Fluctuation and Information in Small Non-equilibrium Systems

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Outline

- Maxwell's demon
  - Introduction
- Demonstration of Information-Energy conversion

  (Toyabe, Sagawa, Ueda, Muneyuki, Sano, Nature Physics, 6, 988, (2010))
- Role of information in different systems
  - Laser cooling
  - Molecular motors
  - Chemotaxis of bacteria

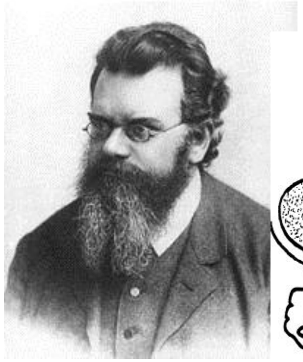
Demons in Thermodynamics

Why does the arrow of time exist?

- Boltzmann's H theorem

Increase of entropy

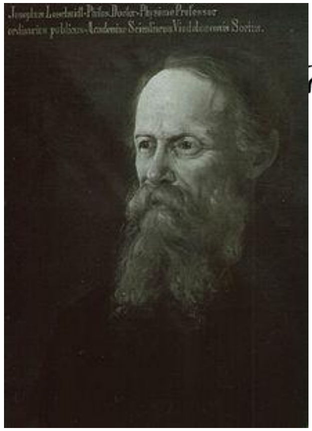
$$\frac{d}{dt}H = \frac{d}{dt}\left(\sum_i p_i \ln p_i\right) \leq 0$$



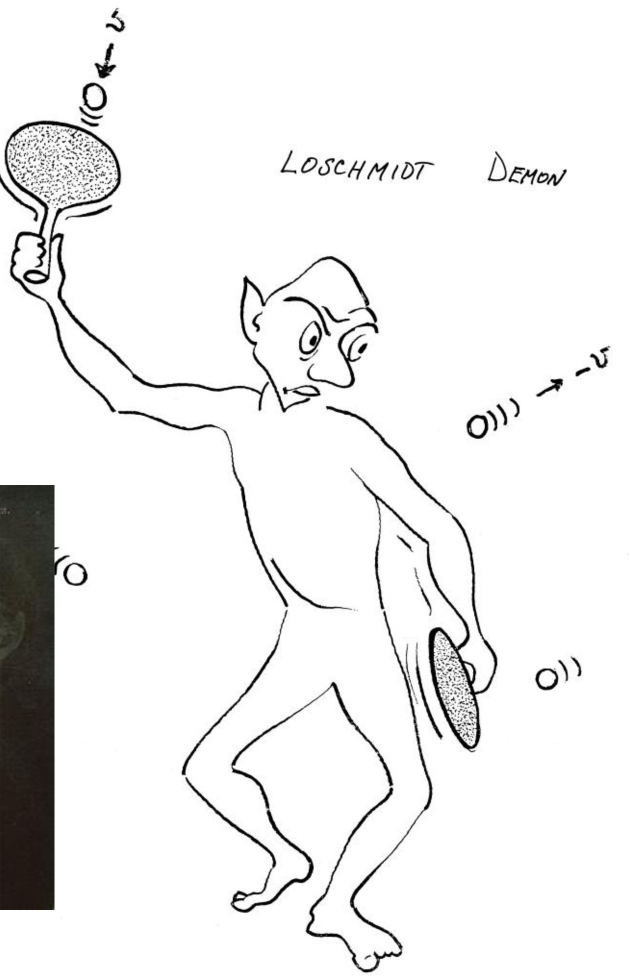
L. Boltzmann

- Loschmidt's demon

Entropy will decrease if the velocities of all atoms are reversed.



Y. Loschmidt



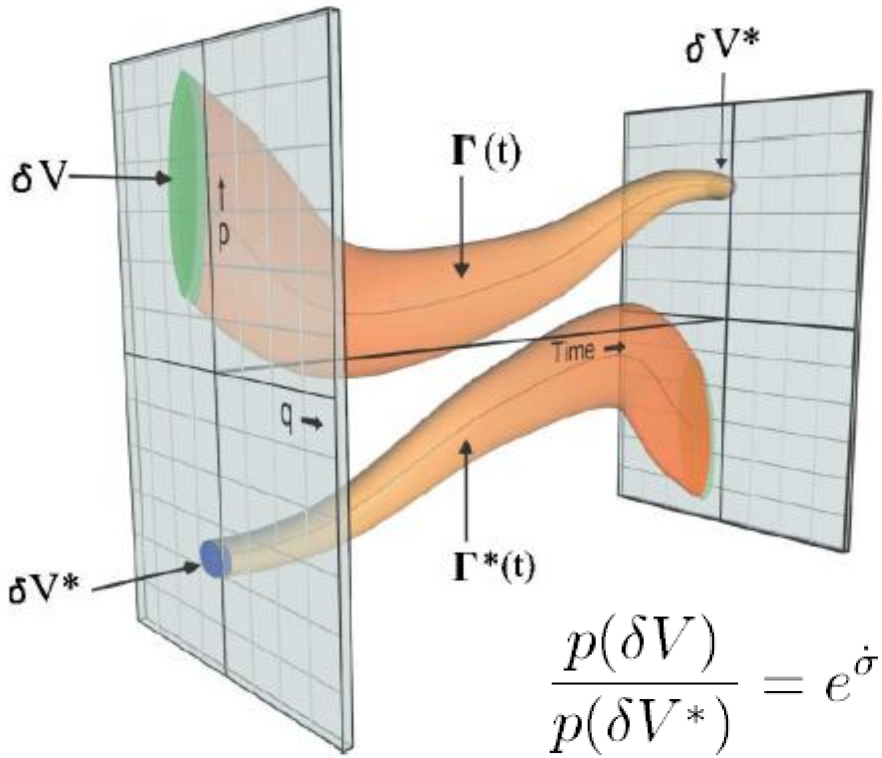
New Theories in Statistical Mechanics

Fluctuation Theorem

- Second law of thermodynamics
- Fluctuation dissipation theorem

$$\frac{p(\sigma)}{p(-\sigma)} = e^{\sigma}$$

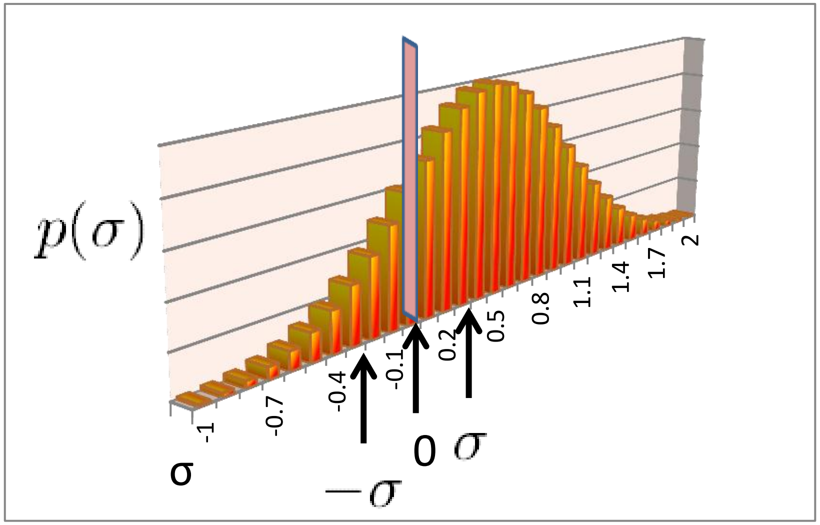
Evans, 1993
Gallavotti, Cohen



$$\frac{p(\delta V)}{p(\delta V^*)} = e^{\dot{\sigma} t}$$

Initial conditions producing positive entropy production is much more frequent than the negative entropy production

Entropy production: $\sigma = \beta(W - \Delta F)$



Confirmed for driven Brownian particles, electric current, etc.

Maxwell’s demon

- Violation of the second law of thermodynamics

(1871)

James Clerk Maxwell (1831-1879)

Opening & closing door do not perform work to atoms.

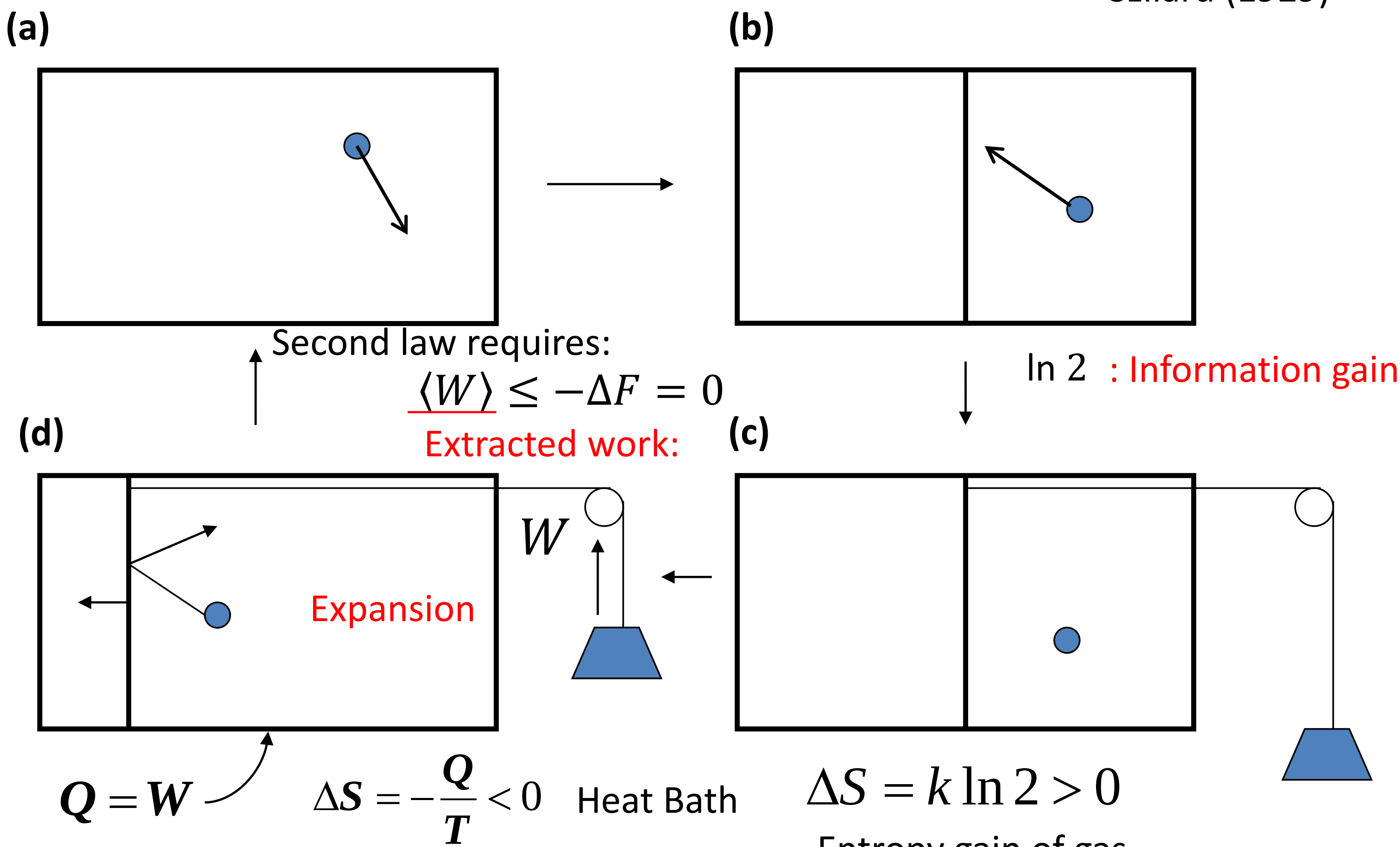
⇒ 2nd law really violate？

⇒ controversial state lasted more than 150 years.

