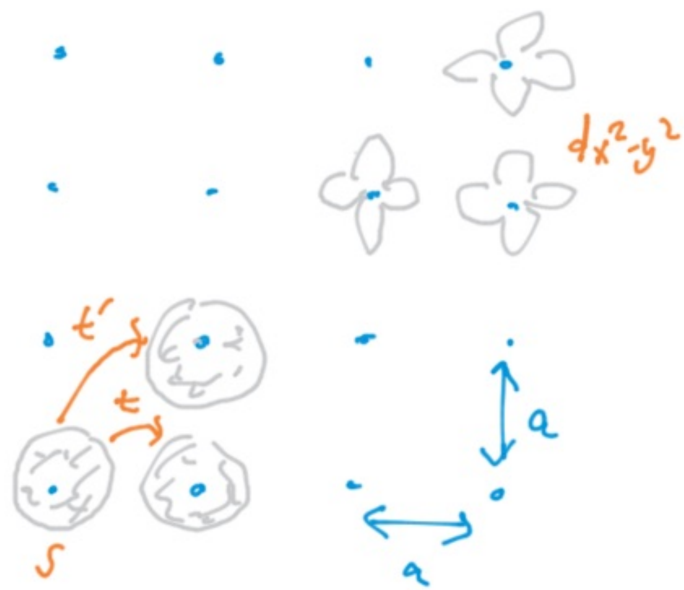
TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

2D Square lattice

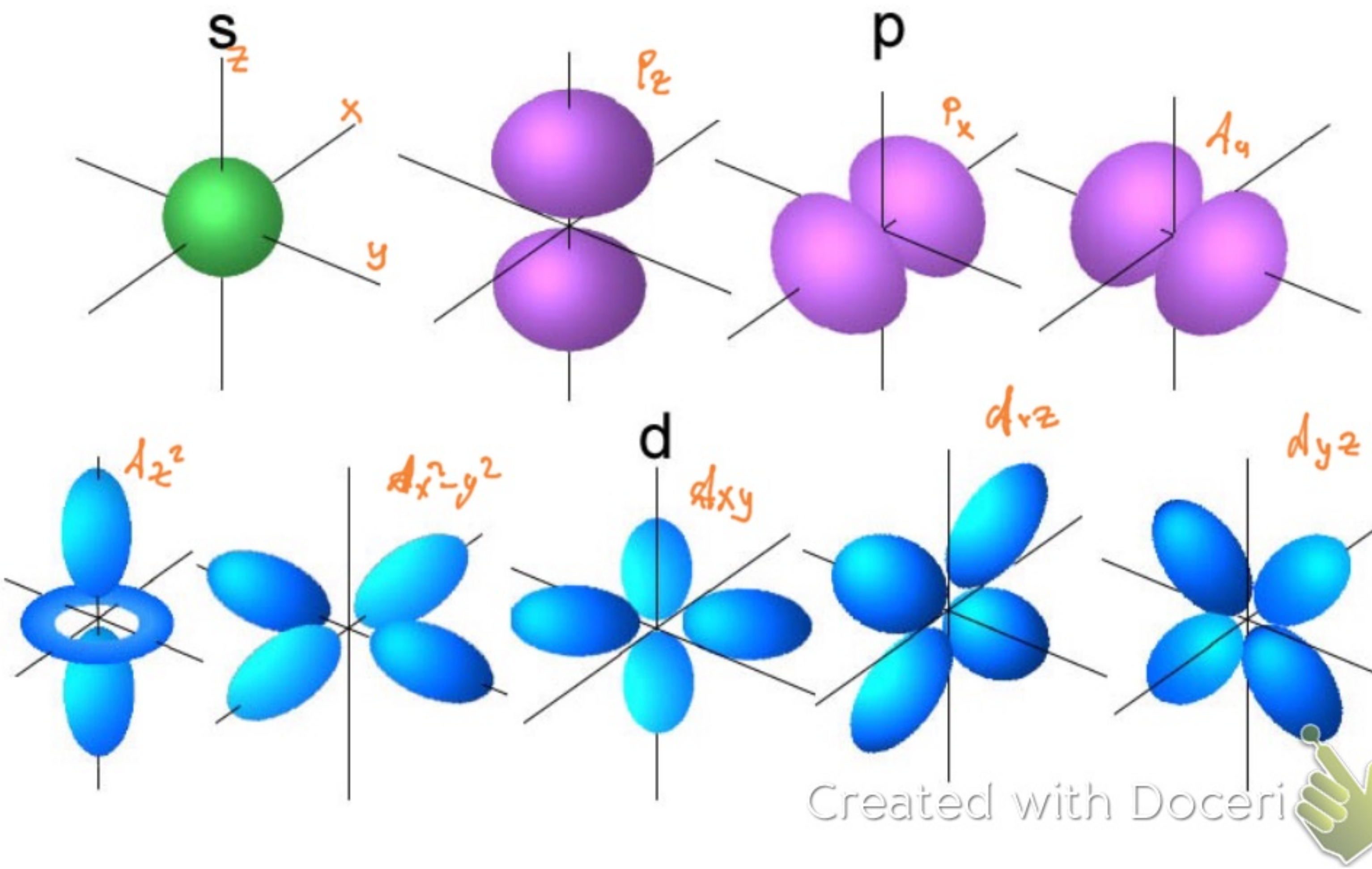
1 electron per atom/site



t = NN hopping prop.

t' = NNN — " —

ELECTRONIC Orbitals



TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

WAVEFUNCTION FOR ELECTRONS AROUND ATOM j

$$\varphi(r - r_j)$$

TB-ASSUMPTION FOR GLOBAL WAVEFUNCT.

$$\psi_k(r) = \sum_j c_{kj}\, \varphi(r - r_j)$$

BLOCH'S THEOREM

BLOCH'S THEOREM

GLOBAL WAVEFUNCTION

$$\psi_k(r) = u_k(r) \cdot e^{ik \cdot r}$$

WHERE

$$u_k(r) = u_k(r+a)$$

$$\Updownarrow$$

$$\psi_k(r+a) = u_k(r+a) \cdot e^{ik(r+a)} = u_k \cdot e^{ikr} \cdot e^{ika}$$

$$= \psi_k(r) \cdot \exp(ika)$$

TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

WAVEFUNCTION FOR ELECTRON AROUND ATOM j

$$\varphi(\bar{r}-\bar{r}_j)$$

TB-ASSUMPTION FOR GLOBAL WAVEFUNCTION

$$\psi_{\bar{k}}(\bar{r}) = \sum_j c_{\bar{k}j}\, \varphi(\bar{r}-\bar{r}_j)$$

TAKE $c_{kj} = N^{-1/2} e^{i\bar{k}\bar{r}_j}$ SUCH THAT

$$\psi_k(\bar{r}) = N^{-1/2} \sum_j \varphi(\bar{r}-\bar{r}_j)\cdot e^{i\bar{k}\bar{r}_j}$$

