Quantum Transport:
Atom to Transistor

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Lecture 31: Transmission
Ref. Chapter 9.5

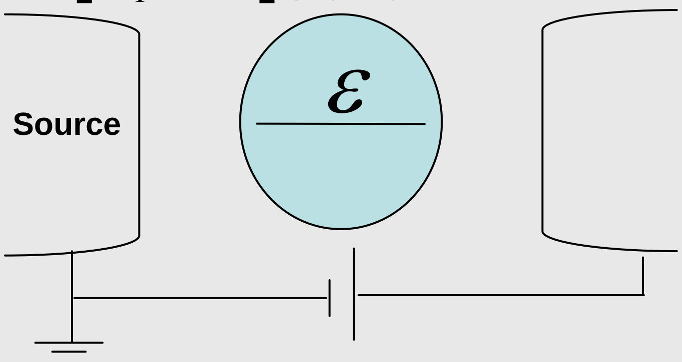
Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

Transmission

00:00

$$\left[\Sigma_1(E)\right] \quad \underset{\text{Channel}}{\left[H\right]} \quad \left[\Sigma_2(E)\right]$$



General Multi-level Devices

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

$$[\rho] = \int \frac{dE}{2\pi}\left(\left[G\Gamma_1 G^+\right] f_1 + \left[G\Gamma_2 G^+\right] f_2\right)$$

$$I = -\frac{q}{h}\int dE \; \bar{T}(E)\,(f_1 - f_2)$$

Transmission Focus of this Lecture

One Level Device

$$N = \int dE D_\varepsilon(E)\,\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

$$I = -\frac{q}{\hbar}\int dE \underbrace{\boxed{D_\varepsilon(E)\,\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}}}_{T(E)/2\pi}(f_1 - f_2)$$

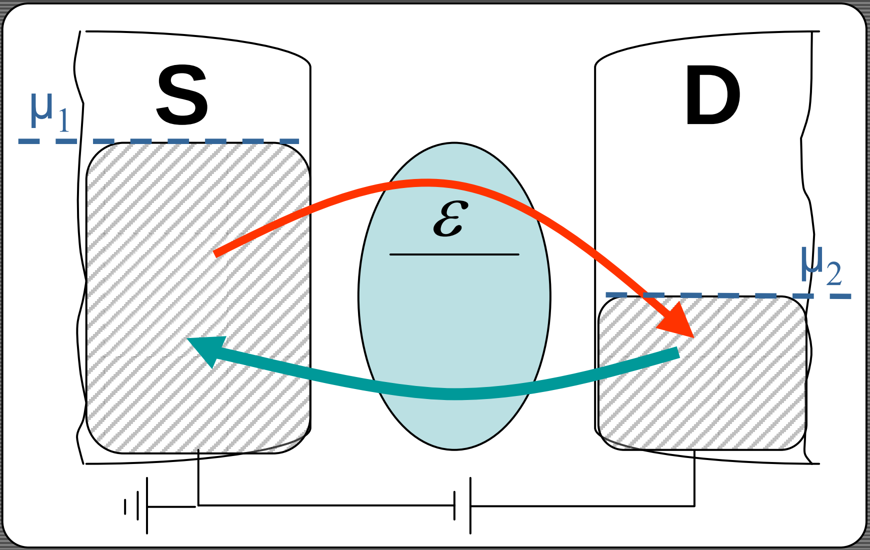
$$\bar{T}(E) = Trace\left(\Gamma_1 G \Gamma_2 G^+\right)$$

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

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

Transmission (physical meaning)

08:40



Two Counter Propagating Fluxes

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

$\overline{T}(E)f1$ **Flux from left to right**

$\overline{T}(E)f2$ **Flux from right to left**

• The way to think of T(E)*f is that T tells us how much electron will flow when there are electrons available in the reservoirs. What tells us the availability of electrons is f.

• **Transmission: How easily an electron transmits from left to right or vice versa.**

• Current is really a measure of how easily electrons can get from left to right or vice versa. Easy transmission should result in low resistance and lots of current. Therefore it makes sense for the current to be proportional to transmission.

Wire with a Delta Function Scatterer

10:30

Incident wave from left

e^{ikx} $\longrightarrow$ $\quad U_0\delta(x)$

re^{-ikx} $\longleftarrow$ $\quad \longrightarrow$ te^{ikx} (x)

t: Transmission amplitude

T: Transmission Probability $T = |t|^2$

Engineering versus Physics

Physics: e^{+ikx} $\quad e^{-i\omega t}$

Engineering: e^{-jkx} $\quad e^{+j\omega t}$

In this course, we use physics convention.

