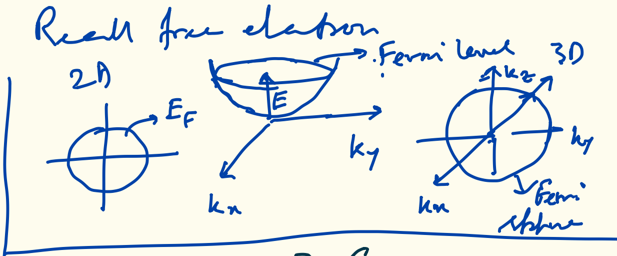
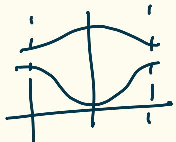


Energy band in higher dimension :

Recall, 1D :



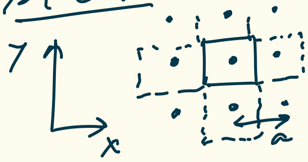
1st BZ

TB in 2D

Recall, $\sum_{R''} e^{i\vec{k}\cdot(R''-R')} \sum_j C_j H_{iR,jR''} = E_{\vec{k}} C_i$ set $R'=0$

$\vec{k} = k_x\hat{x} + k_y\hat{y}$

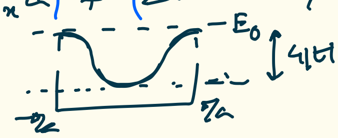
sq. lattice



let $i=j=1$ one orbital per unit cell.

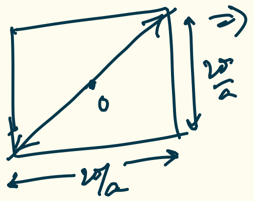
$$E_0 C_1 + \left(e^{ik_x(-a)} C_1 t + e^{k_x a} C_1 t\right) + \left(e^{ik_y a} C_1 t + e^{ik_y(-a)} C_1 t\right) = E_{\vec{k}} C_1$$

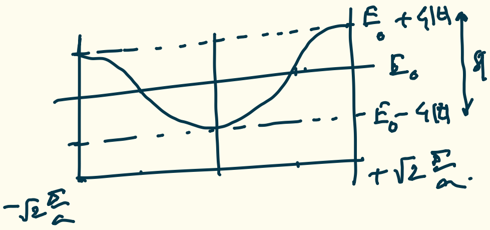
$$\Rightarrow E_{\vec{k}} = E_0 + \left(2t \cos k_x a\right) + \left(2t \cos k_y a\right)$$ plot !

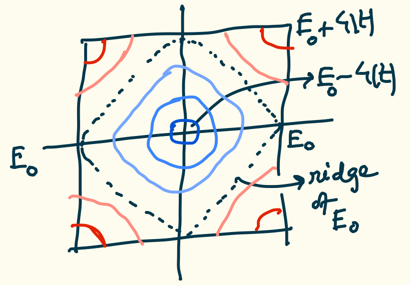


Along (1,0): $E_{\vec{k}} = E_0 + 2t \cos k_x a + 2t$ $t<0$
(also (0,1))

Along (1,1) : $E_{\vec{k}} = E_0 + 2t\cos k_x a + 2t \cos k_y a = E_0 + 4t \cos k_x a$ ∵ $k_x = k_y$ along (11)







Note that (11) will be same as (1,−1), (−1,1), (−1,−1).

From these two band structures along (1,0), (0,1) and (±1, ±1), given the symmetry of cos function it is obvious that E_0 will be Fermi energy in this case.

(Fermi volume)
V_F: Volume enclosed by Fermi surface : $n_{cell} \times N_{BVK} \times \Delta\Omega$

$\Delta\Omega$ is k space volume per allowed crystal momentum. $= \frac{1}{N_{BVK}} \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$

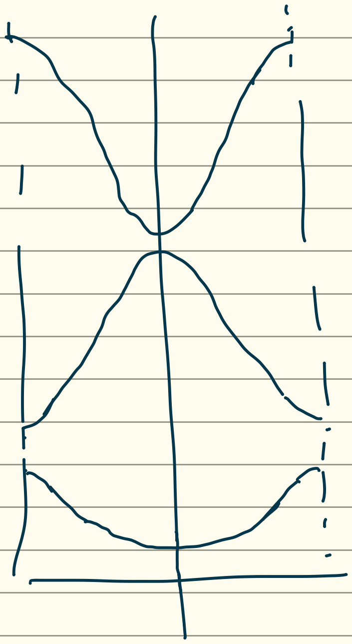
N_{BVK} : the number of unit cell in the BVK cell.