WHERE N = # ELECTRON

CHECK BLOCH'S THEOREM:

$$\psi_k(r) = N^{-1/2} \sum_j \varphi(r - r_j)\, e^{ikr_j}$$

$$-r_i = -r_j + a$$

$$r_j = r_i + a$$

$$\psi_k(r+a) = N^{-1/2} \sum_j \varphi(r + a - r_j)\, e^{ikr_j}$$

$$= \underbrace{N^{-1/2} \sum_i \varphi(r - r_i)\, e^{ikr_i}}_{\psi_k(r)}\, e^{ika}$$

$$= \psi_k(r) \cdot e^{ika}$$

KET - NOTATION :

WAVEFUNCTION: $\psi_k(r) = N^{-1/2} \sum_j \varphi(r - r_j) e^{ik r_j} = |k\rangle$

$\psi_k^*(r) = \langle k|$

EIGEN ENERGY: $\mathcal{E}_k = \langle k | H | k \rangle$

$= \int \psi_k^*(\bar{r})\, H\, \psi(\bar{r})\, d\bar{r}$

TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = \langle k | H | k \rangle = \int \psi_{\bar{k}}^*(\bar{r}) H \psi_{\bar{k}}(\bar{r}) \, d\bar{r}$$

$\varphi_j = \varphi(r - r_j)$

$\varphi_m = \varphi(r - r_m)$

$\rho_m = r_m - r_j$

$$= N^{-1} \int \sum_j e^{-i\bar{k}\bar{r}_j} \varphi^*(\bar{r} - \bar{r}_j) H \sum_m e^{i\bar{k}\bar{r}_m} \varphi(\bar{r} - \bar{r}_m) \, d\bar{r}$$

$$= N^{-1} \sum_j \sum_m e^{ik(r_m - r_j)} \int \varphi_j^* H \varphi_m \, dr$$

$$= N^{-1} \sum_j \sum_m e^{ik\rho_m} \langle \varphi_j | H | \varphi_m \rangle$$

$r_j = 0$

$$= \sum_m e^{ik\rho_m} \int \varphi^*(r) H \varphi(r - r_m) \, dr$$

TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = \sum_m e^{ik\rho_m} \int \varphi^*(r)\, H\, \varphi(r-r_m)\, dr$$

$$= \underbrace{\int \varphi^*(r)\, H\, \varphi(r)\, dr}_{-\mathcal{E}_0} + \sum_{\rho_m = a} e^{i\bar{k}\bar{\rho}_m} \underbrace{\int \varphi^*(r)\, H\, \varphi(r-r_m)\, dr}_{-t} + \dots$$

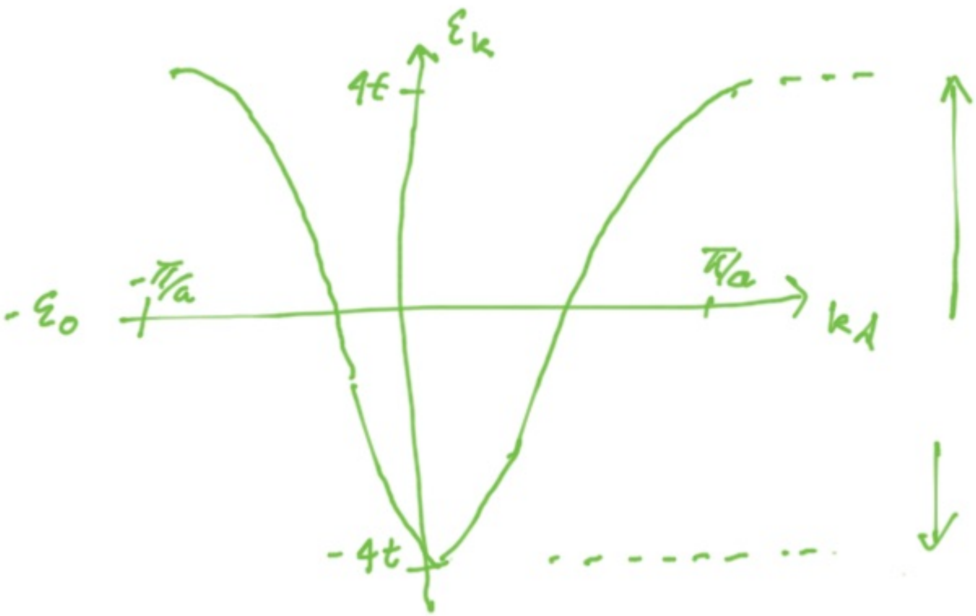
$$= -\mathcal{E}_0 - t\left(\underbrace{e^{ik_x \cdot a} + e^{-ik_x a}}_{2\cos k_x \cdot a} + e^{ik_y a} + e^{-ik_y a}\right)$$

$$= -\mathcal{E}_0 - 2t\{\cos k_x a + \cos k_y a\}$$

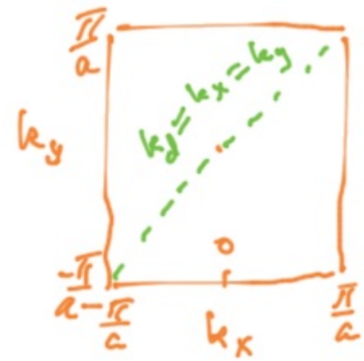
TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = -\mathcal{E}_0 - 2t\{\cos k_x a + \cos k_y a\}$$

