Omega - E_L - E_R + i\eta} \right]$$

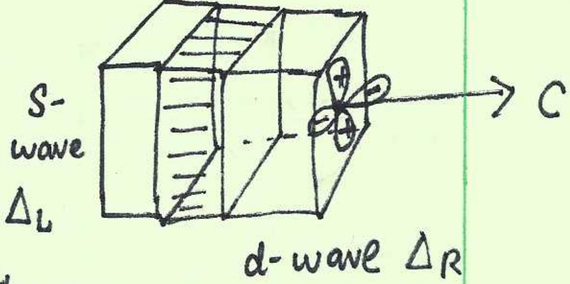
The new property of unconventional SC is the appeareace of angular dependence of

$$\boxed{\int \frac{d\varphi_L}{2\pi} \int \frac{d\varphi_R}{2\pi} \quad \Delta_L(\xi_L, \varphi_R) \, \overset{*}{\Delta_R}(\xi_R, \varphi_R)}$$

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

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



$$\int \frac{d\varphi_R}{2\pi} \Delta_R^*(\xi_R, \varphi_R) = 0 !$$

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?

$\boxed{\text{YBCO is a different story: it's s+d}}$

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

No! this term is not invariant under rotation 90° around c-axis.

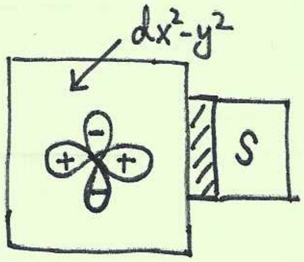
but s and d-wave part do can couple at quartic order as

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

$$\rightarrow \quad I \propto \sin[2(\phi_R - \phi_L + eUt)]$$

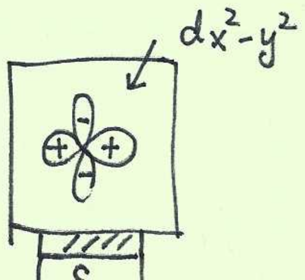
high order Josephson effect, two-pair tunneling.

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



A)

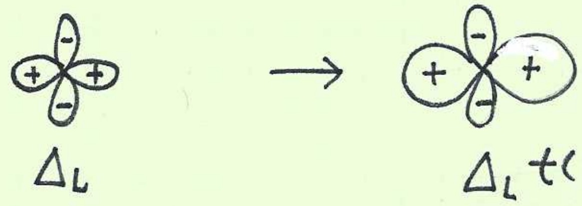
due to geometry, we cannot neglect the momentum dependence of $T_{k,q}$. For example, the tunneling matrix elements for $k \parallel$ surface and $k \perp$ surface are different.



B)

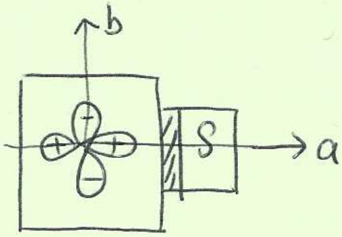
For example, in A) we expect that the tunneling for $\vec{k} \parallel \hat{x}$ is the much stronger than $\vec{k} \parallel \hat{y}$. Thus the d-wave gap function is not averaged evenly, i.e. $\int \frac{d\varphi_L}{2\pi} \Delta_L(\xi_L, \varphi_L)\, t(\varphi_L) \neq 0$.

effect from tunneling matrix element.



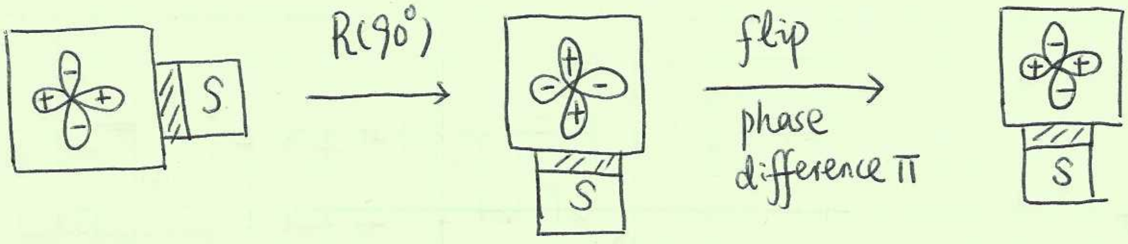
We do have coupling at quadrtic level as

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



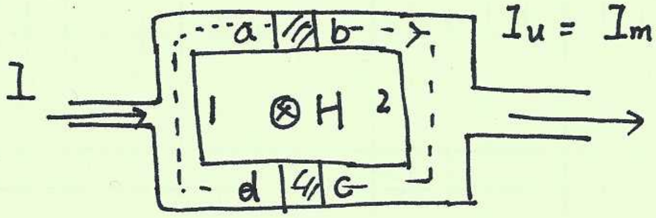
(There's no sysmetry about this set-up which can change the sign of the d-wave part!)

