What Code Is Doing

1. Using Poisson solver to calculate Voltage

2. $H_{Full} = H_0 + V(x,y)$

3. Get list of eigenvectors/values - Energies and wavefunctions

4. Get list of lowest energy eigenstates, using numStates to set how many - This defines ε_{Fermi} *

5. $\sum_n g(n)\,\text{totalDensity}(n)$ $g(n)$ is degeneracies

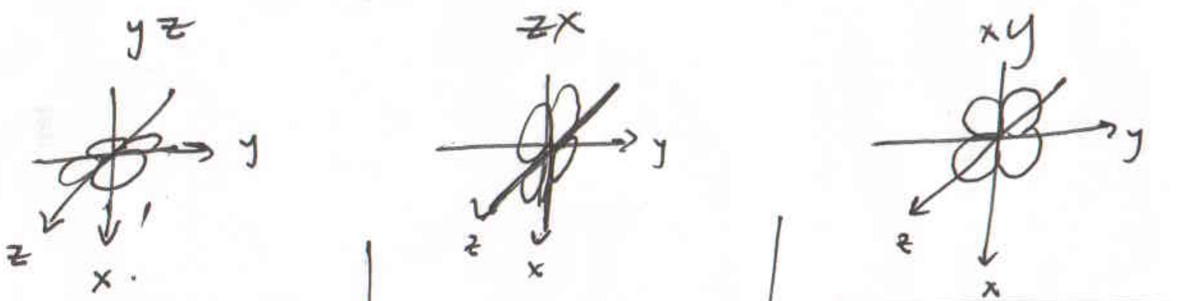
   * $\text{totalDensity}(n) = ?$

   Sum over n states returned by Necessary states
   - Implicit use of step function

   Reconstructs charge distribution

6. Iterate for self consistency - uses mixing for stability

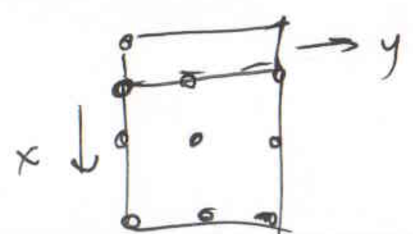
* Each site has three states associated with it, one for each orbital



	yz	zx	xy
X-hoppm	small, t'	large, t	large, t
Y-hoppiy	large, t	small, t'	large, t

$$t_x = \begin{pmatrix} t' & 0 & 0 \\ 0 & t & 0 \\ 0 & 0 & t \end{pmatrix} \begin{Bmatrix} yz \\ zx \\ xy \end{Bmatrix}$$

$$t_y = \begin{pmatrix} t & 0 & 0 \\ 0 & t' & 0 \\ 0 & 0 & t \end{pmatrix} \begin{Bmatrix} yz \\ zx \\ xy \end{Bmatrix}$$



$e^{ik_z a}$

$k_z = 0 \implies 1$

$k_z = \frac{\pi}{2a} \implies e^{i\frac{\pi}{2}}$

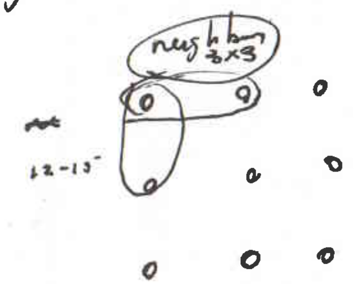
Along z (infinite/periodic)

* use k_z

$\epsilon_{yz}(k_z) = 2t - 2t\cos k_z$

$\epsilon_{zx}(k_z) = 2t - 2t\cos k_z$

$\epsilon_{xy}(k_z) = 2t' - 2t'\cos k_z$

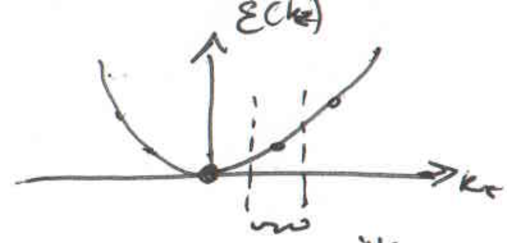


Infinite chain

add a single electron

$$\Rightarrow \rho_R = \frac{1}{L}$$

$$\mathcal{H} = \frac{\hbar^2}{2m} k_z^2$$



fill a single k-state

$$\Rightarrow \rho_k = \frac{2\pi}{L}$$

$$\Rightarrow \rho_R = \frac{1}{2\pi} \rho_k$$

3D (1 infinite dimension)

$$\rho_R = \frac{1}{LWH} = \frac{1}{V}$$

$$\rho_k = \frac{2\pi}{L}$$

$$\Rightarrow \boxed{\rho_R = \rho_k \left(\frac{1}{2\pi}\right)\left(\frac{1}{WH}\right)}$$