$$= -\mathcal{E}_0 - 4t\cos k_d \cdot a$$



BRILLOUIN-ZONE

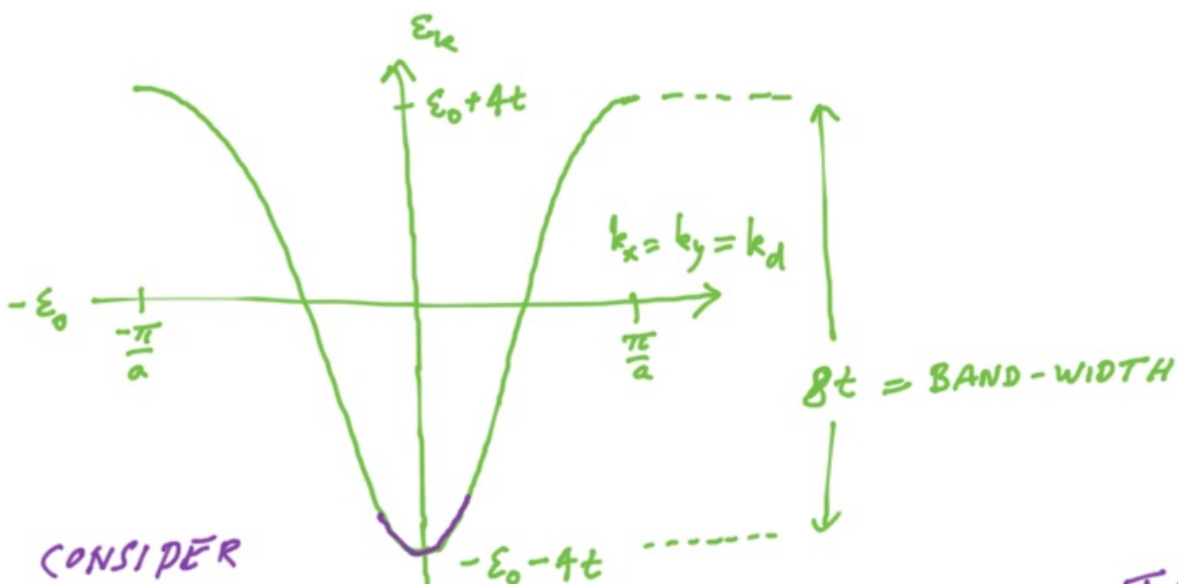


BAND-WIDTH = 8t

TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = -\mathcal{E}_0 - 2t\left\{\cos k_x a + \cos k_y a\right\}$$

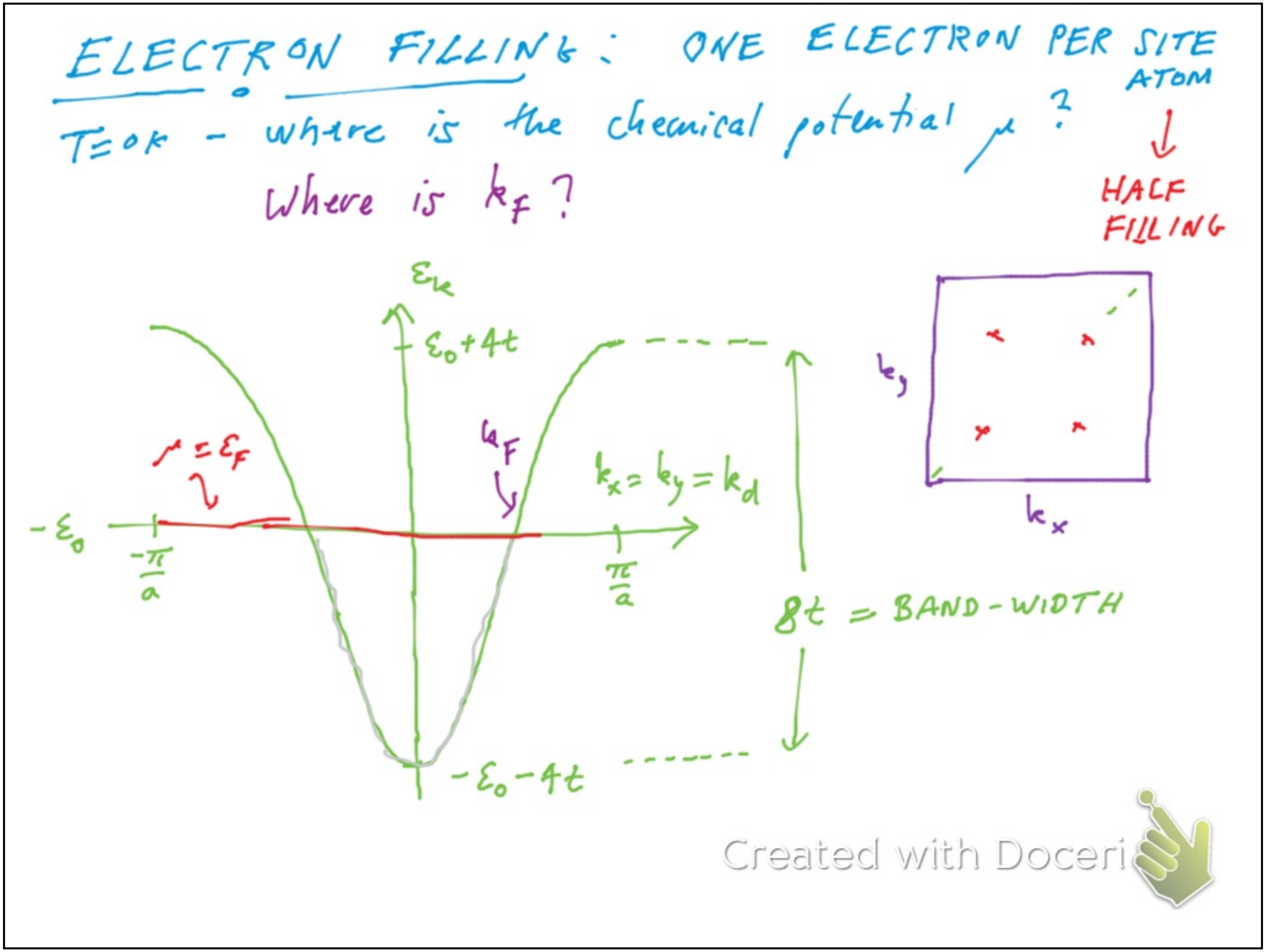
$$= -\mathcal{E}_0 - 4t\cos k_d a = -\mathcal{E}_0 - 4t + 2t a^2 k^2$$