n_{cell} : the " " Bloch state (ψ_k) needed to accommodate electron in a unit cell. As obvious, Fermi surface is a concept applicable in the extended zone scheme when we consider one band per $\vec{k}$ point in k space.

$$\therefore V_F = n_{cell} \cdot \vec{b}_1 \cdot |\vec{b}_2 \times \vec{b}_3|$$

in 2D : $S_F = n_{cell} \, |\vec{b}_1 \times \vec{b}_2|$

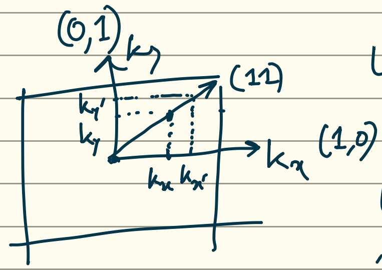
Band structure in folded zone scheme:



In the extended zone scheme

Where is the fermi energy?

1st BZ



Let E_F at k_x along (1,0)

$\therefore\ E_F = E_0 + 2t\cos k_x a + 2t$

Let E_F at (k'_x, k'_y) along (11)

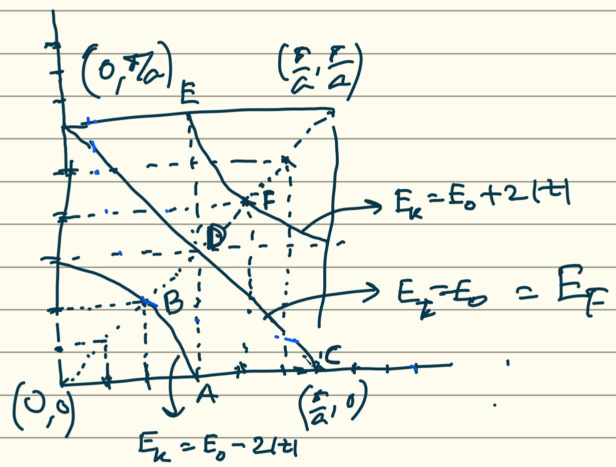
$\therefore\ E_F = E_0 + 2t\cos k'_x a + 2t\cos k'_y a = E_0 + 4t\cos k'_x a$ $[\because k'_x = k'_y$ along (11)$]$

$\therefore\ E_F = E_0 + 2t + 2t\cos k_x a = E_0 + 4t\cos k'_x a$

$\Rightarrow\ 1 + \cos k_x a = 2\cos k'_x a$

	k_x	$\cos k'_x a$	$k'_x a$	k'_x	
(A)	$\frac{1}{2}\frac{\pi}{a}$	$\frac{1+0}{2}$	$\frac{\pi}{3}$	$\frac{1}{3}\frac{\pi}{a}$	(B)
(C)	$\frac{\pi}{a}$	0	$\frac{\pi}{2}$	$\frac{1}{2}\frac{\pi}{a}$	(D)
(E)	$k_x = \frac{\pi}{2a}, k_y = \frac{\pi}{a}$	$-\frac{1}{2}$	$\frac{2\pi}{3}$	$\frac{2}{3}\frac{\pi}{a}$	(F)

(use full expression involving k_x and k_y)



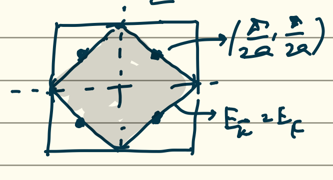
$\therefore$ With only nearest neighbor:

$\therefore$ For single electron per site.

Total N electron

(N cell in BVK cell)

1BZ



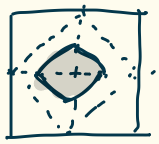
$E_F(N) = E_0$

encloses $\frac{1}{2}$ the area of 1BZ

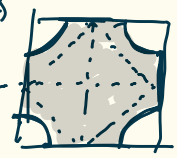
Note that band is fully filled along (1,0), (0,1) → insulator in these directions!