Maxwell's Demon and Szilard Engine

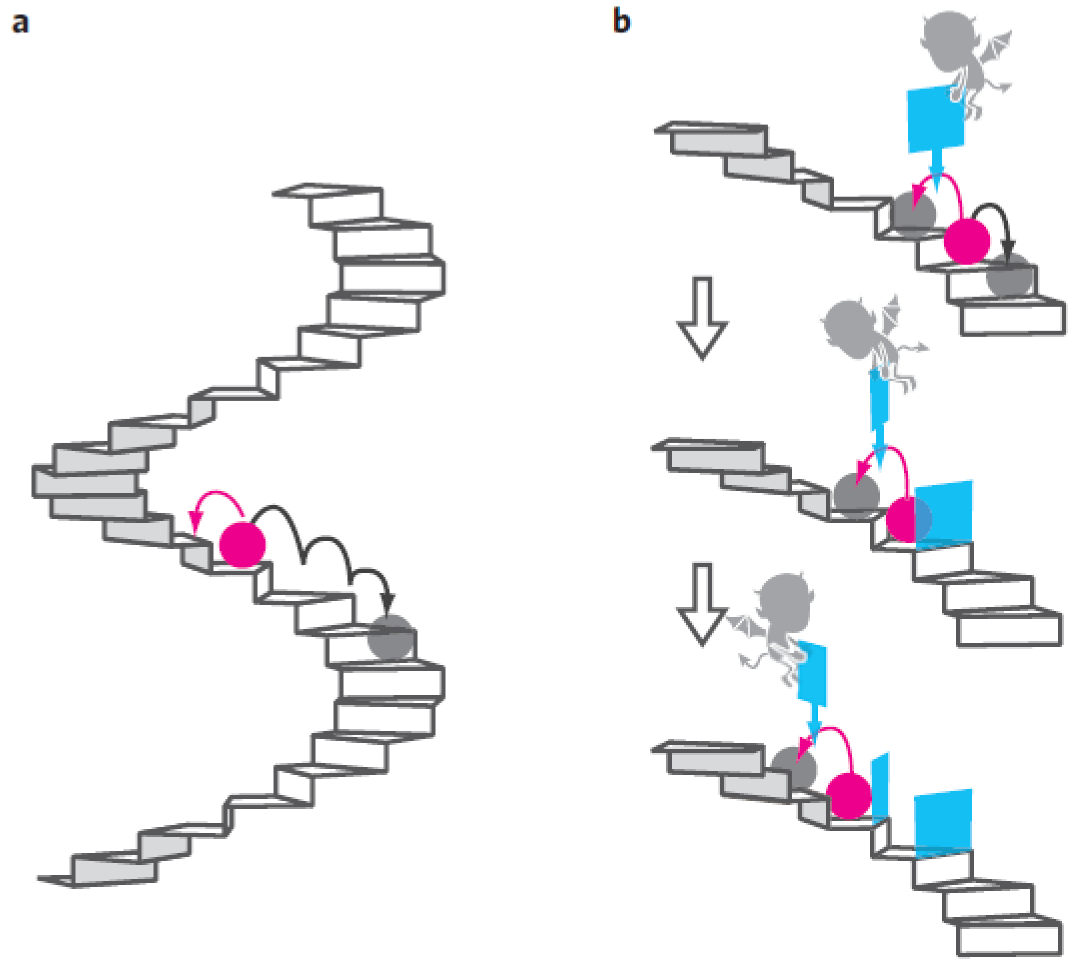
The simplest and analyzable Maxwell's demon

Szilard (1929)



However we gain, $W = k_B T \ln 2$: Information gain → decrease of entropy

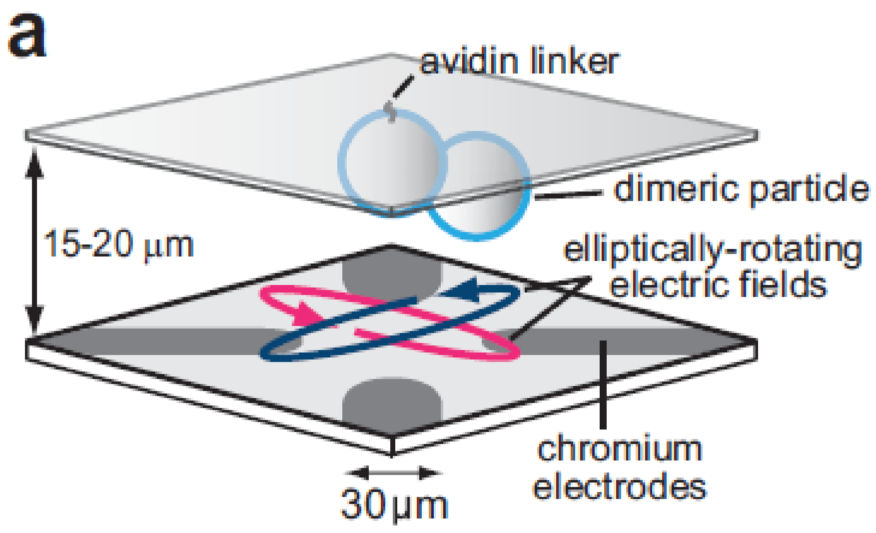
Schematic illustration of the experiment

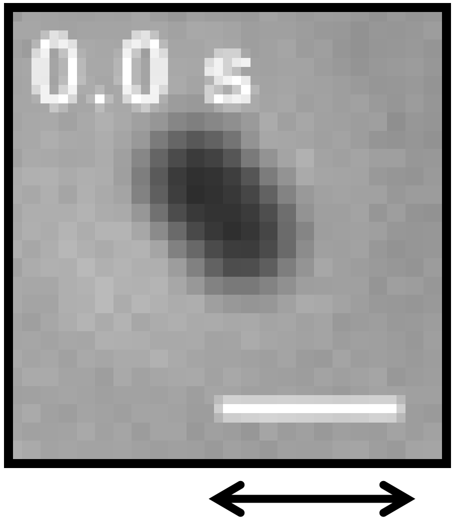


Toyabe, Sagawa, Ueda, Muneyuki, Sano, Nature Physics, 6**,** 988**,** (2010))

Experimental Setup

- Dimeric polystyrene particle (300nm) is linked on the substrate with a biotin.
- Particles exhibit a rotational Brownian motion.

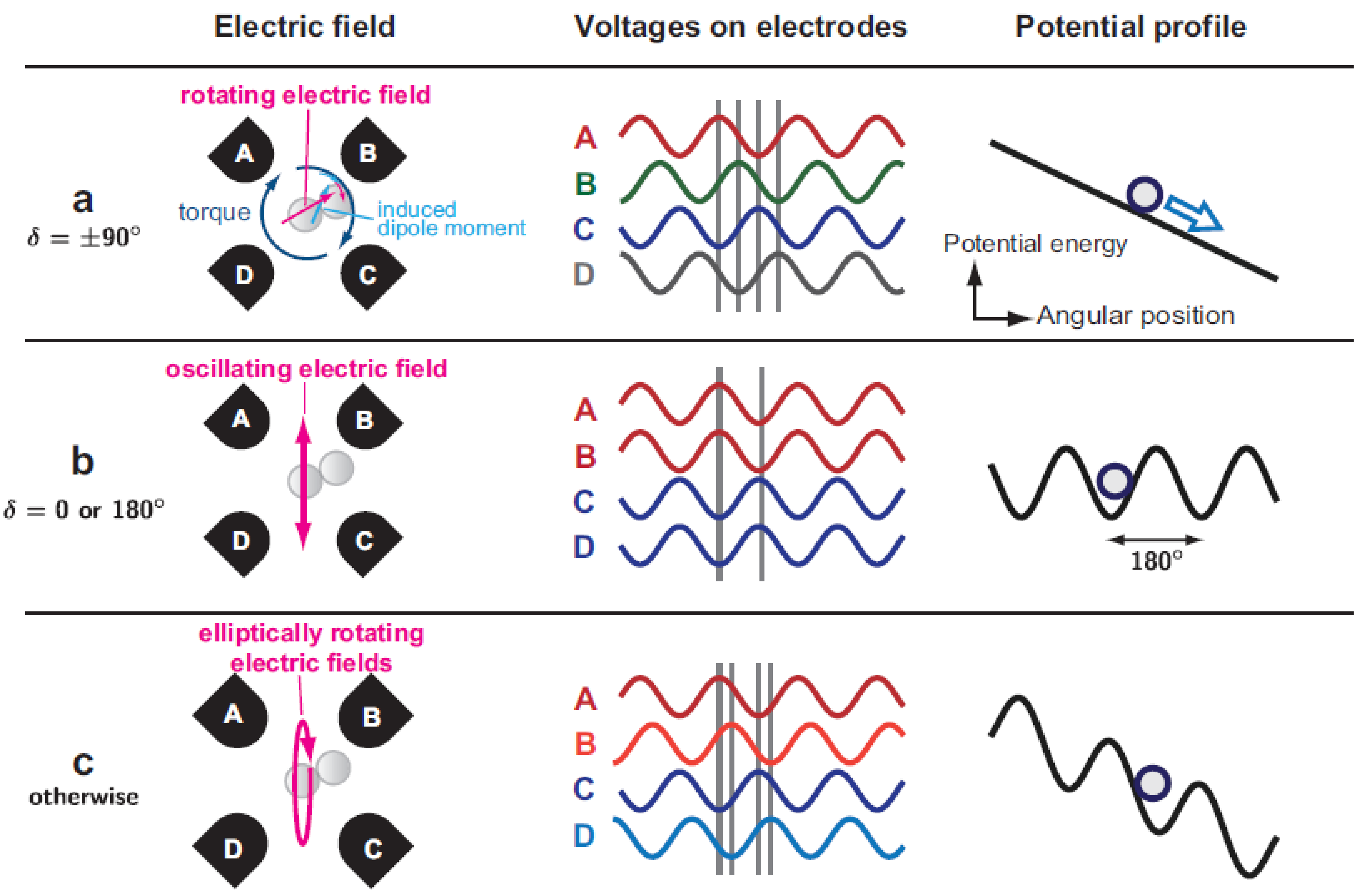




1 µm (1/1000 mm)