CONSIDER BAND BOTTOM
k is small

TAYLOR-EXPANSION

$$\cos x \approx 1 - \frac{x^2}{2} + \ldots$$


ELECTRON FILLING: ONE ELECTRON PER SITE
ATOM
T=0K - where is the chemical potential μ ?
HALF FILLING
Where is k_F ?
ε_k
ε_0+4t
$\mu=\varepsilon_F$
k_F
$k_x=k_y=k_d$
$-\varepsilon_0$
$-\pi/a$
π/a
$8t$ = BAND-WIDTH
$-\varepsilon_0-4t$
k_y
k_x
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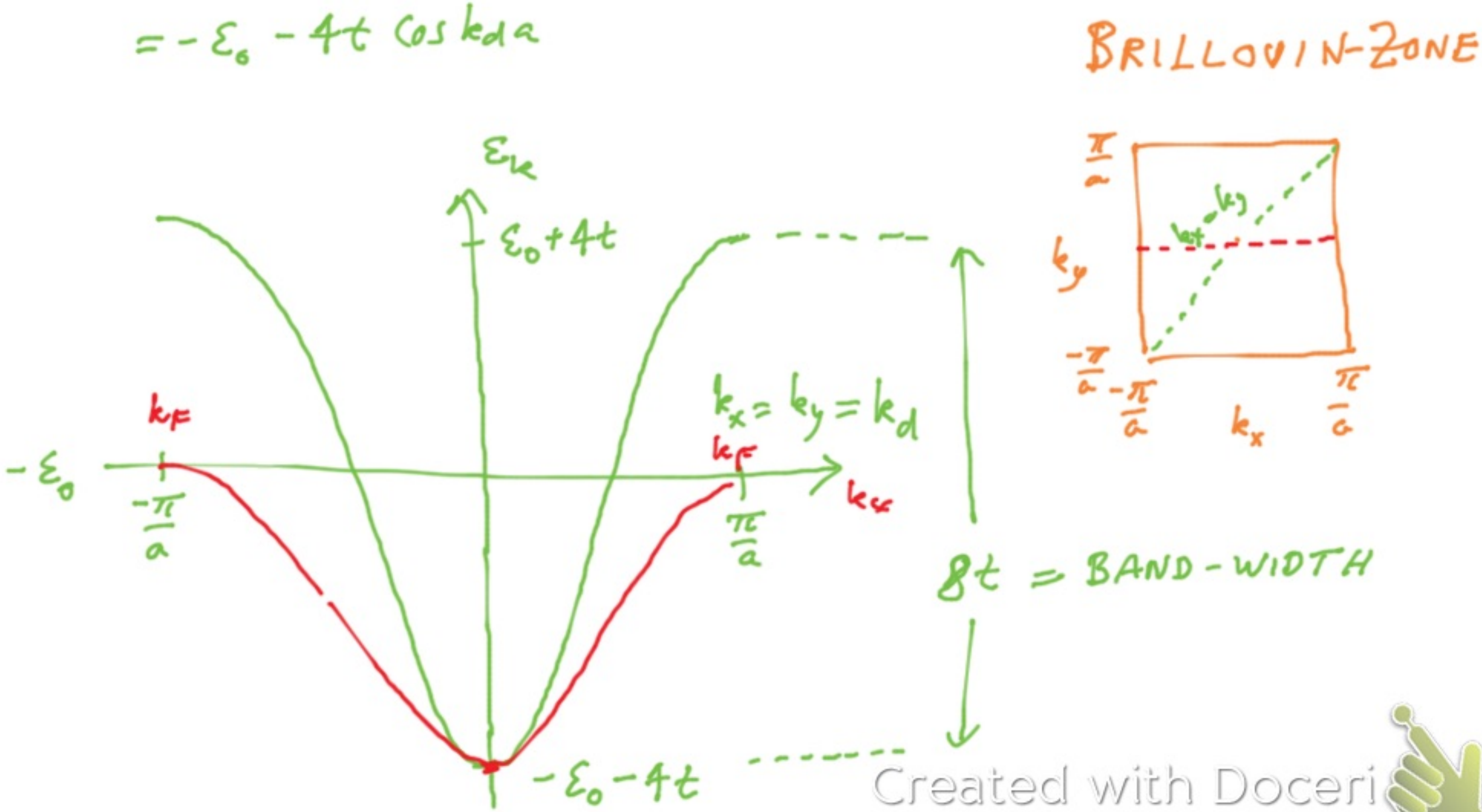
TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\varepsilon_k = -\varepsilon_0 - 2t\{\cos k_x a + \cos k_y a\}$$

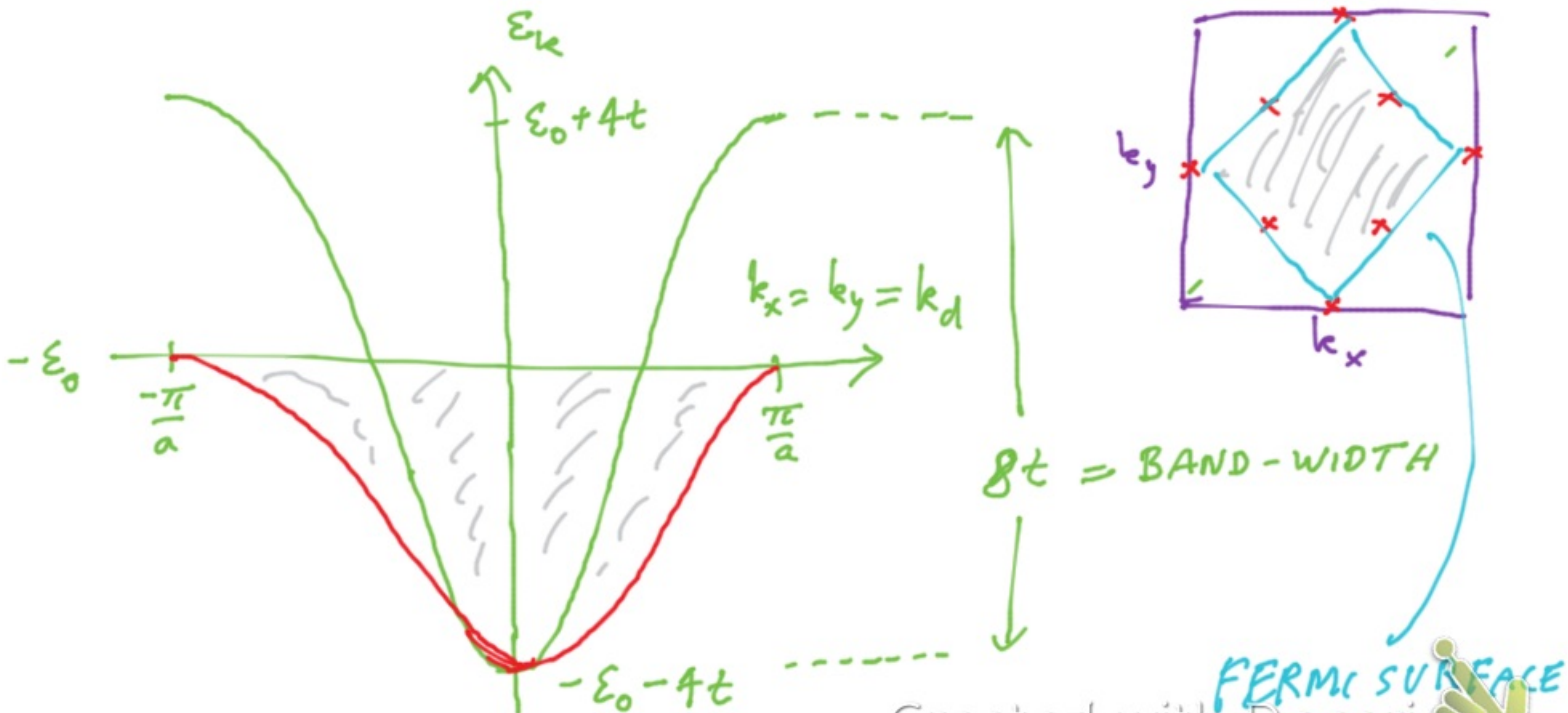
$$= -\varepsilon_0 - 4t \cos k_d a$$



ELECTRON FILLING: ONE ELECTRON PER SITE (ATOM)

T=0K - WHERE IS THE CHEMICAL POTENTIAL? μ

WHERE IS k_F?



TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = \sum_m e^{ik\rho_m} \int \varphi^*(r)\, H\, \varphi(r-r_m)\, dr$$

$$= \underbrace{\int \varphi^*(r)\, H\, \varphi(r)\, dr}_{-\varepsilon_0} + \sum_{\rho_m = a} e^{ik\rho_m} \underbrace{\int \varphi^*(r)\, H\, \varphi(r-a)\, dr}_{-t} + .$$

$$= -\mathcal{E}_0 - t\left(e^{ik_x a} + e^{ik_y a} + e^{-ik_x a} + e^{-ik_y a}\right) -$$

$$= -\mathcal{E}_0 - 2t\{\cos k_x a + \cos k_y a\} -$$

DERIVATION OF SECOND ORDER TERM

$$-t' \cdot \left\{ e^{i(k_x a + k_y a)} + e^{-i(k_x a + k_y a)} + e^{i(-k_x a + k_y a)} + e^{i(k_x a - k_y a)} \right\}$$

$$= -t' \left\{ e^{ik_x a} e^{ik_y a} + e^{-ik_x a} e^{-ik_y a} + e^{-ik_x a} e^{ik_y a} + e^{ik_x a} e^{-ik_y a} \right\}$$

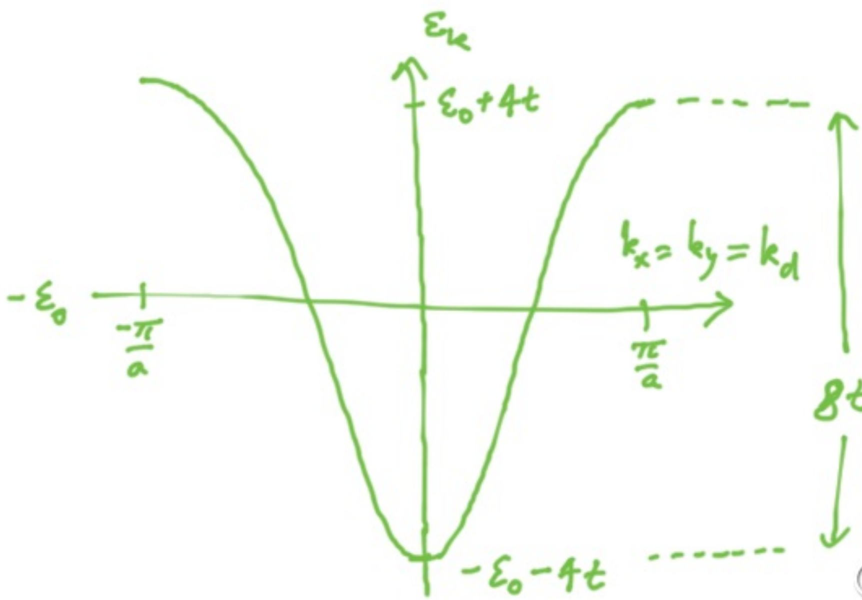
$$= -t' \left[e^{ik_x} \{ 2 \cos k_y a \} + e^{-ik_x a} \{ 2 \cos k_y a \} \right]$$

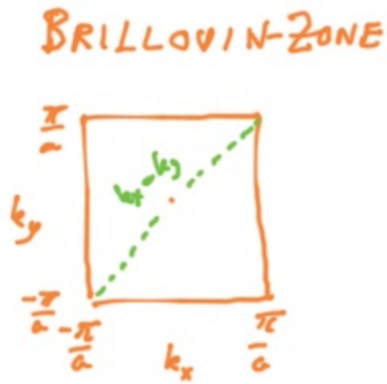
$$= -t' \cdot 2 \cos k_y a \cdot 2 \cos k_x a = -4t' \cos k_x a \cos k_y a$$

TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = -\mathcal{E}_0 - 2t\{\cos k_x a + \cos k_y a\} - \underbrace{4t' \cos k_x a \cos k_y a}_{\text{SECOND ORDER TERM}}$$

WHAT HAPPENS TO THE BAND-WIDTH?



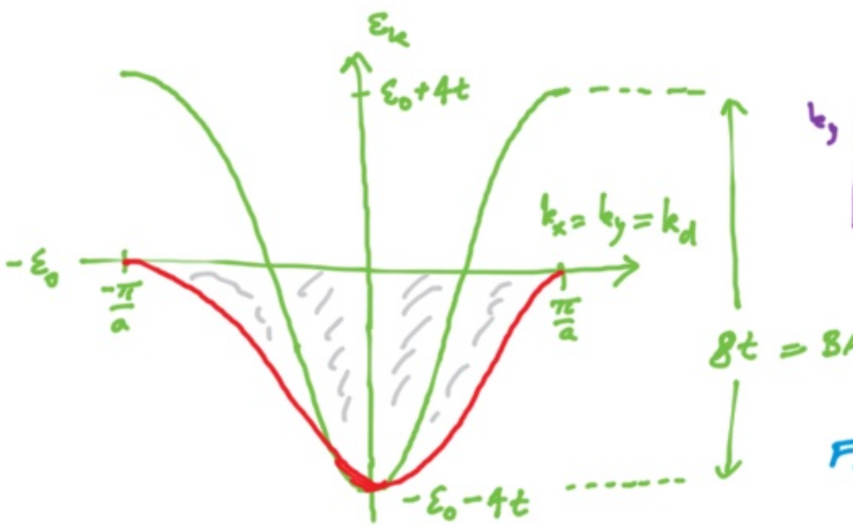


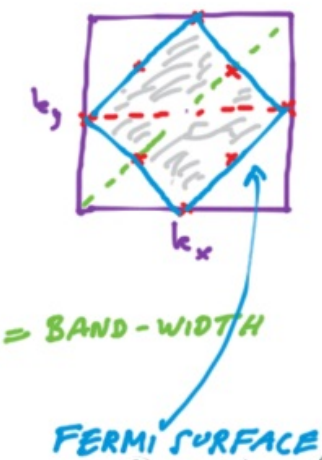
TIGHT-BINDING MODEL: (FOR ELECTRONIC BAND STRUCTURE)

$$\mathcal{E}_k = -\mathcal{E}_0 - 2t\{\cos k_x a + \cos k_y a\} - \underbrace{4t' \cos k_x a \cos k_y a}_{\text{SECOND ORDER TERM}}$$

WHAT HAPPENS TO THE BAND STRUCTURE? DOES IT CHANGE?

WHAT HAPPENS TO THE FERMI SURFACE? DOES IT CHANGE?





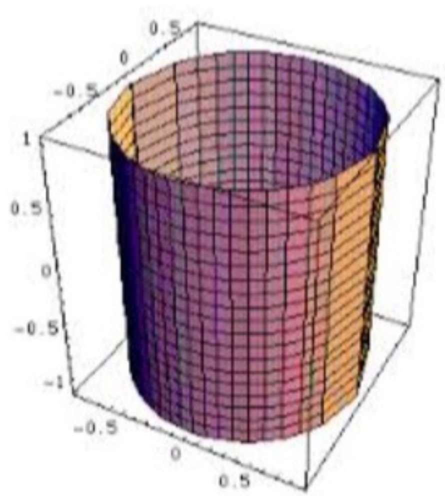
WHAT HAPPENS TO THE FERMI SURFACE AREA? DOES IT CHANGE?

