

Operation of molecular motors

Szabolcs Osváth

Semmelweis University

Properties of nanosystems

- Certain properties are quantized
- Gravity is negligible compared to the other forces
- Surface/mass ratio is very large
- Dissipation of heat is virtually instantaneous
- The role of different binding forces is large
- Molecular level recognition
- Self-organization
- The effect of inertia is negligible
- Increased role of viscosity and thermal movement

Properties of biological motors

- Made of soft material (biopolymers)
- Function is governed by non-covalent forces
- There are no smooth frictionless surfaces
- Fuel: ATP (NADH), transmembrane gradient
- Work in solutions – high viscosity
- Their power is: 100-1000 ATP/s, i.e. $10^{-16} - 10^{-17}$ W
- The power of Brown motion is: 10^{-8} W
- The working principle uses Brown motion

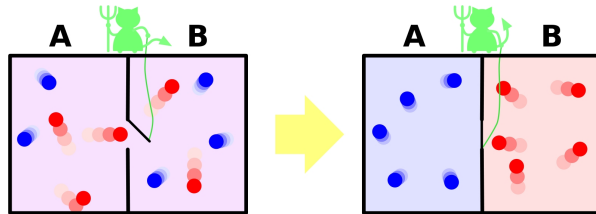
Can the role of the Brownian motion be eliminated?

The importance of the Brownian motion is the consequence of the size and not of the experimental conditions!

The effect of the Brownian motion can not be eliminated.
It does not help if:

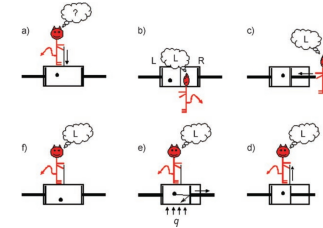
- Pressure is decreased
 - (less frequent collisions, but smaller viscosity)
- Temperature is decreased
 - (the magnitude of the fluctuations is proportional to the square root of the absolute temperature)

Maxwell demon



James Clerk Maxwell
(1871)

The Maxwell demon of Leó Szilárd

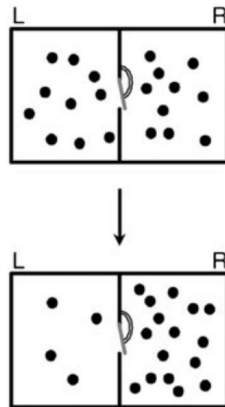


Leó Szilárd : The Maxwell demon has to store information and has to erase information if he wants to return in the initial state.

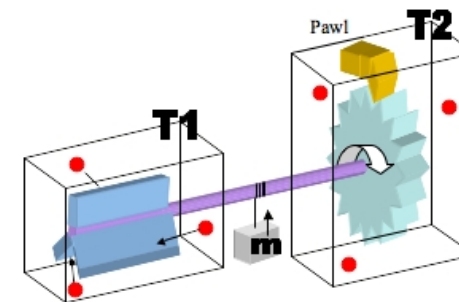
Rolf Landauer (1960): erasing information increases entropy:

– For every bit: $\Delta S = k_B \cdot \ln 2$

Smoluchowski's trapdoor Maxwell demon



Brownian (Smoluchowski, Feynman) ratchet

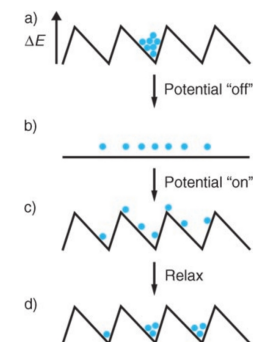


Function of the Brownian ratchet

- Random mixing
- Energy source
- Asymmetric energy surface along the reaction coordinate