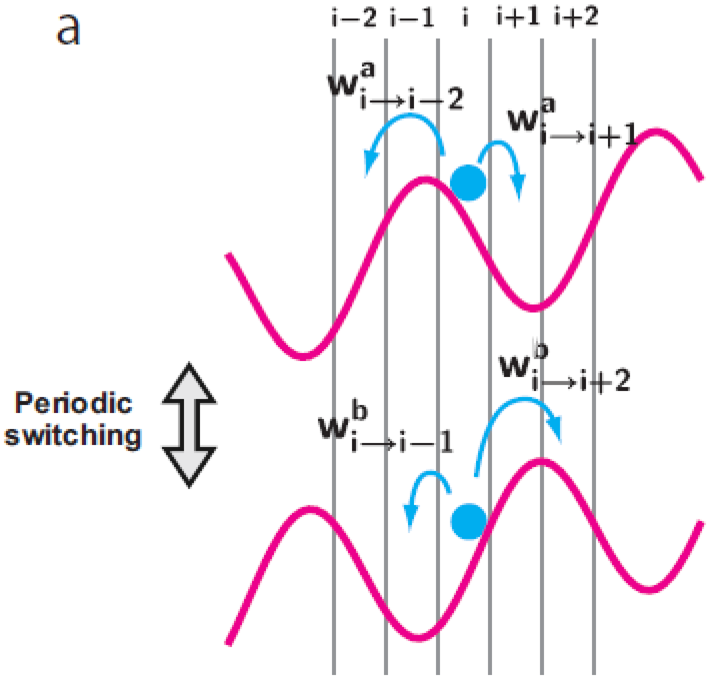
- Quadrant electrodes are patterned on the substrate

How to produce a spiral-stair-like potential

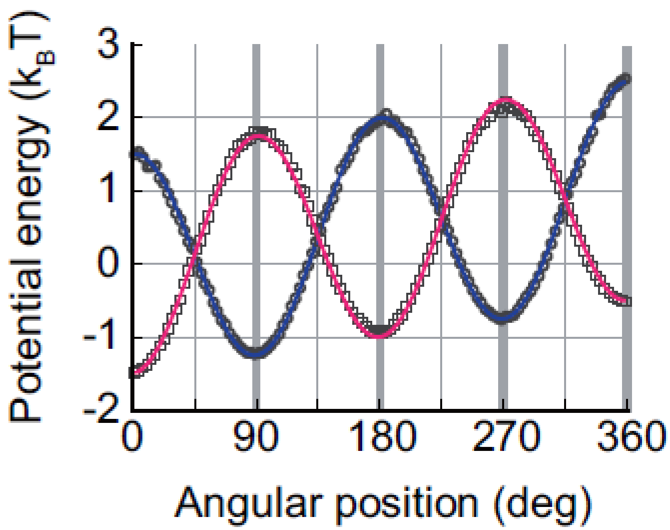


Estimating a potential function

a



b Measured potential function

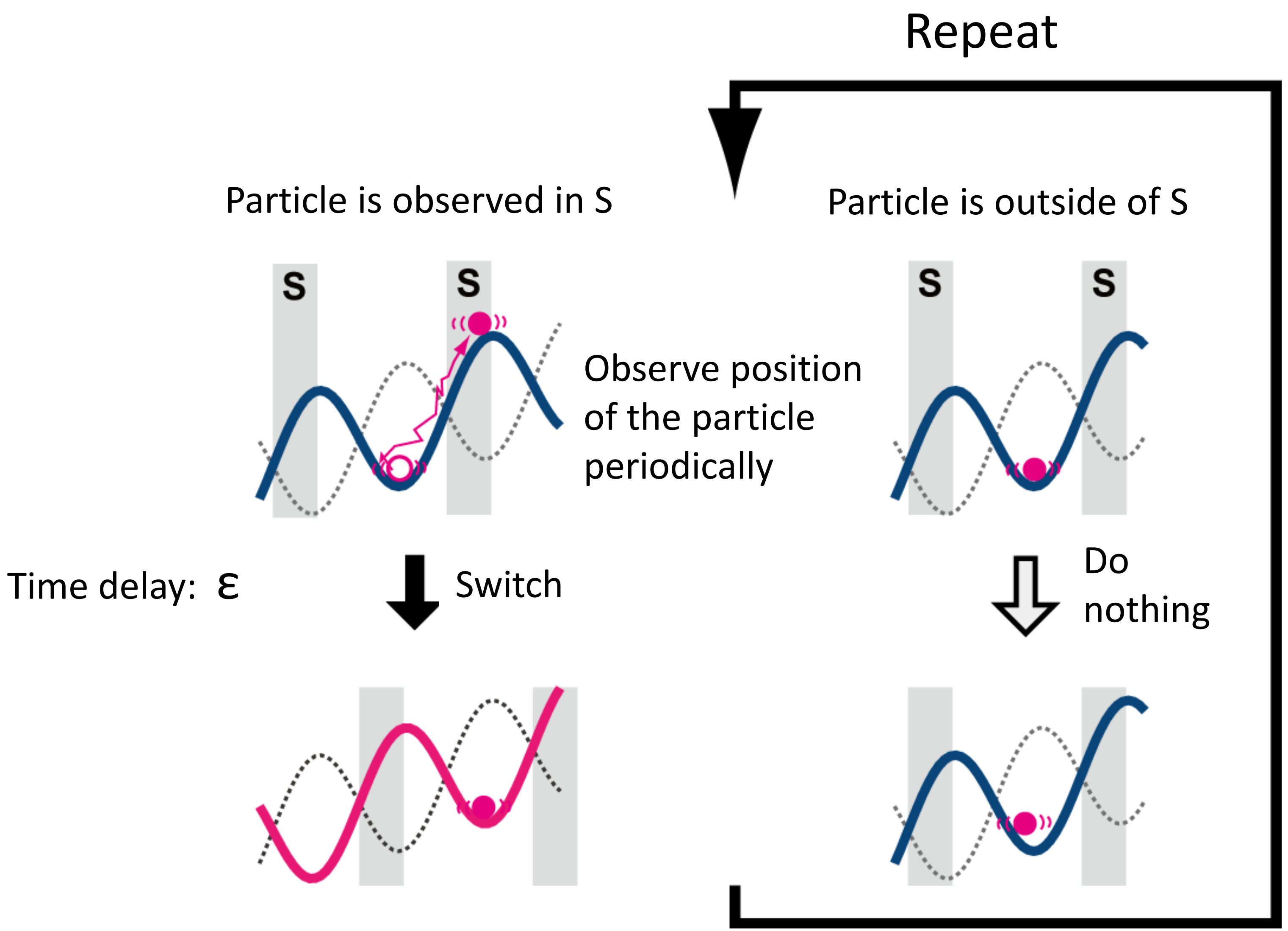


$$\varepsilon^2(\{U_i\}) \equiv \sum_{i<j} \sqrt{n_{i\to j} n_{j\to i}} \left[\Delta U_{i\to j} - \Delta U'_{i\to j}\right]^2,$$

where $\Delta U'_{i\to j} \equiv k_B T \left[\ln w_{j\to i} - \ln w_{i\to j}\right]$

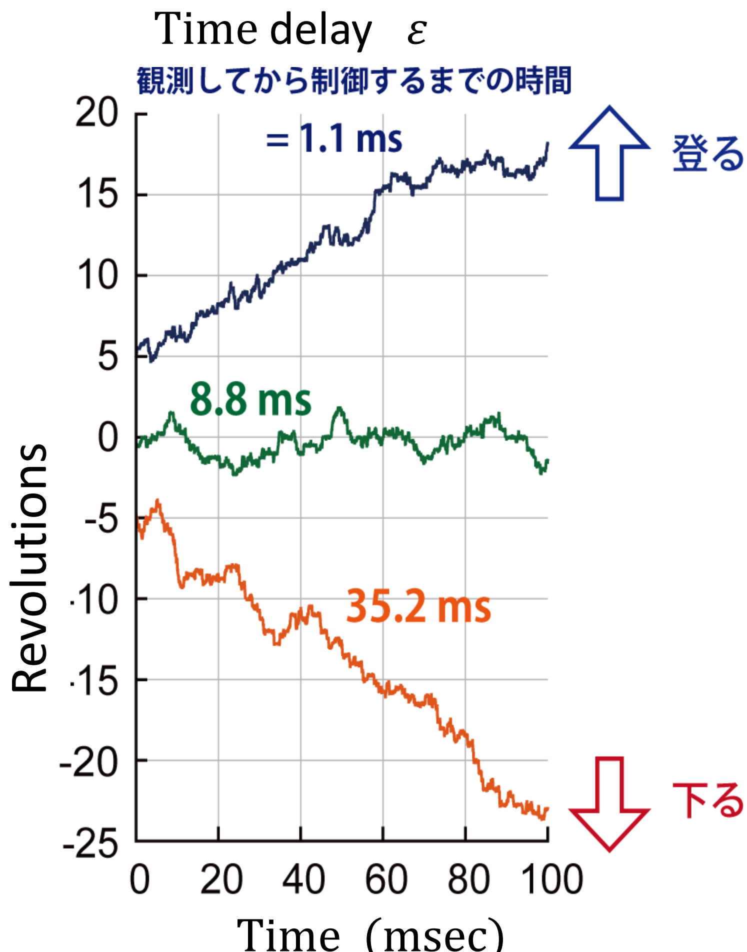
Minimize ε^2

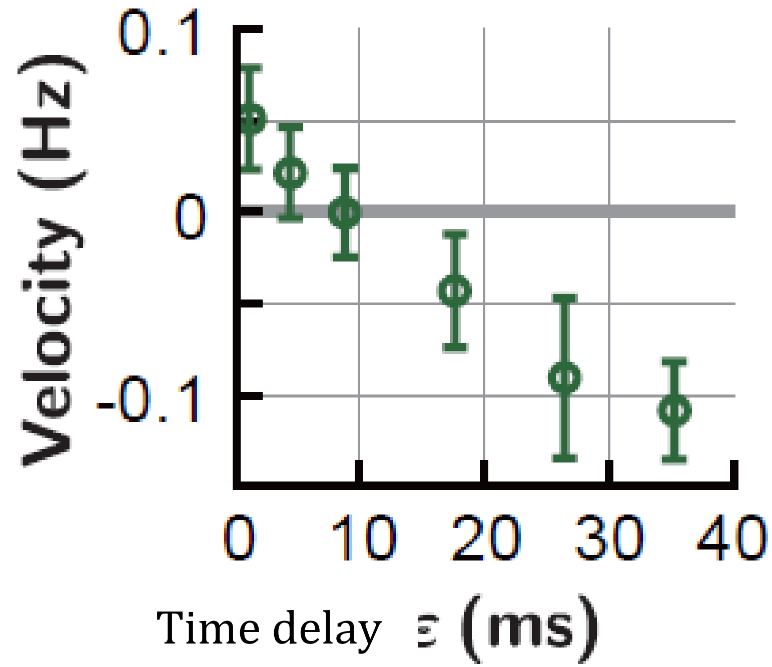
Feedback control based on information contents