- Schrödinger Equation

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

($U(x)=0$ for $x \neq 0$)
With this potential, the wire is uniform and solutions to the Schrödinger equation can be written in the form of plane waves.($e^{\pm ikx}$)

- Note that since both e^{ikx} and e^{-ikx} satisfy Schrödinger equation which is linear, any linear combination of them also satisfies the equation.
- Dispersion Relation: $E = E_c + \hbar^2 k^2 / 2m$
- Now that we have the solution on the left and right, the challenge is to find the solution at x=0. Note that the Schrödinger equation must be satisfied everywhere.

Continuity of the wave function

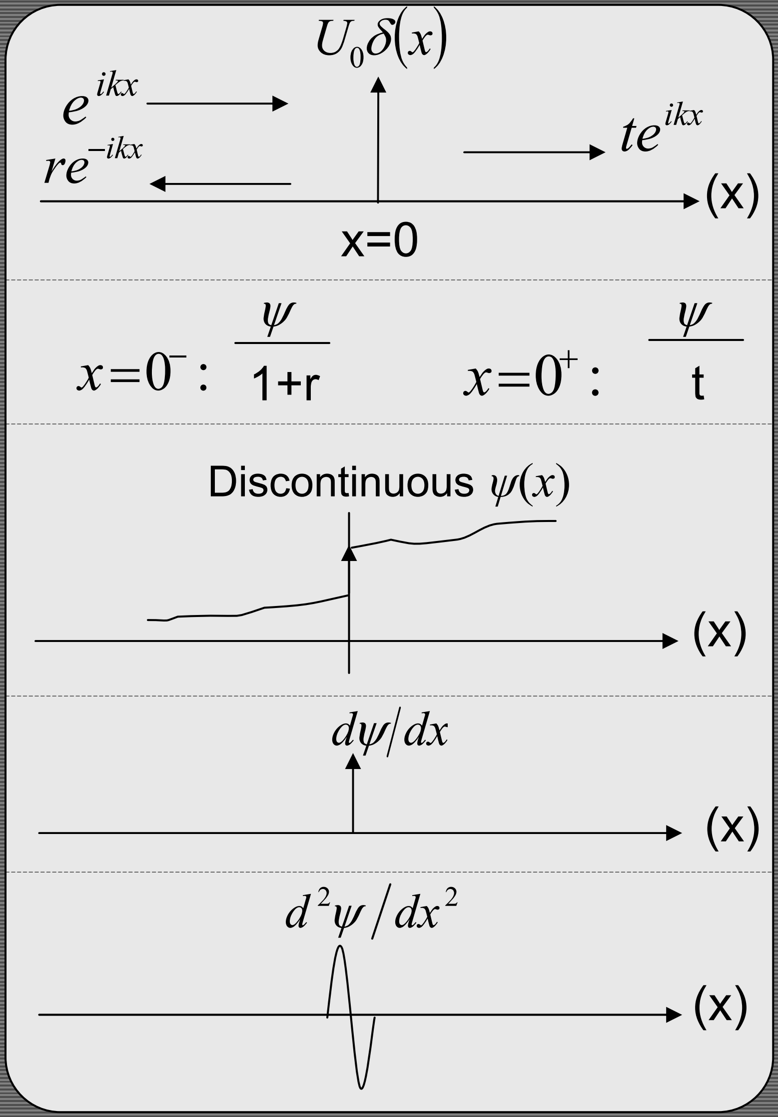
- Here is the key point for solution at x=0:

$$\boxed{\psi \text{ is always continuous.}}$$

- The requirement is that Schrödinger equation must be satisfied every where. What happens if the wave function is not continuous? See the right side:

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

- When ψ is discontinuous, its first derivative is a delta function and its second derivative is a doublet function.
- If the second derivative is a doublet function and the rest of quantities in the Schrödinger Equation are normal functions, then there is no way for the Schrödinger Equation to be satisfied at that point



