

FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

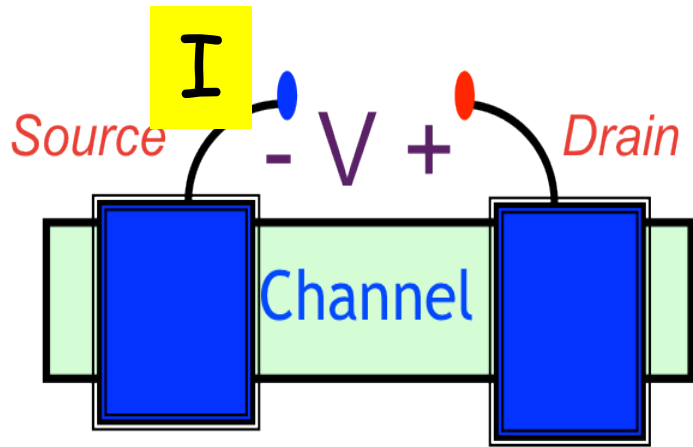
1 Schrodinger Equation



- 2. Contact-ing Schrodinger
- 3. Advanced Examples
- 4. Spin Transport

- 1.1. Introduction
- 1.2. Wave Equation
- 1.3. Differential to Matrix Equation
- 1.4. Dispersion Relation
- 1.5. Counting States
- 1.6. Beyond 1-D
- 1.7. Lattice with a Basis
- 1.8. Graphene
- 1.9. Reciprocal Lattice / Valleys
- 1.10. Summing up ..

1.10a Summing up ..



$$E\psi = H\psi$$

Schrodinger + ⚡ = NEGF

Quantum Transport

Semiclassical Transport



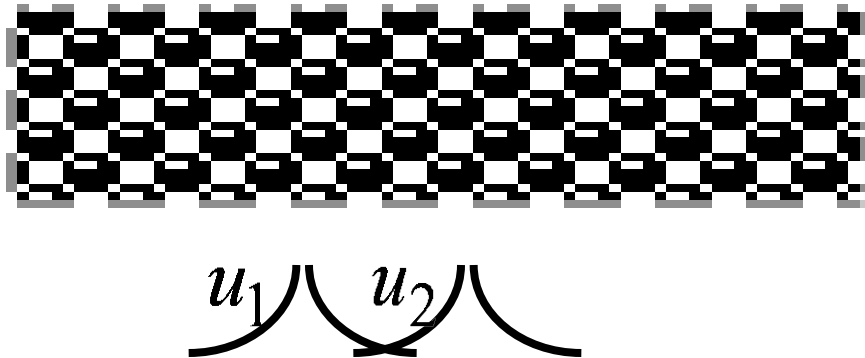
Entropy driven

Force driven

Newton + ⚡ =



1.10b Summing up ..

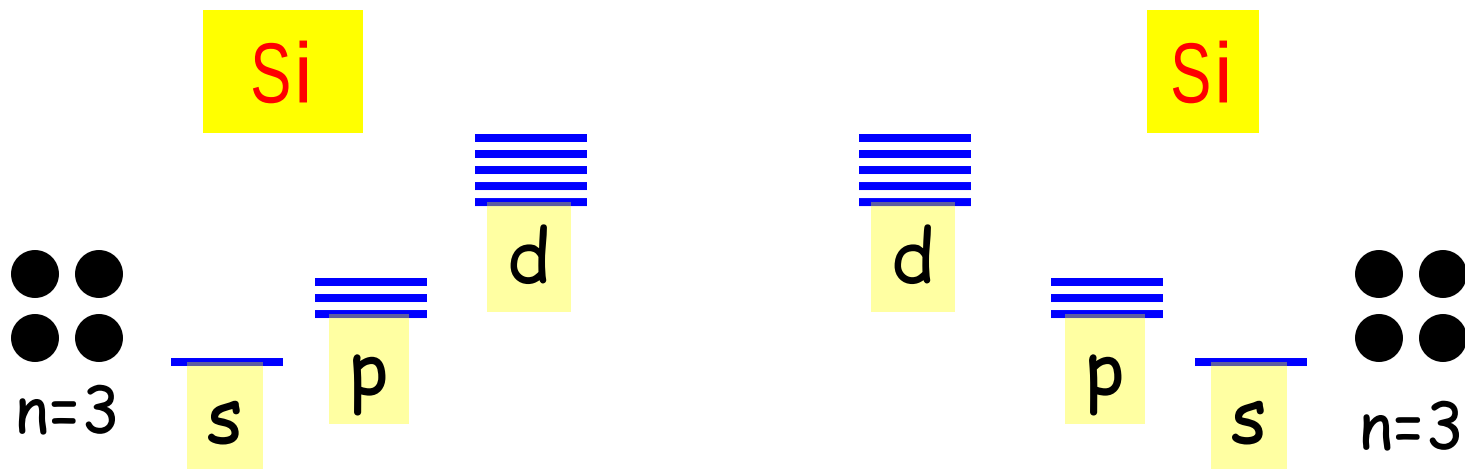


$$E \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \psi_N \end{Bmatrix} = \begin{matrix} \text{N x N} \\ \begin{bmatrix} \dots & \dots & \dots \\ \dots & H & \dots \\ \dots & \dots & \dots \end{bmatrix} \end{matrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \dots \\ \psi_N \end{Bmatrix}$$