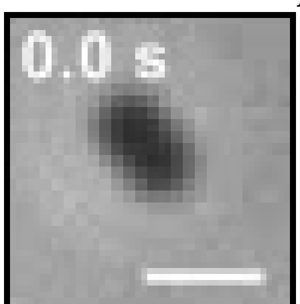


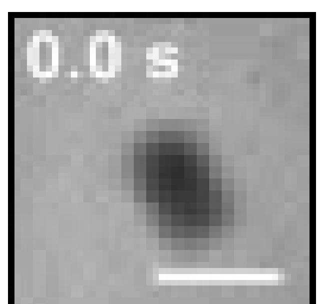
Feedback by Information

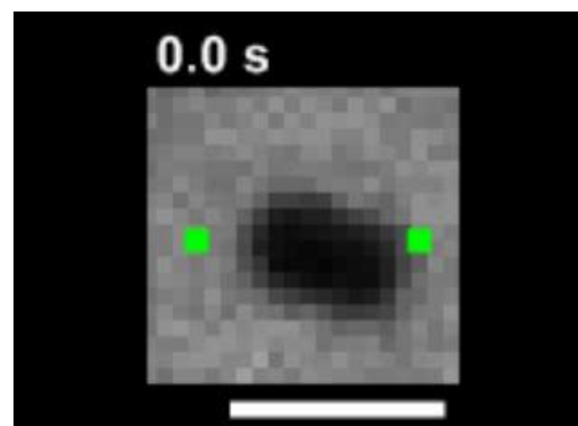
Trajectories under feedback control





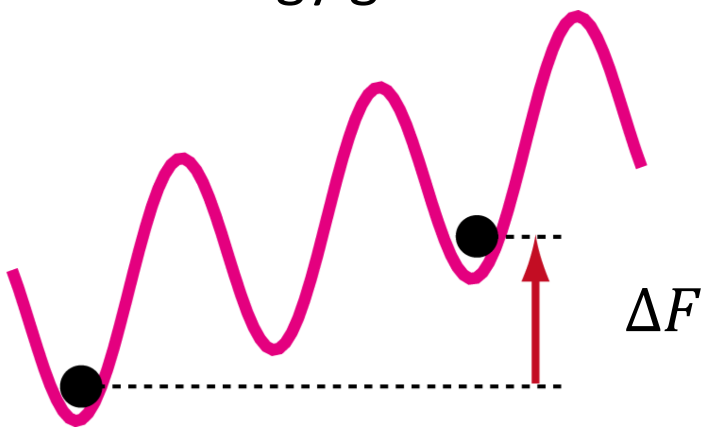






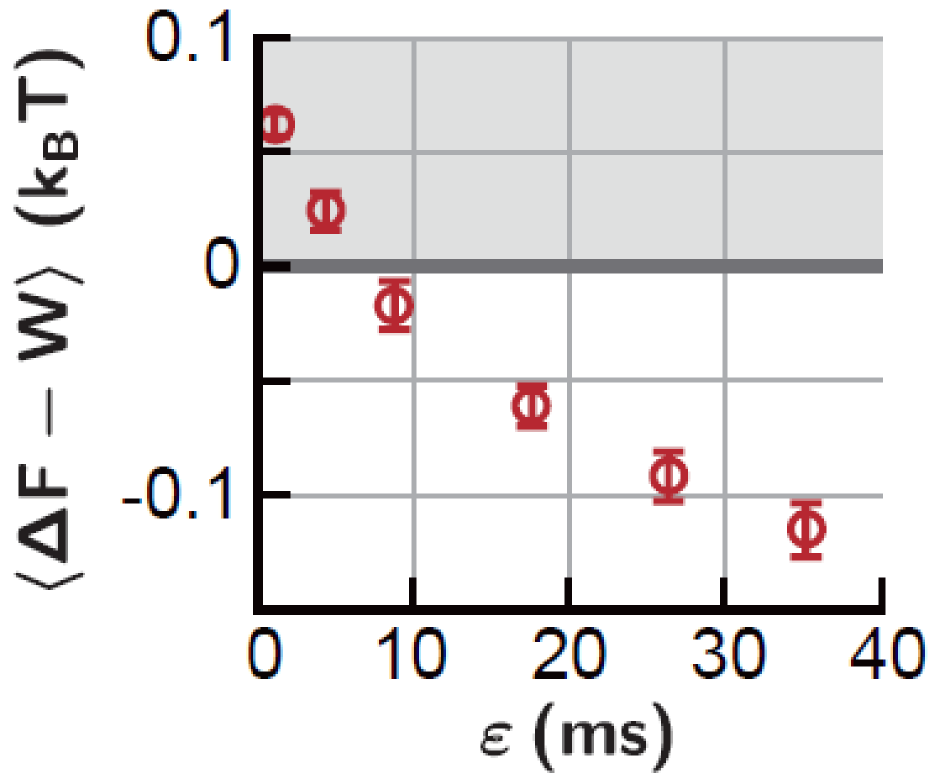
Calculation of Free Energy

- Free energy gain

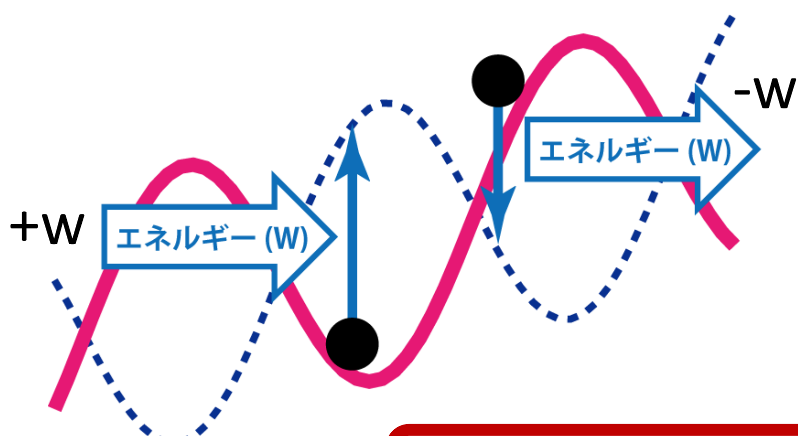


W :Work performed to the system

F :Free energy gain of the system



- Work done to the particle

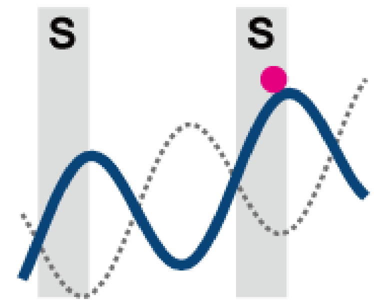


Calculate（ΔF-W）

Efficiency of Information-Energy Conversion

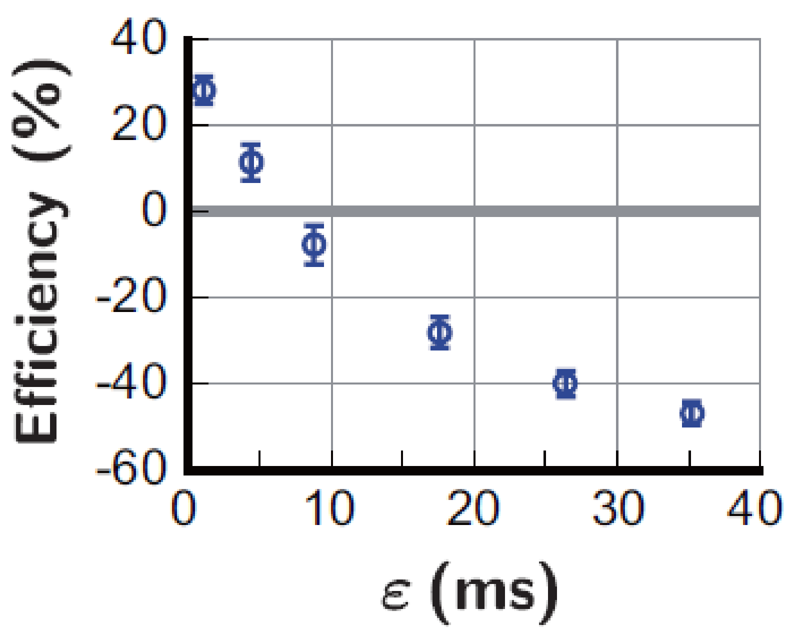
Information gained by the observation:

$$I = -p\ln p \;-(1-p)\ln((1-p)$$



Efficiency of Information-Energy Conversion :

$$\vartheta = \frac{\Delta F - W}{k_B T I}$$



28% Efficiency

Jarzynski equality

Jarzynski equality: $\langle e^{(\Delta F - W)/k_B T} \rangle = 1$

Valid for Liouville equations、ideal chaotic systems
Initial and final distributions are canonical, but path can be out-of-equilibrium

The second law of thermodynamics can be derived:

Jensen's inequality $\langle e^{x} \rangle \geq e^{\langle x \rangle}$ ⇒ $\langle W \rangle - \Delta F \geq 0$

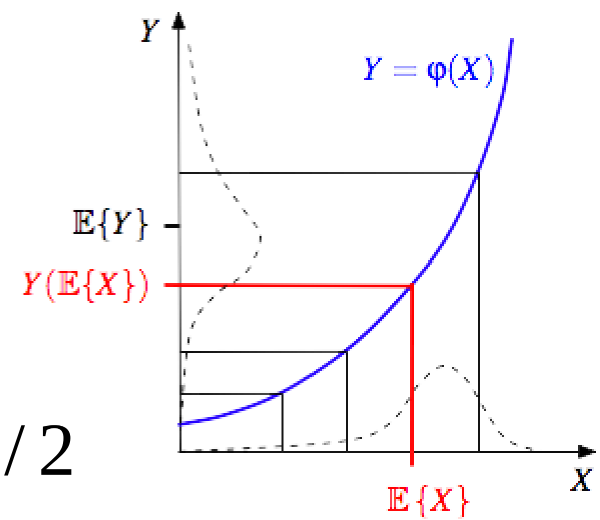
Fluctuation Dissipation Theorem can be derived:

$$\Delta F = -\beta^{-1} \ln < \exp(-\beta w) > = \sum_{n=1}^{\infty} (-\beta)^{n-1} \frac{\omega_n}{n!}$$

1st cumulant: $\Delta F = w_A = < w >$

2nd cumulant:

Fluctuation-dissipation: $\Delta F = < w > - \beta\sigma^2 / 2$



Generalized Jarzynski equality including mutual information

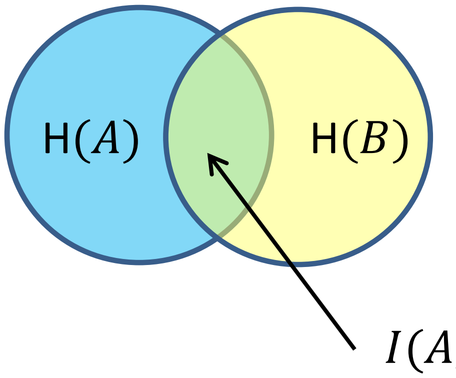
W :Work performed to the system

F :Free energy gain of the system

$$\langle W \rangle \geq \Delta F - kT\langle I \rangle$$

I : mutual information

measurement and control have errors



Correspondingly generalized Jarzynski equality:

$$\langle e^{(\Delta F - W)/k_B T + I} \rangle = 1$$

$$\langle e^{(\Delta F - W)/k_B T} \rangle = \gamma$$

Sagawa & Ueda, PRL (2010)