" " $\frac{1}{2}$ " " $(\pm1, \pm1)$ → Metallic in this direction

"Hole" doping ⇒ N ↓ ⇒ Area enclosed by Fermi surface < $\frac{1}{2}$ of 1BZ ⇒



electron " ⇒ N ↑ ⇒ " " " " " > $\frac{1}{2}$ of 1BZ ⇒



occupying the lower band fully in ←

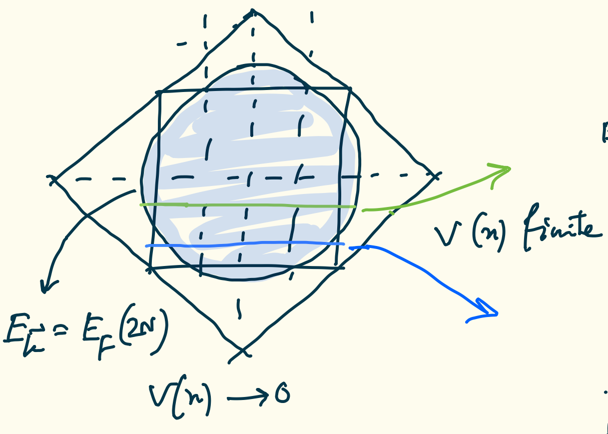
for 2 electron per site: Total 2N electrons with N unit cells in BVK cell.

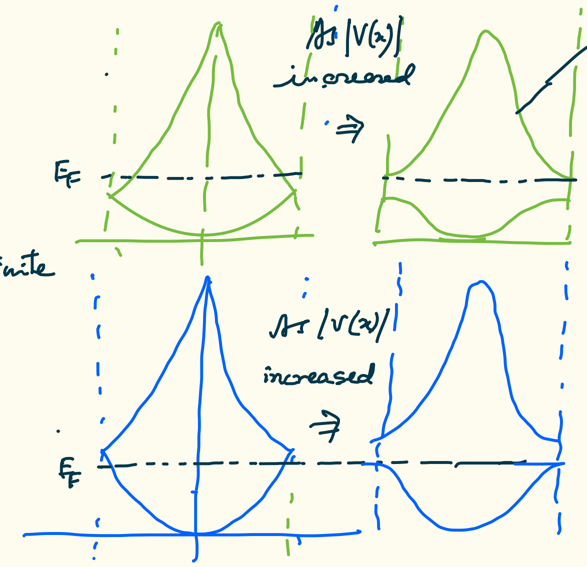
⇒ Need all N ψ_k states each occupied by 2 electrons ↑↓

⇒ Fermi vol: $|\vec{b}_1 \times \vec{b}_2|$

Recall free electron

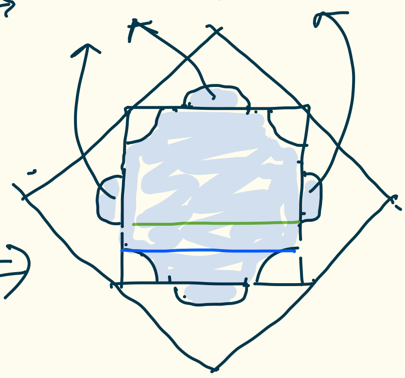
E_F with 2 electron per site: (Total 2N).





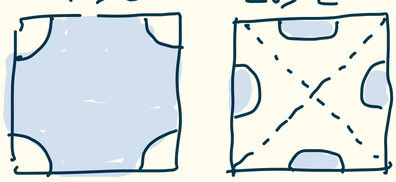
occupying the upper band

⇒



↓

In the folded zone scheme

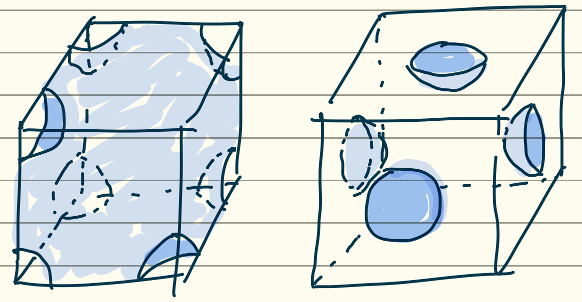


⇒

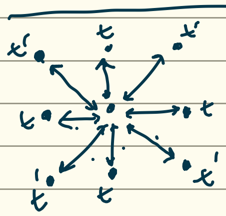
In 3D

1BZ

2BZ folded inside 1BZ



Now let us add next nearest neighbour hopping



$$\therefore E_k = E_0 + 2t\cos k_x a + 2t\cos k_y a + t'\left[e^{i(k_x a + k_y a)} + e^{i(-k_x a + k_y a)} + e^{i(k_x a - k_y a)} + e^{i(-k_x a - k_y a)}\right]$$

