

ECE 659 Quantum Transport: Atom to Transistor

Lecture 14: Coherent Transport I

Supriyo Datta

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Notes prepared by Samiran Ganguly

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi \rightarrow i\hbar \frac{\partial \psi_n}{\partial t} = \sum_m H_{nm} \psi_m$$

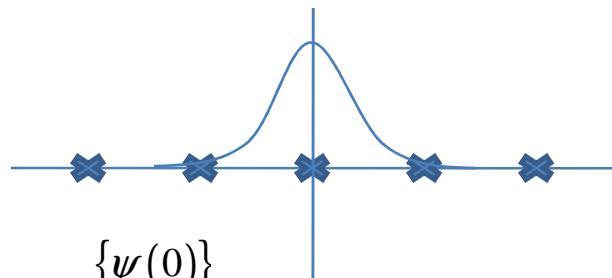
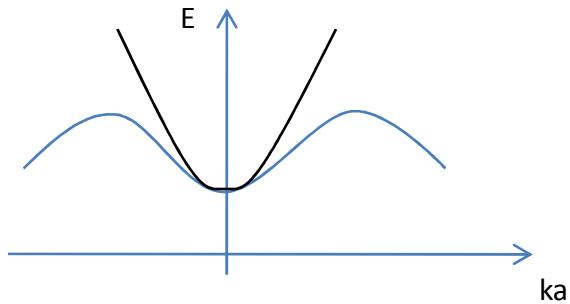
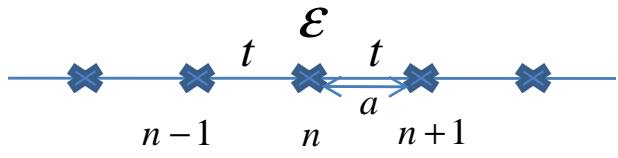
$$E\phi = -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2} + U\phi \rightarrow \phi_n = \sum_m H_{nm} \phi_m$$

$$E = \frac{\hbar^2 k^2}{2m} + U$$

$$E = \epsilon + 2t \underbrace{\cos ka}_{d_n \quad 1 - \frac{k^2 a^2}{2}}$$

$$\psi \sim e^{ikx} e^{-iEt/\hbar} \quad \phi_n = e^{ikna}$$

$$E = \sum_m H_{nm} e^{ik(d_m - d_n)}$$



$$\frac{dx}{dt} = \frac{1}{\hbar} \frac{\partial E}{\partial k}$$

$$\{\psi(0)\} = e^{ikna} e^{-n^2/n_0^2}$$

$$\frac{d\{\psi\}}{dt} = \frac{[H]}{i\hbar} \{\psi\}$$

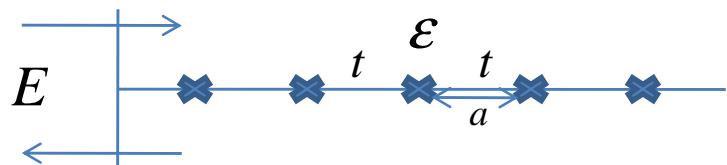
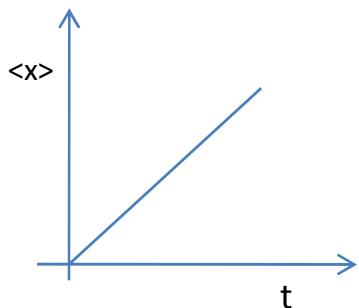
$$\{\psi(t)\} = e^{-i[H]t/\hbar} \{\psi(0)\}$$

Matlab can calculate the exponential using expm() function

The function of a matrix is found by diagonalizing a matrix by a basis transformation, calculating the function of diagonal elements and then using the inverse transform

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \rightarrow \begin{bmatrix} f(a_1) & 0 \\ 0 & f(a_2) \end{bmatrix} \rightarrow \begin{bmatrix} u & v \\ w & x \end{bmatrix}$$

$$\langle x \rangle = \frac{\int dx \psi^* \psi x}{\int dx \psi^* \psi}$$



$$E\phi = H\phi$$

$$[EI - H]\{\phi\} = 0$$

$$\text{In a } 1 \times 1 \text{ case} \quad (E - \varepsilon)\phi = 0$$

$$E = \varepsilon$$

$$[EI - H - \Sigma]\{\phi\} = \{s\}$$

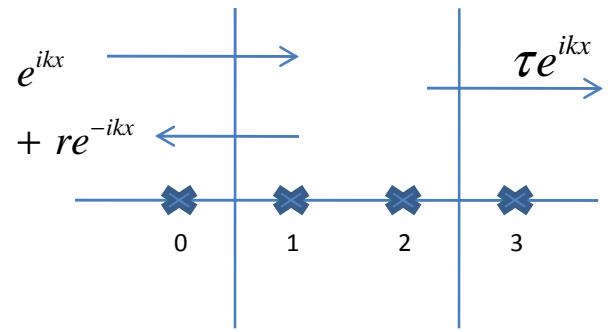
Σ Coupling with two contacts (complex matrix)

H Hamiltonian (real matrix)

S Source matrix

$$\{\phi\} = [G][s]$$

$$[G] = [EI - H - \Sigma]^{-1}$$



$$H = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

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

$$\begin{aligned} E\psi_1 &= \varepsilon\psi_1 + t\psi_2 + t\psi_0 \\ E\psi_2 &= \varepsilon\psi_2 + t\psi_1 + t\psi_3 \end{aligned}$$

$$E \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

$$\psi_2 \sim e^{ik2a}$$

$$\psi_3 \sim e^{ik3a}$$

$$\therefore \psi_3 \sim \psi_2 e^{ika}$$