Quantum point contact simulations

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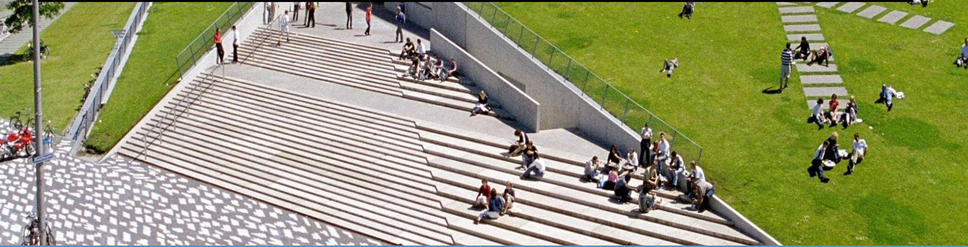


Outline

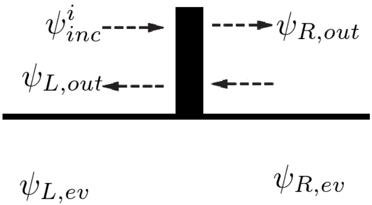
Scattering theory

Definition

Set of incoming and outgoing waves at the leads.

$$\psi_L = \psi_{inc}^i + \Sigma_j r_{ji}\psi_{L,out} + \Sigma_k \beta_{ki}\psi_{L,ev} \quad (1)$$

$$\psi_R = \Sigma_j t_{ji}\psi_{R,out} + \Sigma_k \alpha_{ki}\psi_{L,ev} \quad (2)$$



Quantum Point Contact

- Electrons travel from source to drain.
- Electrons experience potential barrier in the center
- Resulting in reflection and transmission

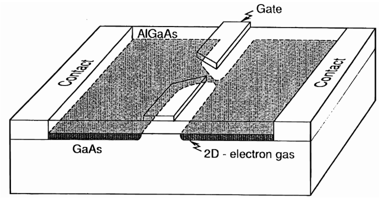


Figure : Experimental set-up.

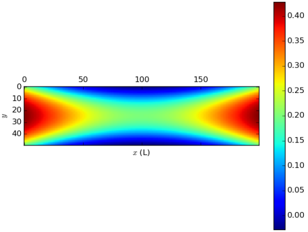
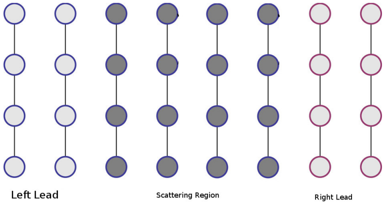


Figure : Simulated potential barrier

Discretize system

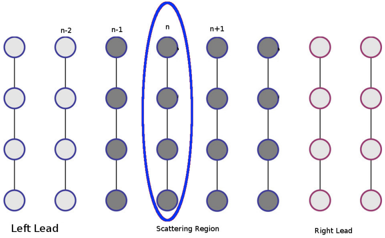
We separate the system into discrete points



Discretize system

We view each column as a single wavefunction

$$\psi_n(y)$$



Tight-binding Hamiltonian

Definition

A tight-binding Hamiltonian only takes neighbours into account
The tight-binding Hamiltonian used in our simulations is given by:

$$H = \begin{bmatrix} \mu_1 & t & & & \\ t & \mu_2 & t & & \\ & t & \mu_3 & \ddots & \\ & & \ddots & \ddots & t \\ & & & t & \mu_N \end{bmatrix} \tag{3}$$

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Transfer Matrix

Definition

A transfer matrix T operates as follows:

$$\begin{pmatrix} \psi_{n+1} \\ t\ \psi_n \end{pmatrix} = T \begin{pmatrix} \psi_n \\ t\ \psi_{n-1} \end{pmatrix} \tag{4}$$

with

$$T = \begin{pmatrix} t^{-1}H & -1 \\ t & 0 \end{pmatrix} \tag{5}$$

Transfer matrices can be multiplied with each other

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Matching conditions

- Plane waves in the left lead Ψ_L and right lead Ψ_R
- Transfer matrices T_i in scattering region can be calculated
- Apply matching condition:

$$\Psi_R = \prod_{i=1} T_i \Psi_L = T_{tot} \Psi_L \tag{6}$$

- Grouping waves together we end up with a system of equations

$$\left(U_{R,out} | U_{R,ev} | - T_{tot} \cdot U_{out} | - T_{tot} \cdot U_{ev} \right) \begin{pmatrix} t \\ \alpha \\ r \\ \beta \end{pmatrix} = T_{tot} \cdot U_{in} \tag{7}$$

