L3 Quantum transport

Sunday, September 5, 2021 12:09 AM

Lecture notes by Ethan Minot, visiting from Oregon State University
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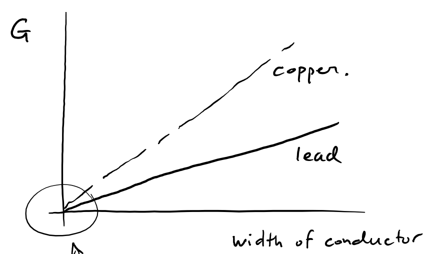
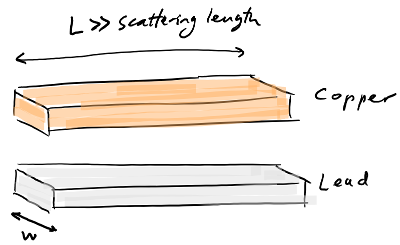
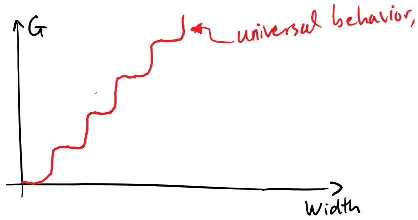
Nanoelectronics Class at Aalto University, Autumn, 2021.

$G = 1/R$





Zoom in to smallest w and make
L < scattering length

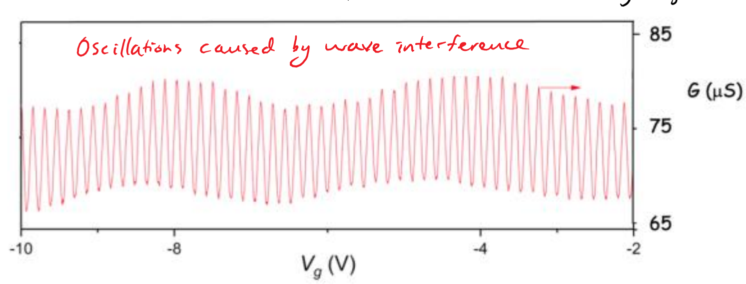


Nanometer size scales

Can't use semiclassical theory in this limit.

Another example of semiclassical treatment being insufficient

Data from a carbon nanotube (1d wire) with L < scattering length



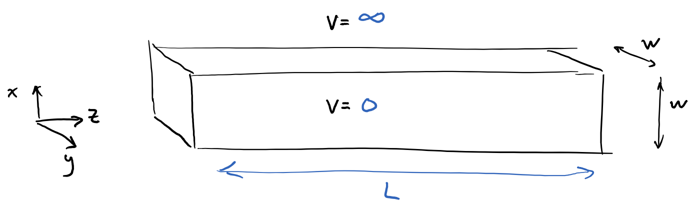
To describe such phenomena, we'll use the Landauer-Buttiker Formalism

$\boxed{\text{Step 1}}$ Use QM to determine the occupied "transverse modes" in a wire

$\boxed{\text{Step 2}}$ Calculate the conductance of each transverse mode when there is no scattering

$\boxed{\text{Step 3}}$ If necessary, account for scattering
- Back-reflection (stays in same mode)
- Scatter into different mode.

Step 1: Wire with square cross-section (easiest example to start with)



current flow

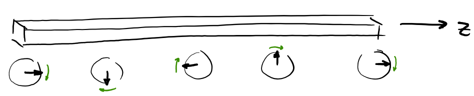
$$\Psi(x,y,z) = X(x)Y(y)Z(z) = \frac{1}{\sqrt{\text{volume}}} \underbrace{\sin\left(\frac{n_x \pi}{w} x\right) \sin\left(\frac{n_y \pi}{w} y\right)}_{\text{pick } n_x \,\&\, n_y} e^{ik_z z}$$

$Z(z) \leftarrow e^{ik_z \cdot z}$

Assume period B.C.s along z-dir

Allowed values of $k_z = \frac{2\pi}{L}, \frac{4\pi}{L}, \frac{6\pi}{L} \dots \quad \frac{2\pi}{L} n_z$

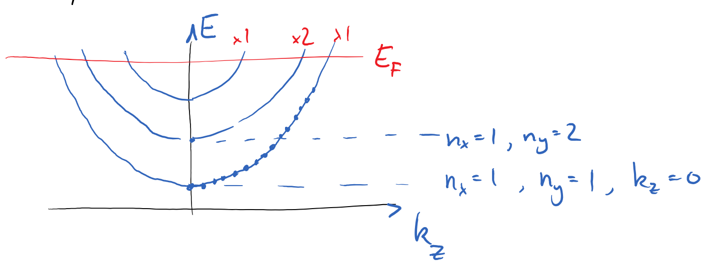
$e^{i\frac{2\pi}{L}z}$



Energy of a particular quantum state in the wire?