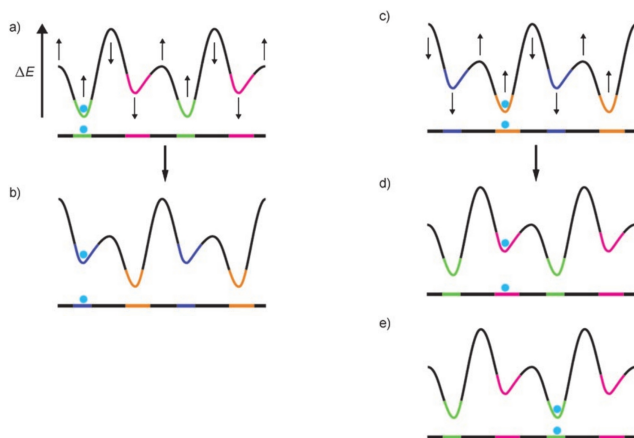
Pulsating ratchet

The potential should be turned off for a short time only, otherwise the transport happens with equal probabilities in both directions.

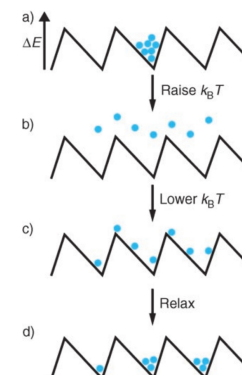


Kay et al. (2007) *Angev. Chem.* 46: 72

Flashing ratchet



Temperature ratchet



Biological application of Nonequilibrium thermodynamics

Evans-Searles FT (revision)

Evans-Searles FT for the entropy production

$$\frac{P(\Omega = A)}{P(\Omega = -A)} = e^A$$

here Ω denotes entropy production

Evans and Searles (2002) Advances in Physics, 51: 1529

Crooks FT (revision)

For a driven system in contact with thermostat:

$$\frac{P_F(A \rightarrow B)}{P_R(A \leftarrow B)} = e^{\frac{W - \Delta G}{k_B T}}$$

W is the work done when the system is driven from the state described by the value A of the control parameter into B

ΔG is the free enthalpy difference between states A and B

G. E. Crooks, J. Stat. Phys. (1998) 90: 1481

Jarzynski equality (revision)

Connects the work measured during non-equilibrium measurements to the free enthalpy difference between the initial and final states.

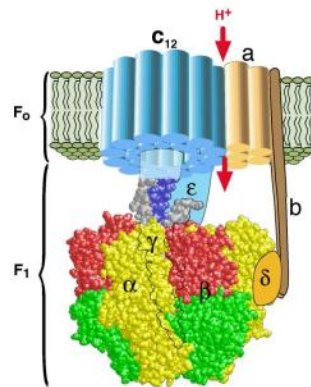
$$\left\langle e^{\frac{-W}{k_B T}} \right\rangle = e^{\frac{-\Delta G}{k_B T}}$$

W is the work done when the system is driven from the state described by the value A of the control parameter into B .

The transition between the initial and final states need not happen through equilibrium states.

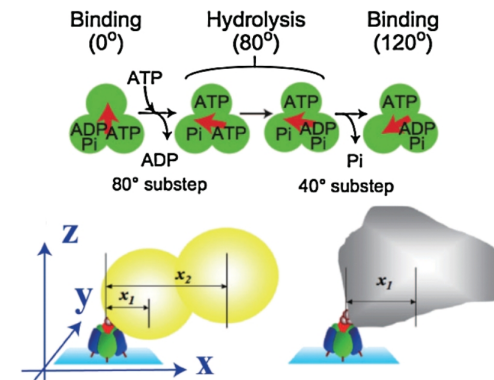
C. Jarzynski, Phys. Rev. Lett. (1997) 78: 2690

Structure of the F₁-ATP-ase motor



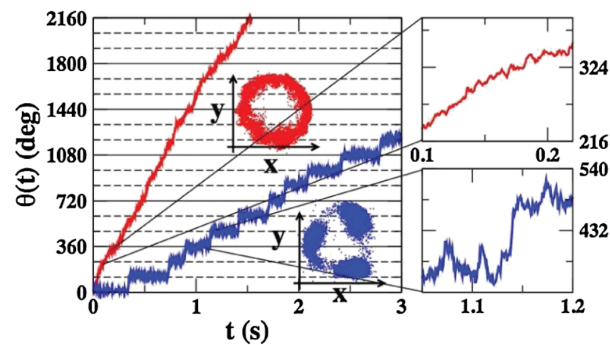
H. Wang and G. Oster (1998). Nature 396:279-282.