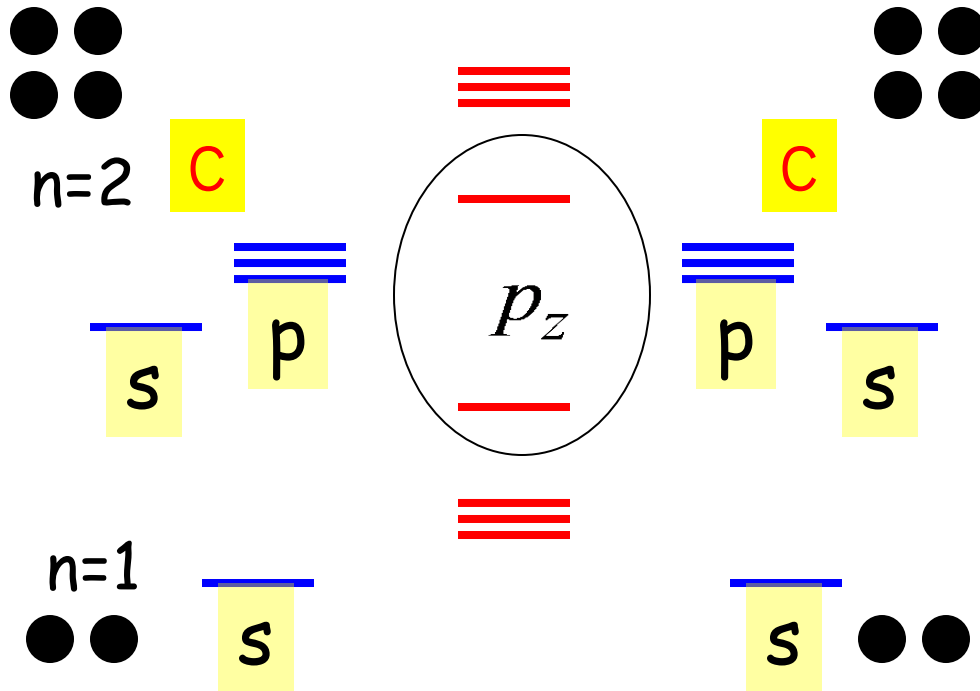
$$E \psi(\vec{r}) = \left(-\frac{\hbar^2}{2m_0} \nabla^2 + U(\vec{r}) \right) \psi(\vec{r})$$

$$\psi(\vec{r}) = \sum_{m=1}^N \psi_m u_m(\vec{r})$$

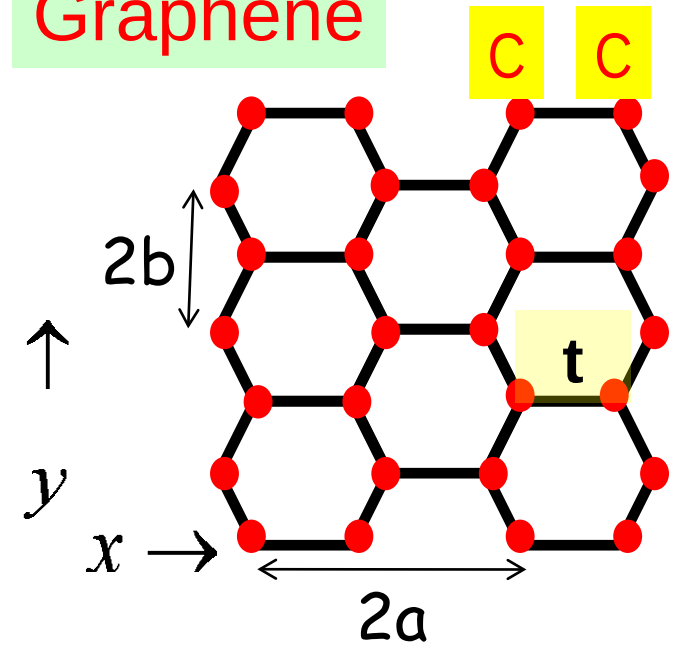
N = number of
“basis functions”



1.10d Summing up

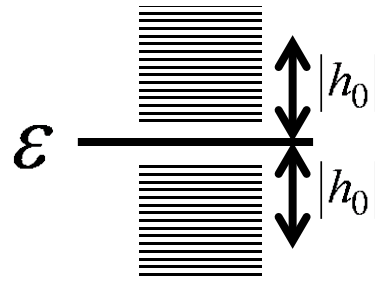


Graphene



1.10e Summing up ..