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left[\left(\frac{\pi n_x}{w}\right)^2 + \left(\frac{\pi n_y}{w}\right)^2 + k_z^2\right]$$

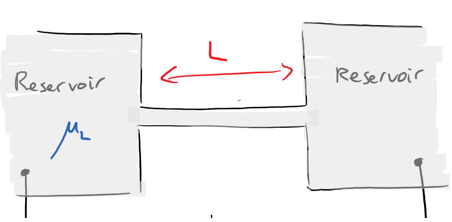
Draw the dispersion relation



n_x	n_y
1	1
1	2
2	1
2	2

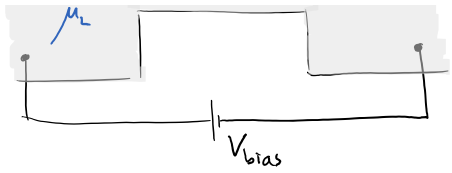
The number of occupied transverse modes depends on E_F.

Step 2: Conductance of via transverse modes (no scattering)

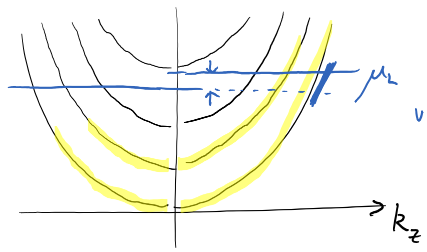


$$G = \frac{I}{V_{bias}}$$

V_{bias}



Occupied states



"Transport window"

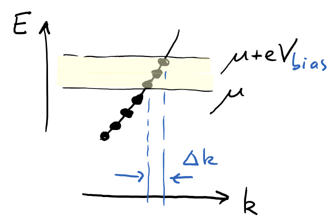
$$v = \frac{1}{\hbar}\frac{dE}{dk}$$

Imbalance of right movers to left movers increases with V_{bias}

Transverse modes with steeper slope ...

but fewer states in the transport window

Start with first mode $(n_x = n_y = 1)$



In the transport window, slope $= \left.\frac{dE}{dk}\right|_{\mu}$

$$\#\text{ of states in transport window} = 2\cdot\frac{\Delta k}{\frac{2\pi}{L}}$$

$$\Delta k = \frac{\Delta E}{\left(\frac{dE}{dk}\right)}$$

$$= \frac{\Delta E}{\left(\frac{dE}{dk}\right)}\,\frac{2L}{2\pi}$$

$$= \frac{2}{\left(\frac{2\pi}{L}\right)}\,\frac{eV_{bias}}{\left(\frac{dE}{dk}\right)}$$

Current carried by one occupied state

$$\frac{ev}{L} = \frac{e}{L}\,\frac{1}{\hbar}\,\frac{dE}{dk}$$

time to traverse the wire is $\frac{L}{v}$

Current carried by the transverse mode

$$I_{mode\,1} = \frac{2}{\left(\frac{2\pi}{L}\right)}\,\frac{eV}{\cancel{\left(\frac{dE}{dk}\right)}}\;\frac{e}{L}\,\frac{1}{\hbar}\cancel{\left(\frac{dE}{dk}\right)}$$

mode 1 $\left(\frac{2\pi}{L}\right)\left(\cancel{\frac{dE}{dk}}\right) \quad L \quad \hbar\left(\cancel{dk}\right)$

$=$

$= \frac{2e^2}{h} V_{bias}$

Current carried by next mode ($n_x = 1 \quad n_y = 2$)

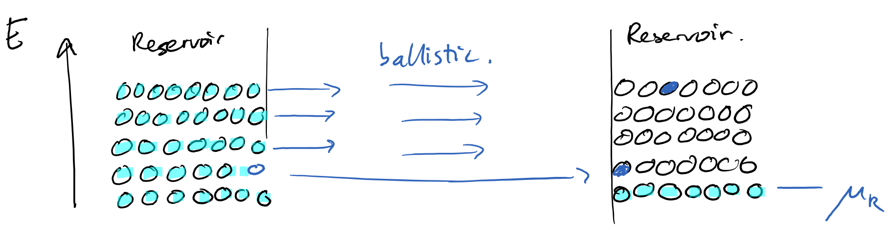
$$I_{mode\,2} = \frac{2e^2}{h} V_{bias}$$

Total current $= \frac{2e^2}{h} M \, V_{bias}$ where M is number of occupied modes.