Rotation of F₁-ATP-ase motor



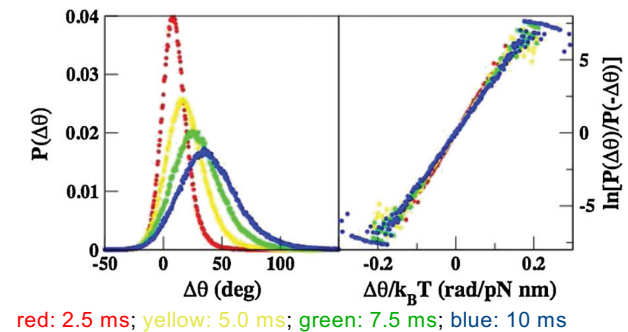
Hayashi et al. (2010) Phys. Rev. Lett. 104: 218103

Rotation of F₁-ATP-ase motor (experiment)



Hayashi et al. (2010) Phys. Rev. Lett. 104: 218103

Fluctuation theorem for the F₁-ATP-ase motor



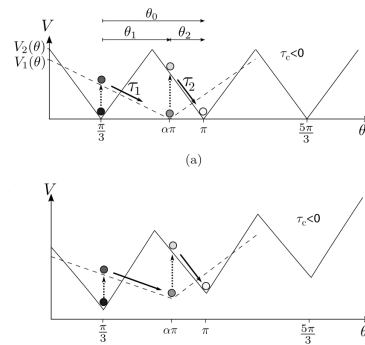
Hayashi et al. (2010) Phys. Rev. Lett. 104: 218103

F₁-ATP-ase flashing ratchet mechanism

Rotation mechanism of the free-rotating and the loaded F₁-ATP-ase motor.

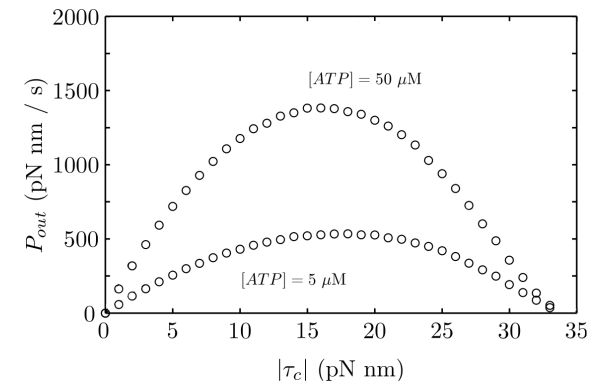
relaxed state:
continuous line

nucleotide binding state:
dashed line



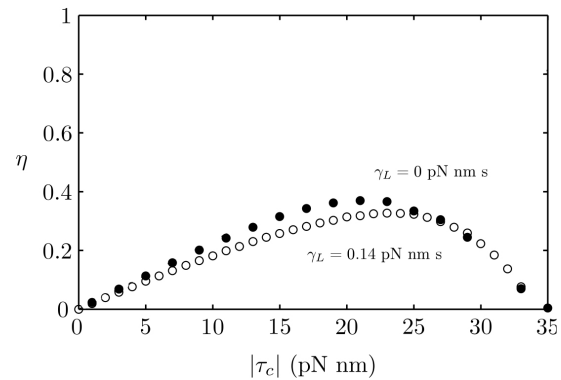
Sancho and Perez-Carrasco (2010) Fluct. Noise. Lett. 11: 1240003

Power release of the F₁-ATP-ase



Sancho and Perez-Carrasco (2010) Fluct. Noise. Lett. 11: 1240003

Efficiency of the F₁-ATP-ase



Sancho and Perez-Carrasco (2010) Fluct. Noise. Lett. 11: 1240003