Discontinuity of dψ/dx

22:00

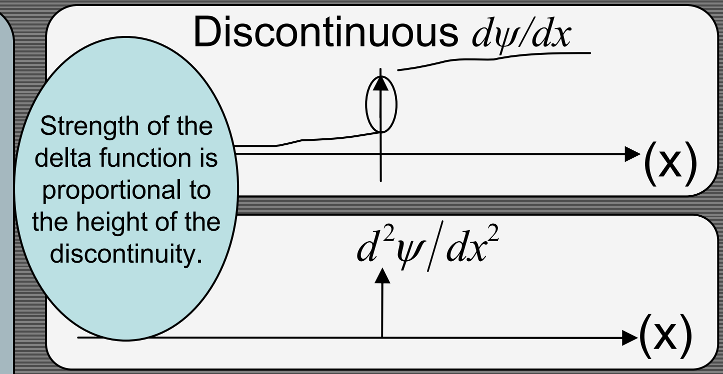
• Since the wave function is continuous across the point x=0, we have: **1+ r = t**

• But what happens to the derivative of ψ? And does it have to be continuous at x=0?

	ψ		ψ
$x = 0^{-}$:	1+r	$x = 0^{+}$:	t
	$d\psi/dx$		$d\psi/dx$
$x = 0^{-}$:	ik(1 - r)	$x = 0^{+}$:	ikt

• Notice that a discontinuous $d\psi/dx$ will result in a delta function for the second derivative which is infinite at x=0. Now if U(x) was a normal function, Schrödinger equation would not be satisfied; hence we would conclude that $d\psi/dx$ has to be continuous at x=0. And therefore we would set ik(1-r) equal to ikt. However,

• U(x) is not a normal function in our example. It is a delta function. So in the case of discontinuous $d\psi/dx$, Schrödinger Equation would have two delta functions in it, which would cancel each other and thus the equation would be satisfied.



• Height of the discontinuity must be such that it results in a delta function with a strength exactly equal to the scatterer so that they would cancel each other out.

Discontinuity of dψ/dx

25:30

- Schrödinger equation for our problem:

$$-\frac{\hbar^2}{2m}\left[ikt - ik(1-r)\right]\cancel{\delta}(x) + U_0\cancel{\delta}(x)\psi(x) = 0$$

- So, $-\frac{\hbar^2}{2m} ik(t-1+r) + U_0 t = 0$
- We also have 1 + r = t.
- Having 2 equations and 2 unknowns, we can solve for r & t.

$$\left.\begin{array}{l}\frac{\hbar^2}{2m} ik(t-1+r) = U_0 t \\ r = t - 1\end{array}\right\} \quad t = \frac{i\hbar v}{U_0 + i\hbar v}, \left(v = \frac{\hbar k}{m}\right)$$

- For an electron with a large velocity, U0 is negligible and t = 1. Low velocity will result in a small transmission.

$$T = |t|^2 = \frac{\hbar^2 v^2}{U_0^2 + \hbar^2 v^2}$$

- A point on dimensions

$$\hbar\omega \to eV$$

$$\hbar v \to eV \cdot m$$

- U_0 has the dimension of eV-m.

$$U(x) = U_0\delta(x)$$

$$\int dx\,\delta(x) = 1 \Rightarrow \delta(x) \to m^{-1}$$

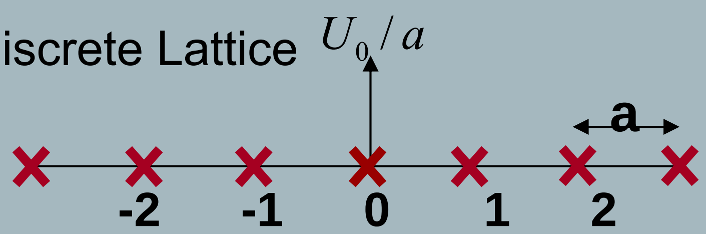
$$U_0 \to eV \cdot m$$

- Thus far we've assumed that x was continuous; however in practice x is discrete. Differential Equations have discrete representations and differential operators become matrix operator.
- We'll solve the same problem for a discrete lattice.

Discontinuous Case
Discrete Lattice

33:30

• Discrete Lattice



• The differential equation now becomes a matrix equation. Also,

Continuous	Discrete

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

• Schrödinger equation at point x=0:

$$\left(E_c + 2t_0 + \frac{U_0}{a}\right)\psi_0 - t_0\psi_{-1} - t_0\psi_1 = E\psi_0$$

$$t_0 = \frac{\hbar^2}{2ma^2}$$

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

• The idea is that out in the lead, we know how ψ_{-1} and ψ_{+1} look like and by relating them to ψ_0, we eliminate them to find an expression for ψ_0.

$$\left(E_c + 2t_0 + \frac{U_0}{a}\right)\psi_0 - t_0\psi_{-1} - t_0\psi_1 = E\psi_0$$

At x = 0$^+$

$$\left.\begin{aligned}\psi_0 &= t \\ \psi_{+1} &= te^{ika}\end{aligned}\right\} -t_0\psi_{+1} = -t_0 e^{ika}\psi_0$$

$$\left(E_c + 2t_0 + \frac{U_0}{a} - t_0 e^{ika}\right)\psi_0 - t_0\psi_{-1} = E\psi_0$$

• Eliminating ψ-1 is harder because of the presence of both the incident and the reflected wave.