Conductance $= \frac{\text{Total current}}{V_{bias}} = \underbrace{\frac{2e^2}{h}}_{\text{quantum of conductance.}} M$

The idea Power $= I V_{bias}$ there is power being dissipated in this system (Joule heating).

Not the wire itself.

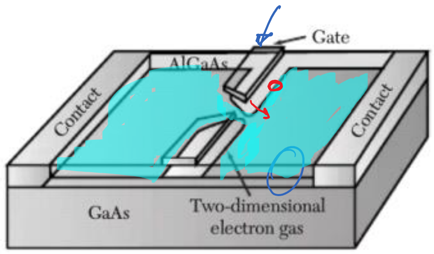


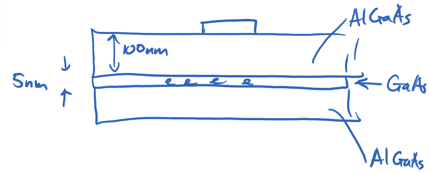
Summary: Energy dissipation happens around the contact between the ballistic wire and the reservoir.

2 famous experiments tuning the number of transverse modes.

2 famous experiments tuning the number of transverse modes.

2DEG





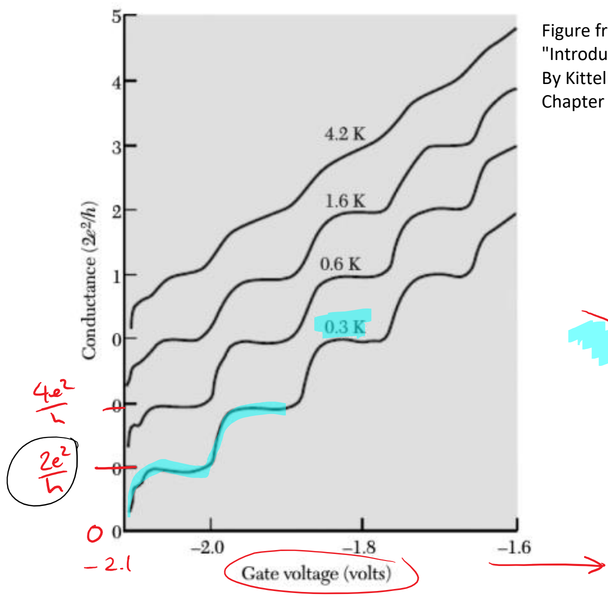
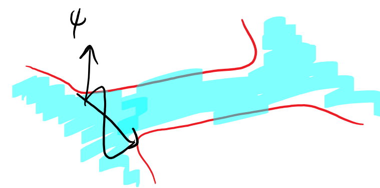


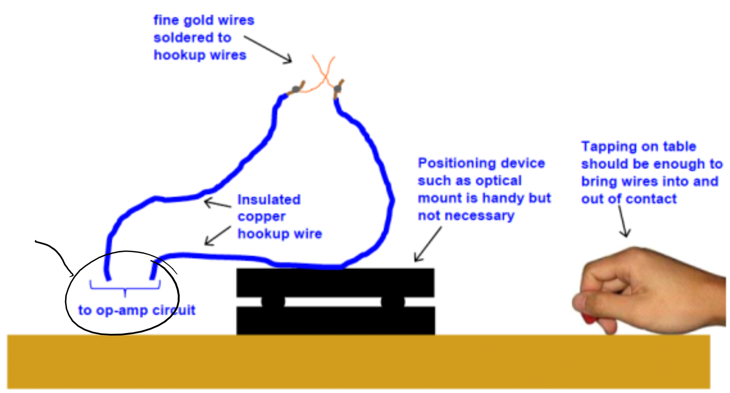
Figure from
"Introduction to Solid State Physics"
By Kittel
Chapter 18, Nanostructures

