Fundamentals of Nanoelectronics

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Lecture 37: Wave Function vs. Green's Function

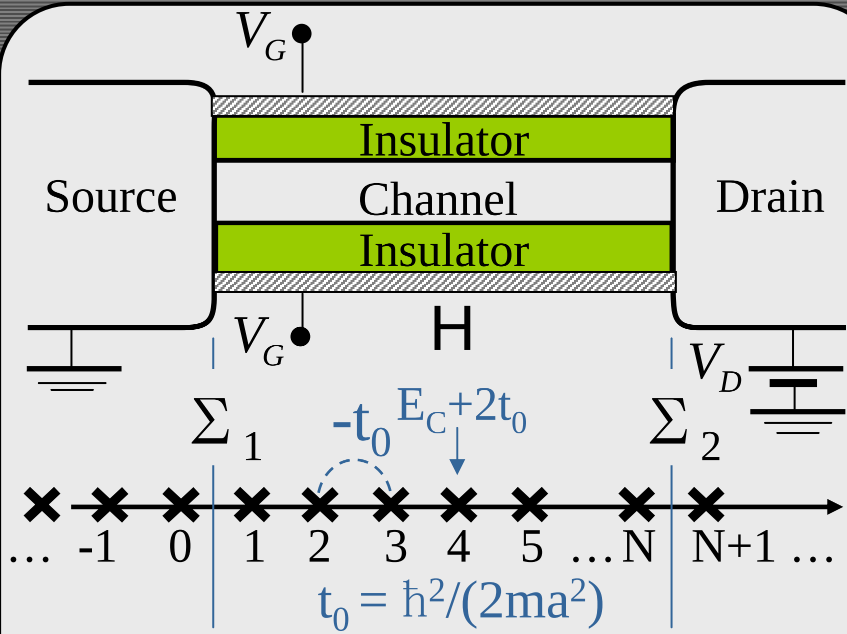
Ref. Chapter 9.1

Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

Review

00:05



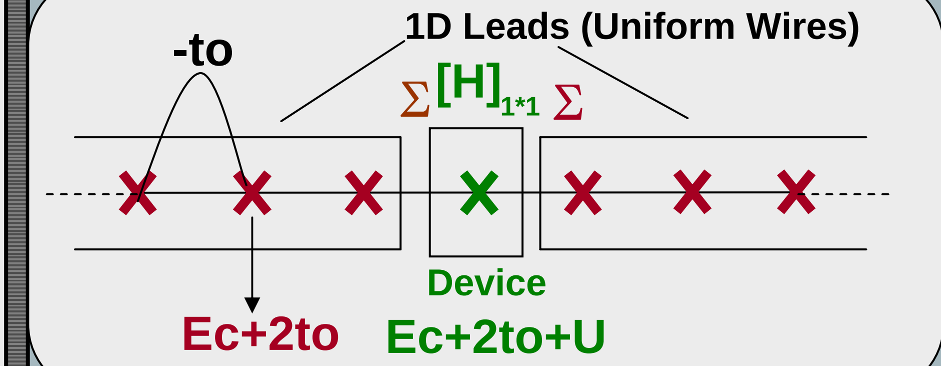
$$I = \frac{2q}{h}\int dE\,\overline{T}(E)\big(f_1(E) - f_2(E)\big)$$

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

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

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

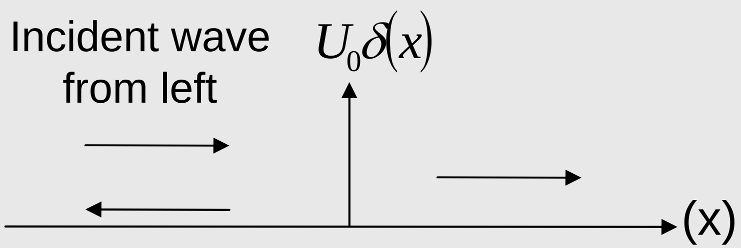
- In the last few lectures we've been discussing coherent transport where electrons go through the channel without loosing energy or dissipating heat. For such a condition we calculated the current (please see left). That in turn requires calculating the transmission T. IN the last session we computed this for a simple case of a uniform wire with one delta function potential at x=0:



