

2020年 清华大学 理论物理+原子分子物理优秀大学生暑期学校  
2020.08.17--2020.08.20

# Stochastic Thermodynamics and Fluctuation Theorem

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Physics School, PKU

# Outline

- Thermodynamics in the 19<sup>th</sup> and the 21<sup>st</sup> century
- Stochastic thermodynamics
- Fluctuation Theorems
- Maxwell's demon
- Summary

# Outline

- Thermodynamics in the 19<sup>th</sup> and the 21<sup>st</sup> century
- Stochastic thermodynamics
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- Perspective

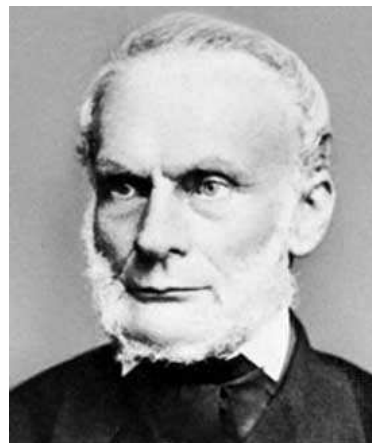
1820 $\simeq$ 1850	classical thermodynamics	$dW = dU + dQ$ $dS \geq 0$
$\simeq$ 1900	eq stat phys	$p_i = \exp[-(E_i - F)/k_B T]$
1930 $\simeq$ 1960	non-eq: linear response	Onsager Green-Kubo, FDT
$\geq$ 1993	non-eq: beyond linear response stochastic thermodynamics	Fluctuation theorem Jarzynski relation

# Background: Thermodynamics of the 19<sup>th</sup> century

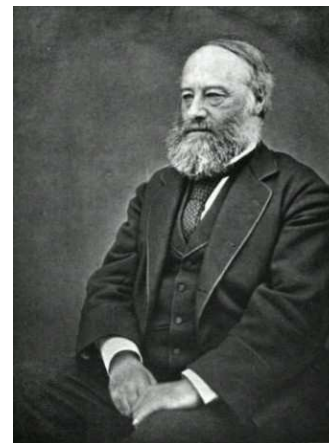
Large system: many degrees of freedom,  
many particles,  
average values,  
vanishingly small fluctuation,  
near equilibrium process,



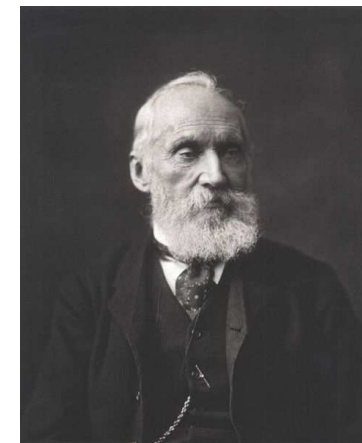
Sadi Carnot



Rdolf Clausius



James Joule



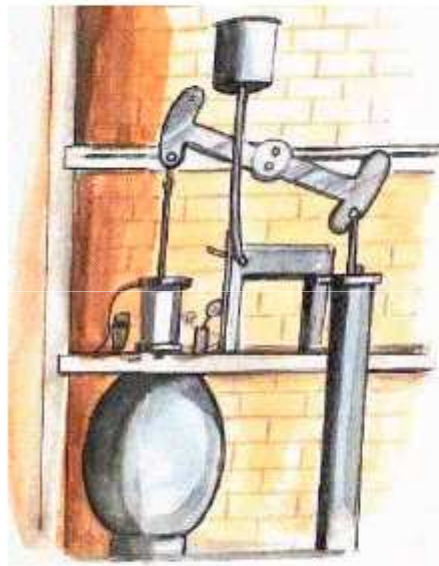
William Thomson

# Laws of thermodynamics

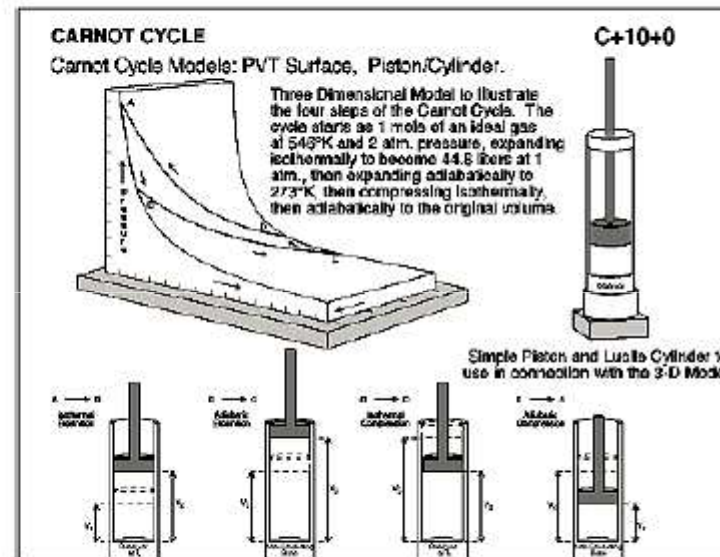
- [Zeroth law of thermodynamics](#): If two systems are in thermal equilibrium separately, with a third system, they must be in thermal equilibrium with each other. This law helps define the notion of [temperature](#).
- [First law of thermodynamics](#): When energy passes, as work, as heat, or with matter, into or out from a system, its internal energy changes in accord with the law of [conservation of energy](#). Equivalently, [perpetual motion machines](#) of the first kind are impossible.
- [Second law of thermodynamics](#): The entropy of any isolated system never decreases. Such systems spontaneously evolve towards [thermodynamic equilibrium](#) — the state of maximum [entropy](#) of the system. Equivalently, [perpetual motion machines](#) of the second kind are impossible.
- [Third law of thermodynamics](#): The entropy of a system approaches a constant value as the temperature approaches [absolute zero](#).<sup>[2]</sup> With the exception of [glasses](#) the entropy of a system at absolute zero is typically close to zero, and is equal to the log of the multiplicity of the quantum [ground state](#).