Experimental test of generalized Jarzynski equality

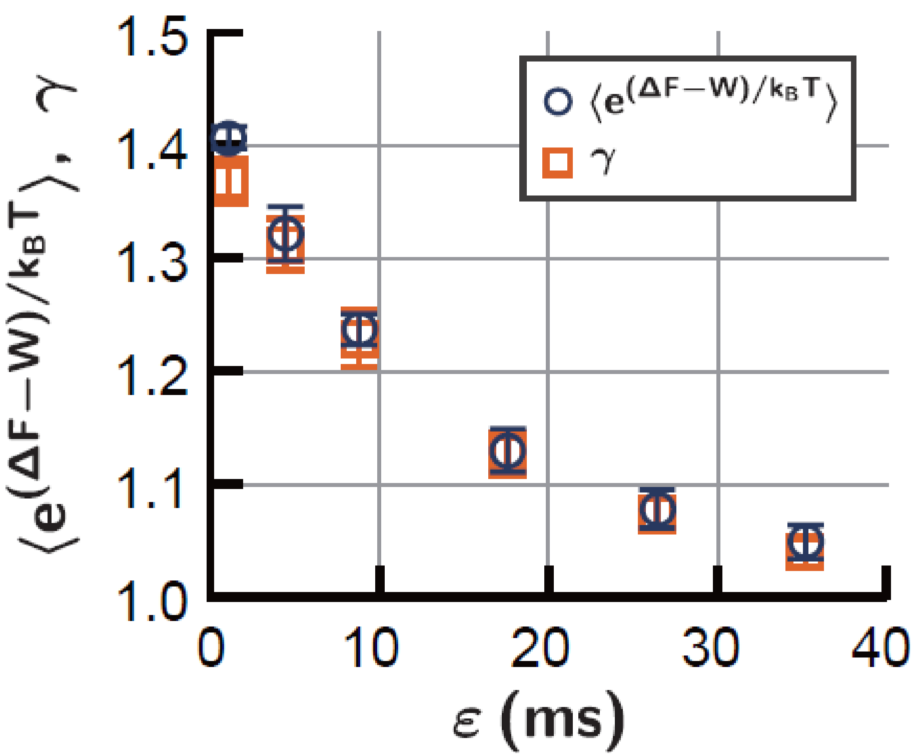
- Entropy Production

$$\langle e^{\beta(\Delta F - W)} \rangle = \gamma$$

generalized Jarzynski equality
Sagawa, Ueda, PRL (2010)

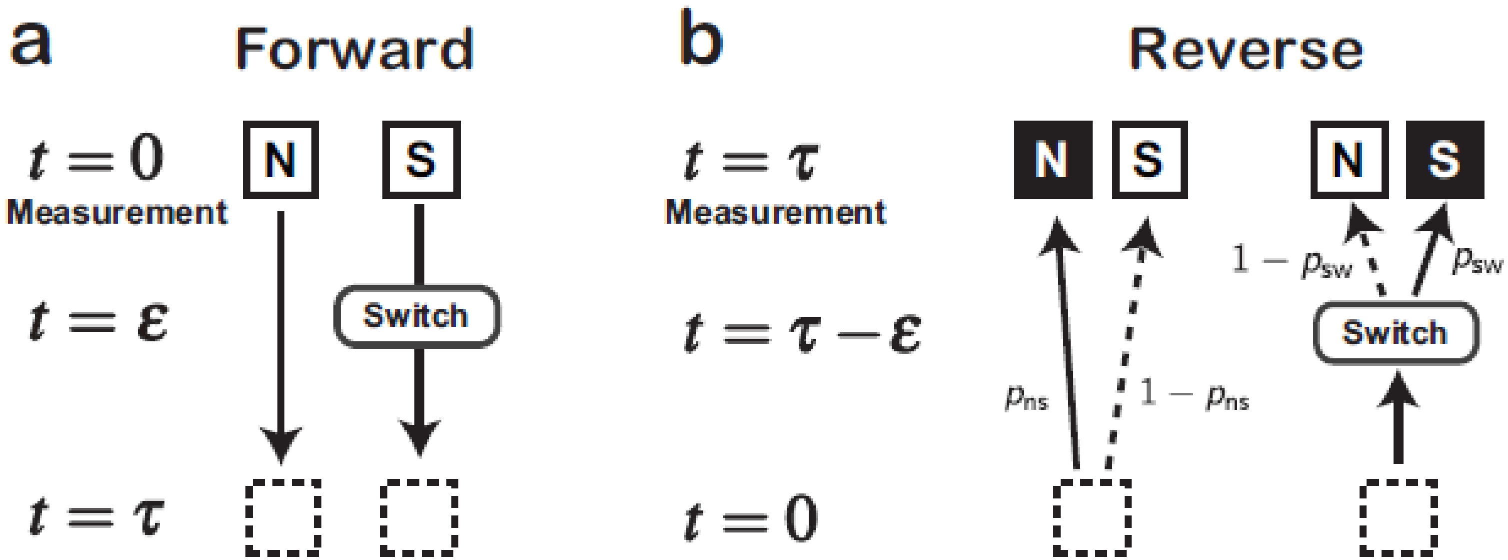
Feedback Efficacy

- **A fundamental principle to relate energy and information feedback**



Agrees within measurement accuracy

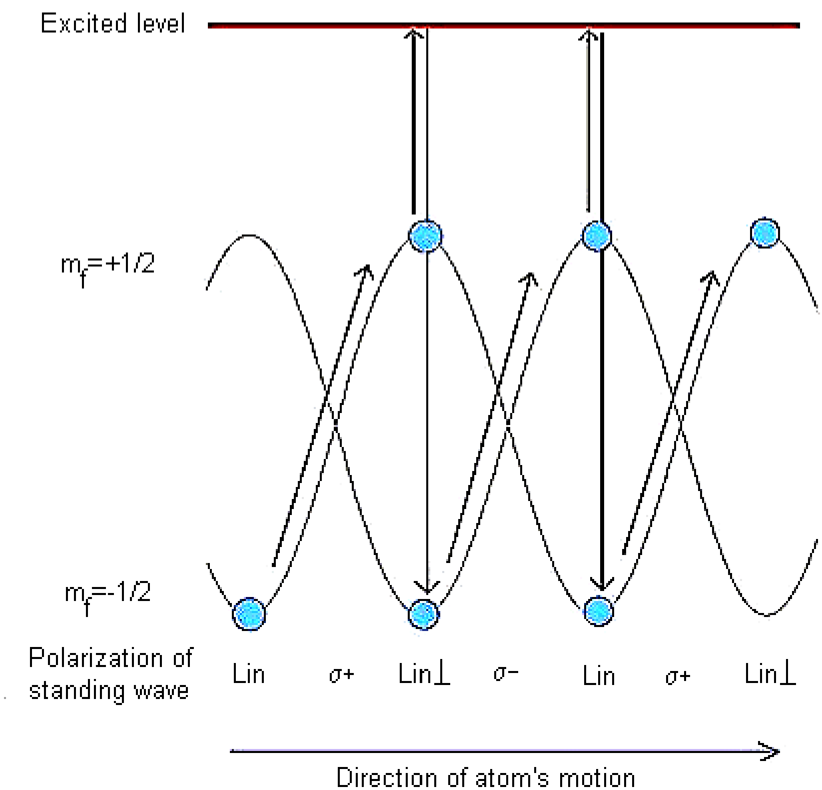
How to measure the feedback efficacy

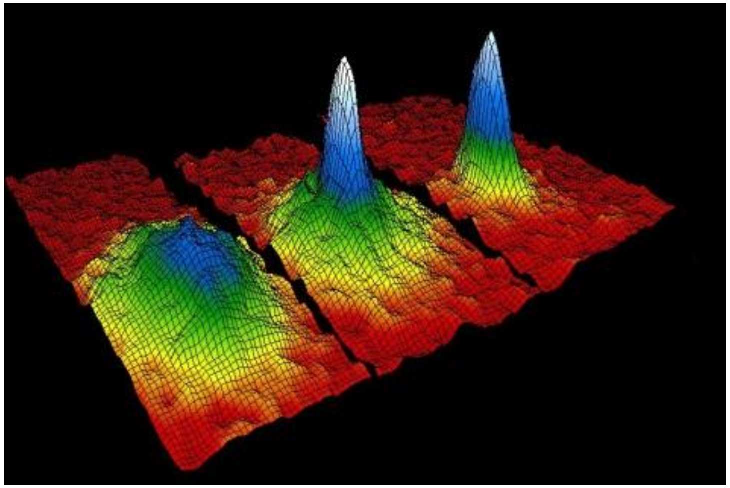


$\gamma = p_{sw} + p_{ns} \leq\geq 1$

Laser Cooling: Sisyphus Cooling

Polarization Gradient Cooling

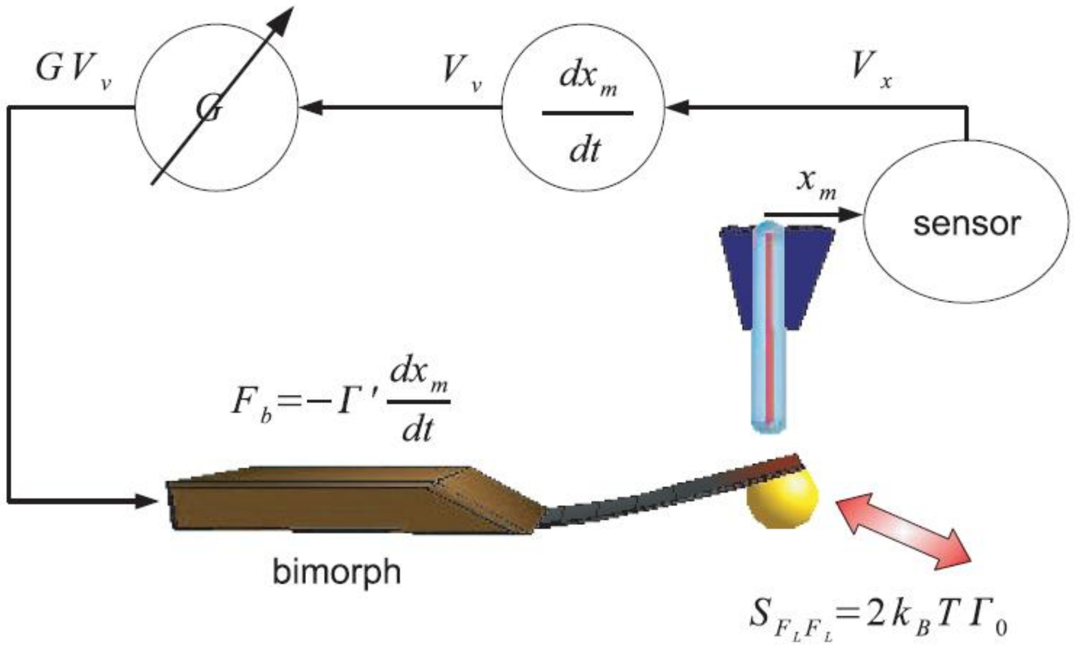




Cohen-Tannoudji

http://www.nobelprize.org/nobel_prizes/physics/laureates/1997/

Cooling limit with feedback control



Reducing thermal fluctuations of lever of Atomic Force Microscope (AFM)

What is the limit of cooling?