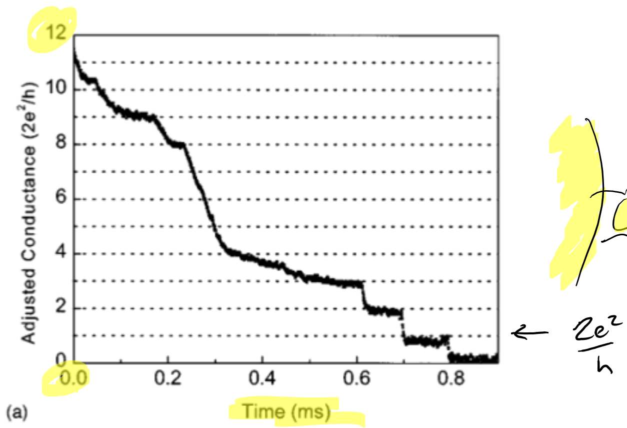


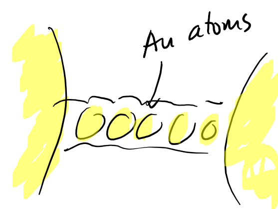
1989

10 year later.

Gold wire break junction



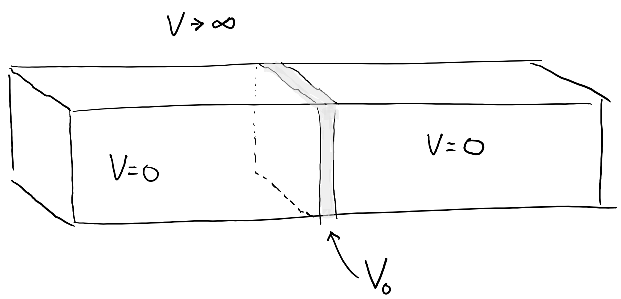


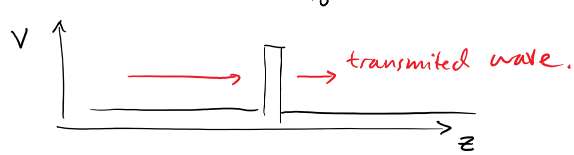


"An undergraduate laboratory experiment on quantized conductance in nanocontacts" Am. J. Phys. (1998)

"Formation and manipulation of a metallic wire of single gold atoms" Nature (1998)

What happens when there is a barrier in the conduction channel



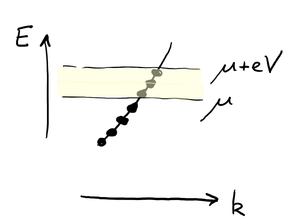


Transmission probability $\quad 0 < T < 1$

Each mode will have different T_n

$$G = \frac{2e^2}{h} M$$

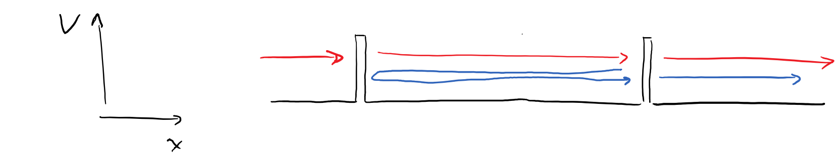
$$G = \frac{2e^2}{h} \sum T_n(E_F)$$



Sometimes an electron has a choice of 2 or more "paths" as it is transmitted through a wire.

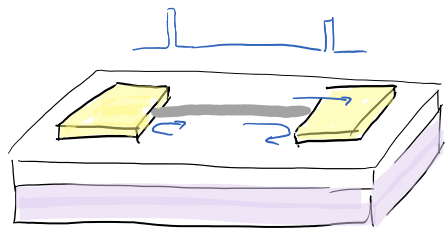
In such cases, $T_n(E_F)$ includes wave interference

Example 1



calculations must use probability amplitudes because relative phase accumulated on each path is critical.

Experimental realization
"Fabry - Perot interference in a nanotube electron waveguide"
Nature 2001



e.g. Two barries in series:

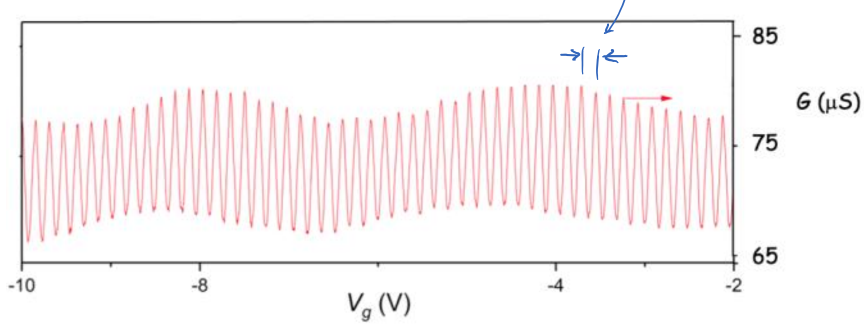
$$T(E_F) = \frac{|t_1|^2 |t_2|^2}{1 + |r_1|^2 |r_2|^2 - 2|r_1||r_2| \cos\phi}$$