# Thermodynamic cycles and Carnot engine

steam engine

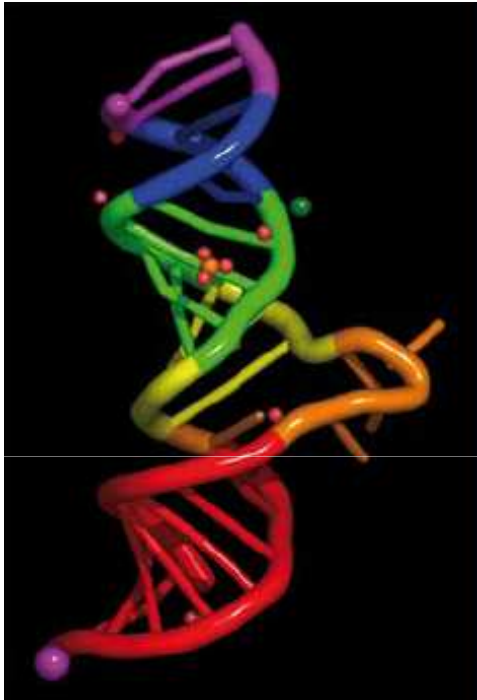


Carnot cycle



textbook thermodynamics

# Thermodynamics of the 21<sup>th</sup> century



Mark Haw, *Physics World*, **20**, No 11, 25, 2007.

Small system: few degrees of freedom,  
few particles,  
prominent fluctuations,  
quantum effects,  
non-equilibrium process,

