Fundamentals of Nanoelectronics

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Lecture 36: Coherent Transport

Ref. Chapter 9.1

Network for Computational Nanotechnology

nanoHUB
online simulations and more

Coherent Transport
General Current Equation

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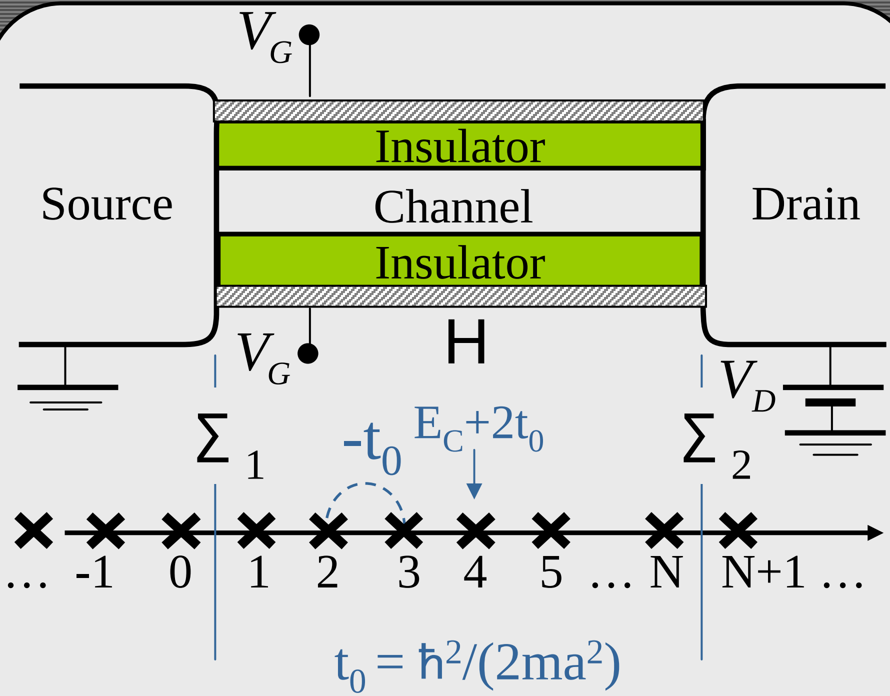

Minimum Contact Resistance

$$R = \frac{h}{2q^2 M}$$

- In the last few lectures we've been discussing coherent transport where electrons go through the channel without loosing energy or dissipating heat.
- Using the general form, current can be calculated as follows:

$$G(E) = \left(EI - H - \Sigma_1 - \Sigma_2\right)^{-1}$$

$$A = i(G - G^+)$$

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^+)$$

$$\Gamma_2 = i(\Sigma_2 - \Sigma_2^+)$$

$$\boxed{I = \frac{2q}{h}\int dE\,\overline{T}(E)\left(f_1(E) - f_2(E)\right)}$$

$$\overline{T}(E) = Trace\left(\Gamma_1 G \Gamma_2 G^+\right)$$

Wire With a Delta Function Potential

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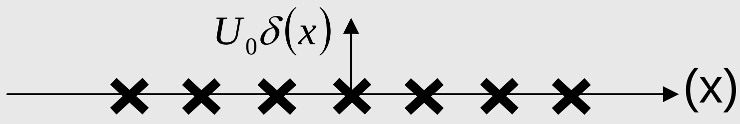
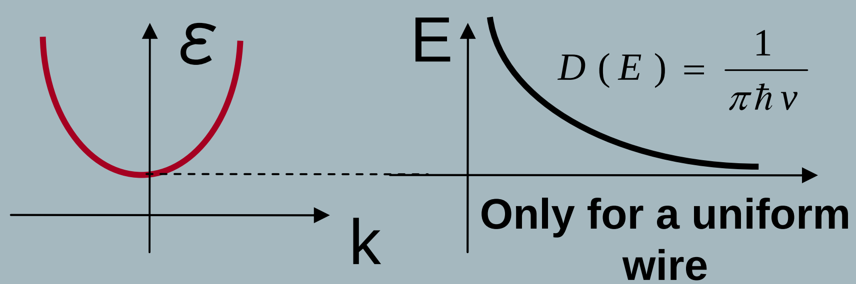




Schrödinger Equation

$$\left[E_c-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right]\psi(x)=E\psi(x)$$

Since there is a non-zero potential at x=0, the general solution for the wire cannot be written as plane waves. Every where else the wire is uniform and solutions to the Schrödinger equation can be written in the form of plane waves.($e^{\pm ikx}$)