← derive this total probability by using probability amplitudes t & r for each barrier

$$\phi = \phi_{r_2} + \phi_{r_1} + 2Lk_F$$

the value of ϕ changes when E_F changes.

$2Lk_F$ changes by 2π



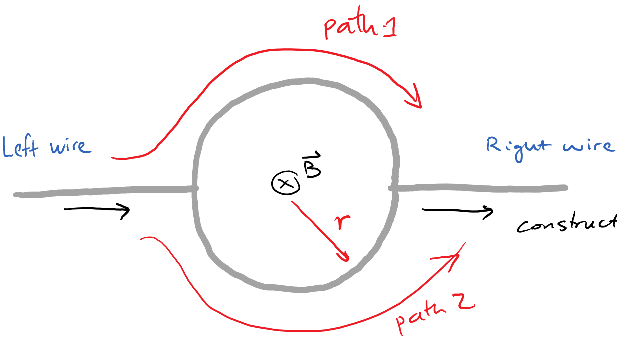
From the paper "Quantum Interferences in ultraclean CNTs" PRL (2021)

$|t_1|^2$ & $|t_2|^2 \simeq 1$ "open system"

Example 2 oscillating T with respect to B.

Known as Aharonov-Bohm effect, §4.1 of textbook.

(foundational idea that will come back for flux qubits & transmon qubits)



constructive or destructive ?

Calculate phase accumulated in path 1 & path 2

dynamic phase

Path 1 $\displaystyle\int_{\text{path 1}} \vec{k}\cdot d\vec{l} = \frac{\sqrt{2mE}}{\hbar}\pi r$ when $B = 0$

$$\frac{\sqrt{2mE}}{\hbar}\pi r - \frac{e}{\hbar}\int_{\text{path 1}} \vec{A}\cdot d\vec{l} \quad \text{when } B \neq 0$$

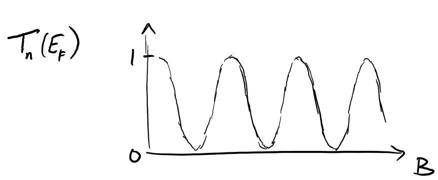
Phase from vector potential

Path 2 $\displaystyle\int_{\text{path 2}} \vec{k}\cdot d\vec{l} = \frac{\sqrt{2mE}}{\hbar}\pi r - \frac{e}{\hbar}\int_{\text{path 2}} \vec{A}\cdot d\vec{l}$

$$\phi_2 - \phi_1 = \frac{e}{\hbar}\oint \vec{A}\cdot d\vec{l}$$ closed loop

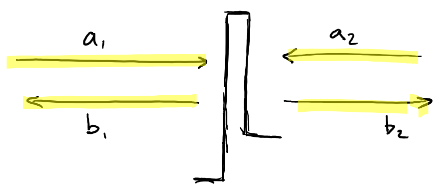
$$= \frac{e}{\hbar}\int_{\text{surf}} \nabla\times\vec{A}\, d\vec{a} = \frac{e}{\hbar}\overbrace{B\,\pi r^2} = \frac{\Phi}{\Phi_0}$$

$$= 2\pi\frac{\Phi}{\Phi_0} \qquad \Phi_0 = \frac{h}{e}$$



Theoretical machinery for generalizing this approach (keeping track of various transmission/reflection amplitudes).