Magnetic domains in ferromagnets: less than 300nm

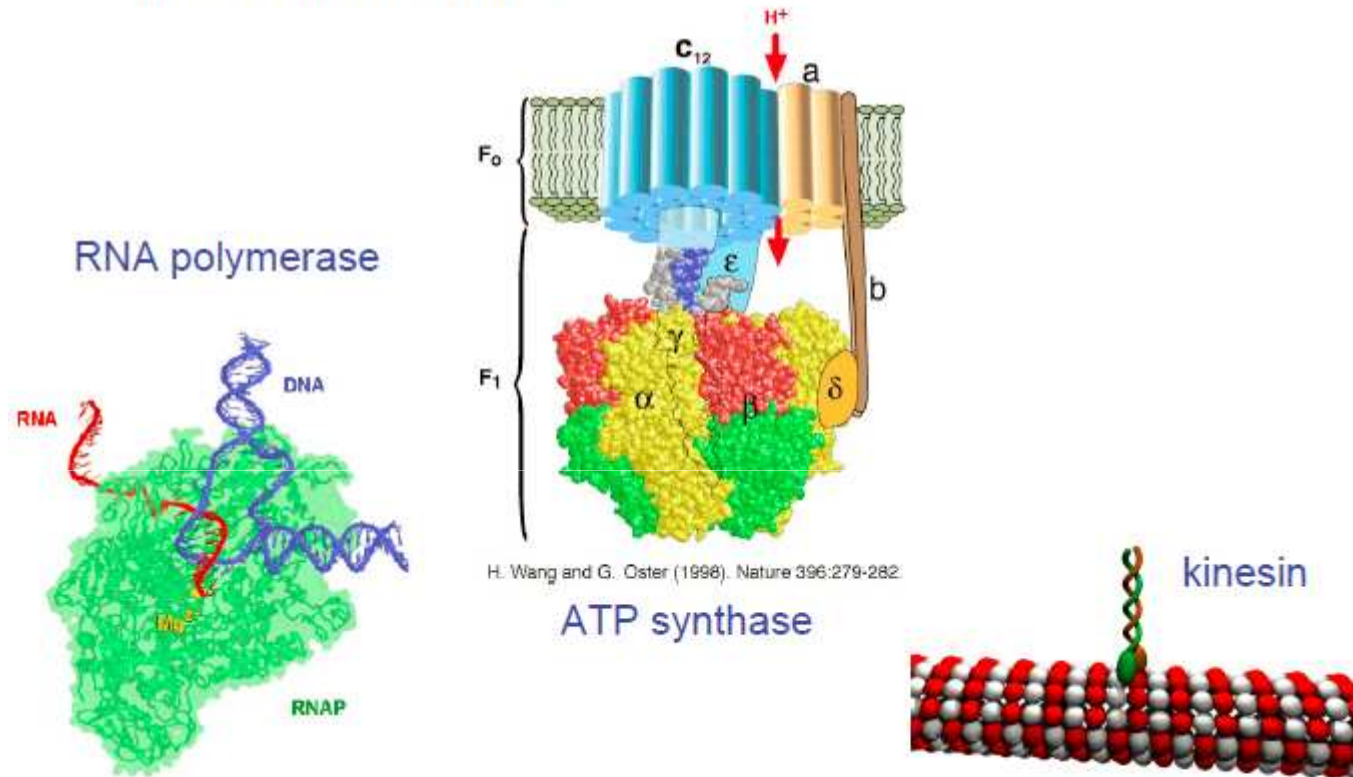
Quantum dots: less than 100nm

Biological molecular machines: range from 2 to 100nm

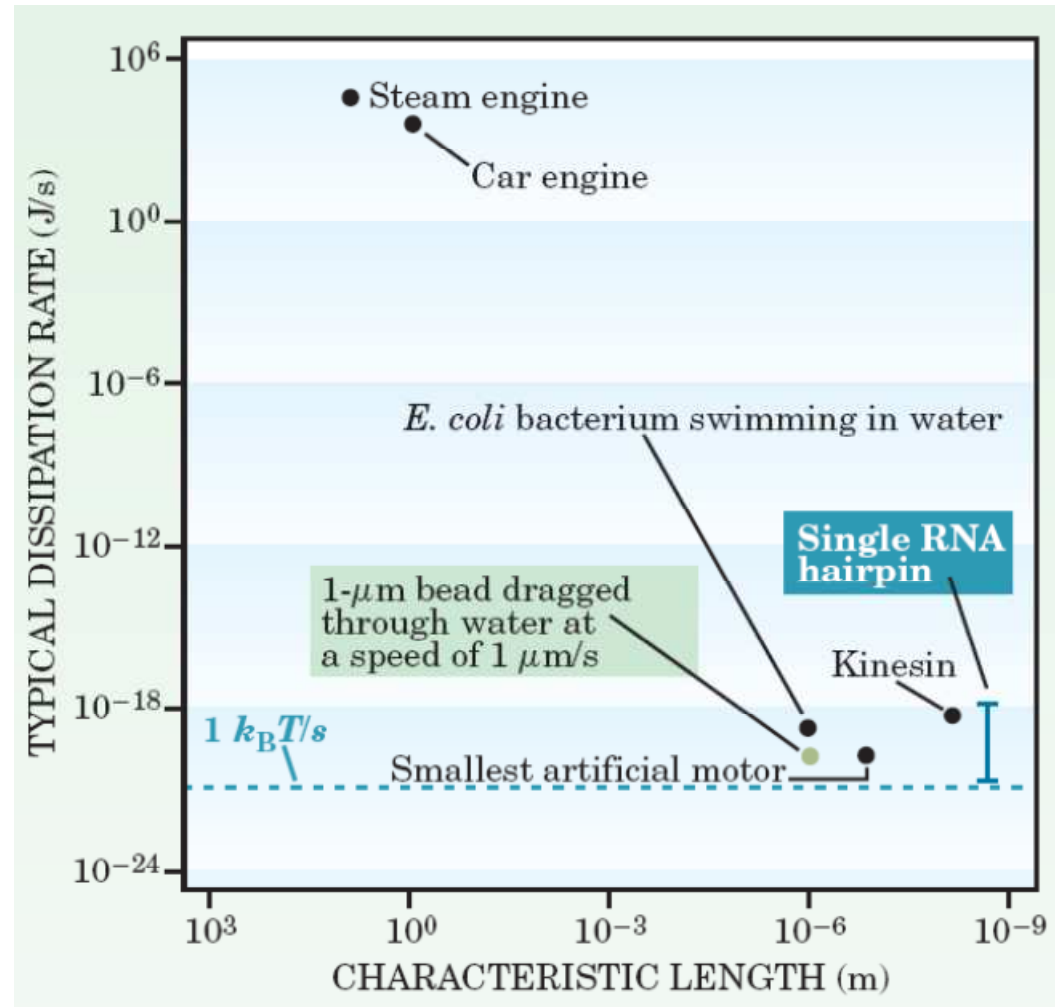


# Stochastic molecular machines based on fluctuations

## Molecular machines



What are the underlying thermodynamics?  
How is chemical energy converted to mechanical motion?



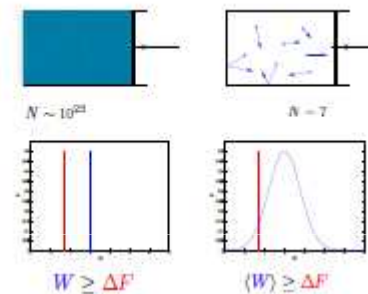
C. Bustamante, J. Liphardt, and F. Ritort, *Physics Today*, **58**, no 7, page [43-48](#), 2005.

Thermodynamics of small systems are important and interesting!

# Features of small system thermodynamics

$$W \simeq \Delta F \simeq k_B T, \Delta S \simeq k_B$$

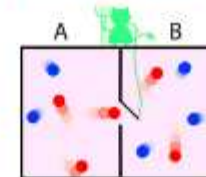
1. **Fluctuating** thermodynamic quantities, in particular in **non-equilibrium** processes.



2. **Strong coupling** to the reservoir(s).



3. **Information** acquired in measurements becomes **thermodynamically relevant**.



# Outline

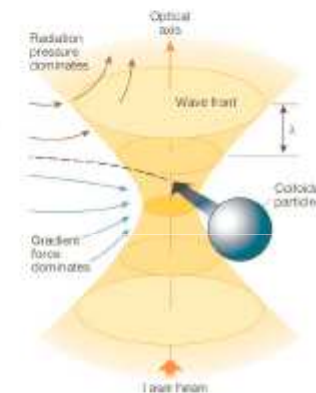
- Thermodynamics in the 19<sup>th</sup> and the 21<sup>st</sup> century
- **Stochastic thermodynamics**
- Fluctuation Theorems
- Maxwell's demon
- Summary

## Quantitative analysis: Langevin dynamics



- select relevant degrees of freedom
- subsume the rest into a **heat bath**
- model the interaction with the bath by **friction** and **noise** (FDT)

works nicely if **timescales** separate,  
Here: overdamped version



$$\dot{x} = -V'(x, \lambda) + \sqrt{2/\beta} \xi(t) \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t')$$