- 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



$I_u = I_{mu} \sin \tilde{\Delta}\phi_u$

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

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

should be gauge invariant phase difference

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

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

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

The phase difference across the up and down junction

gauge invariant phase: $\boxed{\tilde{\Delta}\phi_u = \phi_b - \phi_a - \left(\int_a^b \vec{A}\cdot d\vec{l}\right)2\pi/\Phi_0}$

that enters the formula of current.

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

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

(phase arcoss the junction).

$\Phi_0 = \frac{hc}{2e} = 2.07\times10^{-7}$ Gauss. cm^2

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

inside superconductor

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

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

$= 2n\pi$

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

exclude the insulater junction

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

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

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

If the inductance of the loop ~~is~~ is considered, the flux Φ consists two part: $\quad \Phi = \Phi_{ex} + L I_{cir} \qquad (2)$

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

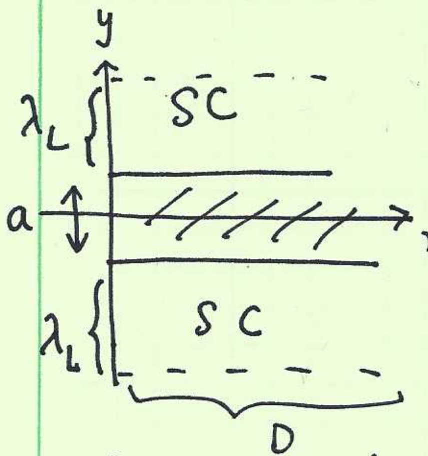
In principle (1), (2), (3) should be solved consistently. If the self-inductance can be neglected, we have

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

$$\Rightarrow I_{max} = 2I_m\left|\cos\frac{\pi\Phi_{ex}}{\Phi_0}\right|,$$

the maximum supercurrent desity oscillatite with Φ_{ex}/Φ_0.

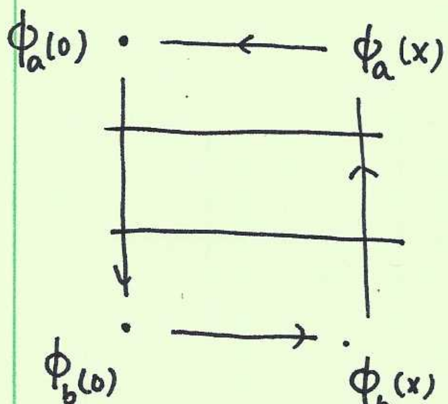
Digression ②: Fraunhofer pattern : a single planar Josephson junction.



$$A_x = 0,$$

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

the gauge-independent phase difference



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

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

$$\left\{ \oint \nabla\phi\, dl = (\phi_a(x) - \phi_b(x)) + (\phi_a(0) - \phi_a(x)) + (\phi_b(0) - \phi_a(0)) + (\phi_b(x) - \phi_b(0)) = 2n\pi \right.$$

$$\left.\begin{aligned} \tilde{\Delta}\phi_a(x) &= \phi_a(x) - \phi_b(x) - \frac{2\pi}{\Phi_0}\int_{bx}^{ax} \vec{A}\cdot d\vec{l} \\ \tilde{\Delta}\phi(0) &= \phi_a(0) - \phi_b(0) - \frac{2\pi}{\Phi_0}\int_{b0}^{a0} \vec{A}\cdot d\vec{l} \\ \Rightarrow \quad \phi_a(0) - \phi_a(x) &= -\frac{2\pi}{\Phi_0}\int_{ax}^{a0} \vec{A}\cdot d\vec{l} \quad \cdots \\ \phi_b(x) - \phi_b(0) &= -\frac{2\pi}{\Phi_0}\int_{b0}^{bx} \vec{A}\cdot d\vec{l} \end{aligned}\right\}$$

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

$$= j_m D \int_0^1 d\,{}^{x}\!/_{D} \, \sin\!\left(\tilde{\Delta}\phi(0) - \frac{2e}{\hbar c} BD(a+2\lambda_L) \, {}^{x}\!/_{D}\right)$$