- Using the general form, current can be calculated as follows:

$$G(E)=\left(EI-H-\Sigma_1-\Sigma_2\right)^{-1}$$

$$A=i(G-G^+)$$

$$\Gamma_1=i(\Sigma_1-\Sigma_1^+)$$

$$\Gamma_2=i(\Sigma_2-\Sigma_2^+)$$

$$\boxed{I=\frac{2q}{h}\int dE\bar{T}(E)\left(f_1(E)-f_2(E)\right)}$$

$$\bar{T}(E)=Trace\left(\Gamma_1 G\Gamma_2 G^+\right)$$

Wire With a Delta Function Potential

17:30

- For a uniform 1-D wire we have:

$$\left[E_c - \frac{\hbar^2}{2m_c}\frac{d^2}{dx^2} + U(x)\right]\psi(x) = E\psi(x)$$

- Based on the discrete lattice above Schrödinger equation becomes a matrix equation.

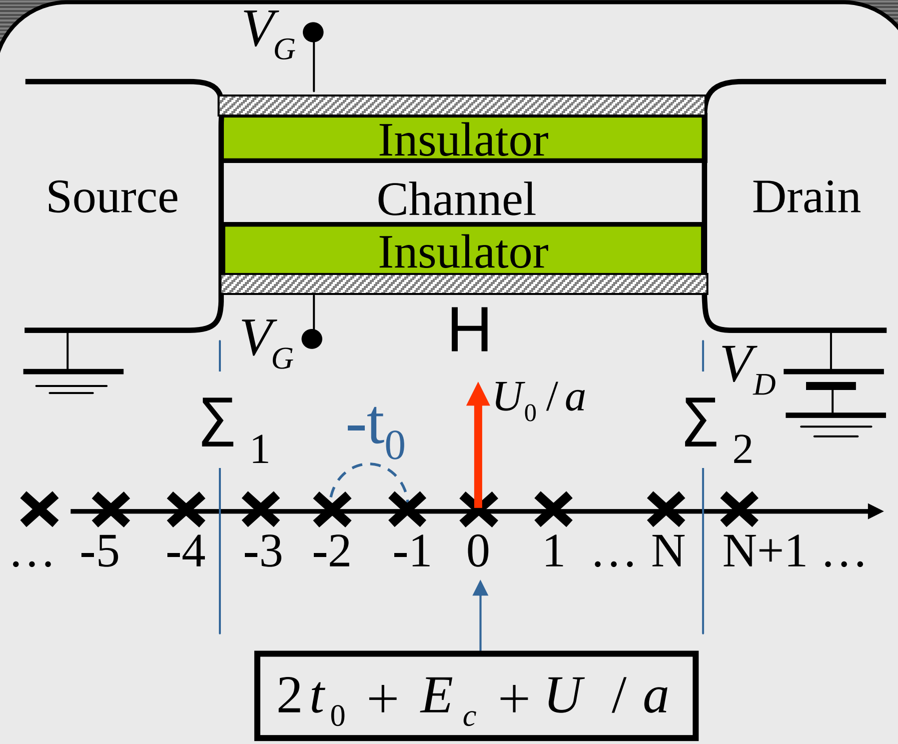
Continuous	Discrete

$$\psi(x) \rightarrow \psi_{-1}, \psi_0, \psi_1, etc.$$

- The Hamiltonian is tri diagonal

$$H = \begin{bmatrix} 2t_0 & -t_0 & 0 & \cdots & \cdots & -t_0 \\ -t_0 & 2t_0 & -t_0 & 0 & \cdots & \vdots \\ 0 & -t_0 & \ddots & \ddots & & \vdots \\ \vdots & 0 & \ddots & \ddots & & \vdots \\ \vdots & \vdots & & & \ddots & -t_0 \\ -t_0 & \cdots & \cdots & \cdots & -t_0 & 2t_0 \end{bmatrix}$$