# Continuous stochastic processes

Stochastic differential equation:

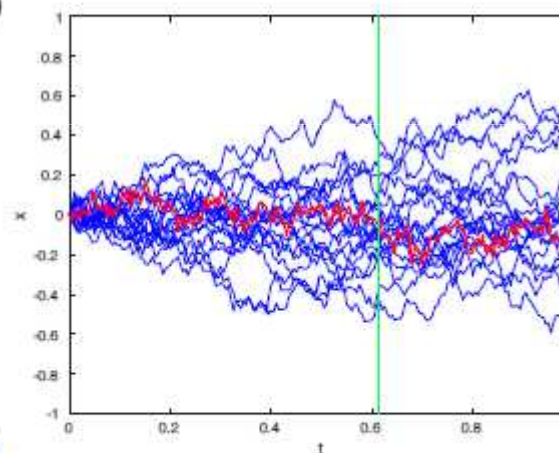
$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t) + \sqrt{\frac{2}{\beta}} \boldsymbol{\xi}(t) \quad \langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$$

Fokker-Planck equation:

$$\partial_t P(\mathbf{x}, t) = -\nabla \cdot \left( \mathbf{f}(\mathbf{x}, t) P(\mathbf{x}, t) - \frac{1}{\beta} \nabla P(\mathbf{x}, t) \right)$$

Path measure in function space:

$$P_T[\mathbf{x}(\cdot)] = \mathcal{N}_T[\mathbf{x}(\cdot)] \exp \left( -\frac{\beta}{4} \int_0^T dt \left( \dot{\mathbf{x}} - \mathbf{f}(\mathbf{x}, t) \right)^2 \right)$$



# Stochastic thermodynamics

Let  $f(x, t) = -\nabla V(x, \lambda(t))$  with some protocol  $\lambda(t)$  (driven system).

Change of energy of the system:

$$dU = dV = \frac{\partial V}{\partial \lambda} d\lambda + \frac{\partial V}{\partial x} dx = dW + dQ$$

First Law of thermodynamics for a single fluctuating trajectory.  
(Sekimoto, 1994)

Work and heat become stochastic variables  $W[x(\cdot)], Q[x(\cdot)]$ .

What are their distributions?



## Langevin equation

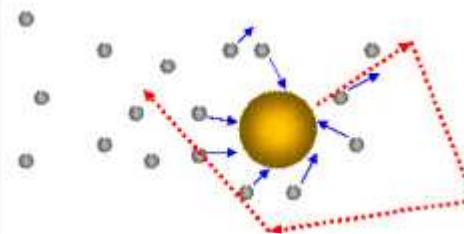
Observation time  $\tau \gg \tau_{H_2O}$

$$m\ddot{x} = f(x, t) + [-\gamma\dot{x} + \xi(t)]$$

effect from the fast  
water molecules

$$\langle \xi(t)\xi(\tau) \rangle = 2\gamma k_B T \delta(t - \tau)$$

relating fluctuating force to friction



Observation time  $\tau \gg m/\gamma$

$$0 = f(x, t) + [-\gamma\dot{x} + \xi(t)]$$

Over-damped Langevin equation

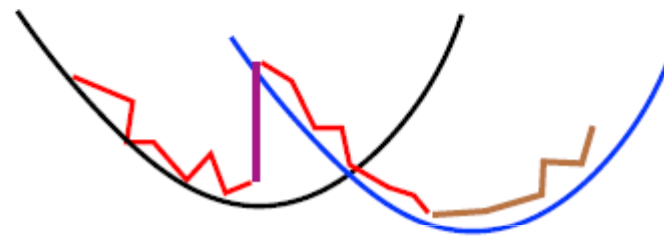
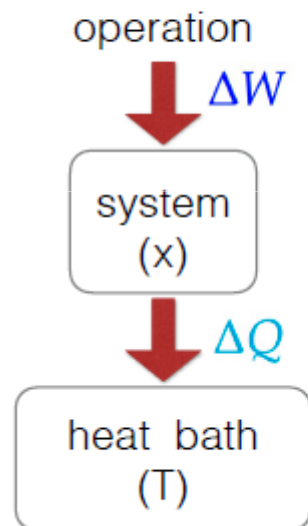
discretization

$$x' = x + \delta t f(x, t) + \sqrt{2D\delta t} \eta$$

$$P(\eta) \sim \exp\left(-\frac{\eta^2}{2}\right) \quad D = \frac{k_B T}{\gamma}$$



## Energy transduction along a stochastic process



potential energy  $\rightarrow$  heat

work  $\rightarrow$  potential energy

heat  $\rightarrow$  potential energy

heat  $\rightarrow$  work?

First Law: energy balance for a trajectory

$$m\ddot{x} = -\frac{\partial U(x, \lambda)}{\partial x} + [-\gamma\dot{x} + \xi(t)]$$

↓ for a small step  $dx$

$$d\left[\frac{1}{2}m\dot{x}^2 + U(x, \lambda)\right] = \frac{\partial U(x, \lambda)}{\partial \lambda}d\lambda + [-\gamma\dot{x} + \xi(t)]dx$$

$$dE = \Delta W + \Delta Q$$

change of  
internal energy

work by external  
operation

heat production  
in the medium

K. Sekimoto, *Progr. Theor. Exp. Phys.*, 130:17–27, 1998

## Transformation of probability

$$W[\mathbf{x}(\cdot)] = \int_0^T dt \frac{\partial V}{\partial \lambda}(\mathbf{x}(t), \lambda(t)) \dot{\lambda}(t)$$
$$Q[\mathbf{x}(\cdot)] = \int_0^T dt \nabla V(\mathbf{x}(t), \lambda(t)) \cdot \dot{\mathbf{x}}(t)$$

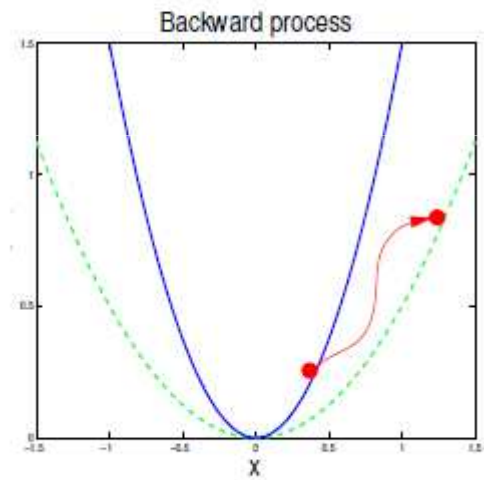
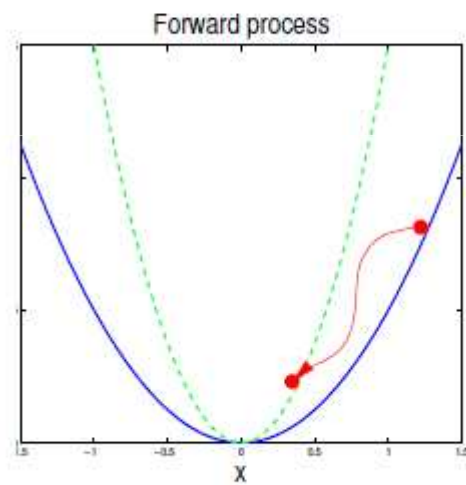
$$P_T[\mathbf{x}(\cdot)] = \mathcal{N}_T[\mathbf{x}(\cdot)] \exp \left( -\frac{\beta}{4} \int_0^T dt \left( \dot{\mathbf{x}} + \nabla V(\mathbf{x}, \lambda) \right)^2 \right)$$

$$P(W) := \int_{(\mathbf{x}_0, 0)}^{(\mathbf{x}_T, T)} \mathcal{D}\mathbf{x}(\cdot) P_T[\mathbf{x}(\cdot)] \delta(W - W[\mathbf{x}(\cdot)])$$
$$P(Q) := \int_{(\mathbf{x}_0, 0)}^{(\mathbf{x}_T, T)} \mathcal{D}\mathbf{x}(\cdot) P_T[\mathbf{x}(\cdot)] \delta(Q - Q[\mathbf{x}(\cdot)])$$

What to do with it?

## Time inversion

Reverse process:  $\bar{\lambda}(t) := \lambda(T - t)$  , mirror trajectory:  $\bar{x}(t) := x(T - t)$



## The detailed fluctuation theorem

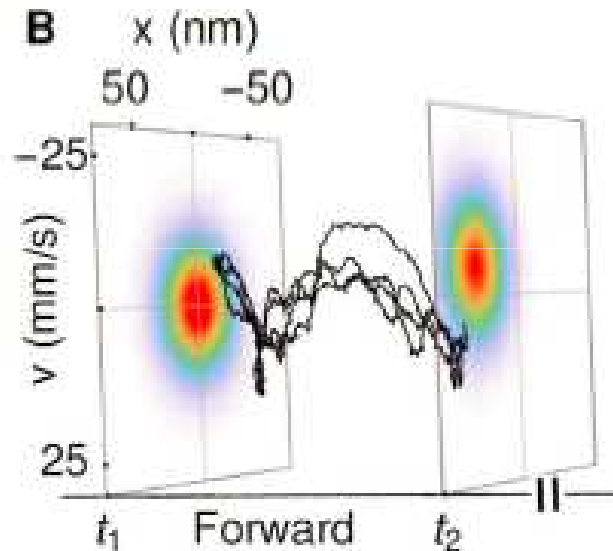
$$\begin{aligned}\frac{P_T[\mathbf{x}(\cdot)]}{\bar{P}_T[\bar{\mathbf{x}}(\cdot)]} &= \frac{\mathcal{N}_T[\mathbf{x}(\cdot)] \exp\left(-\frac{\beta}{4} \int_0^T dt \left(\dot{\mathbf{x}} + \nabla V(\mathbf{x}, \lambda)\right)^2\right)}{\mathcal{N}_T[\bar{\mathbf{x}}(\cdot)] \exp\left(-\frac{\beta}{4} \int_0^T dt \left(\dot{\bar{\mathbf{x}}} + \nabla V(\bar{\mathbf{x}}, \bar{\lambda})\right)^2\right)} \\ &= \frac{\mathcal{N}_T[\mathbf{x}(\cdot)] \exp\left(-\frac{\beta}{4} \int_0^T dt \left(\dot{\mathbf{x}} + \nabla V(\mathbf{x}, \lambda)\right)^2\right)}{\mathcal{N}_T[\mathbf{x}(\cdot)] \exp\left(-\frac{\beta}{4} \int_0^T dt \left(-\dot{\mathbf{x}} + \nabla V(\mathbf{x}, \lambda)\right)^2\right)} \\ &= \exp\left(-\beta \int_0^T dt \dot{\mathbf{x}} \cdot \nabla V(\mathbf{x}, \lambda)\right) = e^{-\beta \Delta Q}\end{aligned}$$