Bands in infinite periodic solid

1 atom, 1 orbital

Hamiltonians

Atoms

(1) $H = \varepsilon_0$

(2) $H = \begin{pmatrix} \varepsilon_0 & -t \\ -t & \varepsilon_0 \end{pmatrix} \begin{Bmatrix} a \\ b \end{Bmatrix}$ $\quad -t$

(3) $H = \begin{pmatrix} \varepsilon_0 & -t & \\ -t & \varepsilon_0 & -t \\ & -t & \varepsilon_0 \end{pmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix}$ $\quad -t, -t$

(∞)

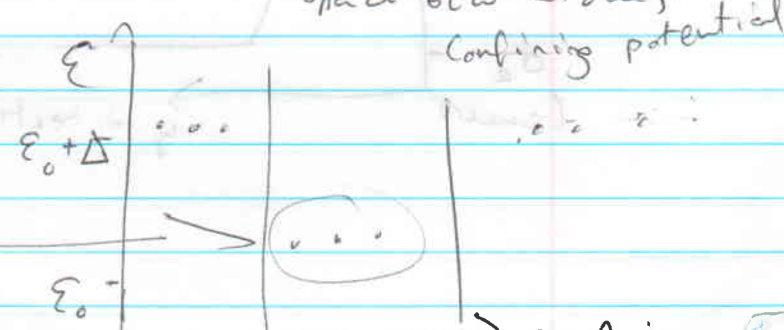
$$H = \begin{pmatrix} \varepsilon_0 & -t & & \\ -t & \varepsilon_0 & -t & \\ & -t & \ddots & \\ & & & \ddots \end{pmatrix} \begin{Bmatrix} a \\ b \\ \vdots \\ \vdots \end{Bmatrix}$$

→ Bloch's Theorem.

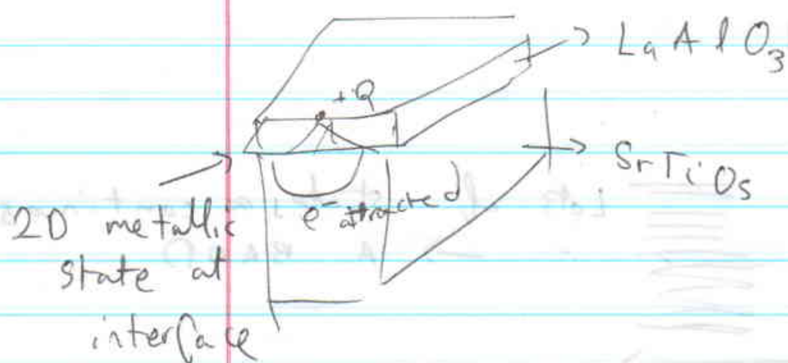
$$H(k) = \varepsilon_0 - 2t\cos(k_x \ell) \quad (\text{one } D)$$