$$t_0 = \hbar^2 / 2ma^2$$



$$\int \delta(x)dx = 1$$

Continuous	Discrete
$\delta(x) \rightarrow$	$\frac{1}{a}$

Sigma Matrices For 1D Leads

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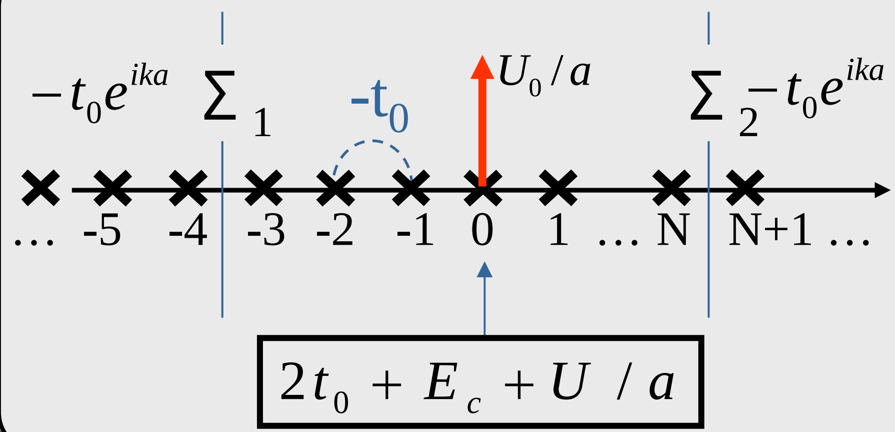


$$\Sigma_1 = \begin{bmatrix} -t_0 e^{ika} & & \\ & & \\ & & \end{bmatrix}$$

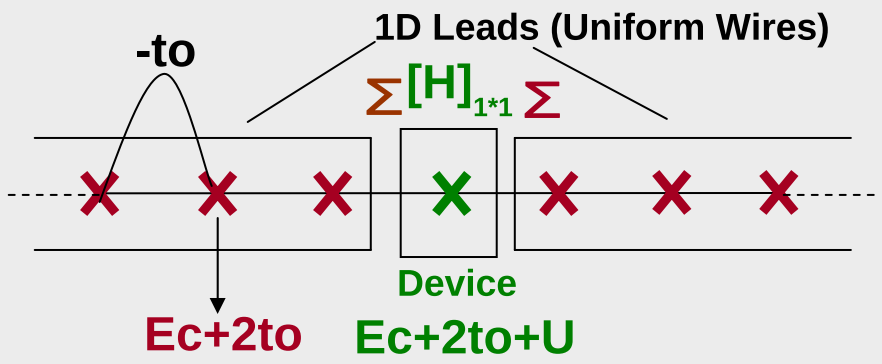
$$\Sigma_2 = \begin{bmatrix} & & \\ & & \\ & & -t_0 e^{ika} \end{bmatrix}$$

- The sigma's can be written as:

Example

Simple example of a device with only one lattice point:

- **Small One Level Device**



$$[H] = E_c + 2t_0 + \frac{U_0}{a}$$

$$\left.\begin{aligned}[\Sigma_1(E)] &= -t_0 e^{ika} \\ [\Sigma_2(E)] &= -t_0 e^{ika}\end{aligned}\right\} \quad \text{where: } \begin{aligned} E &= E_c + 2t_0(1-\cos ka) \\ &= E_c + 2t_0 - t_0 e^{ika} - t_0 e^{-ika} \qquad (1)\end{aligned}$$

$$G(E) = \left(EI - H - \Sigma_1 - \Sigma_2\right)^{-1} = \frac{1}{E - E_c - 2t_0 - \frac{U}{a} + t_0 e^{ika} + t_0 e^{ika}}$$

Using (1) →

$$= \frac{1}{-t_0 e^{ika} - t_0 e^{-ika} - \frac{U}{a} + t_0 e^{ika} + t_0 e^{ika}} = \frac{1}{-\frac{U}{a} + 2it_0 \sin ika}$$

Example: Green's Function

$$[H] = E_c + 2t_0 + \frac{U_0}{a}$$

$$\left.\begin{aligned}[\Sigma_1(E)] &= -t_0 e^{ika} \\ [\Sigma_2(E)] &= -t_0 e^{ika}\end{aligned}\right\} \text{where: } \begin{aligned} E &= E_c + 2t_0(1-\cos ka) \\ &= E_c + 2t_0 - t_0 e^{ika} - t_0 e^{-ika} \qquad (1)\end{aligned}$$

$$G(E) = \left(EI - H - \Sigma_1 - \Sigma_2\right)^{-1} = \frac{1}{E - E_c - 2t_0 - \frac{U}{a} + t_0 e^{ika} + t_0 e^{ika}}$$

Using (1) →

$$= \frac{1}{-t_0 e^{ika} - t_0 e^{-ika} - \frac{U}{a} + t_0 e^{ika} + t_0 e^{ika}} = \frac{1}{-\frac{U}{a} + 2it_0 \sin ika} \qquad (2)$$