At x = 0$^-$

$$\left.\begin{aligned}\psi_0 &= 1 + r \\ \psi_{-1} &= e^{-ika} + re^{+ika}\end{aligned}\right\} \psi_{-1} = \psi_0 e^{+ika} + e^{-ika} - e^{+ika}$$

• Substituting for ψ-1, we have:

Discontinuous Case
Discrete Lattice

- Finally, putting ψ^{-1} and ψ^{+1} in terms of ψ^{0} will give us:

$$\left(E_c + 2t_0 + \frac{U_0}{a} - t_0 e^{ika} - t_0 e^{ika}\right)\psi_0 - t_0(e^{-ika} - e^{+ika}) = E\psi_0$$

- Grouping the similar terms, we have:

$$\left[E - \left(E_c + 2t_0 + \frac{U_0}{a} - t_0 e^{ika} - t_0 e^{ika}\right)\right]\psi_0 = t_0\left(e^{ika} - e^{-ika}\right)$$

$$t_0\left(e^{ika} - e^{-ika}\right) = 2it_0 \sin ka$$

- But sin(ka) is really the velocity in a discrete lattice because:

$$E = E_c + 2t_0(1 - \cos ka)$$

- And

$$\hbar v = \frac{\partial E}{\partial k} = 2at_0 \sin ka$$

- We then have: $2it_0 \sin ka = i\hbar v$

$$\underbrace{\left[E - \left(E_c + 2t_0 + \frac{U_0}{a} - t_0 e^{ika} - t_0 e^{ika}\right)\right]}_{\frac{U_0 + i\hbar v}{a}}$$

- Finally, $\psi_0 = t = \dfrac{i\hbar v}{U_0 + i\hbar v}$

Same as before

- The important thing to note is that the matrix equations mentioned earlier generalize the procedure that was done here. Therefore, one does not have to go through this again and again.
- See next page to find out about the correspondence and similarities.

Use of General Matrix Equations

$$G = (EI - H - \Sigma_1 - \Sigma_2)^{-1} \longrightarrow \left[\underbrace{E}_{\mathrm{E}} - \left(\underbrace{E_c + 2t_0 + \frac{U_0}{a}}_{\mathrm{H}} \underbrace{- t_0 e^{ika}}_{\Sigma_1} \underbrace{- t_0 e^{ika}}_{\Sigma_2}\right)\right]^{-1}$$

- We've just derived the equations for a 1D wire. What we want is to derive the general equations for any device with a specified Hamiltonian which is in contact with some two contacts having any general Σ_1 and Σ_2.

- Once we have the general equations, it is then easy to directly get answers. For instance if we want transmission, what we'll do is:

$$\boxed{2t_0 \sin ka = \hbar v} \quad \overline{T}(E) = Trace\,(\Gamma_1 G \Gamma_2 G^+) \quad \boxed{\hbar v = 2t_0 \sin ka}$$

$$\times\,\mathbf{-1} \qquad \hbar v \left(\frac{1}{U_0 + i\hbar v} \; \frac{1}{U_0 - i\hbar v} \right) \hbar v \qquad \times\,\mathbf{-1}$$

$$\Gamma_1 = i(\Sigma_1 - \Sigma_1^+),\ \Gamma_2 = i(\Sigma_2 - \Sigma_2^+)$$

Green's Function Method

- So if we'd just made a use of $\overline{T}(E) = Trace(\Gamma_1 G \Gamma_2 G^+)$ and applied it blindly to this problem we would have gotten the right answer, namely:

$$T = \frac{\hbar^2 v^2}{U_0{}^2 + \hbar^2 v^2}$$

- The power of using Green's function is that once one has derived the equations and is familiar with them, the they can be used to solve any problem in a fairly straight forward manner.

Green's Function Method

- 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.

- Next day, we'll derive:

$$[\rho] = \int \frac{dE}{2\pi}\left(\left[G\Gamma_1 G^+\right]f_1 + \left[G\Gamma_2 G^+\right]f_2\right)$$