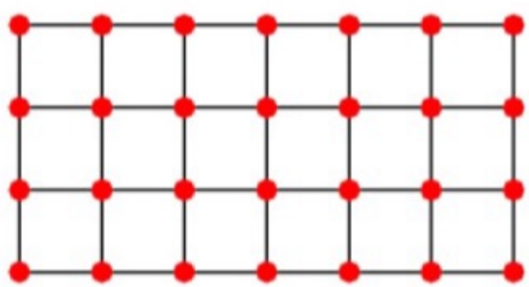
BACK TO MAGNETIC FIELD EXPERIMENTS:

- HALL EFFECT
- MAGNETO-RESISTANCE EFFECT
- QUANTUM OSCILLATIONS

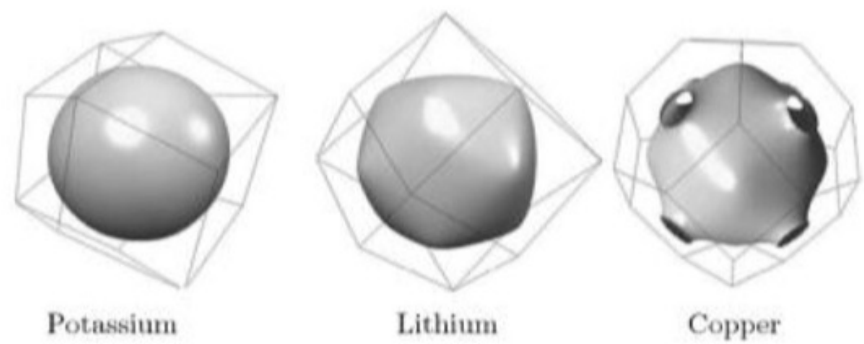
2D and 3D Fermi surfaces

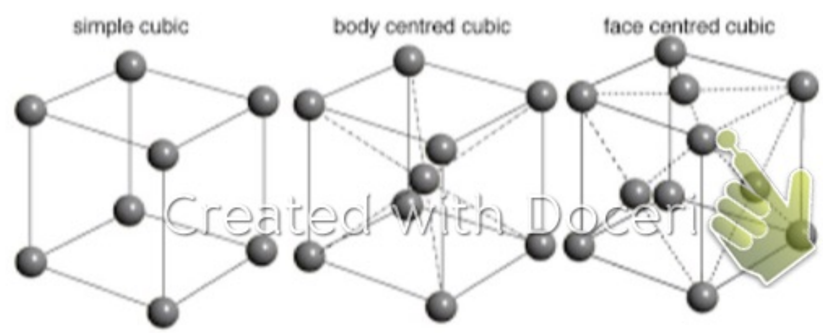
Layered Materials

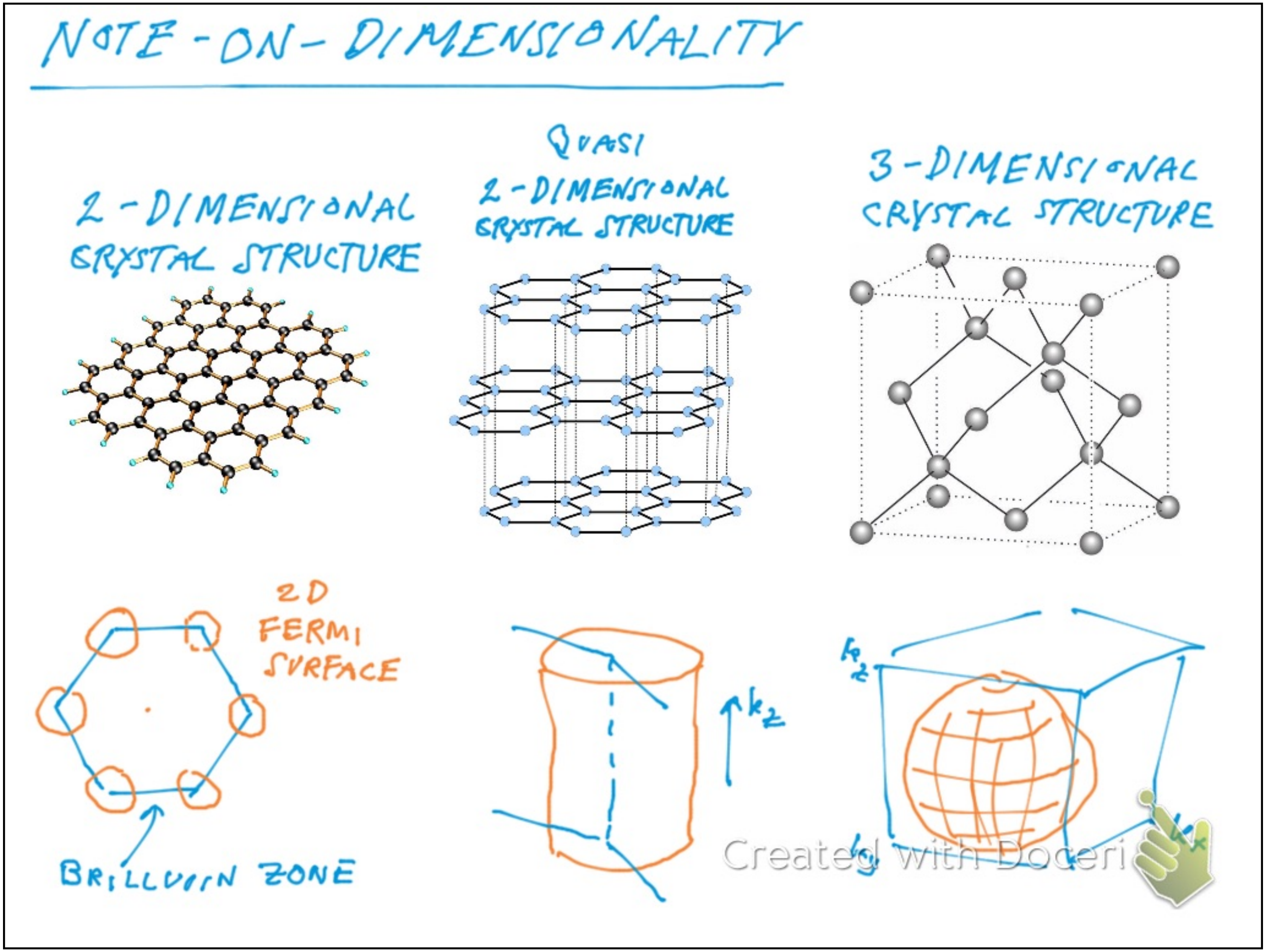




Cubic Materials






NOTE-ON-DIMENSIONALITY
2-DIMENSIONAL CRYSTAL STRUCTURE
QUASI 2-DIMENSIONAL CRYSTAL STRUCTURE
3-DIMENSIONAL CRYSTAL STRUCTURE
2D FERMI SURFACE
BRILLUOIN ZONE
k_z
k_z
k_x
k_y
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QUANTUM OSCILLATIONS: ONSAGER'S RELATION