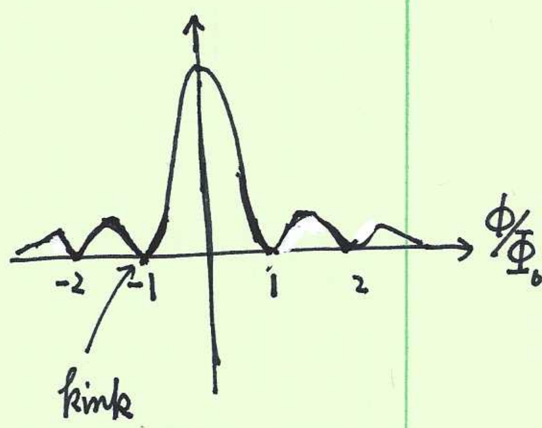
define $\phi = BD(a+2\lambda_L)$

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

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

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

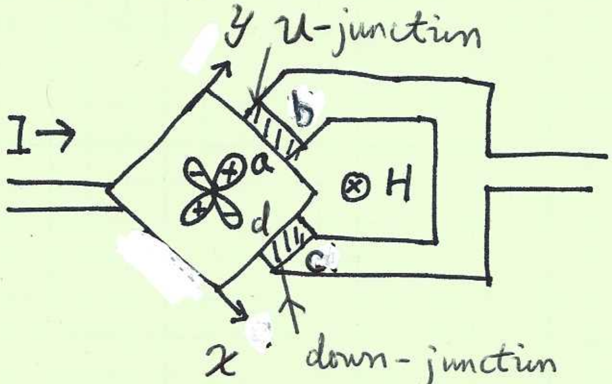
$$\Rightarrow I_{max} = j_m D \left| \frac{\sin \pi \, \Phi/\Phi_0}{\pi \, \Phi/\Phi_0} \right|$$



Now let us apply it to the d-wave case

① d-S SQUID:

The two junctions have opposit sign of coupling constants



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

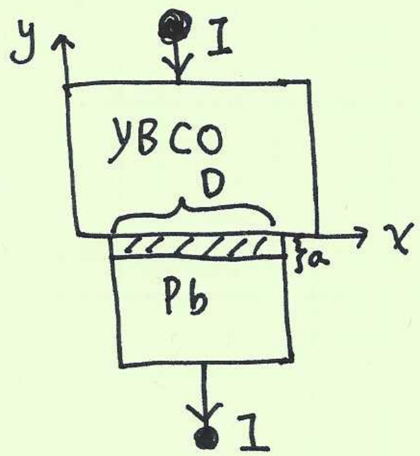
$$= 2I_m \sin\frac{\tilde{\Delta}\phi_u - \tilde{\Delta}\phi_d}{2}\cos\frac{\tilde{\Delta}\phi_u + \tilde{\Delta}\phi_d}{2} = 2I_m \sin\frac{\pi\Phi}{\Phi_0}\cos\left(\Delta\phi_u + \frac{\pi\Phi}{\Phi_0}\right)$$

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

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

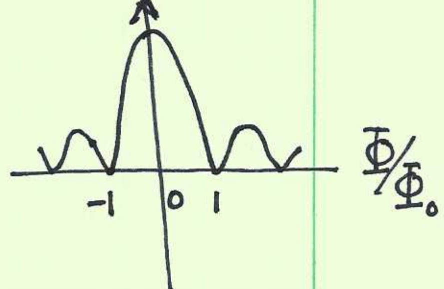
② Corner junction

if we make a planar Josephsun junction



This planar junction will exhibit the same Fraunhofer pattern as two s-wave one, i.e

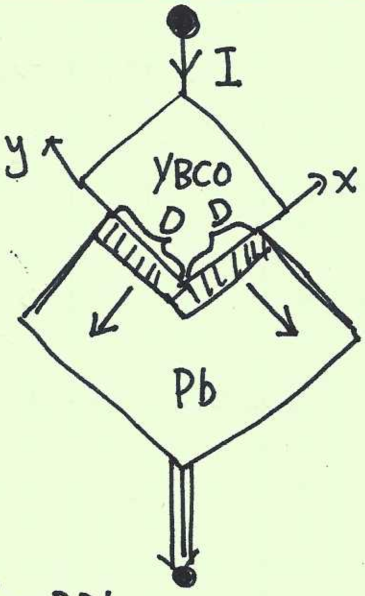
$$I_{max} \propto \left|\frac{\sin\pi\Phi/\Phi_0}{\pi\Phi/\Phi_0}\right|$$



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

a: is the width of insulating regin

L: is effective width of junction



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

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

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

$$A_y = 0, \quad A_x = By \qquad \left(\text{c.f. the odd gauge } \begin{matrix} A_x = 0 \\ A_y = -Bx \end{matrix} \right).$$

$\Rightarrow$ current along $45°$: $-\frac{1}{\sqrt{2}} j_m \int_0^1 dy' \sin\left(\tilde{\Delta}\phi(0) + \frac{2\pi\Phi}{\Phi_0} y'\right)$