**Exact** for arbitrarily large deviations from equilibrium!

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# Path integral over all classical trajectories

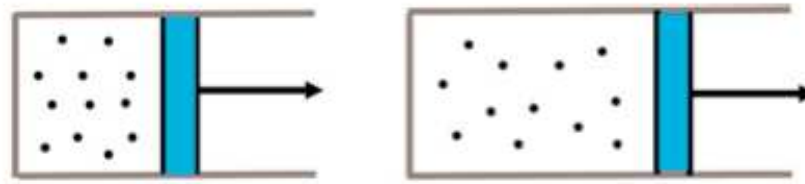


$$\begin{aligned}
 \langle e^{-\beta W[x(\tau)]} \rangle &\equiv \int dx_0 dx_t D[x(\tau)] \frac{e^{-\beta H_0(x_0)}}{Z_0} P[x(\tau) | x_0] e^{-\beta W[x(\tau)]} \\
 &= \frac{Z_1}{Z_0} \int dx_0 dx_t D[x(\tau)] \frac{e^{-\beta H_1(x_t)}}{Z_1} P[x(\tau) | x_0] e^{-\beta Q[x(\tau)]} \\
 &= \frac{Z_1}{Z_0} \int dx_0 dx_t D[x(\tau)] \frac{e^{-\beta H_1(\tilde{x}_0)}}{Z_1} \tilde{P}[\tilde{x}(\tau) | \tilde{x}_0] \\
 &= \frac{Z_1}{Z_0} = e^{-\beta \Delta F} \quad \Longrightarrow \quad \langle W[x(\tau)] \rangle \geq \Delta F
 \end{aligned}$$

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

- Jarzynski equality (1997):  $\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$   
 equilibrium information from non-equilibrium processes.

# Jarzynski equality: relation between nonequilibrium work and equilibrium free energy difference



The second law of thermodynamics  
(equality for quasistatic process only)

$$\langle W \rangle \geq \Delta F$$

J. Gibbs, (1876)

Jarzynski equality  
(always equality, no matter slow or fast)

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

C. Jarzynski, PRL, 78, 2690  
(1997)

(cited for 4437 times)





## 2019 Lars Onsager Prize Recipient

**Christopher Jarzynski**  
**University of Maryland,**  
**College Park**

**Citation:**

*"For seminal contributions to non-equilibrium thermodynamics and statistical mechanics that have had remarkable impact on experimental research in single-molecule and biological physics, engendering whole new fields of theoretical, numerical, and laboratory research, as well as for groundbreaking work on the thermodynamics of small systems."*



## Past Recipients

2018: [Subir Sachdev](#)

2017: [Natan Andrei](#)

[Paul B.](#)

[Wiegmann](#)

2016: [Giorgio Parisi](#)

[Marc Mezard](#)

[Riccardo](#)

[Zecchina](#)

2015: [Franz Wegner](#)

2003: [Pierre Claude](#)

[Hohenberg](#)

2002: [Anatoly Larkin](#)

2001: [Bertrand I.](#)

[Halperin](#)

2000: [David James](#)

[Thouless](#)

[John Michael](#)

[Kosterlitz](#)

1999: [Chen Ning Yang](#)

1998: [Leo P. Kadanoff](#)

1997: [Robert H.](#)

[Kraichnan](#)

1995: [Michael E. Fisher](#)

# Timeline of the second law

- Maximum Work Principle (1876)

$$\langle W \rangle \geq \Delta F$$

- Fluctuation-Dissipation relation (1950)

$$\langle W \rangle - \Delta F = \frac{1}{2} \beta \sigma_W^2$$

- Jarzynski equality (1997)

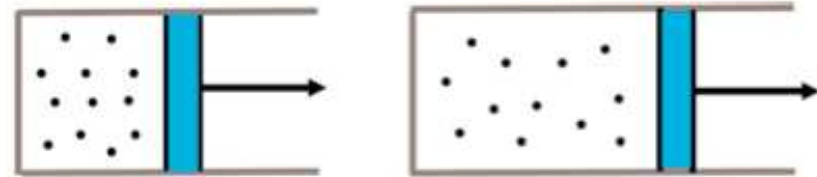
$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$

$$\Downarrow \langle e^x \rangle \geq e^{\langle x \rangle}$$

$$\langle W \rangle \geq \Delta F$$

- Hummer-Szabo relation (2001)

$$\langle \delta(\tilde{\Gamma} - \Gamma_\tau) e^{-\beta W} \rangle = \frac{e^{-\beta U_\tau(\tilde{\Gamma})}}{Z_0}$$



- Crooks Fluctuation Theorem (1998)

$$\frac{P_R(-W)}{P_F(W)} = e^{-\beta(W-\Delta F)}$$

- Differential Fluctuation Theorem (2008)

$$P_F(W, \Gamma_0 \rightarrow \Gamma_\tau) e^{-\beta(W-\Delta F)} = P_R(-W, \Gamma_\tau^* \rightarrow \Gamma_0^*)$$