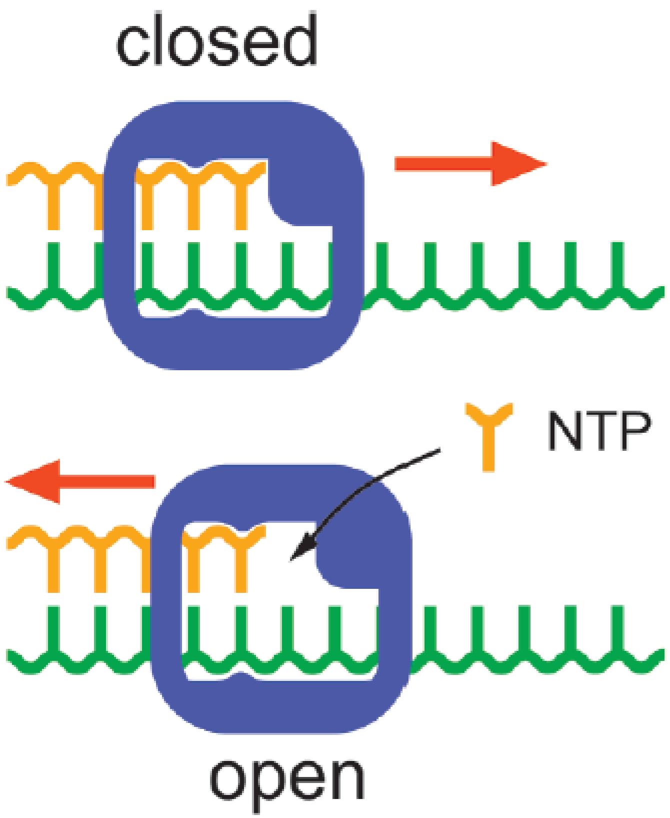
G. Jourdan et al., Nanotechnology, (2007)

Cooling Limit:

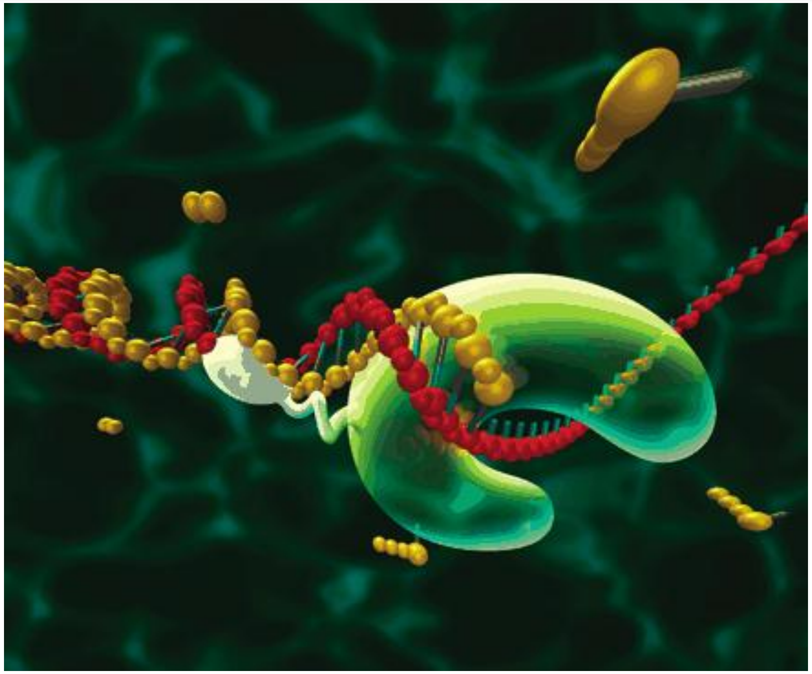
$$\frac{T - T_{\rm eff}}{T} \geq \frac{\sum_i \langle I_i \rangle_0}{\tau} t_r .$$

S. Ito and M. Sano, PRE (2011)

Are molecular motors Maxwell's demon?

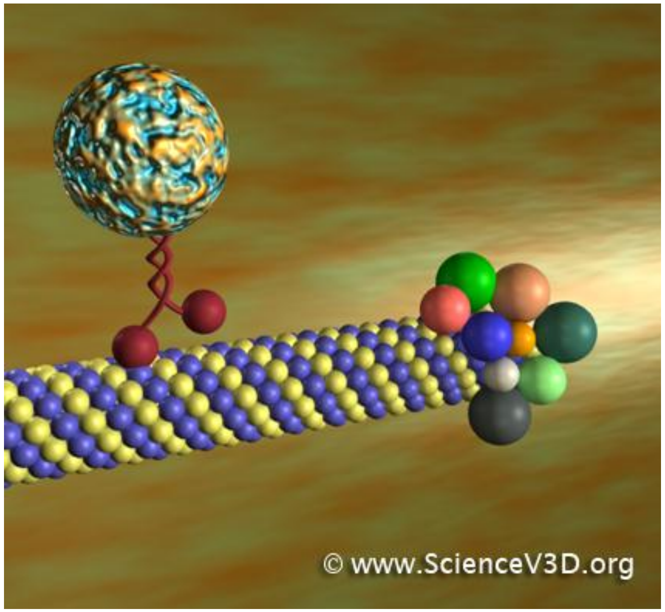


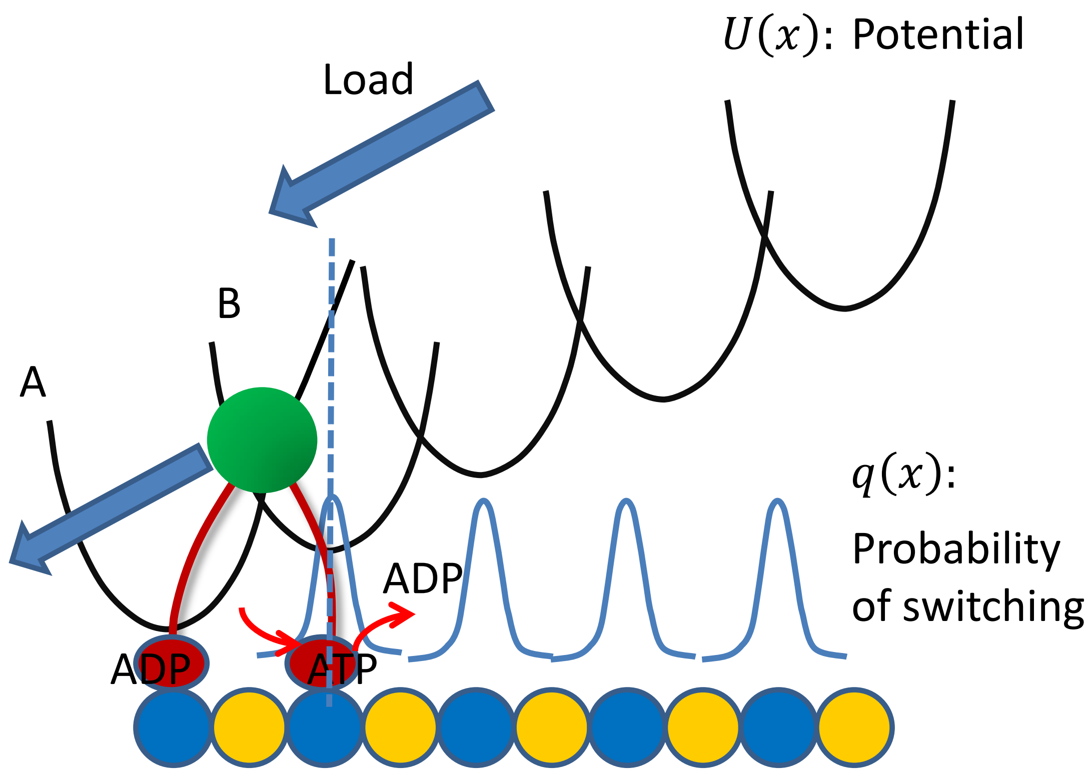
DNA Polymerase behaves like a thermal ratchet



- Polymerase binds to DNA
- each process is reversible
- Moves back and forth by thermal fluctuations
- NTP can bind in the open space
- NTP concentration is higher than equilibrium

Are molecular motors Maxwell's demon?





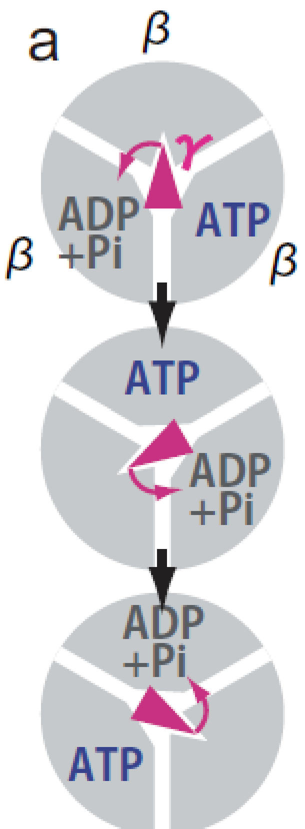
$$p_A(x) = \frac{e^{-\beta U_A(x)}}{Z}$$

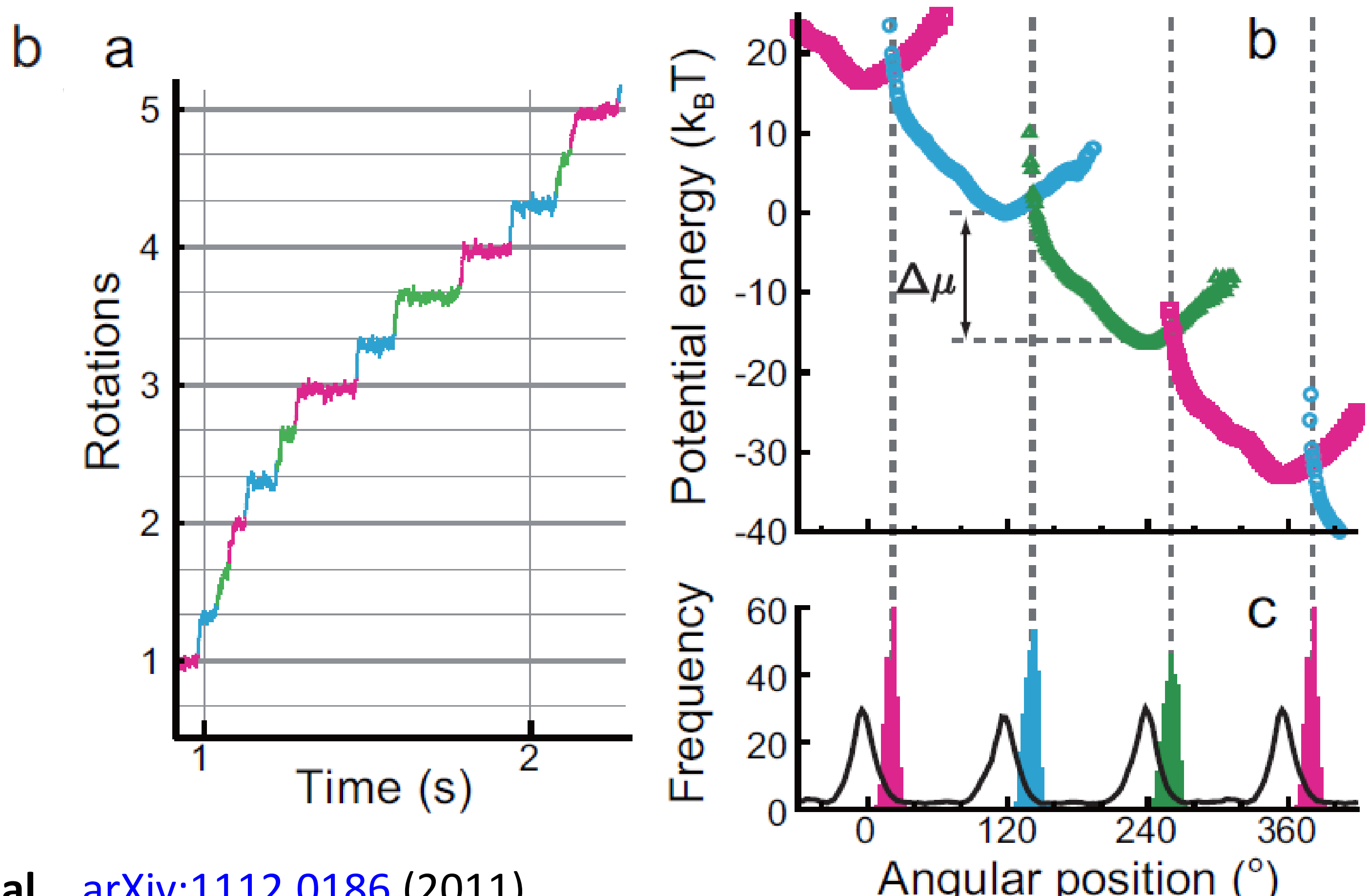
$$\langle e^{-\beta(W-\Delta F)} \rangle = \gamma = \int q(x) \frac{p_A(x)}{p_B(x)} dx$$