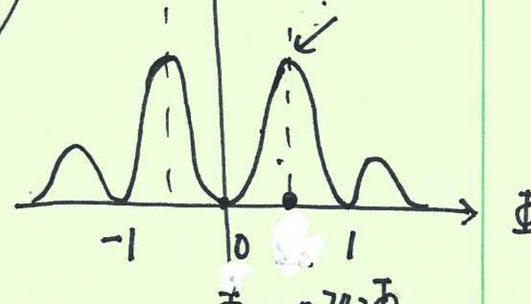
the overall "$-$" sign comes from the d-wave symmetry

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

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

$$\pi\Phi_a = \tan\left(\frac{\pi\Phi_a}{2\Phi_0}\right)$$

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



$\Phi_a = 0.742\Phi_0$

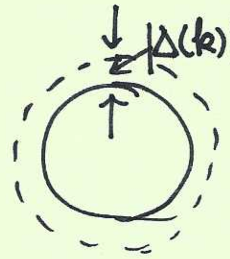
p-wave Cooper pairing and more

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 istropic - B phase $J = L + S = 0$.

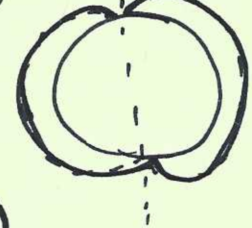
fully gapped, 3D topological pairing

$|\Delta(k)|$ const



2 anisotropic - A phase J is not well-defined,

nodal quasi-particle

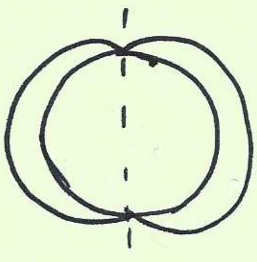


$\Delta(k) \propto \sin\theta_k$

3 J-triplet pairing (Y. Li and C. Wu)

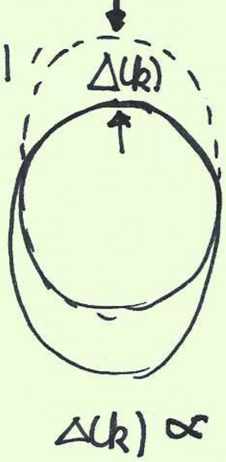
a new pairing pattern $J = L = S = 1$ due to dipolar interaction

$J_z = 0$



$\Delta(k) \propto \sin\theta_k$

$J_z = \pm 1$



$\Delta(k) \propto 1 \pm \cos\theta_k$

scientific report 2, 392 (2012).

we use the continuum model

$$H = \sum_k (\varepsilon(k)-\mu)\, a^\dagger_{k\sigma} a_{k\sigma} + \frac{1}{2\,Vol} \sum_{kk'} V(kk')\, a^\dagger_{-k'\beta}\, a^\dagger_{k'\alpha}\, a_{k\alpha}\, a_{-k\beta}$$

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

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

define order parameter

$$\Delta^a_{\sigma\sigma'} = -\sum_{k'} V_t\, k'_a \langle a_{k'\sigma}\, a_{-k'\sigma'}\rangle$$

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

μ – spin channel

a – orbital channel

Thus the p-wave order parameter 3x3 complex matrix, which has 18 real parameters.

we can also define the pairing matrix $\Delta_{\sigma\sigma'}(k) = k_a \Delta^a_{\sigma\sigma'}$.

$$\Delta_{\sigma\sigma'}(k) = \Delta_{\mu a}\, k_a\, (\sigma_\mu i\sigma_2)_{\sigma\sigma'} = \Delta(k)\, \hat{d}_\mu(k)\, (\sigma_\mu i\sigma_2)_{\sigma\sigma'}$$

the tensor $\Delta_{\mu a}$ maps the momentum $\vec{k}$ vector into a vector in spin channel — d-vector.

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

The $\hat{d}(k)$ vector is normalized as $\boxed{\hat{d}^*(k)\, \hat{d}(k) = \sum_\mu d^*_\mu(k) d_\mu(k) = 1}$

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

☆ $\Delta_{\sigma\sigma'}(k)$ is a symmetric matrix, (triplet)

in comparison, the singlet channel pairing $\Delta_{\sigma\sigma'} = \Delta_s (i\sigma_2)_{\sigma\sigma'} = \begin{pmatrix} 0 & \Delta_s \\ -\Delta_s & 0 \end{pmatrix}$

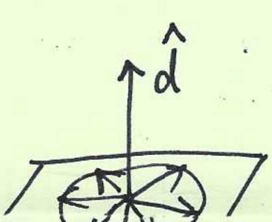
is anti-symmetric.