- In a 1D wire we find the velocity ca be written as: $\begin{cases} E = E_c + 2t_0(1-\cos ka) \\ v = \frac{1}{\hbar}\frac{dE}{dk} = \frac{a}{\hbar} 2t_0 \sin ka \quad (3) \end{cases}$

- Finally substituting 3 in 2 we can write G as: $G = \frac{1}{-\frac{U}{a} + \frac{\hbar}{a} iv} \Rightarrow$

$$\boxed{G(E) = \frac{a}{i\hbar v - U}}$$

Spectral Function
Transmission

- The spectral function can be found from G: $\boxed{G(E) = \dfrac{a}{i\hbar v - U}}$

$$A = i(G - G^{+}) = ia\left(\frac{1}{i\hbar v - U} - \frac{1}{-i\hbar v - U}\right) = ia\left(\frac{1}{i\hbar v - U} + \frac{1}{i\hbar v + U}\right)$$

$$\boxed{A(E) = \frac{2a\hbar v}{\hbar^2 v^2 + U^2}}$$

- We can find transmission using: $\overline{T}(E) = Trace\left(\Gamma_1 G \Gamma_2 G^{+}\right)$

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^{+}) \qquad \Gamma_2 = i(\Sigma_2 - \Sigma_2^{+}) \qquad \sum_1 = \sum_2 = -t_0 e^{ika}$$

$$\Gamma_1 = \Gamma_2 = i\left(-t_0 e^{ika} + t_0 e^{-ika}\right) = -it_0\left(2i \sin ka\right) \overset{\textbf{(3)}}{=} \frac{\hbar v}{a}$$

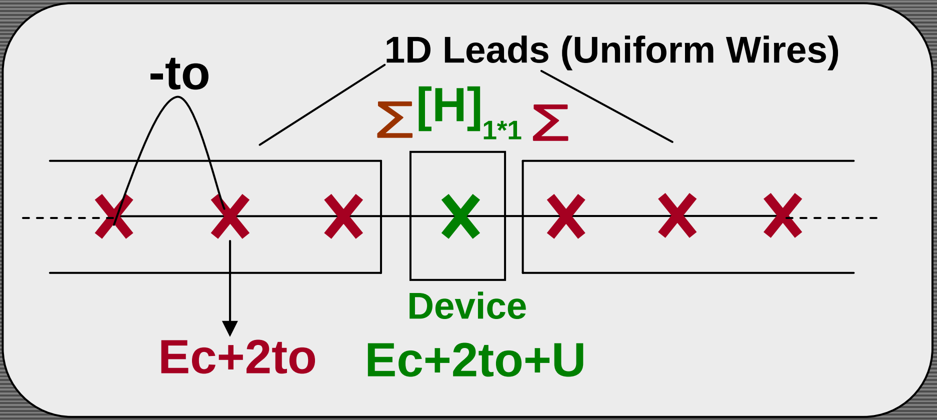
$$\boxed{\begin{aligned} E &= E_c + 2t_0\left(1 - \cos ka\right) \\ v &= \frac{1}{\hbar}\frac{dE}{dk} = \frac{a}{\hbar} 2t_0 \sin ka \quad \textbf{(3)} \end{aligned}}$$

$$\overline{T}(E) = Trace\left(\Gamma_1 G \Gamma_2 G^{+}\right) = \left(\frac{\hbar v}{a}\right)^2 \frac{a^2}{\hbar^2 v^2 + U^2} \Rightarrow \boxed{T = \frac{\hbar^2 v^2}{U^2 + \hbar^2 v^2}}$$

What happens to transmission when U=0?

44:55

$$T = \frac{\hbar^2 v^2}{U^2 + \hbar^2 v^2}$$



- When U=0, T=1 from the formula above. Physically, electron is really passing through a uniform wire and we expect the transmission to be 1.

• <u>Green's Function Method</u>

- Advantage: Having a new problem, one can derive the answers quickly without having to go through the detailed physics.

- Disadvantage: One can calculate every thing without really understanding anything.

What happens to spectral function when U=0?

46:10

- Local density of states can be found from the spectral function:

$$A(E) = \frac{2a\hbar v}{\hbar^2 v^2 + U^2}$$

$$LDOS\ (E) = \frac{A(E)}{2\pi} = \frac{1}{\pi}\frac{a\hbar v}{\hbar^2 v^2 + U^2}$$

- Again if we set U=0 we get the old result that we found for a 1D wire:

$$D(E) = \frac{1}{\pi\hbar v}$$