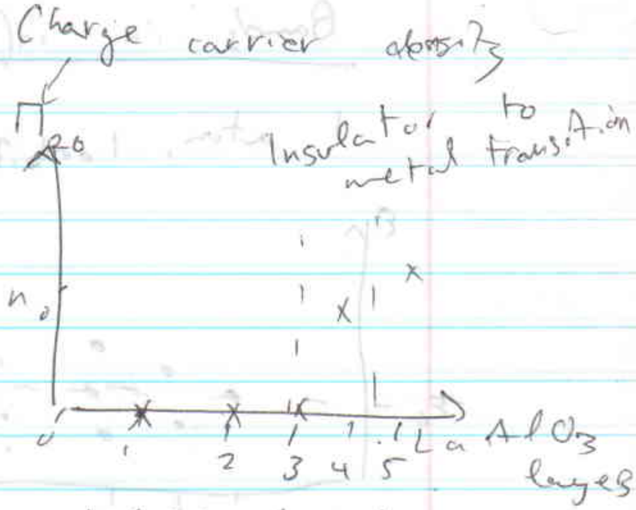
k: crystal momentum; ℓ: space btw atoms

Quantum confinement



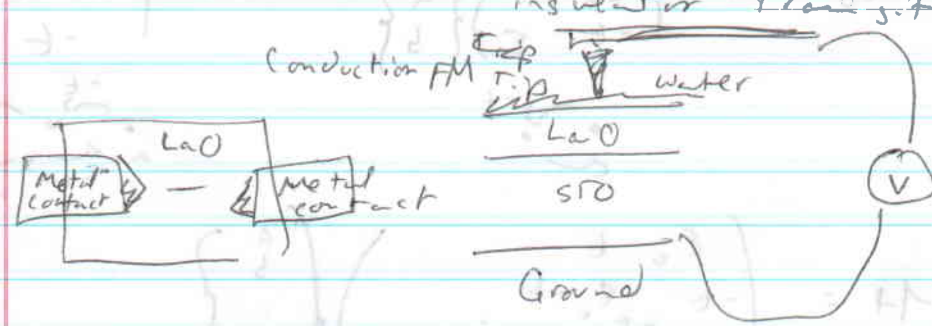
Use as system, accurate within nt^2/Δ → Perturbation theory



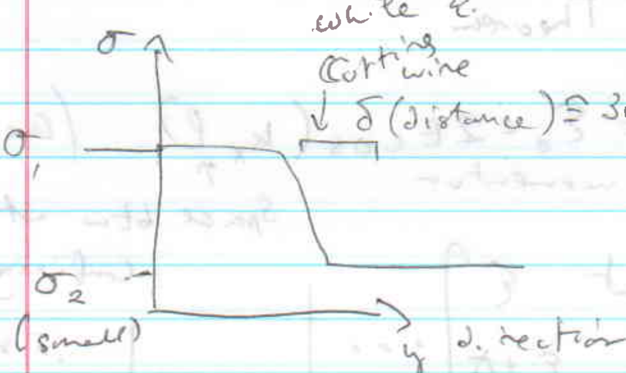


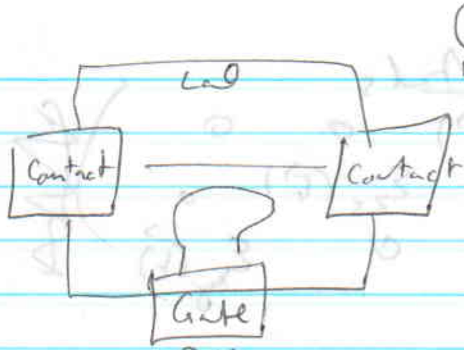
\# charge carriers depends on LaAlO$_3$ thickness

Jeremy Levy : 3 layers LaAlO$_3$
Altered surface to induce metal/insulator transition



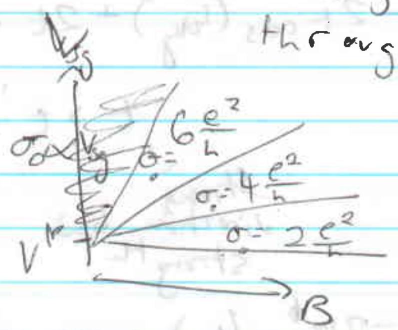
Can find conductivity $\sigma = \frac{I}{V}, \frac{\partial I}{\partial V}$ (ohm's)



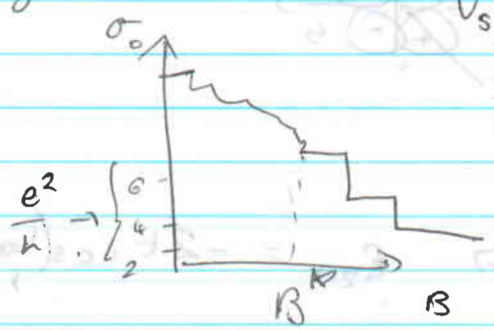


Side gate voltage (V_{sg}) $\Rightarrow$ increases wire charge ρ

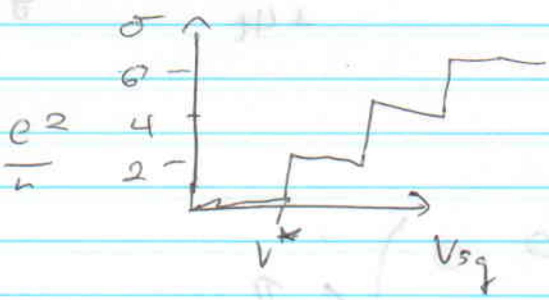
Pulls charge out through gate



V_{sg} fixed



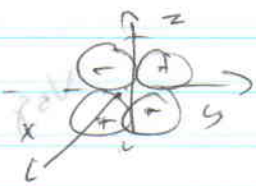
fixed $B > B^*$



H With multiple orbitals

$$H_0(\vec{k}) = \begin{pmatrix} \varepsilon_{yz}(\vec{k}) & 0 & 0 \\ 0 & \varepsilon_{zx}(\vec{k}) & 0 \\ 0 & 0 & \varepsilon_{xy}(\vec{k}) \end{pmatrix} \otimes \underbrace{\mathbb{1}_{2\times 2}}_{\text{Spin}}$$