⊗ physical meaning of d-vecter

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

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

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 $\Delta_{\sigma\sigma'} = \Delta_z \langle a_{k\uparrow} a_{-k\downarrow} + a_{k\downarrow} a_{-k\uparrow} \rangle$ 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, $\mathrm{Re}\,\hat{d} \not\parallel \mathrm{Im}\,\hat{d}$, then the angular momentum expectation value of Cooperpair is nonzero. Let us consider pairing $a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\uparrow}$, which corresponding to $\hat{d} = \frac{-1}{\sqrt{2}}(1, i, 0)$, then $S_z = 1$.

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

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

for a triplet Cooper pair described by $\Delta_{\sigma\sigma'}(k) = \Delta(k)\,\hat{d}_a(k)\,(\sigma^a i\sigma_2)_{\sigma\sigma'}$

⊛ Bogoliubov - spectra (mean-field Hamiltonian)

$$H_{MF} = \sum_{k\sigma} (\varepsilon_k - \mu)\, a^{\dagger}_{k\sigma} a_{k\sigma} - \frac{1}{2} \sum_{k\sigma\sigma'} a^{\dagger}_{k\sigma} a^{\dagger}_{-k\sigma'}\, k_a \Delta^{a}_{\sigma\sigma'}$$

$$- \frac{1}{2} \sum_{k,\sigma\sigma'} a_{-k\sigma'} (\Delta^{\dagger,a} k_a)_{\sigma'\sigma}\, a_{k\sigma}$$

$$+ \frac{\mathrm{Vol}}{2V_t} \sum_{\sigma\sigma',a} |\Delta^{a}_{\sigma\sigma'}|^2$$

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

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

$\sum'$ means only sum over half of the momentum space

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

$$+ \frac{Vol}{2V_t} \sum_{\sigma\sigma', a} | \Delta^{a}_{\sigma'\sigma} |^2$$

$$H_{\alpha\beta}(k) = \begin{bmatrix} \varepsilon(k) - \mu & \Delta(k)_{\sigma\sigma'} \\ \Delta^{+}(k) & -(\varepsilon(k) - \mu) \end{bmatrix},$$

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 Γ-matrix

$$\boxed{\begin{gathered} H_{\alpha\beta}(k) = (\varepsilon(k) - \mu)\,\Gamma^1 + \Delta(k)\left[d_x(k)\,\Gamma^3 + d_y(k)\,\Gamma^4 + d_z(k)\,\Gamma^5\right] \\ \Gamma^1 = I \otimes \tau_3,\quad \Gamma^2 = \sigma_2 \otimes \tau_1,\quad \Gamma^3 = \sigma_3 \otimes \tau_1,\quad \Gamma^4 = I \otimes \tau_2,\quad \Gamma^5 = -\sigma_1 \otimes \tau_1 \end{gathered}}$$

τ – refers to the particle-hole channel

σ – refers to spin

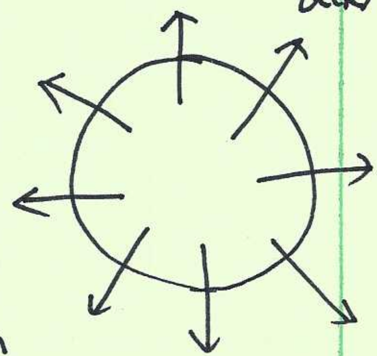
$$H^2(k) = (\varepsilon(k) - \mu)^2 + \Delta^2(k) \Rightarrow E(k) = \pm\sqrt{(\varepsilon(k) - \mu)^2 + \Delta^2(k)}$$

1 For the B-phase, the d-vector: $\Delta_{\sigma'\sigma}(k) = \Delta(k)\, \hat{d}_\mu(k)\, (\sigma_\mu i\sigma_2)_{\sigma'\sigma}$

and $\Delta(k)\, \hat{d}_\mu(k) = \Delta_{\mu a} k_a$. Thus $\Delta_{\mu a}$ maps the momentum space vector $\vec{k}$ to a vector in spin space. If $\Delta_{\mu a}$ is proportional to a $O(3)$ matrix, i.e., $\Delta_{\mu a} \propto d_{\mu a} \leftarrow O(3)$ matrix, then it realizes a connection between two triads. In the simplest case $d_{\mu a} \propto \delta_{\mu a}$

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

$\hat{d}(k) \parallel \hat{k}$



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

$$J = L + S = 0.$$

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 $\quad SO_L(3) \otimes SO_S(3) \,/\, SO_J(3)$

