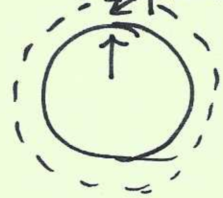
P-wave Cooper pairing and moore

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

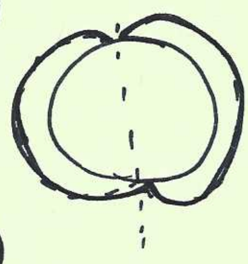
   fully gapped, 3D topological pairing

$|\Delta(k)|$ const



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

   nodal quasi-particle

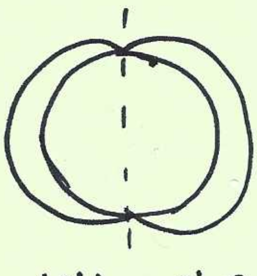


$\Delta(k) \propto \sin\theta_k$

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

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

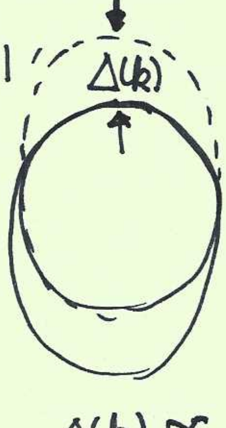
$J_z = 0$



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

$J_z = \pm 1$

$\Delta(k)$



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

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)

$\boxed{\text{define order parameter}}$

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

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

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 $\underbrace{\vec{k}}_{\text{vector}}$ 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

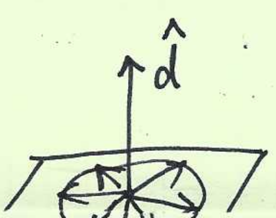
In many situation, $\vec{d}(k)$ up to an overall phase can be choosen as real, and we attribute the phase to $\Delta(k)$. Nevertheless, the direction of $\hat{d}(k)$ is not well-defined: if we set $\begin{cases} \hat{d}(k) \to -\hat{d}(k) \\ \Delta(k) \to e^{i\pi}\Delta(k) \end{cases}$ then $\vec{\Delta}(k)$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

Thus d-vecter is actually a directer, not a really vecter.

The physical meaning of d-vecter: 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 $\frac{1}{2}\sum_{k\sigma\sigma'} a^{+}_{k\sigma}\,\Delta_{\sigma\sigma'}(k)\,a^{+}_{-k\sigma} = {\sum_{k\sigma\sigma'}}' a^{+}_{k\sigma}\left(\Delta^{a}_{\sigma\sigma'}\cdot k_a\right) a^{+}_{-k\sigma'}$

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

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

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

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

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

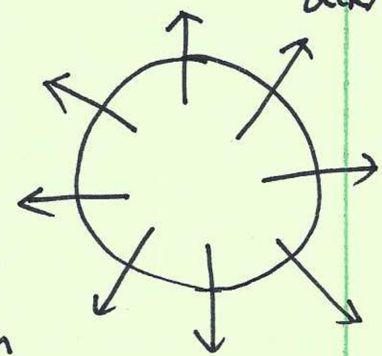
$$H^2(k) = (\varepsilon(k)-\mu)^2 + \Delta^2(k) \Rightarrow E(k) = \pm\sqrt{(\varepsilon(k)-\mu)^2 + \Delta^2(k)}$$

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

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

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



^3He-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 $\sum_{\mu a} d_{\mu a} \cdot d_{\mu a} = 1$.

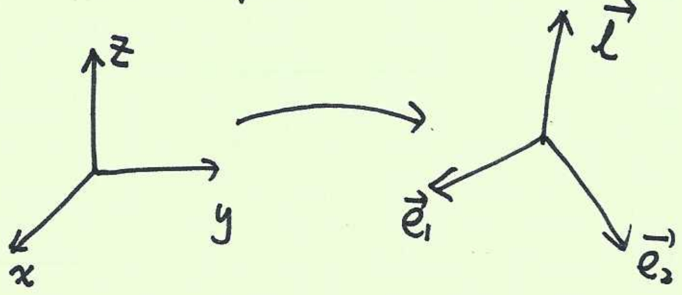
The spectra is fully gapped: $E(k) = \pm \sqrt{(\varepsilon(k) - \mu)^2 + |\Delta|^2}$.