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Transmission, Reflection, and Conductance

For each mode i the sum of transmissions and reflections must add up to unity:

$$\sum_{j=1}^{N} |r_{ij}|^2 + |t_{ij}|^2 = 1 \tag{8}$$

The conductance of the system is then given by Landauers formula:

$$G = G_0 \sum_{i,j} |t_{ij}|^2 \tag{9}$$

Results

Transfer matrix method shows expected behaviour

However...

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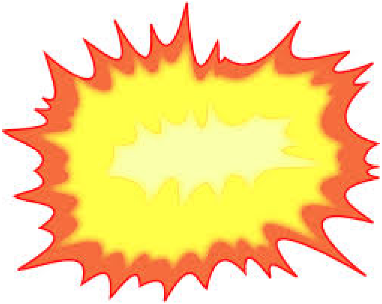
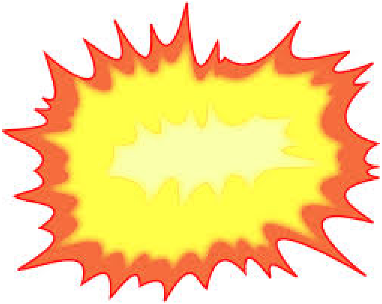
Transfer matrix method shows expected behaviour

However... Transfer matrix blows up after ± 20 iterations!



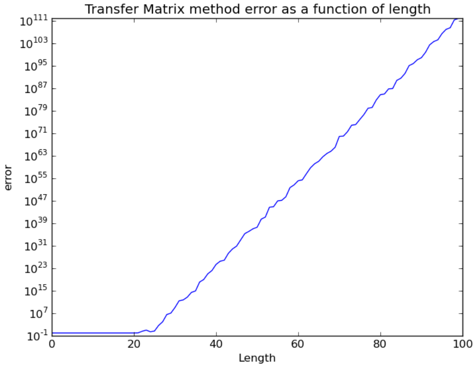


Results

Transfer matrix method shows expected behaviour

Transfer matrix blows up after ± 20 iterations!

- Plot of $\sum_{j=1}^{N} |r_{ij}|^2 + |t_{ij}|^2 = 1$ as a function of length of the system.



Scattering Matrix Method

- Cause: eigenvalues of transfer matrices have different values
  - Resulting elements behave exponentially
- Solution: transform transfer matrices into scattering matrices
  - All eigenvalues in scattering matrices have unity magnitude
  - No exponential behaviour!
- Scattering matrices transform incoming waves into outgoing waves
- Downsides of scattering matrices:
  - Scattering matrices are multiplied in a complex way
  - Must transform transfer matrix to scattering matrix at every step

Results

Quantized conductance

Conductance is quantized according to the number of modes available

- Depends on chemical potential μ of leads

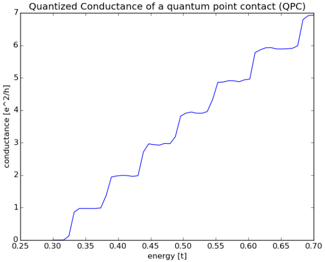


Figure : Our simulation.

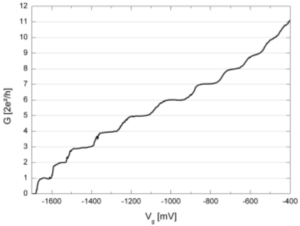


Figure : Experiment [1]

1

[1] B J van Wees, H van Houten, C W J Beenakker, J G Wdhamson, L P Kouwenhoven, D van der Marel, and C T Foxon, *Phys Rev Lett 60*, 848 (1988)

Optimization

1. Transfer matrix method
   1. (+) Easy implementation
   2. (+) Fast algorithm
   3. (-) Error grows exponentially
2. Scattering matrix method
   1. (+) Very stable
   2. (-) Slow algorithm

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Best of both worlds:

- <3 Scatter matrix $+ <3$ Transfer matrix
- Speed up of 2.5x
- C++ (401 lines of code, 6.40s) and Python (160 lines, 5.01s)
- LaTeX presentation (341 lines of code)