$$\overline{T}(E) = \frac{\hbar^2 v^2}{U^2 + \hbar^2 v^2}$$

Overview

- There is another approach to the simple example that we did last time. In this method, we view electrons as waves incident on the delta function potential (located at x=0) from left (right). We then use the Schrödinger equation calculate the transmission amplitude. Transmission probability is the squared module of transmission amplitude. Although this method gives us good physical insight about the problem, it won't be convenient for real practical problems.



t: Transmission amplitude

T: Transmission Probability

$$T = |t|^2$$

From last time:

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

Incident Wave From Left

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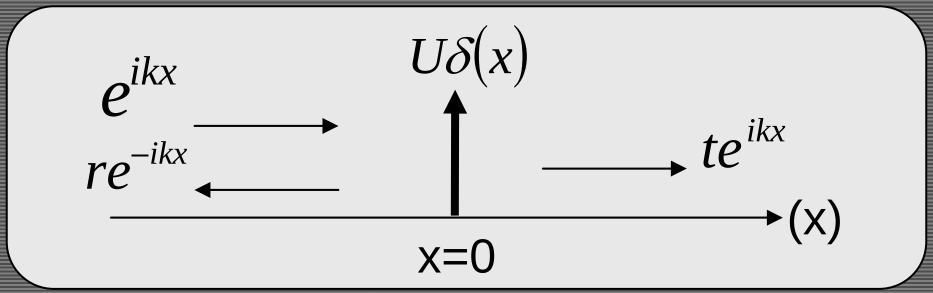


- **Schrödinger Equation**

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

($U(x)=0$ 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 given that the following holds:
- Dispersion Relation: $E=\hbar^2k^2/2m$
- 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.**

Can The Wave Function Be Discontinuous?

14:16

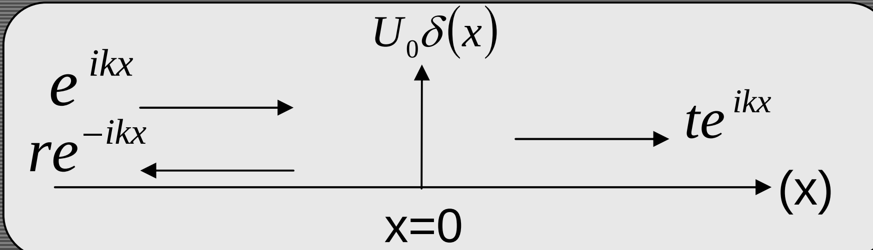
- Here is the key point for solution at x=0:

ψ 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:

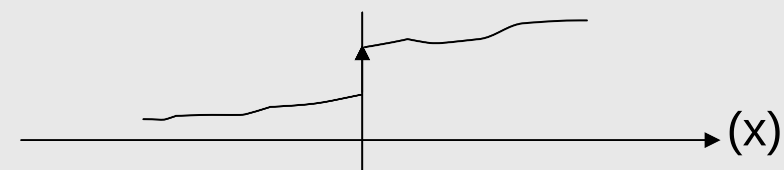
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right]\psi(x)=E\psi(x)$$

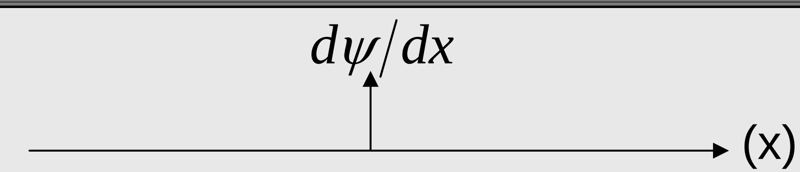
- When ψ is discontinuous, its first derivative is a delta function and its second derivative is a doublet function.
- If the second derivative is a doublet function and the rest of quantities in the Schrödinger Equation are normal functions, then there is no way for the Schrödinger Equation to be satisfied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

