Transport: quantization of the conductance.

Conductance

\[ G = \frac{I}{V} \]

Quasi-1D systems with width \( w \) comparable to the de Broglie wavelength

Diffusive transport regime \( \Lambda \ll \omega, L \)

Ballistic transport regime \( \Lambda \gg \omega, L \)

\[ \Lambda = \text{mean free path} \]
**Quantized conductance discovery**

**Quantized Conductance of Point Contacts in a Two-Dimensional Electron Gas**

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Ballistic point contacts, defined in the two-dimensional electron gas of a GaAs-AlGaAs heterostructure, have been studied in zero magnetic field. The conductance changes in quantized steps of $e^2/h$ when the width, controlled by a gate on top of the heterojunction, is varied. Up to sixteen steps are observed when the point contact is widened from 0 to 360 nm. An explanation is proposed, which assumes quantized transverse momentum in the point-contact region.

**FIG. 1.** Point-contact resistance as a function of gate voltage at 0.6 K. Inset: Point-contact layout.

**FIG. 2.** Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/h$.
Transport: quantization of the conductance.

Quantization of conductance

Ballistic regime

SIMPLIFIED DERIVATION OF QUANTIZED CONDUCTANCE

Left reservoir \[ I_D \] Right reservoir

No inelastic scattering!
Chemical potential difference \( \delta \mu = e V_{bias} \)

Density of \( e^- \)'s in channel \( n \) contributing to the current : \( n_e = \frac{1}{2} \sum g_v(r_f) \delta V_{bias} \)

Current \( I_n = n_e e V_{bias} = \frac{1}{2} g_v(r_f) V_{bias} \)

1D - density of states : \( g_v(r_f) = \frac{1}{2} \sqrt{V_{bias}} \)

\[ I_n = \frac{2e^2}{h} V_{bias} \]

\[ G = \sum_{n=1}^{N} \frac{2e^2}{h} T_n \]

\( G \) = Conductance

\( T_n \) = Transmission of channel \( n \); \( N \) = open channels

Landauer Formula
• Transport: quantization of the conductance.

More precise calculations.. (pdf-notes Bruus, Datta...)

The chemical potential can be changed in a controlled manner by applying a voltage \( V \):

\[
\mu = \mu_0 - eV.
\]

The probability \( \mathbb{P} \) that a given quantum state with energy \( \varepsilon \) is occupied by an electron is determined by the Fermi-Dirac distribution

\[
\mathbb{P}(\varepsilon, \mu_0, V, T) = \frac{1}{\exp \left[ \frac{\varepsilon - \mu_0 + eV}{k_B T} \right] + 1}
\]

• Transport: quantization of the conductance.

Current density and transmission of electron waves

• Electron waves in constant potentials in 1D

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_\varepsilon(x)}{\partial x^2} + V \psi_\varepsilon(x) = E \psi_\varepsilon(x)
\]

\[
\psi_\varepsilon(x) = e^{\pm ikx}, \quad k = \frac{1}{\hbar} \sqrt{2m(\varepsilon - V)}.
\]

\[
\varepsilon = \frac{\hbar^2 k^2}{2m} + V
\]

\[
\psi_{+k}(x, t) = e^{i(kx - \frac{\hbar}{2m} t)}, \quad \text{(right-moving wave)}
\]

\[
\psi_{-k}(x, t) = e^{i(-kx - \frac{\hbar}{2m} t)}, \quad \text{(left-moving wave)}
\]

• Work with time-independent solutions

\[
\psi_{+k}(x) = e^{ikx}, \quad \text{(right-moving wave)}
\]

\[
\psi_{-k}(x) = e^{-ikx}, \quad \text{(left-moving wave)}
\]
Transport: quantization of the conductance.

The current density $\mathbf{J}$

$$\mathbf{J} = n \mathbf{v} = n \mathbf{p}/m$$

$$\mathbf{J} = \psi^* \psi \mathbf{p}/m.$$  

$$\mathbf{J}(r) = \frac{i}{m} \text{Re}[\psi^*(\mathbf{p}\psi)] = \frac{i}{m} \text{Im}[\psi^*(\nabla\psi)]$$

The electric current $I$ passing through the $yz$ plane in the $x$ direction

$$I = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz (-e)J_x = -\frac{e\hbar}{m} \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \text{Im}[\psi^*(\frac{\partial\psi}{\partial x})]$$

But $\psi_{k\alpha}(\mathbf{r}) = \chi_k(x) \phi_\alpha(y, z)$.

$I_{k\alpha}$ carried by the quantum state $\psi_{k\alpha}$

$$I_{k\alpha} = \frac{e\hbar}{m} \text{Im}[\chi_k(x)^* \frac{\partial}{\partial x}(\chi_k(x))].$$

Electron channels

• For a given quantum number $\alpha$ there are many possible quantum states, namely two (spin up and spin down) for each $k$

$$\varepsilon_k = \hbar^2 k^2 / 2m.$$  

$$\varepsilon_{k\alpha} = \varepsilon_k + \varepsilon_\alpha \quad \Rightarrow \quad k = \frac{1}{\hbar} \sqrt{2m(\varepsilon_{k\alpha} - \varepsilon_\alpha)}.$$  

• $I_{k\alpha}$ carried by an electron in state $\psi_{k\alpha}$ in channel $\alpha$

$$I_{k\alpha} = -\frac{2e\hbar}{Lm} \text{Im}\left[ e^{-ikx} \frac{\partial}{\partial x} (e^{ikx}) \right] = -\frac{2e\hbar k}{Lm} = -2e \frac{v_{k\alpha}}{L}.$$  

$v_{k\alpha}$ is the velocity of an electron in the state $\psi_{k\alpha}$

• Current $I_{k\alpha}$ running from the left reservoir $L$ into the right reservoir $R$ through the nanostructure
• Transport: quantization of the conductance.

Current $I_{L\rightarrow R}$ running from the left reservoir $L$ into the right reservoir $R$ through the nanostructure

$$I_{L\rightarrow R} = \sum_\alpha \sum_k [n^L_\alpha(\varepsilon)] \times [ - 2e \frac{\varepsilon}{L} \nu_k] \times [T_\alpha(\varepsilon)].$$

sum for all channels and wave vectors

Fermi-Dirac probability

transmission probability of an electron at energy $\varepsilon$ making it through to the reservoir to the right

$$\sum_k \rightarrow (L/2\pi) \int dk. \quad \text{(in 1D)}$$

$$\int \frac{dk}{\hbar} \rightarrow \int \frac{d\varepsilon}{h} \frac{dk}{\hbar}. \quad \text{But,} \quad \frac{dk}{d\varepsilon} = \frac{1}{\hbar}$$

Then,

$$I_{L\rightarrow R} = -\frac{2e}{\hbar} \int_\infty^\infty \frac{d\varepsilon}{h} n^L_\alpha(\varepsilon) T_\alpha(\varepsilon).$$

$$I = I_{L\rightarrow R} - I_{R\rightarrow L} = -\frac{2e}{\hbar} \int_{-\infty}^\infty \frac{d\varepsilon}{h} n^L_\alpha(\varepsilon) \left[ n^L_\alpha(\varepsilon) - n^R_\alpha(\varepsilon) \right]$$

• Transport: quantization of the conductance.

$$n^L_\alpha(\varepsilon) - n^R_\alpha(\varepsilon) = n^L_\alpha(\varepsilon, \mu_0 - eV) - n^L_\alpha(\varepsilon, \mu_0) \approx \frac{\partial n^L_\alpha}{\partial \mu} \bigg|_{\mu_0} (-eV) = \left( -\frac{\partial n^L_\alpha}{\partial \varepsilon} \right) (-eV)$$

$$I = \frac{2e^2}{\hbar} \sum_\alpha \int_{-\infty}^\infty \frac{d\varepsilon}{h} T_\alpha(\varepsilon) \left( -\frac{\partial n^L_\alpha}{\partial \varepsilon} \right) V.$$  

Temperature dependent conductance $G(T)$

$$G(T) = \frac{I}{V} = \frac{2e^2}{\hbar} \sum_\alpha \int_{-\infty}^\infty \frac{d\varepsilon}{h} T_\alpha(\varepsilon) \left( -\frac{\partial n^L_\alpha}{\partial \varepsilon} \right)$$

$$-\frac{\partial n^L_\alpha}{\partial \varepsilon} = \delta(\varepsilon_F - \varepsilon)$$

All information about the nanostructure lies in the transmission coefficient

The zero temperature conductance

$$G(T = 0) = \frac{2e^2}{\hbar} \sum_\alpha T_\alpha(\varepsilon_F)$$

Landauer Formula

$$\frac{2e^2}{\hbar}$$

Conductance quantum
Transport: quantization of the conductance.

More precise treatments: Non-equilibrium Green’s function method (see e.g. Datta’s book) Implemented in ab-initio calculation packages as TRANSIESTA

M. Bradbyge et al. PRB 65,165401 (2002)

Transport: quantization of the conductance.

Conductance as a function of radius from cylindrical infinite wire calculations

\[
\frac{G}{G_0} = \left( \frac{\pi R}{\lambda_F} \right)^2 \left( 1 - \frac{2\alpha \lambda_F}{\pi R} \right)
\]

A. García et al. PRB 49, 16581 (1994)
• Quantum size effects (from conductance measurements)

• Conductance histograms

Geometrical information can be obtained from the conductance histograms

Conductance histograms for alkali metals
• Quantum size effects (from conductance measurements)

• Shell and supershell structure of nanowires from conductance histograms

Increasing the temperature, the atoms can move and reorganize to the positions which minimize the energy.

Quantum beat structure in stability

Calculations with jellium model

M.J. Puska, E. Ogando, N. Zabala, PRB 64, 033401 (2001)

M.I. Yanson et al. PRL 84, 5834 (2000); Nature 400, 144 (1999)

Surface energy

Radius

M.J. Puska, E. Ogando, N. Zabala, PRB 64, 033401 (2001)

Semiclassical model

explain existence of more stable radii

Semiclassical orbit closes when its length \( L \) is an integer times the Fermi wavelength

\[ L = n\lambda_F \]

Two states whose quantum numbers fulfill

\[ \Delta m = p \quad \Delta n = q \]

belongs to the same orbit

M.J. Puska, E. Ogando, N. Zabala, PRB 64, 033401 (2001)
**Quantum size effects (from conductance measurements)**

The Fourier transform reveals the connection with the semiclassical approach.

The pendular and triangular orbits are the most important ones.

Interference of two waves of similar frequencies produce beat structure.

**Quantum size effects (from conductance measurements)**

- Shell and supershell for other metals

Frequencies do not change.
• Quantum size effects (from conductance measurements)

• Potential softness effect

\[ V_{\text{eff}}(n(r)) = V_{XC} \]

This model represents the ultimate limit in which the positive background is completely deformed until its charge density is the same as the electron density.

1. Free parameter model
2. Lowest energy by deformation
3. Optimal shape from electrons point of view

\[ 2 + 8 \neq 10 \]
• Quantum size effects (from conductance measurements)

• Ultimate jellium wire breaking simulations

Liquid-like shape

Cluster derived structure

Straight wire structure

Cluster derived structure

• Summary of properties

(ultimate jellium wire breaking simulations)
• Quantum size effects (from conductance measurements)

Atomic shell and supershell

A.I. Yanson et al. PRL 87, 216805 (2001)

• Other hot topics

MOLECULAR ELECTRONICS

Molecular rectifiers: Tour wires

Taylor et al. PRL ’02

See also:
Aviram and Ratner. Chem. Phys. Lett. ’74
Tour et al. J. Am. Chem. Soc. ’01
• Other hot topics

• Magnetism in nanowires and the 0.7 conductance anomaly
  Materials which are non-magnetic can exhibit magnetism in small dimensions
  - Experiments: non-integer values of conductance quanta

Wires on surfaces can also exhibit magnetism.

• Kondo effect in QPC and quantum dots

• Luttinger liquid effects, important for 1D systems
  These effects belong to cutting edge of modern nanoscience and nanotechnology.

• Summary

• We have studied some important systems with 1D behaviour, as 1D metals, polymers, semiconductor wires formed at heterostructures and nanowires formed by contact breaking.

• We have adressed some important phenomena taking place in these systems as the Peierls transition and the quantization of the conductance. For the later we have obtained the Landauer formula describing the conductance in ballistic regime.

• Using a cylindrical jellium model we have obtained some of these properties and described the oscillations occurring in the physical properties and in particular in the stability, giving rise to quantum size effects.

• Finally we have pointed out some hot topics related to 1D systems.