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

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

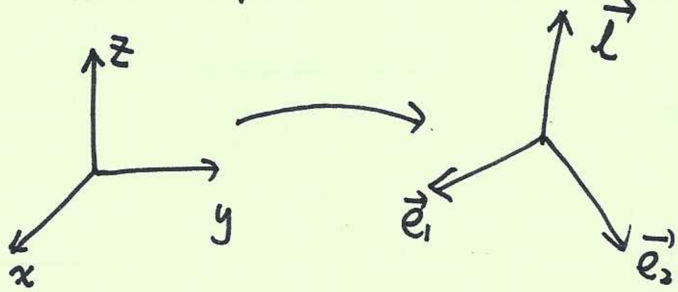
The spectra is fully gapped: $E(k) = \pm\sqrt{(\varepsilon(k) - \mu)^2 + |\Delta|^2}.$

② The A-phase : $\Delta_{\sigma\sigma'}(k) = \Delta(k)\,\hat{d}_\mu(k)\,(\sigma_\mu i\sigma_2)_{\sigma'\sigma}$

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

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

$(p_x + ip_y \xrightarrow{\text{rotate}}$



$\vec{l} = \hat{e}_1 \times \hat{e}_2$

direction of orbital angular momentum.

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

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

$$\rightarrow \quad \Delta_\mu'(k) = \Delta_\mu(k)\,e^{i\alpha}$$

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

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

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

Dirac fermion at $\theta = 0$, and π.

Green's function (Matsubara)

$$\begin{bmatrix} -T_\tau \langle a_\sigma(k\tau)\, a^\dagger_{\sigma'}(k,0)\rangle, & -T_\tau \langle a_\sigma(k\tau)\, a_{\sigma'}(-k,0)\rangle \\ -T_\tau \langle a^\dagger_\sigma(-k,\tau)\, a^\dagger_{\sigma'}(k,0)\rangle, & -T_\tau \langle a^\dagger_\sigma(k\tau)\, a_{\sigma'}(-k,0)\rangle \end{bmatrix}$$

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

$$G(k, i\omega_n) = \begin{bmatrix} \mathcal{G}_{\sigma\sigma'}(k, i\omega_n) & \mathcal{F}_{\sigma\sigma'}(k, i\omega_n) \\ \mathcal{F}^\dagger_{\sigma\sigma'}(k, i\omega_n) & -\mathcal{G}_{\sigma\sigma'}(-k, -i\omega_n) \end{bmatrix}$$

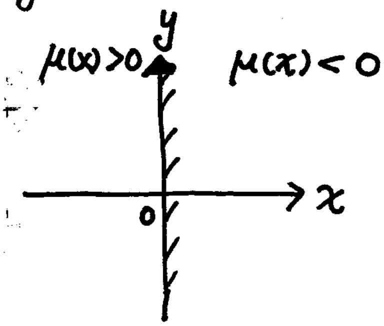
$$= \frac{i\omega_n + (\varepsilon(k)-\mu)\,\Gamma^1 + \Delta(k)\left(d_x\Gamma^3 + d_y\Gamma^4 + d_z\Gamma^5\right)}{(i\omega_n)^2 - E^2(k)}$$

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

① Simplified model

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

$$\begin{cases} ① -\mu(x)\, u_n + \frac{\Delta}{k_f}(-i\partial_x v_n + ik_y v_n) = E_n(k_y)\, u_n \\ ② \frac{\Delta}{k_f}(-i\partial_x u_n - ik_y u_n) + \mu(x)\, v_n = E_n(k_y)\, v_n \end{cases}$$



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

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

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

but actually only one is possible.

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

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

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

$\Rightarrow$ these two Eqs are consistent

$$\frac{1}{k_f}\partial_x u_0 = \frac{\mu(x)}{\Delta} u_0 \Rightarrow \boxed{u_0(x) \sim e^{-\int_0^{|x|} dx' \frac{k_f}{\Delta}|\mu(x')|}} \quad ②$$

For the current set up, that $\mu(x)<0$ at $x>0$, we do have exponetial 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 $\underbrace{H_0 = f_y(k_y) + f_x(-i\hbar\nabla_x) - \mu(x)}_{\text{I want to be general!}}$

we have

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

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

still try the solution
$$\begin{cases} \frac{\Delta}{k_f} i k_y v_0 = E_0(k_y) u_0 \\ \frac{\Delta}{k_f}(-i) k_y u_0 = E_0(k_y) v_0 \end{cases}$$
(let's choose $u_0 = -i v_0$)

and the x-direction

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

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

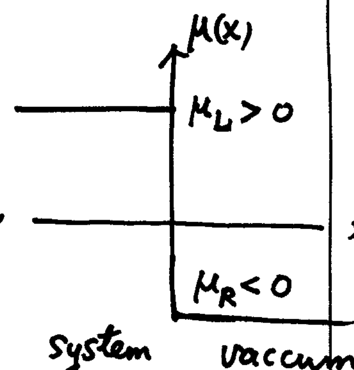
consistent! $\Rightarrow$ the edge spectra is not affected, which $E_0(k_y)$ is still determined by the off-diagonal term $E_0(k_y) = -\frac{\Delta k_y}{k_f}$.