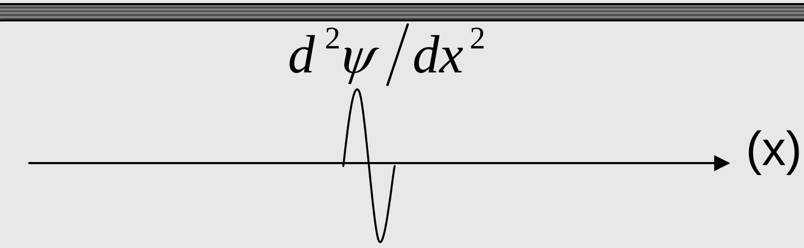


$x=0^-:\ \dfrac{\psi}{1+r}\qquad x=0^+:\ \dfrac{\psi}{t}$

Discontinuous







Discontinuity Of $d\Psi/dx$

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

$x = 0^-$: ψ = 1+r $x=0^+$: ψ = t

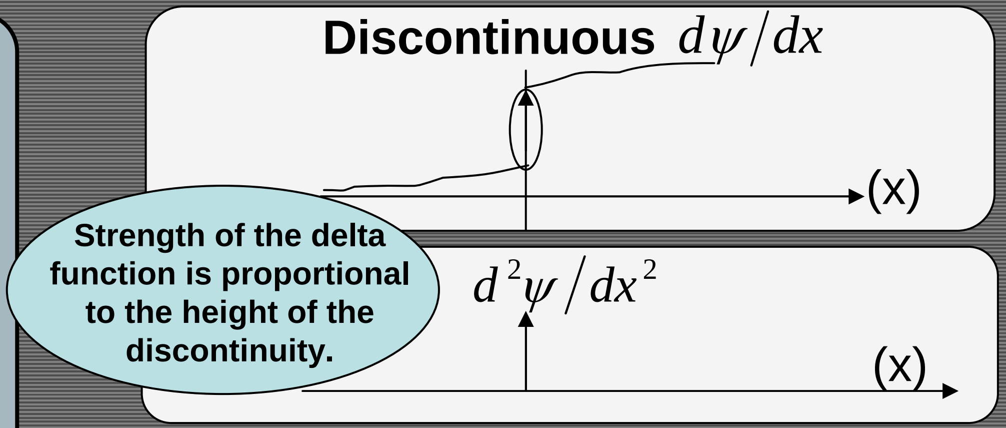
- But what happens to the derivative of ψ ?

And does it have to be continuous at x=0?

$x = 0^-$: $d\psi/dx$ = ik(1 - r) $x=0^+$: $d\psi/dx$ = 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.

2 Equations, 2 Unknowns

24:30

- Schrödinger equation for our problem:

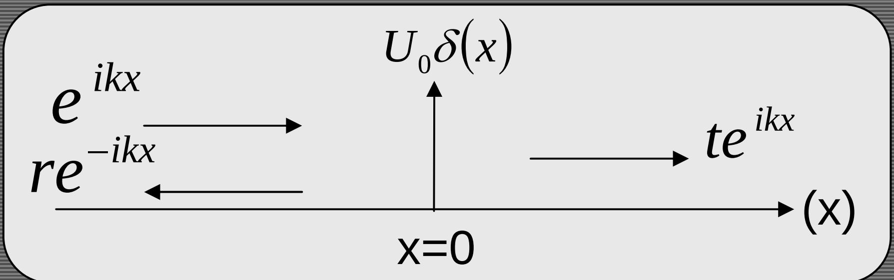
$$-\frac{\hbar^2}{2m}\left[ikt - ik(1-r)\right]\cancel{\delta(x)} + U\cancel{\delta(x)}\psi(x) = 0$$