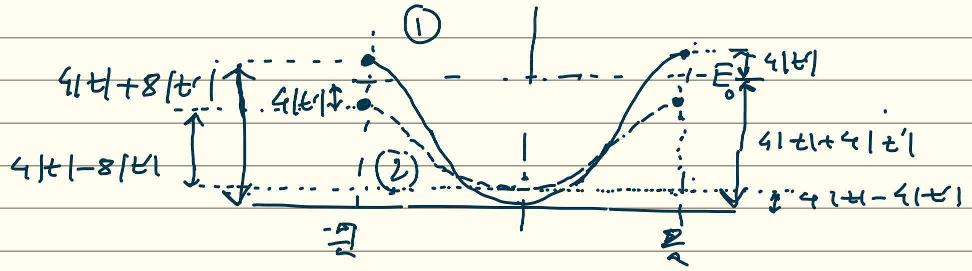
$$= E_0 + 2t\cos k_x a + 2t\cos k_y a + 4t'\cos k_x a \cos k_y a$$

Consider two realistic scenarios:

1. $t<0,\ t'<0,\ |t|>|t'|$
2. $t<0,\ t'>0,\ |t|>|t'|$

$\therefore$ Along $(1,0)$: $E_k = E_0 + 2t + 2t\cos k_x a + 4t'\cos k_x a$

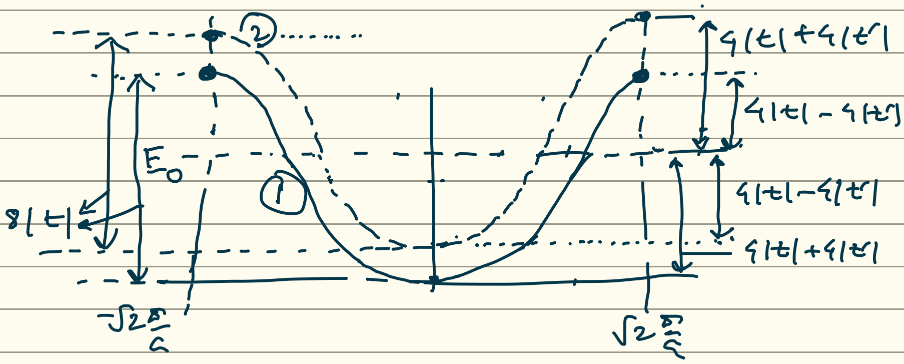
	Scenario 1	Scenario 2
$k_y=0,\ k_x=0$: $E = E_0 + 4t + 4t' \Rightarrow$	$E = E_0 - 4\lvert t\rvert - 4\lvert t'\rvert$	$E = E_0 - 4\lvert t\rvert + 4\lvert t'\rvert$
$k_y=0,\ k_x=\frac{\pi}{a}$: $E = E_0 - 4t' \Rightarrow$	$E = E_0 + 4\lvert t'\rvert$	$E = E_0 - 4\lvert t'\rvert$



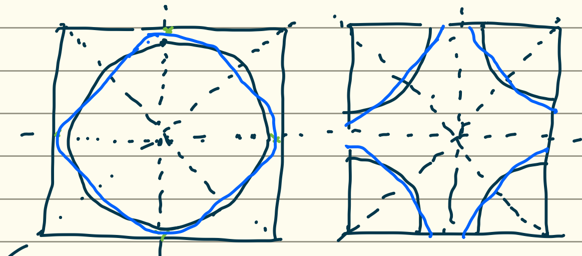
Along $(1,1)$: $E_k = E_0 + 4t\cos k_x a + 4t'\cos^2 k_x a$

$\because k_x = k_y$ along $(1,1)$

	1	2
$k_y=0,\ k_x=0$: $E = E_0 + 4t + 4t' \Rightarrow$	$E = E_0 - 4\lvert t\rvert - 4\lvert t'\rvert$	$E = E_0 - 4\lvert t\rvert + 4\lvert t'\rvert$
$k_y=\frac{\pi}{a},\ k_x=\frac{\pi}{a}$: $E = E_0 - 4t + 4t' \Rightarrow$	$E = E_0 + 4\lvert t\rvert - 4\lvert t'\rvert$	$E = E_0 + 4\lvert t\rvert + 4\lvert t'\rvert$



Scenario 1 Scenario 2



plot of $E_k = E_0$

$|t'| < |t'|$
(blue) (black)

Numerical assignment: Plot E_F with "hole" and electron doping.

E_F :

with

One electron per site: