Nanodevices and Maxwell's Demon

Electronic demon

For a detailed write-up of this lecture
See arXiv:condmat/0704.1623
Unified viewpoint: Materials

Quantum Transport Far from Equilibrium

\[ \Gamma = i \left[ \Sigma - \Sigma^+ \right] \]
Unified viewpoint: Ballistic to Diffusive

Quantum transport far from equilibrium

\[ \Gamma = i \left[ \Sigma - \Sigma^+ \right] \]
$G = \sigma A / L$

$\sigma = e^2 n \tau / m$

$\tau = ?$

“Very complicated”

$m = ?$  $n = ?$

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\[
G = \sigma \frac{A}{L}
\]

\[
\gamma \sim \frac{2\hbar D}{L^2} \quad \rightarrow \quad D\gamma \sim A/L
\]

\[
G = (\frac{e^2}{h})(\pi D\gamma), \quad D \sim AL
\]

\[
\gamma \sim \frac{\hbar v}{L} \quad \rightarrow \quad D\gamma \sim A
\]

\[
G = \left(\frac{e^2}{h}\right) \frac{1}{1/25.8 \, K\Omega}
\]

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Equilibrium Energy Level Diagram

- **Vacuum Level**: Shows the energy levels in the absence of an applied voltage.
- **No states**: Indicates the absence of energy levels.
- **Filled states**: Represents energy levels that are occupied.
- **Electrochemical Potential**: The Fermi level (µ) indicates the energy level at which the probability of finding an electron is 0.5.
- **Gate Voltage (V_G)**:
  - **V_G < 0**: Insulator region with no states.
  - **V_G > 0**: Channel region with filled states.

Symbols:
- S (Source)
- D (Drain)
- Channel

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What makes electrons flow?

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Current through a 1-level conductor

\[ \text{Normalized Current} \]

\[ V \Rightarrow \]

\[ I = \frac{e \gamma_1}{2 \hbar} \]

\[ \gamma_1 / \hbar \]

\[ \gamma_1 / \hbar \]
\[ \frac{dI}{dV} \sim \frac{e\gamma_1 / 2\hbar}{4kT/e} \]

\[ V \Rightarrow \]

Normalized Current

Normalized Conductance

Conductance?
Conductance quantum

\[
\frac{d I}{d V} \sim \frac{e \gamma_1 / 2 \hbar}{(2 \gamma_1 + 4kT)/e}
\]

\[
\sim e^2 / 4\hbar \quad \text{if} \quad \gamma_1 \gg kT
\]

Conductance quantum

\[
\sim e^2 / 2\pi\hbar \sim 1/25.8 \text{ K}\Omega
\]
Conductance quantum

Measurement of the conductance of a hydrogen molecule

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Importance of electrostatics

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Current-Voltage Characteristics of Self-Assembled Monolayers
by Scanning Tunneling Microscopy

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(Received 9 June 1997)

Theory with proper electrostatics

“Standard” theory
Electrostatics of a Nanotransistor

- Diagram of a nanotransistor with labeled components:
  - $V_G$ (Gate voltage)
  - $S$ (Source)
  - $D$ (Drain)
  - $D(E-U)$
  - $\mu_1$ and $\mu_2$
  - $\gamma_1$ and $\gamma_2$

- Graph showing current ($I$) and voltage ($V_D$) with
  - No gate
  - Perfect Gate

- Equation: $\mu_1 \frac{h}{\gamma_1}$ and $\mu_2 \frac{h}{\gamma_2}$
Conductance: for any DOS, $D$

$I \sim \frac{e \gamma_1}{2 \hbar}$

$D \text{ eV}$

Current per state

$\frac{1}{V} = \frac{e^2}{2 \pi \hbar} \rho_1$ Transmission

$\rho_1$ Quantum

$\rho_1$ Conduction

$D$: Density of states
\[ I = \int dE \ D(E) \ \frac{e\gamma_1}{2\hbar} \left[ f_1(E) - f_2(E) \right] \]
Current versus temperature

\[ I = \int dE \ D(E) \ \frac{e\gamma_1}{2\hbar} \left[ f_1(E) - f_2(E) \right] \]
Thermoelectricity in Molecular Junctions