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

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

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

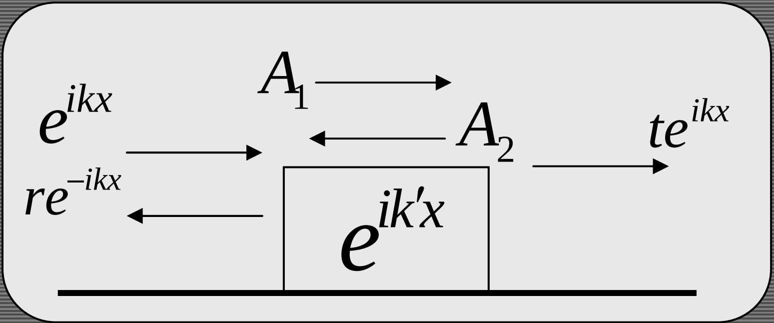
$$T = |t|^2 = \frac{\hbar^2 v^2}{U^2 + \hbar^2 v^2}$$



Arbitrary Potentials

32:45

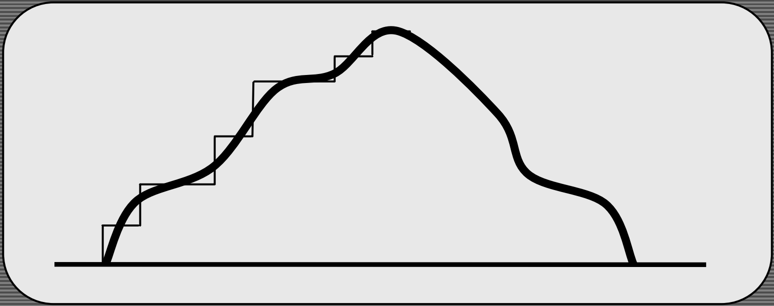
• For a potential barrier like the figure, again we have an incident wave from left. Parts of it transmits and parts of gets reflected. Since the potentials in the 3 different regions are constant, the solution can be written as plane waves in each region. Then by matching the boundary conditions at each boundary we can find the proper constants that multiply plane waves. Note that the boundary conditions at each boundary are that the wave function and its derivative must be continuous.



In each region

$$E = \hbar^2 k^2 / 2m + U$$

• For a complicated potential like the figure on the right, we first approximate it as piecewise constant potentials. Then it is the same story as above: the solutions at each region can be written as plane waves multiplied by unknown constants. The constants can be determined from the proper boundary conditions at each boundary.



Importance Of Transmission

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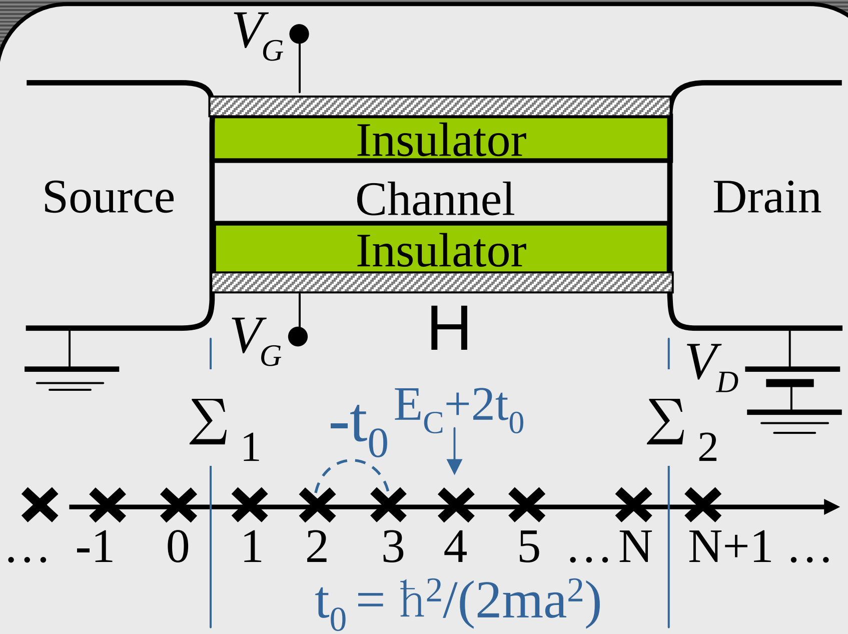