Probability of switching

If the switching position is much shifted to forward direction, γ can exceed 1, otherwise not.

Autonomous switching of F1 molecular motor





Toyabe_S et al., arXiv:1112.0186 (2011)

But efficiency of free energy transduction is much smaller than 1.

$$\sigma_f \equiv \frac{\Delta F}{\Delta G} \leq \frac{D(q||p_0)}{D(q||p_0) + D(p_0||q)} \leq 1.$$

Kawaguchi, Sano JPSJ (2011).

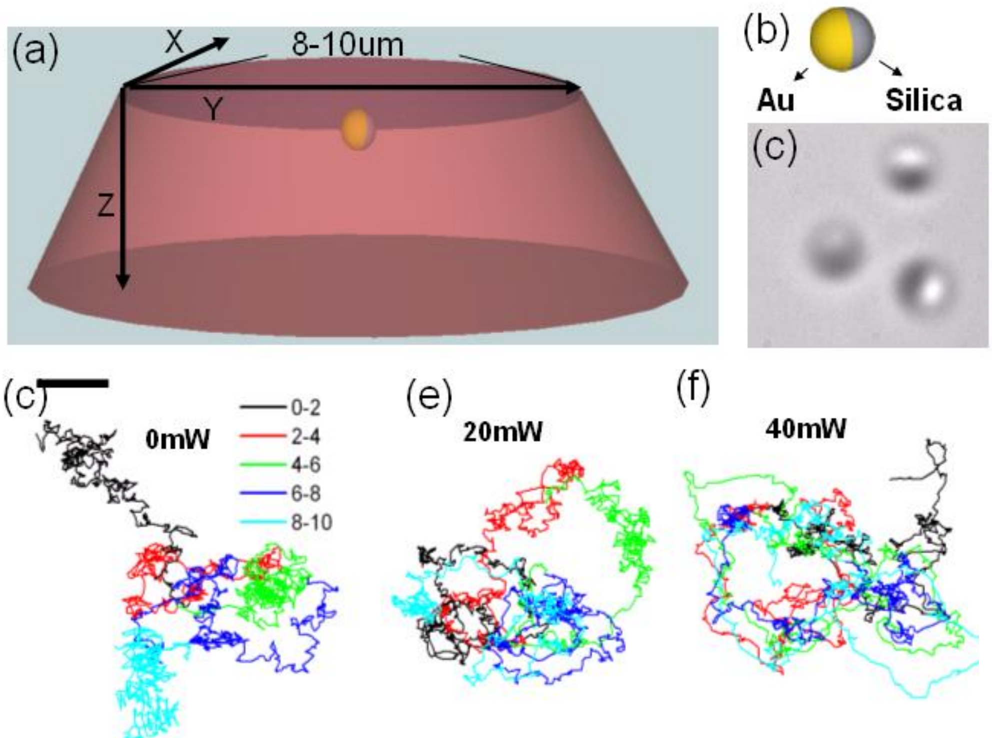
D: Kullback-Leibler Information

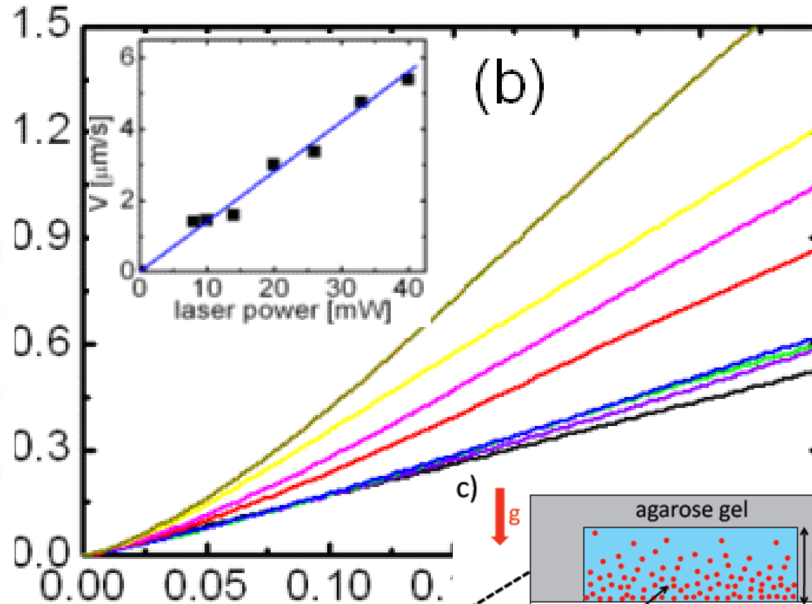
Information and Feedback in Different Systems

	Fluctuation	Information	Feedback	Outcome
Maxwell's demon	Thermal	Speed, position	Biased Choice of fluctuations	Gain Free Energy
Active Particle	Thermal	-------	--------	Enhance Diffusion
Bacteria (*Escherichia coli*)	tumbling	Chemotactic Signal	Change tumbling freq.	Chemotaxis
Amoeboid cell (*Dictyostelium Discoideum*)	Instability of cell shape	Chemotactic Signal	Biased Choice of random protrusion	Chemotaxis

Self-propulsion of Janus hot particle

Jiang, Yoshinaga, Sano, PRL (2010).



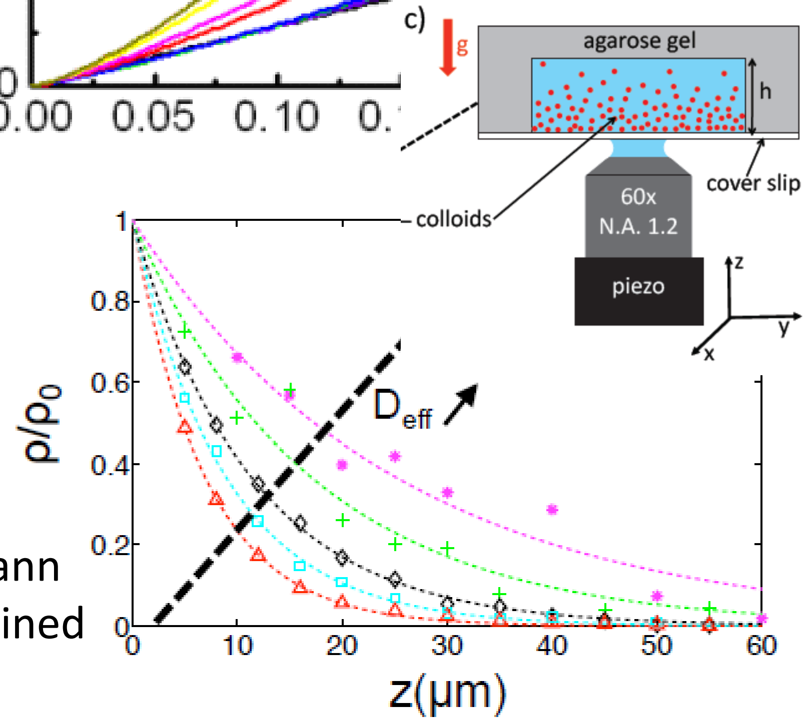


$$\langle \Delta r^2(t) \rangle = 2\tau V^2[t - \tau(1 - e^{-t/\tau})]$$

$$\langle \Delta r^2(t) \rangle \sim V^2 t^2, \qquad t << \tau$$

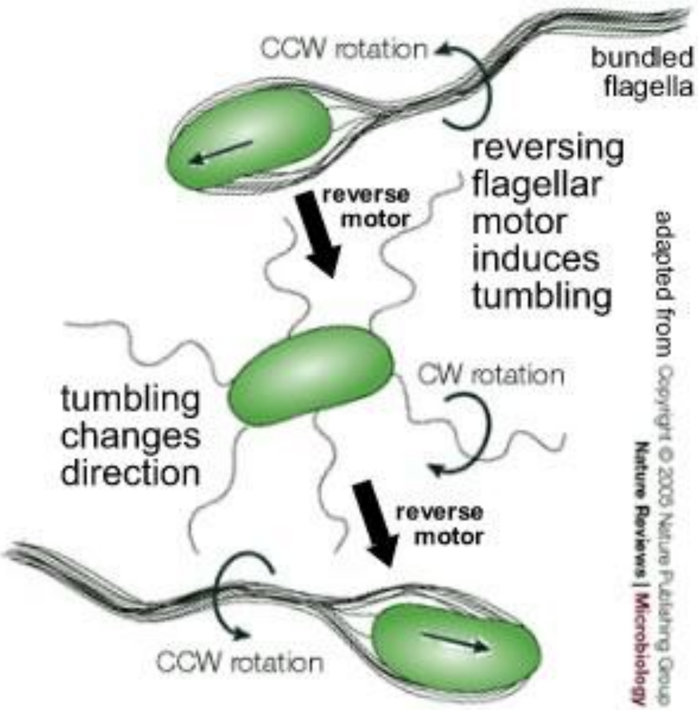
$$\langle \Delta r^2(t) \rangle \sim \tau V^2 t, \qquad t >> \tau$$

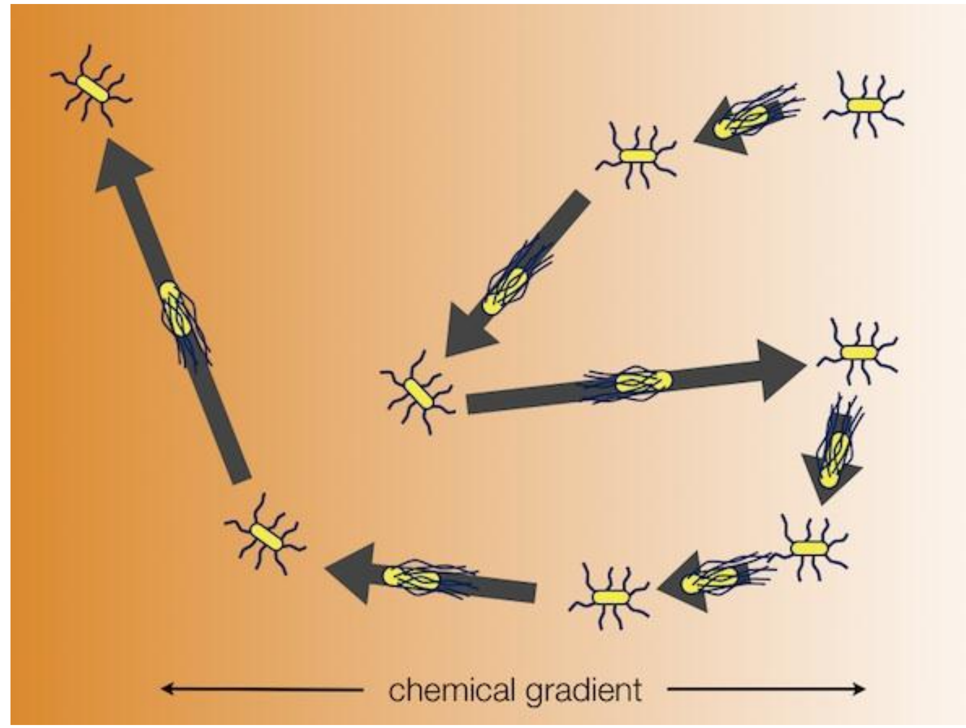
Effectively, Boltzmann distribution is obtained Under gravity.