Pramod Reddy, Sung-Yeon Jang, Rachel A. Segalman, Arun Majumdar

By trapping molecules between two gold electrodes with a temperature difference across them, the junction Seebeck coefficients of 1,4-benzenedithiol (BDT), 4,4'-dibenzenedithiol, and 4,4'-tribenzenedithiol in contact with gold were measured at room temperature to be +8.7 ± 2.1 microvolts per kelvin (μV/K), +12.9 ± 2.2 μV/K, and +14.2 ± 3.2 μV/K, respectively (where the error is the full width half maximum of the statistical distributions). The positive sign unambiguously indicates p-type (hole) conduction in these heterojunctions, whereas the Au Fermi level position for Au-BDT-Au junctions was identified to be 1.2 eV above the highest occupied molecular orbital level of BDT. The ability to study thermoelectricity in molecular junctions provides the opportunity to address these fundamental unanswered questions about their electronic structure and to begin exploring molecular thermoelectric energy conversion.

Experiment:

Theory:
Paulsson and Datta, PRB 67, 241403 (2003),
From ballistic to diffusive transport

Separate dynamics + dissipation

Dissipation

\{ \}

\gamma

Dynamics

\{ \}

\gamma

Landauer model

Mixed dynamics + dissipation

Boltzmann

\gamma

\gamma_s

\gamma

NEGF

Newton's law

Schrodinger equation

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Maxwell’s demon as an energy conversion device

Need two groups of states:

“Red” & “Blue”
Anti-parallel (AP) Spin Valve

Source    Channel    Drain

Perfect AP
Imperfect AP

Current
Voltage

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Perfect AP with Spin-flip Impurities

![Diagram of a transistor with spin-flip impurities](image)

**Insulating substrate**

**Source** | **Channel** | **Drain**
---|---|---

**Current**

- **w/o spin-flip**
- **with spin-flip**

**Voltage**

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nanoHUB.org

online simulations and more
Perfect AP with Spin-polarized gate

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Current at zero voltage!!

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Device as a “demon”

Normalized current ---\rightarrow

Voltage ---\rightarrow

No further current
Where did the energy come from?

Answer: From the contacts
Second law?

\[ S = 0 \]

\[ S = k \ln W \]

\[ S = Nk \ln 2 \]

Energy up to \( T \Delta S \) may be extracted.
Resetting the demon takes energy

No energy needed

Need > N kT to “Erase”
Flipping a spin costs energy
Carnot’s principle

\[
\frac{Q_1}{kT} < \frac{Q_2}{kT_D}
\]

Q₁: heat from contacts
Q₂: heat to “magnet”
Q₁ - Q₂: useful work
Nanoscale Refrigerator

Cooled by device

Heat from surroundings

Source \[ T \]

Channel

Drain \[ T \]

\[ T_D \]
Back to the unified viewpoint

Dynamic demons

\[ \mu_1 \quad \Sigma_1 \quad H+U \quad \Sigma_2 \quad \mu_2 \]

\[ \Sigma_s(\vec{M}) \]

<----- LLG equation ----->

\[ \mu_1 \quad \Sigma_1 \quad H+U \quad \Sigma_2 \quad \mu_2 \]

\[ \Sigma_s(\vec{M}) \]

Current

Voltage

Pentalayer Spin-Torque Device

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Quantum Transport far from Equilibrium

Materials

Transport Regimes

0.1 mm
10 μm
1 μm
0.1 μm
10 nm
1 nm
0.1 nm

Macroscopic dimensions

Atomic dimensions

Correlated/Entangled!

Reference:
For a detailed write-up see arXiv:cond-mat/0704.1623
Correlated/Entangled "demon"

Entangled!

\[ * A \]

\[ * B \]

Source \( \rightarrow \) Channel \( \rightarrow \) Drain

\[ A^2 \]

\[ B^2 \]