$$I = \frac{2q}{h}\int dE\,\bar{T}(E)\left(f_1(E) - f_2(E)\right)$$

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

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- Finally calculating the current for coherent transport boils down to calculating the transmission function. Once we have the transmission we can calculate the current form the equation on the left.

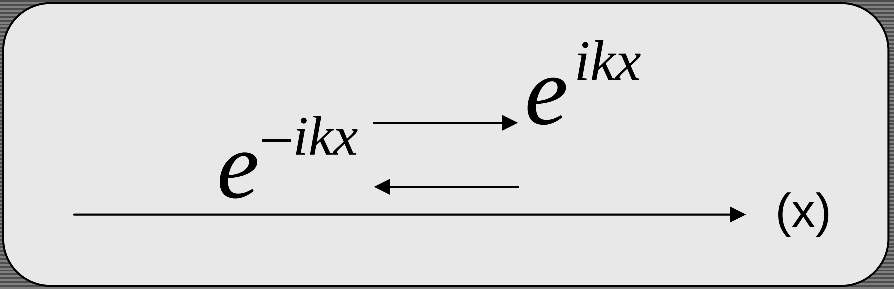
Two Different Conventions

40:28

- How do we figure put which plane wave goes to the right and which one goes to the left?
- Associates with each plane wave there is a time dependent part. If we represent the time dependent part as $e^{-iEt/\hbar}$ then the traveling wave functions can be written as:

$$\rightarrow e^{ik(x-vt)}$$

$$\leftarrow e^{-ik(x+vt)}$$



Engineering versus Physics

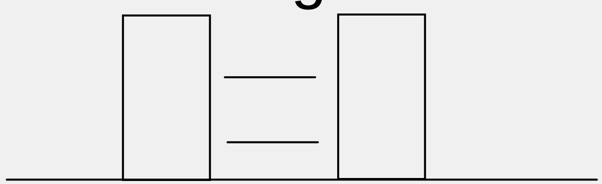
Physics:	e^{+ikx}	$e^{-iEt/\hbar}$
Engineering:	e^{-jkx}	$e^{+jEt/\hbar}$

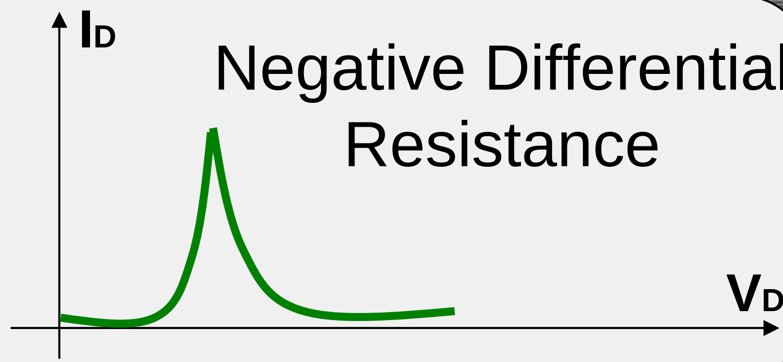
In this course, we use physics convention.

Negative Differential Resistance

45:42

Resonant Tunneling Diode





- Why does negative differential resistance happen?
- A voltage is applied to the two barrier device, the barrier and the Fermi level on the right start going down. Initially current increases for higher voltages. But there comes a point where the allowed energy levels in between the two barriers falls under the bottom edge of the allowed energy levels in the left contact. In this case since there is no energy level available for the electron coming from the left contact, current will drop to 0.