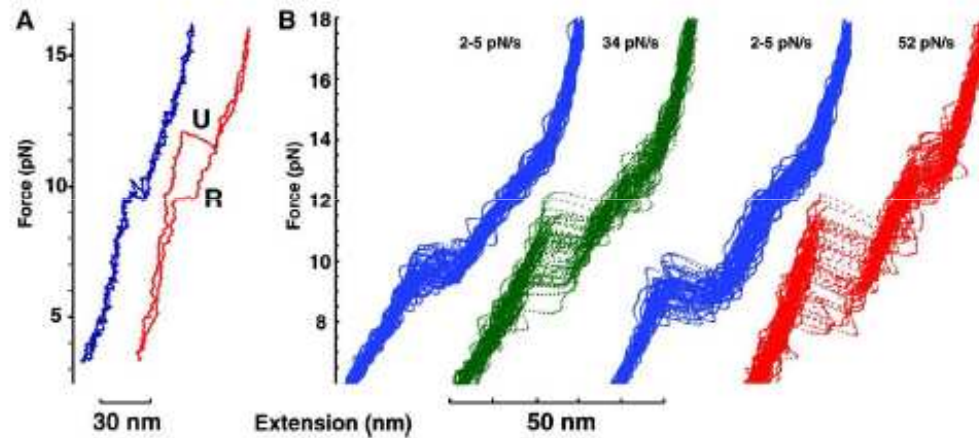
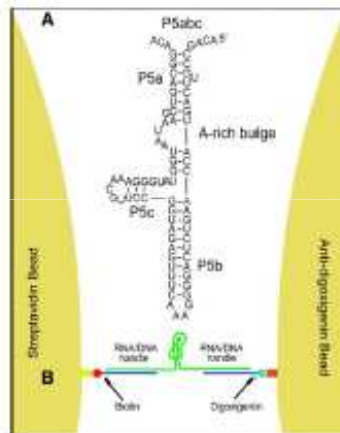
Time reversed:

$$\overline{\lambda}_t = \lambda_{26t}$$

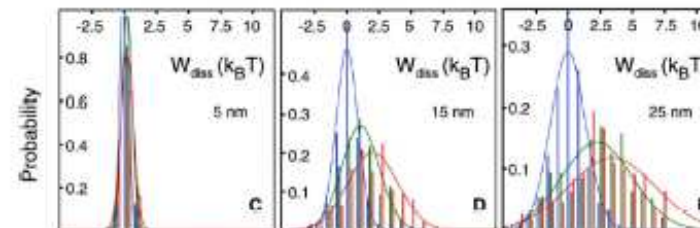
# Experimental test of Jarzynski's equality

- Nano-world Experiment: Stretching RNA

[Liphardt et al, Science 296 1832, 2002.]

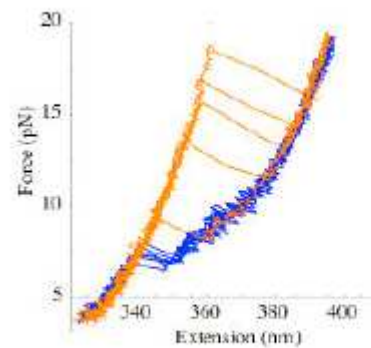


– distributions of  $W_{\text{diss}}$ :

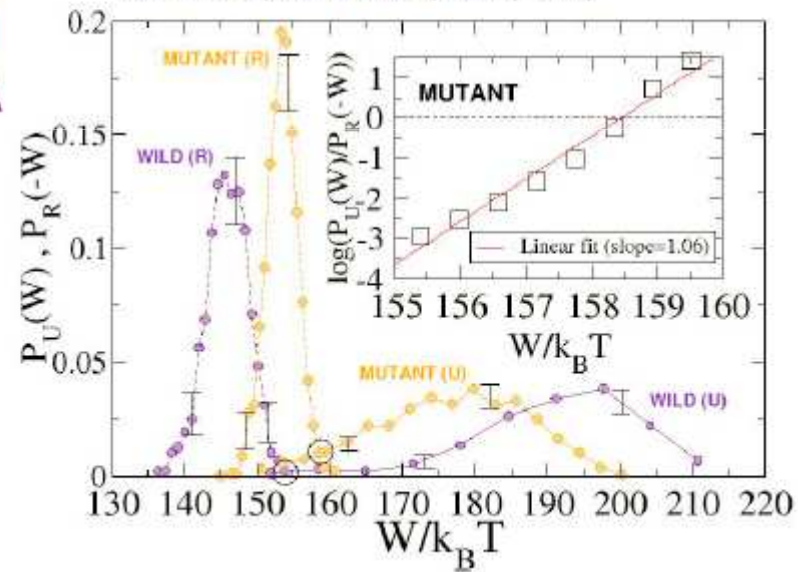


## Unfolding & refolding of ribosomal RNA

$$\frac{\rho_{\text{unfold}}(+W)}{\rho_{\text{refold}}(-W)} = \exp[\beta(W - \Delta F)]$$



Collin et al, *Nature* **437**, 231 (2005)