$$\hbar \frac{dk}{dt} = -e \cdot \vec{v} \cdot \vec{B}$$

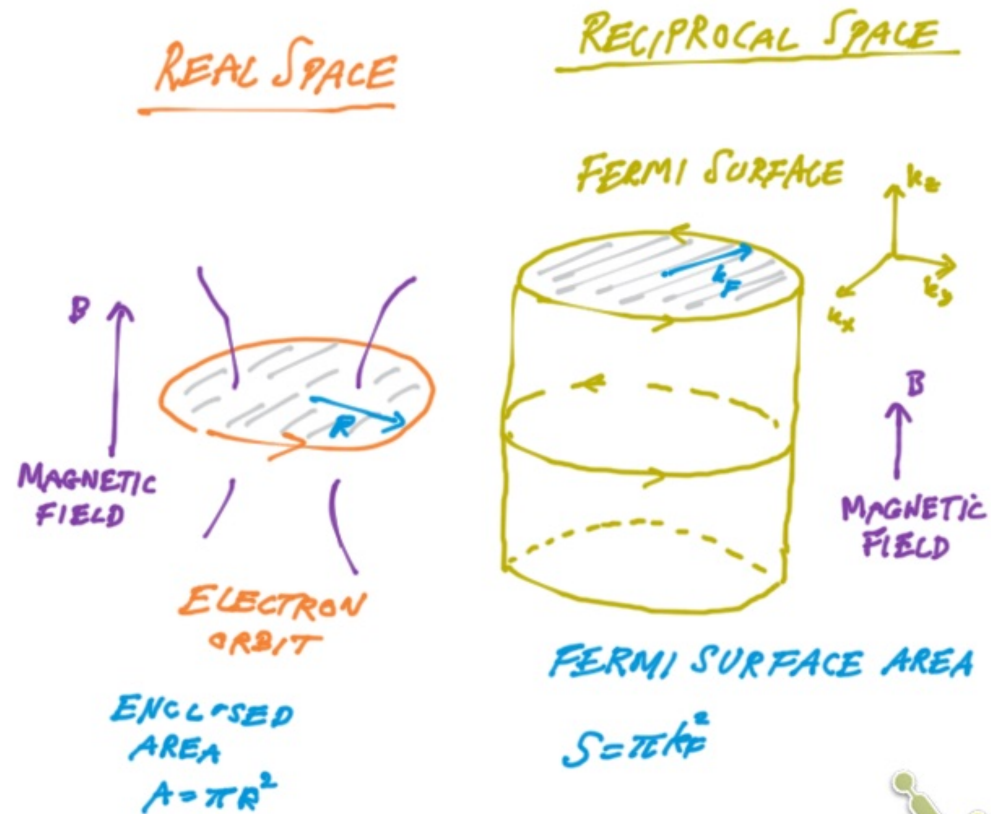
$$= -e|B| \cdot \frac{d\bar{r}}{dt}$$

$\Downarrow$

$$d\bar{k} = -\frac{e|B|}{\hbar} d\bar{r}$$

$\Downarrow$

$$A = \left(\frac{\hbar}{eB}\right)^2 S$$



QUANTUM OSCILLATIONS: ONSAGER'S RELATION

MAGNETIC FLUX CONSIDERATIONS

$$\Phi = \text{FLUX} = |B| \cdot A = |B| \left(\frac{\hbar}{e|B|}\right)^2 \cdot S = \left(\frac{\hbar}{e}\right)^2 \frac{S}{|B|}$$

$$\Downarrow$$

$$S = \left(\frac{e}{\hbar}\right)^2 \cdot B \cdot \Phi$$

MAGNETIC FLUX QUANTIZATION

$$\Phi_n = \left(n + \frac{1}{2}\right) \frac{h}{e} \quad \text{with} \quad n = 0, 1, 2, 3, \ldots$$

$$S_n = \left(\frac{e}{\hbar}\right)^2 B_n \left(n + \frac{1}{2}\right) \frac{\hbar \cdot 2\pi}{e} = \frac{2\pi e}{\hbar} \left(n + \frac{1}{2}\right) B_n$$

Quantum Oscillations: Onsager's Relation

$$S_n = \underbrace{\frac{2\pi e}{\hbar}}_{\alpha}(n+\tfrac{1}{2})B_n = \alpha \cdot (n+\tfrac{1}{2})B_n$$

DEFINE: $\Delta B = B_{n+1} - B_n$ SUCH THAT

$$(n+1+\tfrac{1}{2})\cdot\alpha B_{n+1} = (n+\tfrac{1}{2})\alpha B_n = (n+\tfrac{1}{2})\alpha(B_{n+1} - \Delta B)$$

$$\Downarrow$$

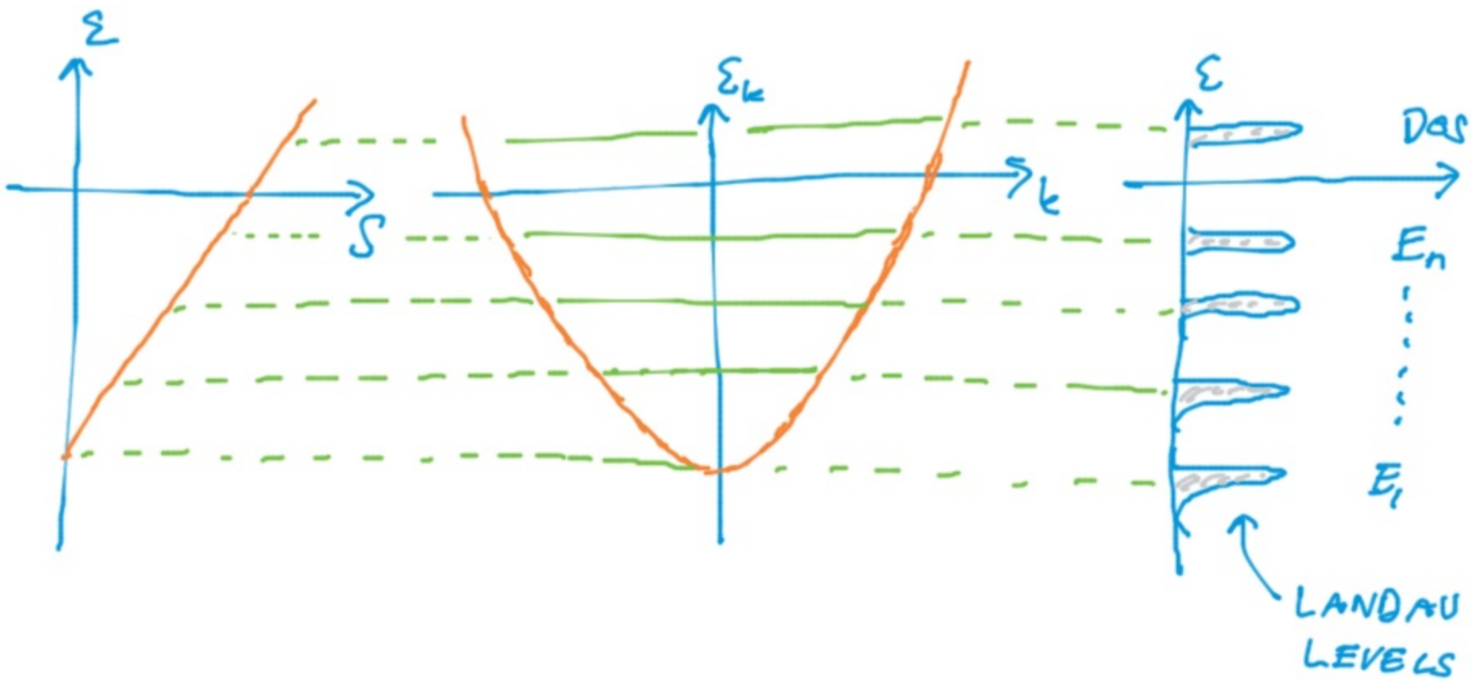
$$-\Delta B(n+\tfrac{1}{2}) = B_{n+1} \Rightarrow (n+\tfrac{1}{2}) = \frac{-B_{n+1}}{\Delta B}$$