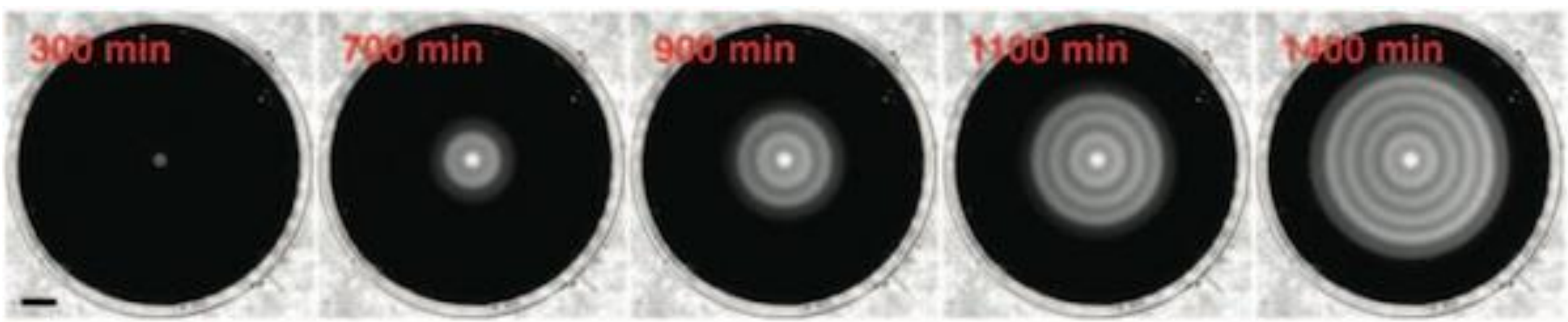


L. Bocquet, PRL (2010)

Chemotaxis of Bacteria







http://www.sciencemag.org/content/334/6053/238.abstrac
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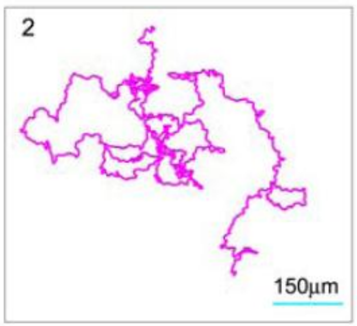
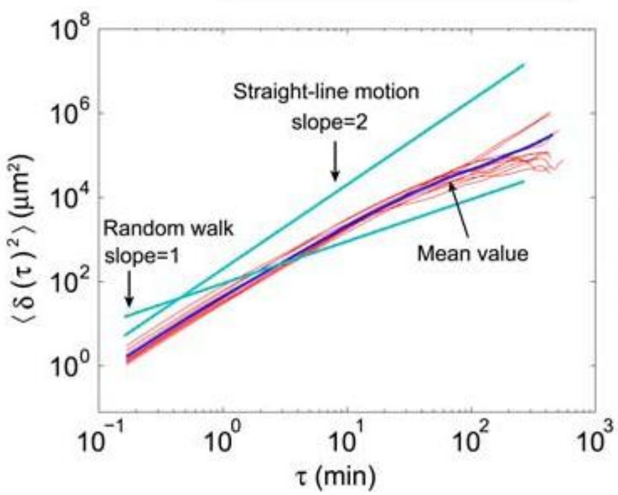
- Long term migration behaviors of Bacteria and Amoeboid cells result in an enhanced diffusion.

→

- Final distribution approaches to an equilibrium distribution





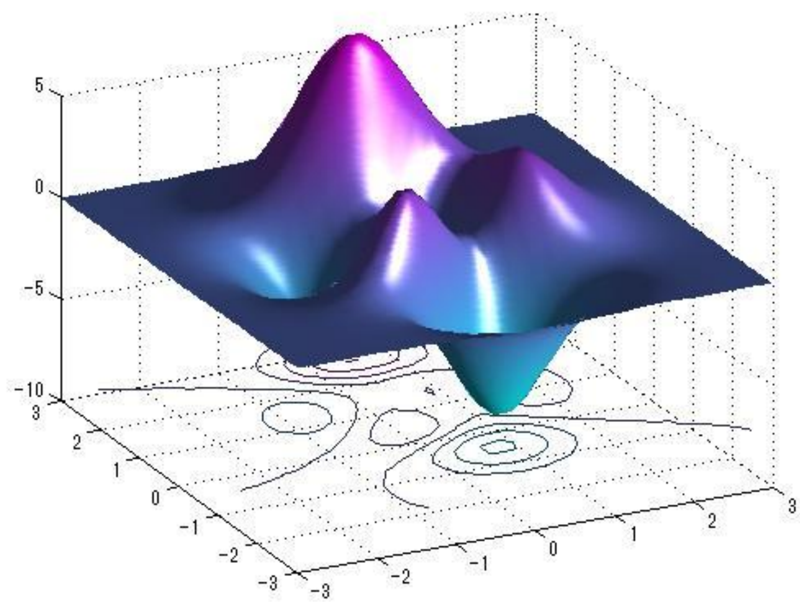
Li, Cox, PLos One (2008)

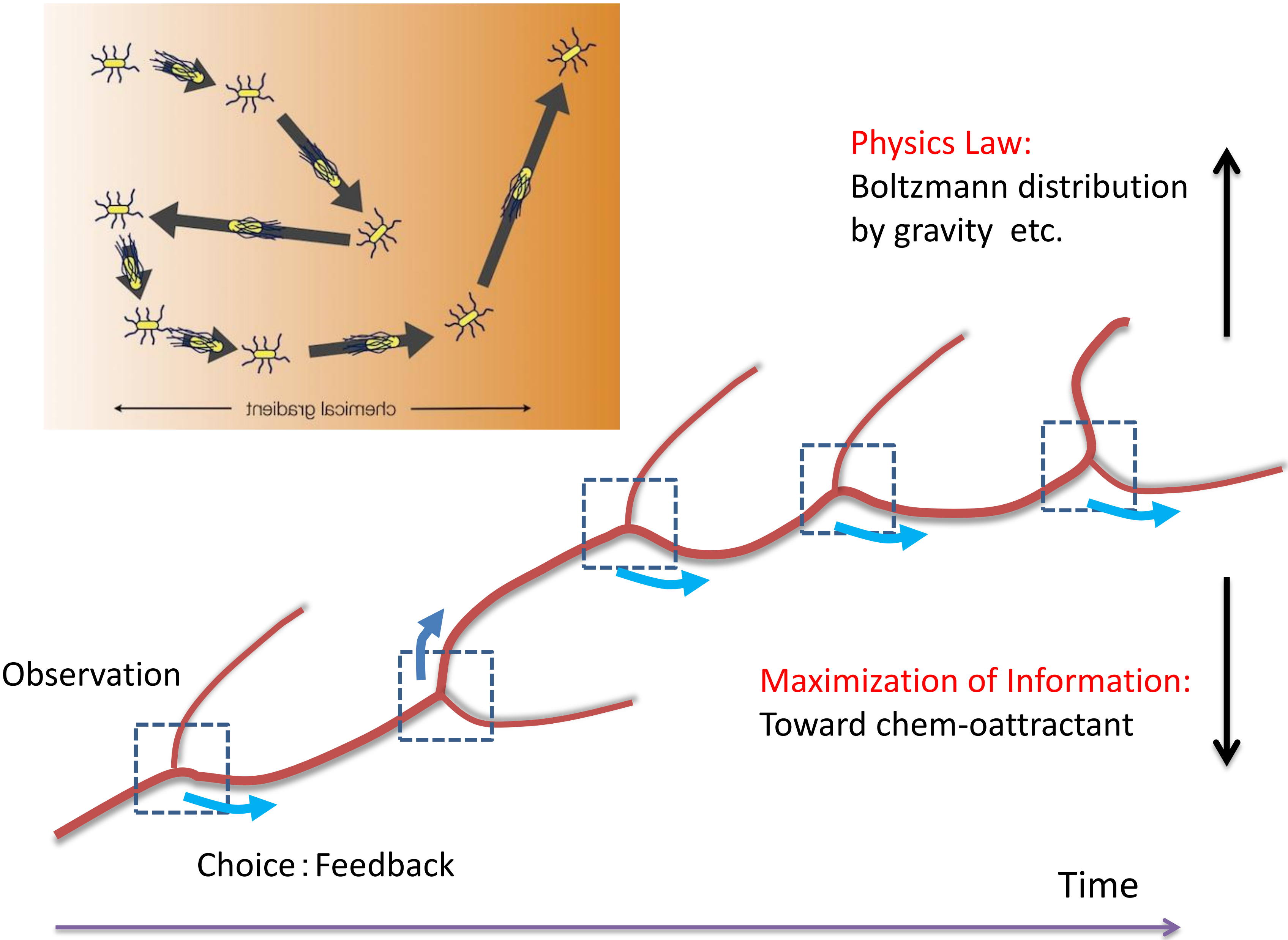
Sufficient Condition: Master equation + detailed balance

→ H Theorem like（～2^{nd} Law of Thermodynamics）

$$P(x) = \frac{e^{-\beta U(x)}}{Z}$$

$U(x)$: Potential by obstacles




chemical gradient
Physics Law:
Boltzmann distribution
by gravity etc.
Observation
Maximization of Information:
Toward chem-oattractant
Choice : Feedback
Time

Summary

- Maxwell's demon
- Demonstration of Information-Energy conversion

  (Toyabe, Sagawa, Ueda, Muneyuki, Sano, Nature Physics, 6, 988, (2010))

- Some of molecular motors utilize information of thermal fluctuations.
- Chemotaxis is a process of information feedback

  Active Colloids (Colloidal particles with asymmetry)