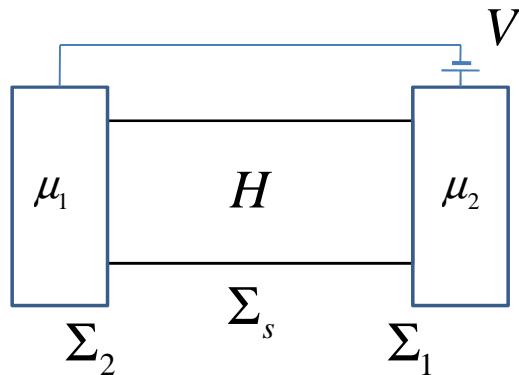


# ECE 659 Quantum Transport: Atom to Transistor

Lecture 29: Hamiltonian including Spin  
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$$E\{\psi\} = \left( \frac{p^2}{2m^*} I + \frac{\eta}{\hbar} \vec{\sigma} \cdot (\vec{E} \times \vec{p}) \right) \{\psi\}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

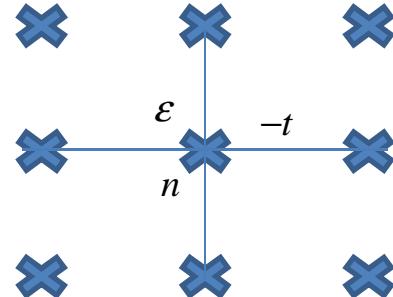
$$p = -i\hbar\nabla$$

$$p_x = -i\hbar \frac{\partial}{\partial x} \quad p_y = -i\hbar \frac{\partial}{\partial y} \quad p_z = -i\hbar \frac{\partial}{\partial z}$$

Any 2x2 Hermitian matrix can be written as linear combination of Identity and Pauli matrices

Usually the Rashba term contains the magnitude of Electric field so:  $E\{\psi\} = \left( \frac{p^2}{2m^*} I + \frac{\eta}{\hbar} \vec{\sigma} \cdot (\vec{z} \times \vec{p}) \right) \{\psi\}$

If there is no spin orbit coupling we use:  $\epsilon I$  and  $-tI$



$$E\{\psi_n\} = \sum_m [H_{nm}] \{\psi_m\}$$

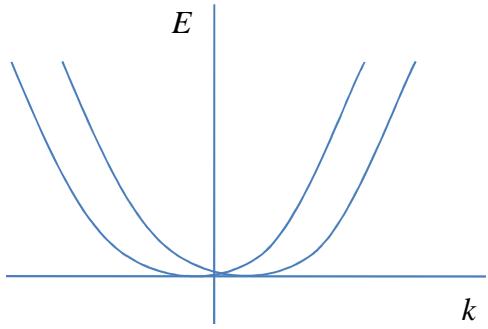
$$\{\psi(\vec{r})\} = \{\phi\} e^{i\vec{k}\cdot\vec{r}}$$

$$E\{\phi\} = [h(\vec{k})] \{\phi\}$$

$$p_x e^{i\vec{k}\cdot\vec{r}} = -i\hbar \frac{\partial}{\partial x} e^{i\vec{k}\cdot\vec{r}} = \hbar k_x e^{i\vec{k}\cdot\vec{r}}$$

$$\text{so } \vec{p} e^{i\vec{k}\cdot\vec{r}} = \hbar \vec{k} e^{i\vec{k}\cdot\vec{r}}$$

In a 1-D system we can write the E-k relation easily but it cannot be done so easily now