$$S_n = \frac{2\pi e}{\hbar}\,\frac{-B_{n+1}B_n}{\Delta B} \Rightarrow S \cdot \frac{-\Delta B}{B_{n+1}B_n} = S\left(\frac{1}{B_{n+1}} - \frac{1}{B_n}\right) = \frac{2\pi e}{\hbar}$$

DEFINE: $F \equiv \left(\frac{1}{B_{n+1}} - \frac{1}{B_n}\right)^{-1}$

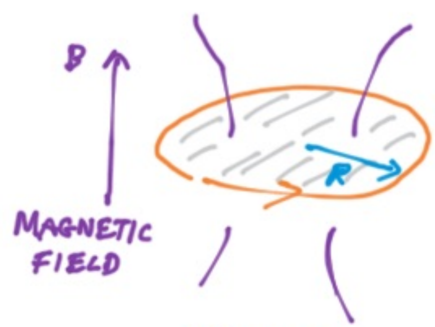
$$F = \frac{\Phi_0}{2\pi^2} S$$

QUANTIZATION - OF - ENERGY



CYCLOTRON - FREQUENCY

REAL SPACE



ELECTRON ORBIT

ENCLOSED AREA

$A = \pi R^2$

CENTRIPETAL FORCE

$$\frac{mv^2}{R} = e \cdot B \cdot v$$

ORBIT PERIOD

$$T = \frac{2\pi R}{v}$$

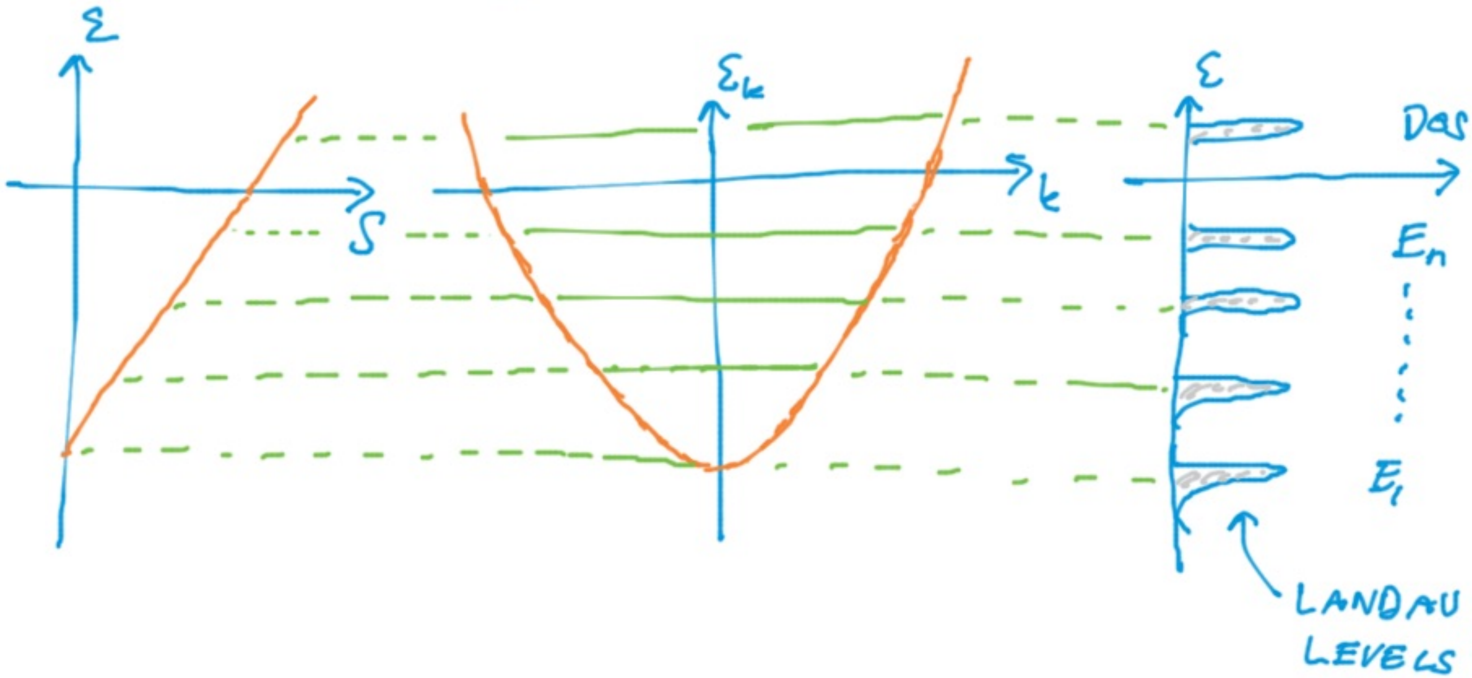
FREQUENCY

$$F = 1/T$$

CYCLOTRON - FREQUENCY

$$\omega_c = 2\pi F = \frac{eB}{m}$$

QUANTIZATION - OF - ENERGY



ESTIMATION OF $\hbar\omega_c$

$\hbar\omega_c = 1 \cdot 10^{-4}\,eV$ @ 1 Tesla

$E_F \approx 1eV$

$$E_n = \hbar\omega_c \left(n + \tfrac{1}{2}\right)$$