$$h(\vec{k}) = \begin{bmatrix} \varepsilon & h_0^* \\ h_0 & \varepsilon \end{bmatrix}$$



$$E = \varepsilon \pm |h_0|$$

$$= \varepsilon \pm at \sqrt{k_x^2 + \beta_y^2}$$

$$h_0 = t \left(1 + 2e^{ik_x a} \cos k_y b \right)$$

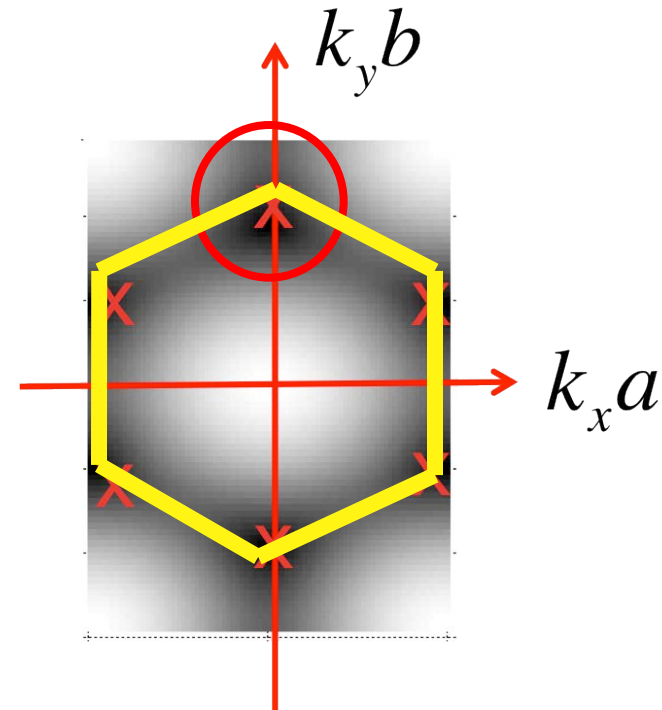
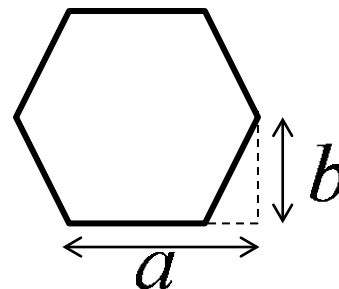
$$\approx -iat (k_x + i\beta_y)$$

$$v = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{at}{\hbar}$$

$$a \approx 0.2 \text{ nm}$$

$$\sim 10^6 \text{ m/sec}$$

$$t \approx 3 \text{ eV}$$



Coming up next ..

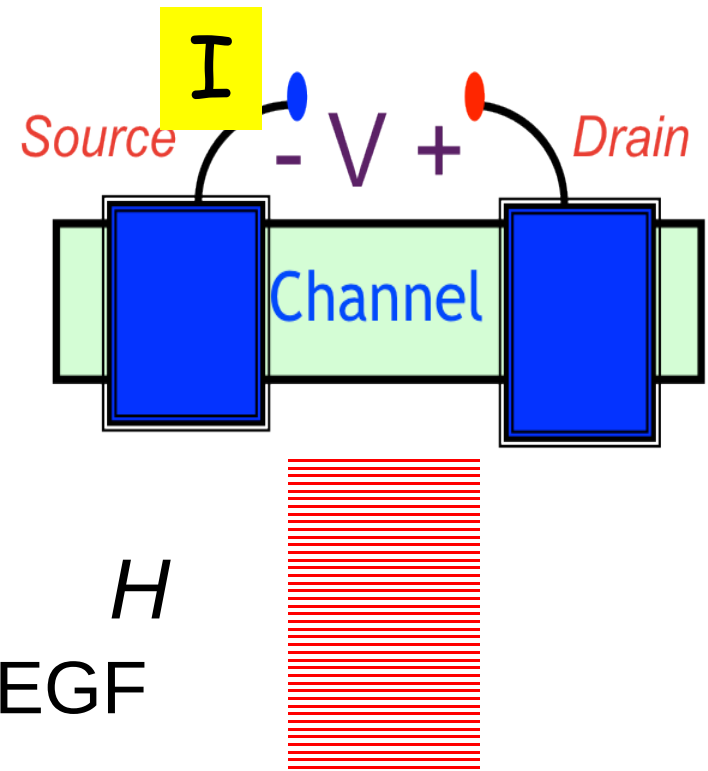
B. Quantum Transport

1. Schrodinger Equation $E\psi = H\psi$

2. Contact-ing Schrodinger

3. Advanced Examples

4. Spin Transport



Schrodinger +  = NEGF

H