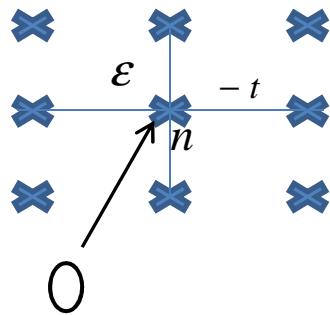
$$\{\psi_n\} = \{\phi_0\} e^{i\vec{k} \cdot \vec{d}_n}$$

$$E\{\psi_n\} = \sum_m [H_{nm}] \{\psi_m\}$$

$$E\{\phi\} e^{i\vec{k} \cdot \vec{d}_n} = \sum_m [H_{nm}] e^{i\vec{k} \cdot \vec{d}_m} \{\phi\}$$

$$E\{\phi\} = \underbrace{\sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)}}_{h(\vec{k})} \{\phi\}$$

$$h(\vec{k}) = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)}$$



For 1D lattice:

$$\epsilon \quad -t$$

$$\begin{aligned} h(\vec{k}) &= \epsilon - t e^{ik_x a} - t e^{-ik_x a} \\ &= \epsilon - 2t \underbrace{\cos k_x a}_{1 - \frac{k_x^2 a^2}{2}} \\ \therefore E &= (\epsilon - 2t) + ta^2 k_x^2 \end{aligned}$$

Now:

$$E\{\phi\} = \left( \frac{\hbar^2 k^2}{2m^*} I + \eta \vec{\sigma} \cdot (\vec{z} \times \vec{k}) \right) \{\phi\}$$

$k_x \hat{x} + k_y \hat{y}$

$$h(\vec{k}) = \frac{\hbar^2 k^2}{2m^*} I + \eta [\sigma_y k_x - \sigma_x k_y]$$

$$\cos k_x a \approx 1 - \frac{k_x^2 a^2}{2}$$

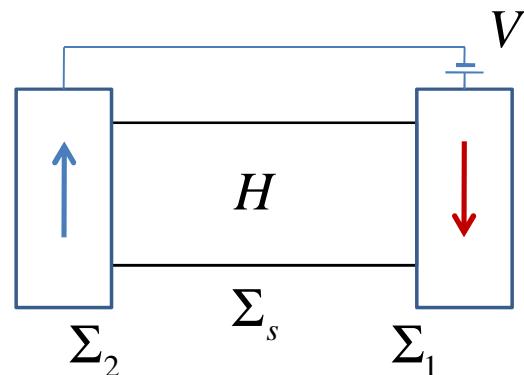
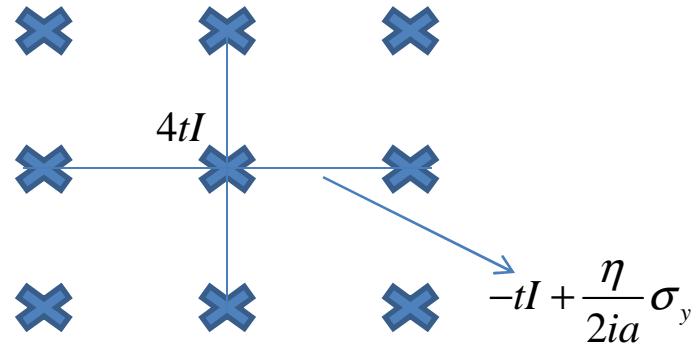
$$\begin{aligned} & 2 \frac{\hbar^2}{2m^*} \left( \frac{k_x^2 + k_y^2}{2} \right) I \\ & = 2t(1 - \cos k_x a + 1 - \cos k_y a) I \\ & = (4t - te^{ik_x a} - te^{-ik_x a} - te^{ik_y a} - te^{-ik_y a}) I \end{aligned}$$

For spin-orbit term:

$$\sin k_x a \approx k_x a$$

$$\begin{aligned} & \eta [\sigma_y k_x - \sigma_x k_y] \\ & = \frac{\eta}{a} [\sigma_y \sin k_x a - \sigma_x \sin k_y a] \\ & = \frac{\eta}{2ia} [\sigma_y (e^{ik_x a} - e^{-ik_x a}) - \sigma_x (e^{ik_y a} - e^{-ik_y a})] \end{aligned}$$

These terms allow us to write the couplings:



$$\begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix}$$