$\varepsilon_{yz} = \cancel{-2t\cos}$

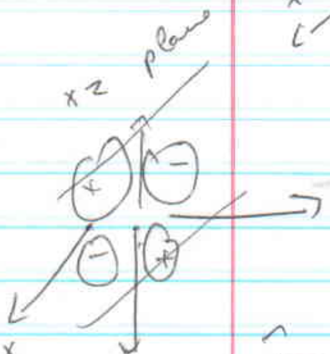


$$-2t'\cos(k_x a) - 2t\cos(k_y) + 2t + 2t'$$

$t > t'$

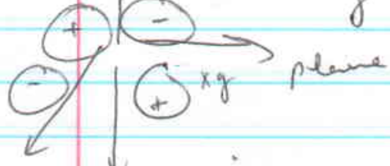
Strong direction bond strength

weak direction



$$\varepsilon_{zx} = -2t\cos(k_x a) - 2t'\cos(k_y a) + 2t + 2t'$$

$$\varepsilon_{xy} = -2t\cos(k_x a) - 2t\cos(k_y a) + 4t$$



$$H_{\text{confined}} = \begin{pmatrix} \Delta_z & 0 & 0 \\ 0 & \Delta_z & 0 \\ 0 & 0 & 0 \end{pmatrix} \otimes \mathbb{1}_{2\times 2}$$

Perpendicular to surface

Pushes up $\{yz, zx\}$ bands energywise

H_{so} (spin orbit) = complicated 6x6

$$H_{\text{Rashba}}(\vec{k}) = \begin{pmatrix} 0 & 0 & 2t_R i\sin(k_x a) \\ 0 & 0 & 2t_R i\sin(k_y a) \\ \multicolumn{2}{c}{\underbrace{\text{Complex conjugates}}_{\text{Hermitian}}} & 0 \end{pmatrix} \otimes \mathbb{1}_{2\times 2}$$

$\mathcal{E}_x$

Adding confinement

$$\mathcal{E}_{xy}^{\not{c}} = -2t\cos(k_x a) - 2t\cos(k_y a) + 4t$$

Confined along y

1) Assume k_y is small, $-2t\cos(k_y a) \simeq \cancel{-2t + ta^2 k_y^2}$
$-2t + ta^2 k_y^2$

2) k_y goes to $\partial/\partial y$

$$\frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{-\hbar^2}{2m}\partial_y^2$$

$$p_y = -i\hbar\, \partial/\partial t$$

$$\left(\frac{\hbar^2}{2m} \Rightarrow ta^2\right)$$

3) Add confining potential, solve (Particle in a box)

$$\mathcal{E}_{xy}\varphi = \left[2t - 2t\cos(k_x a) + ta^2\partial_y^2\right]\varphi$$

$$\mathcal{E}_k\varphi_k = \cancel{H}\,\varphi_k \quad + \frac{\Delta_{SO}}{3}$$

$$ta^2\partial_y^2\varphi_k = \left(\mathcal{E}_k - 2t + 2t\cos k_x a - \frac{\Delta_{SO}}{3}\right)\varphi_k$$

$$= \tilde{\mathcal{E}}_k\varphi_k$$

$-2t + 2t\cos k_x a$
$= -2t(1 - \cos k_x a)$
$\approx -2t\left(\frac{a^2 k_x^2}{2}\right)$
$\approx -ta^2 k_x^2$

When you angle the wire

$$\mathcal{E}_{xy} \approx ta^2(k_x^2 + k_y^2) \quad \text{Circle}$$

$$\mathcal{E}_{yz} = t' a^2 k_x^2 + ta^2 k_y^2$$

$$\mathcal{E}_{zx} = ta^2 k_x^2 + t' a^2 k_y^2$$

$$ta^2\partial_y^2\varphi_k = \left(\mathcal{E}_x - ta^2 k_x^2 - \frac{\Delta_{SO}}{3}\right)\varphi_k$$

$$\mathcal{E}(k_x, k_y) \xrightarrow{\text{Rotate}} \mathcal{E}(k_\parallel, k_\perp) \xrightarrow[k_\perp \to \partial_\perp]{} \text{Diff eq}$$