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

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

$\hat{d}$-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 $\hat{e}_1 = \hat{x}$, $\hat{e}_2 = \hat{y}$, $\hat{l} = \hat{z}$, $\hat{d}_\mu = \hat{z}$ $\Rightarrow$

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

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

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

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

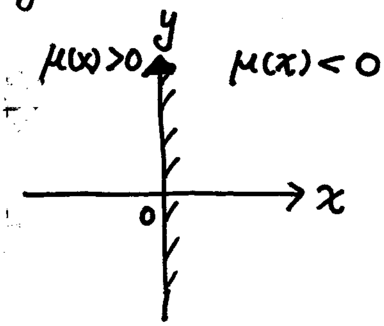
$$= \frac{i\omega_n + (\varepsilon(k) - \mu)\Gamma^1 + \Delta(k)(d_x\Gamma^3 + d_y\Gamma^4 + d_z\Gamma^5)}{(i\omega_n)^2 - E^2(k)}$$

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

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

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

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

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

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

and the x-direction

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

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

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

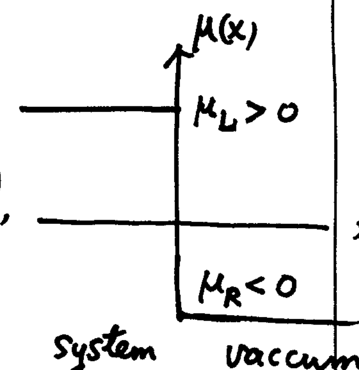
but the zero mode Eq along the x-direction $\longrightarrow$

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

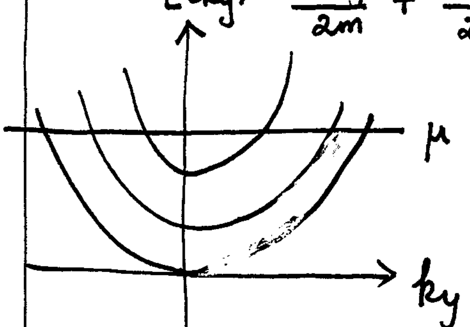
or

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

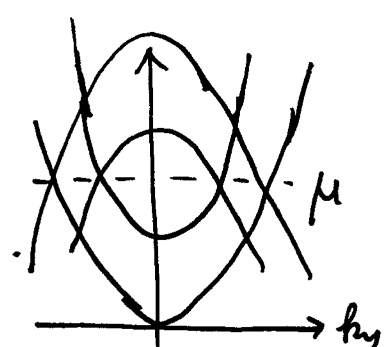
This Eq is more realistic compared with the oversimplified one $\frac{\Delta}{k_f}\partial_x u_0 = \mu(x) u_0$. In that case, all the states (plane wave) (k_x, k_y) in the bulk are occupied, i.e. $k_f \to +\infty$. Now, if for the value of k_y, such that $\frac{\hbar^2 k_y^2}{2m} > \mu_L$ (see figure),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



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

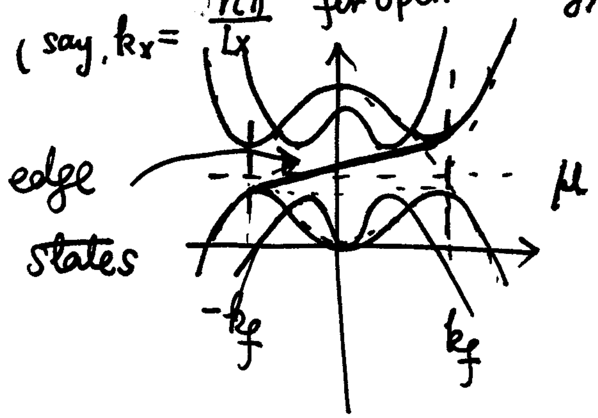


$\xrightarrow{\Delta = 0}$



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

$\rightarrow \Delta \neq 0$



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:

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

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

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

~~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. $\phi_1 = i\sigma_2\phi_2$

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

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

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

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

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

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

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

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

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

$\Rightarrow$ consistent

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

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

which is the same as before

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

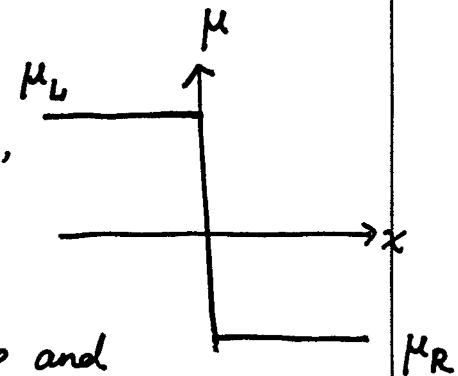
$$\hbar\Delta(k_x\sigma_1 + k_y\sigma_2)\, i\sigma_2(\mp i\sigma_1)\phi_1 = E_0(k_x, k_y)\phi_1$$

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

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 $\mu_L \gg \mu_R$, 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 $\mu_R \to -\infty$, which corresponses 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, $= \int_{0^-}^{0^+} dx\, u'' \to \epsilon\, \underbrace{u''}_{\text{may be}}$ 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 $\frac{\Delta}{E_f} \ll 1$.

(a) 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.

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

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

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

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

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

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

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

$\nwarrow$ 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 $1/\beta_2 k_f$.