Simplest case



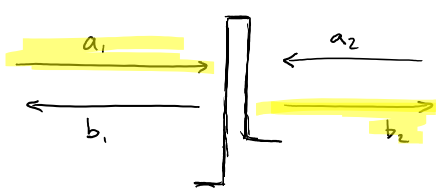
$$\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \underbrace{\begin{bmatrix} r & t' \\ t & r' \end{bmatrix}}_{S} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

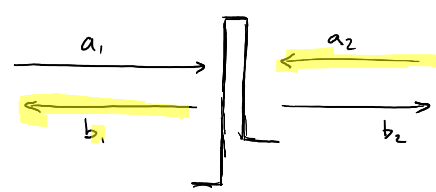
a) Note time reversal symmetry $S = S^T$

b) And unitaryness $S^\dagger S = I$

a)

Time reversal





described by t described by t'

at $B=0$ $t = t'$, $S_{nm} = S_{mn}$

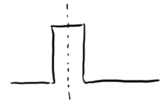
b) Probability going in $|a_1|^2 + |a_2|^2$

going out $|b_1|^2 + |b_2|^2$

$\vec{a}^\dagger \vec{a} = \vec{b}^\dagger \vec{b}$ and $\vec{b} = S\vec{a}$

$$= \vec{a}^\dagger \underbrace{S^\dagger S}_{I} \vec{a}$$

Consider a barrier with mirror symmetry

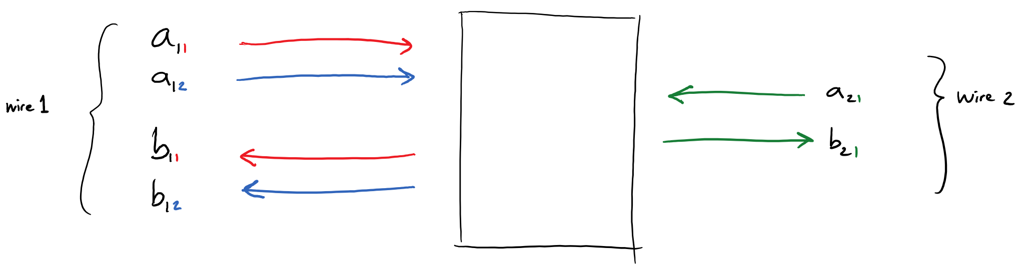


Check if this scattering matrix is possible

$$\begin{bmatrix} r & t' \\ t & r' \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}$$

The scattering matrix formalism can be expanded to handle arbitrary # of modes on left & right.

Example Extra mode on the left (shown in red)



$$\begin{bmatrix} b_{11} \\ b_{12} \\ b_{21} \end{bmatrix} = \begin{bmatrix} r_{11} & t & \cdots \\ \cdots & r_{12} & \cdots \\ \cdots & \cdots & r_{11} \end{bmatrix} \begin{bmatrix} a_{11} \\ a_{12} \\ a_{21} \end{bmatrix}$$

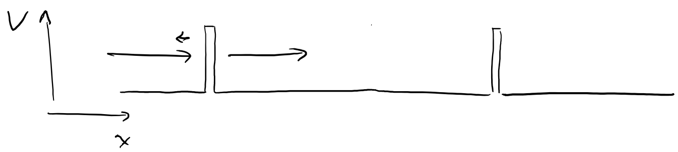
Scattering matrix S

This scattering matrix machinery will return later in the course.

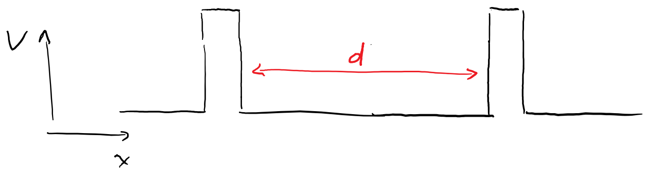
Quantum Dots

I already discussed an "open" pair of barriers

A special case that can be described by the Landauer-Buttiker formalism - or an equivalent description that we formulate below.



Now try a "closed" pair of barriers



Crucial element in the charge qubit, Cooper-pair box qubit, transmon qubit

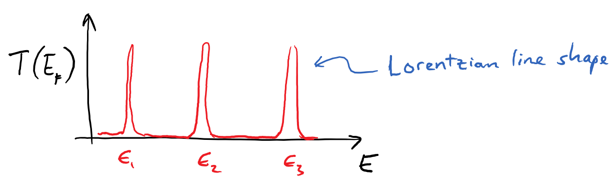
The barriers are very reflective.