but the zero mode Eq along the x-direction $\longrightarrow$

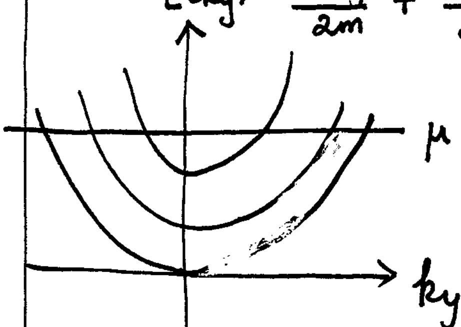
$$\left[f_x(-i\hbar\partial_x) + \frac{\Delta}{k_f}\partial_x \right] u_0 = \left[\mu(x) - f_y(k_y) \right] u_0$$

$$\text{or} \quad \boxed{\left[\frac{-\hbar^2\partial_x^2}{2m} + \frac{\Delta}{k_f}\partial_x \right] u_0 = \left[\mu(x) - \frac{\hbar^2 k_y^2}{2m} \right] u_0}$$

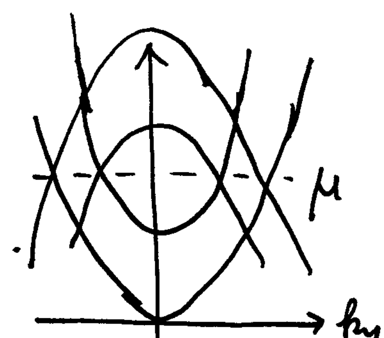
This Eq is more realistic compared with the oversimplified one $\frac{\Delta}{k_f}\partial_x u_0 = \mu(x) u_0$. In that case, all the states (plane wave) (k_x, k_y) in the bulk are occupied, i.e. $k_f \to +\infty$. Now, if for the value of k_y, such that $\frac{\hbar^2 k_y^2}{2m} > \mu_L$ (see figure), we have no edge states, (because $\mu(x) - \frac{\hbar^2 k_y^2}{2m}$ always negative).



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

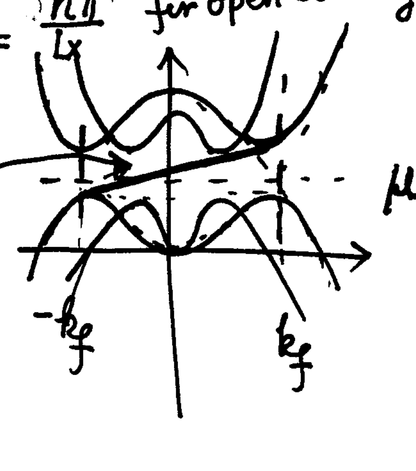


$\Delta = 0$ $\longrightarrow$



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

$\rightarrow \Delta \neq 0$



estimation of edge state velocity

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

Surface states of the BW state

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

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

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

seek surface state spectra:

$$\begin{cases} \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu(x)\right]\phi_1 + \Delta(\hbar k_x\sigma_1 + \hbar k_y\sigma_2 - i\hbar\partial_z\sigma_3)\underbrace{}_{i\sigma_2}\phi_2 = E_0(k_x k_y)\,\phi_1 \\ \Delta(-i\sigma_2)(\hbar k_x\sigma_1 + \hbar k_y\sigma_2 - i\hbar\partial_z\sigma_3)\,\phi_1 + \left(-\frac{\hbar^2 k_{\parallel}^2}{2m} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \mu(x)\right)\phi_2 = E_0(k_x k_y)\,\phi_2 \end{cases}$$

we want
$$\begin{cases} \Delta\hbar(k_x\sigma_1 + k_y\sigma_2)\, i\sigma_2\,\phi_2 = E_0(k_x, k_y)\,\phi_1 & (1) \\ \Delta(-i\sigma_2)\hbar(k_x\sigma_1 + k_y\sigma_2)\,\phi_1 = E_0(k_x, k_y)\,\phi_2 & (2) \end{cases}$$

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

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

$2 \Rightarrow \Delta\hbar\,\underline{(-i\sigma_2)(k_x\sigma_1 + k_y\sigma_2)\, T}\,\phi_2 = E_0(k_x k_y)\,\phi_2$

~~we need~~

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

also need to be Hermitian

$$\Rightarrow T^{-1} i\sigma_2 \underbrace{(-k_x\sigma_1 + k_y\sigma_2)} = (-i\sigma_2)\, T \quad \underbrace{T^{-1}(k_x\sigma_1 + k_y\sigma_2)\, T}$$

