CQT, Lecture#1: Nanodevices and Maxwell's Demon

Objective:
To illustrate the subtle interplay of dynamics and thermodynamics that distinguishes transport physics.

Reference:
http://arxiv.org/abs/0704.1623

“QTAT”
Datta, Quantum Transport: Atom to Transistor, Cambridge (2005)
Maxwell’s demon

Electron demon

Source

Channel

Drain

\[ V = 0 \]

\[ \text{current} \]
Top-down view

\[ V = I R \quad \text{or} \quad I = V G \]

Conductance, \( G = \frac{1}{R} \)

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

Conductivity

\[ \sigma = \frac{q^2 n \tau}{m} \]

\( \tau = ? \)

\( m = ? \quad n = ? \)

“Very complicated”
Ohm’s law

\[ I = GV , \quad G = \sigma A / L \]

Density of states

\[ G = (q^2 / h) (\pi D \gamma) \]

Escape rate

\[ G = \left( \frac{q^2}{h} \right) \frac{1}{25.8 \, k\Omega} \]
Equilibrium Energy Level Diagram

- **Vacuum Level**
  - **No states**
  - **FILLED**

- **Electrochemical Potential**
  - **S Channel D**

- **Gate**

- **Insulator**

- **$V_G$**
  - $V_G < 0$
  - $V_G > 0$
What makes electrons flow?

\[ \mu_1, \mu_2 \]

\[ V \]

\[ I \]
\[ \gamma / \hbar : \text{Escape Rate} \]

\[ \gamma \text{ has dimensions of energy} \]

Current depends on Density of states, \( D(E) \) around the contact electrochemical potentials.

AND

on escape rates

\[ \gamma_1 \quad \gamma_2 \]
Where is the power dissipated?

\[ \text{Power} = V I \]

- \( \text{Dissipation} \)
- \( \text{D}(E) \)
- \( \text{Contacts assumed to remain in equilibrium} \)
- \( \text{Thermodynamics} \)
- \( \text{Newton's law} \)
- \( \text{Schrodinger equation} \)
- \( \text{Dynamics} \)
Dynamics and dissipation

Separate dynamics + dissipation

Landauer model

Mixed dynamics + dissipation

Boltzmann NEGF

Dissipation

Dynamics

Dissipation

Newton’s law

Schrodinger equation

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Spin Valves

Anti-parallel (AP)

Current

Imperfect

Perfect

Voltage

Source Channel Drain

Insulating substrate

Source Drain

nanoHUB.org

online simulations and more

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Network for Computational Nanotechnology

Faulty  

Perfect  

AP

AP

AP
Perfect AP with Spin-flip Impurities

Insulating substrate

Source Channel Drain

Spin flip

Current with spin-flip w/o spin-flip

Voltage

Source Drain

nanoHUB.org
online simulations and more

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Perfect AP with Spin-polarized gate

- Source
- Channel
- Drain

Insulating substrate

Spin flip

Source

Drain

Current

Voltage

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Current at zero voltage!!

**Figure 1A**

- **Normalized current --> Voltage --> Current**
- **Source** → **Channel** → **Drain**

Normalized current vs Voltage

Current vs Voltage

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Device to “demon”

Source

Channel

Drain

Normalized current ---→

Voltage ---→

No further current
Where did the energy come from?

Answer: From the contacts
Second law?

\[ S = 0 \]

Energy upto \( T \Delta S \) may be extracted

\[ S = k \ln W \]

\[ S = Nk \ln 2 \]
Resetting the demon takes energy

No energy needed

Need > N kT to "Erase"

Maxwell's demon, ed. H.S. Leff and A.F. Rex,
ISBN 0-691-08727-X pbk
.. A finite-sized demon .. gets so hot that he cannot see very well after a while ..", Feynman lectures, Vol.1, 46-5.

Flipping a spin costs energy
The cool demon as a heat engine

Cooled

T_D

Source

Channel

Drain

300K

Carnot’s principle

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

Q_1: heat from contacts
Q_2: heat to demon
Q_1 - Q_2: useful work

TD = 60K

Voltage --->

Current --->

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Cooling the demon: Refrigerator

Q₁: heat delivered to contacts
Q₂: heat taken from demon

Battery delivers Q₁ - Q₂

Carnot’s principle

\[
\frac{Q_1}{kT} > \frac{Q_2}{kT_D}
\]
Why is the flow unidirectional?

\[ S = Nk \ln 2 \]

No energy needed

\[ S = 0 \]

Need > \( N kT \) to "Erase"
Entropy as a driving force

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Entropy-driven vs. dynamic processes

"Reservoir" vs. "System"

Density of states

Down > Up

Entropy: $S = \mu_1 \Sigma_1 - \mu_2 \Sigma_2$

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Entangled "demon"

Source Channel Drain

A^2

B^2

Entangled! +

A

B

A^2

B^2

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Unified model for nanodevices

0.1 mm
Macroscopic dimensions

<--- L -->

10 µm
Diffusion

1 µm

0.1 µm
Boltzmann

10 nm

0.1 nm
Atomic dimensions

“Even simple things .. work .. in only one direction because it has some ultimate contact with the rest of the universe ..”
Feynman lectures, Vol.1, 46-8

Nanowires, nanotubes, molecules ..... Switches, energy conversion ...

“NEGF”

+ “Landauer” =

μ₁

Σ₁

Σ₂

μ₂

Hot

Σₚ

Macroscopic dimensions

Atomic dimensions