To apply Landauer-Buttiker, we can show that when $|r_1|^2$ & $|r_2|^2 \approx 1$

$$T(E_F) = \frac{|t_1|^2|t_2|^2}{1+|r_1|^2|r_2|^2 - 2|r_1||r_2|\cos\phi} \approx \frac{\Gamma_1\Gamma_2}{(E-\epsilon_n) + (\Gamma_1+\Gamma_2)^2/4}$$

see §3.4 of txbk Eqn 3.74

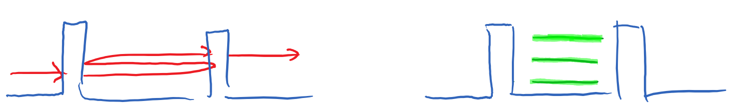
where $\Gamma_i = \frac{|t_i|^2 \hbar v_n}{2d}$, ϵ_n are the energies of maximum transmission and v_n is velocity associted n^{th} state.



Then the conductance would be

$$G = T(E_F)\,\frac{2e^2}{h}$$

This result suggests a different (and rewarding) way of thinking about the physical system

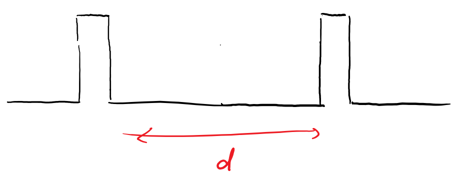


Original picture:
Summation of different paths

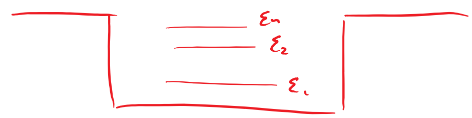
New Picture:
Discrete electron orbitals that have some finite uncertainty in energy. Probability of tunneling will depend on energy detuning between incoming electron and the nearest ϵ_n

This new picture is a lot like atomic energy levels.
For this reason, quantum dots are called "artificial atoms".

- What are the energy eigenstates, ϵ_n, inside the two barriers?



$\Rightarrow$



Treat the system like a finite quantum well.

- What is the uncertainty in energy, ΔE_n of the n^{th} quantum level?

Use the Heisenberg Uncertainty relation $\Delta E \approx \dfrac{\hbar}{\underbrace{\Delta t}_{\text{dwell time of an electron in the electron orbital.}}}$

- What is the average dwell time Δt of an electron in the orbital?

Escape rate from left barrier $\dfrac{|t_1|^2}{(\text{round trip time})} = \dfrac{|t_1|^2}{\left(\frac{2d}{v_n}\right)}$

Probability of transmission barrier 1.

v_n is velocity in the n^{th} quantum state

Example rate = (Prob)(Attempt freq) = (0.01)(1 GHz) = 0.01 GHz

Escape rate from right barrier $\dfrac{|t_2|^2}{(\text{round trip time})} = \dfrac{|t_2|^2}{\left(\frac{2d}{v_n}\right)}$

$$\text{Total rate} = \frac{|t_1|^2 v_n}{2d} + \frac{|t_2|^2 v_n}{2d}$$

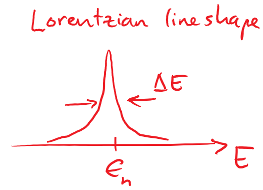
$$\Delta t = \frac{1}{\text{rate}} = \frac{1}{\frac{|t_1|^2 v_n}{2d} + \frac{|t_2|^2 v_n}{2d}}$$

Just like atomic physics, Δt corresponds to an uncertainty in energy

$$\Delta E = \hbar \left(\frac{|t_1|^2 v_n}{2d} + \frac{|t_2|^2 v_n}{2d} \right)$$

Now, resonant tunneling of an electron into the n^{th} state can happen when the electron energy is slightly detuned from ϵ_n.

Probability of electron tunneling into the QD $\propto \dfrac{1}{(E-\epsilon_n)^2 + \frac{\Delta E^2}{4}}$

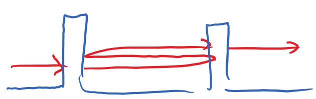


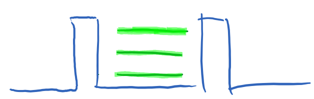
$$\propto \frac{1}{(E-\epsilon_n)^2 + \frac{\hbar^2}{4}\left(\frac{|t_1|^2 v_n}{2d} + \frac{|t_2|^2 v_n}{2d} \right)^2}$$

This matches the result derived from

$$\frac{|t_1|^2 |t_2|^2}{1 + |r_1|^2 |r_2|^2 - 2|r_1||r_2| \cos\phi}$$

Why did we bother coming up with a different, but equivalent, descriptions for this situation?





This new picture (lifetime broadened discrete energy levels in a closed system) is easier to extend to include Coulomb charging. That's a subject for next lecture.