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

$$\Rightarrow T^{-1} i\sigma_2 = (-i\sigma_2)\, T \Rightarrow T = i\sigma_2$$

if $T = i\sigma_2$, i.e. $\phi_1 = i\sigma_2\phi_2$

$$\left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} - \mu(x)\right] i\sigma_2\phi_2 - \Delta(i\hbar\partial_z\sigma_3)\, i\sigma_2\phi_2 = 0 \quad (1)$$

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

$$(1) \Rightarrow \left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} - \mu(x)\right]\phi_2 + \underbrace{i\sigma_2(\sigma_3)\, i\sigma_2}_{\sigma_1}\, i\hbar\Delta\partial_z\phi_2 = 0$$

This means that ϕ_2 has to satisfy another matrix Eq. This is not consis~~tant~~ with

$$(-i\sigma_2)(k_x\sigma_1 + k_y\sigma_2)(i\sigma_2)\,\phi_2 = E(k_x k_y)\,\phi_2$$

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

In other words, we seek a purely scalar equation for the z-direction. ⑥

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

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

$$\left[+\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} - \mu(x)\right] \phi_1 - \overbrace{\Delta(i\hbar\partial_z\sigma_3)(i\sigma_2)(\mp i\sigma_1)\phi_1}^{\mp\Delta\hbar\partial_z\phi_1} = 0 \quad (1)$$

$$\Delta(-i\sigma_2)(-i\hbar\partial_z\sigma_3)\phi_1 + \left[-\frac{\hbar^2 k_{11}^2}{2m} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \mu(x)\right](\mp i\sigma_1)\phi_1 = 0 \quad (2)$$

$$(2) \Rightarrow \left[\frac{\hbar^2 k_{11}^2}{2m} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} - \mu(x)\right]\phi_1 + \underbrace{\Delta(\mp i\sigma_1)(-i\sigma_2)(-i\hbar\partial_z\sigma_3)\phi_1}_{\mp\Delta\hbar\partial_z\phi_1} = 0$$

⇒ consistent

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

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

which is the same as before

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

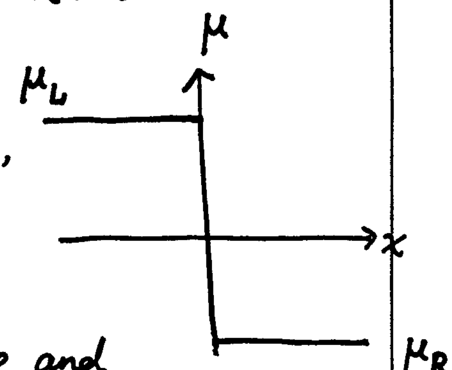
$$\hbar\Delta(k_x\sigma_1 + k_y\sigma_2)\, i\sigma_2(\mp i\sigma_1)\phi_1 = E_0(k_x, k_y)\phi_1$$

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

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

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

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



actually, if both μ_L and $\mu_R>0$, but $\mu_L \gg \mu_R$, there may still exist $\mu_L>\frac{\hbar^2k_y^2}{2m}>\mu_R$, 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 continous at the boundary. Imagine that we set $\mu_R\to-\infty$, which corresponses to open boundary, i.e. $u_0(x)=0$ for $x>0$.

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

but $u_0(x)$ should be continous, $\quad = \int_{0^-}^{0^+}dx\, u'' \to \epsilon\, \underbrace{u''}_{\text{may be}}$ finite

i.e. we seek solution

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

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

β can actually be complex.

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

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

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

or for $\boxed{|k_y/k_f| < \sqrt{1-\left(\frac{\Delta}{2E_f}\right)^2}}$, 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 $\boxed{u_0(x) \sim e^{\frac{k_f}{2}\frac{\Delta}{E_f}x} \cdot \sin\left(\sqrt{\left(1-\left(\frac{k_y}{k_f}\right)^2\right)-\left(\frac{\Delta}{2E_f}\right)^2}\, k_f x\right)}$

in the case of $\frac{k_f}{2}\frac{\Delta}{E_F} \gg \sqrt{\left[1-(k_y/k_f)^2\right]-\left(\frac{\Delta}{2E_f}\right)^2}$, then the oscillation is cut off by the exponential decay. we can approximate $\sin \# x \sim \# x$

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

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

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

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

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

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

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

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

b') as $\left|k_y/k_f\right| \to 1$, $\beta_2 << \beta_1$, thus the decay becomes slow

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

$$= \begin{cases} \propto x\, e^{\beta_2 x} \\ \propto e^{\beta_2 x} \end{cases} \leftarrow \text{decay length } 1/\beta_2 \to \infty$$

and merge to bulk states.

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

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

(c) 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 $1 > |k_y/k_f| > 0$, we always have

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

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