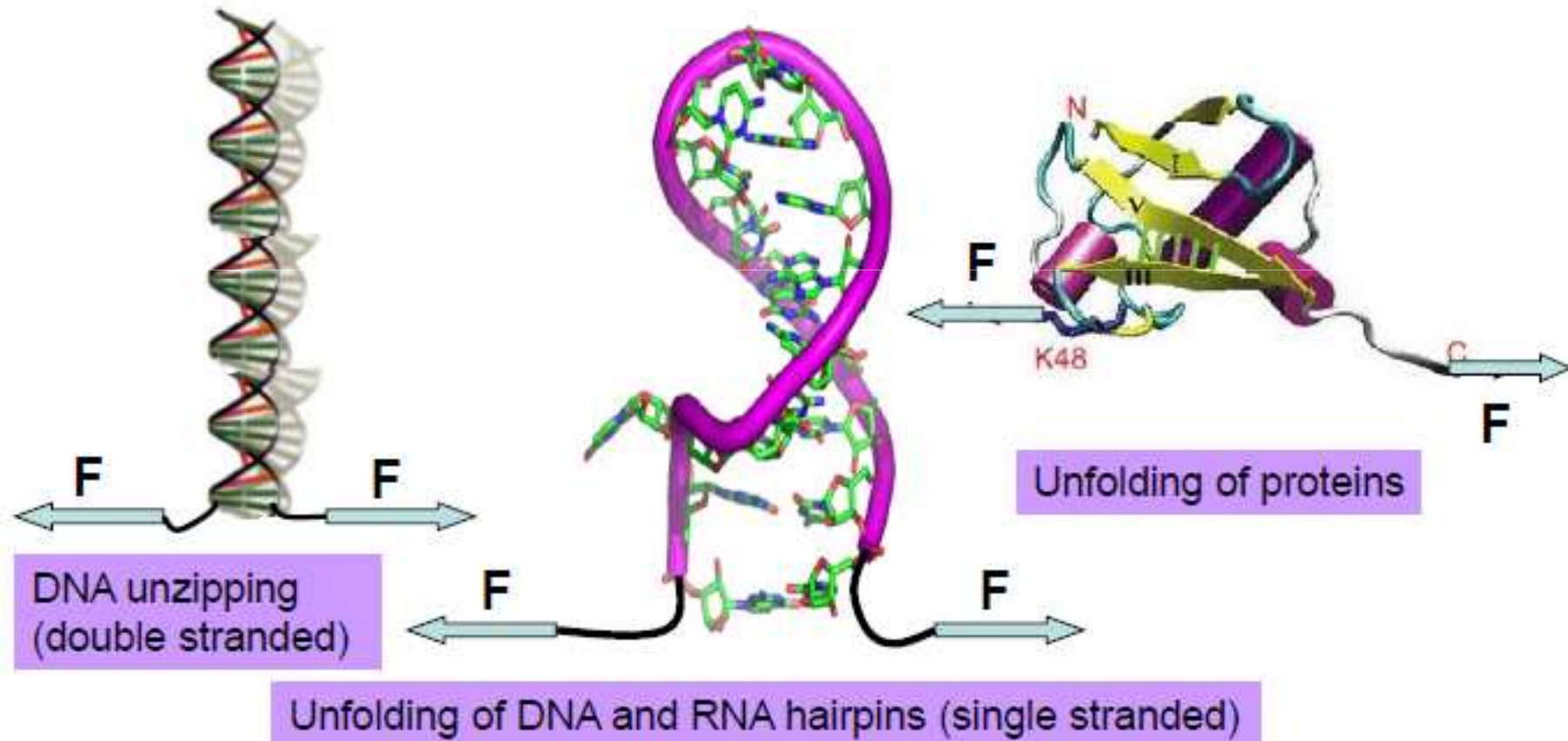
# Molecular unzipping

KTH/CSC

B. Essevaz-Roulet, U. Bockelmann, F. Heslot F (1997) *Proc Natl Acad Sci USA* 94:11935-11940

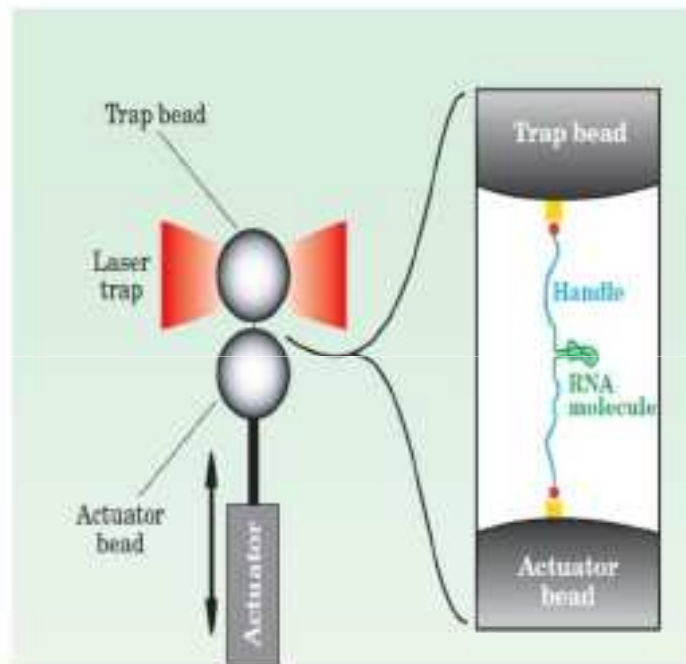
M. Rief, H. Clausen-Schaumann, H.E. Gaub (1999) *Nat Struct Biol* 6:346-349

C. Danilowicz et al. (2003) *Proc Natl Acad Sci USA* 100:1694-1699

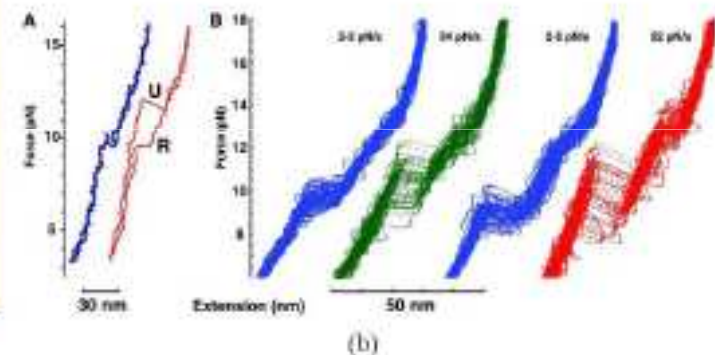
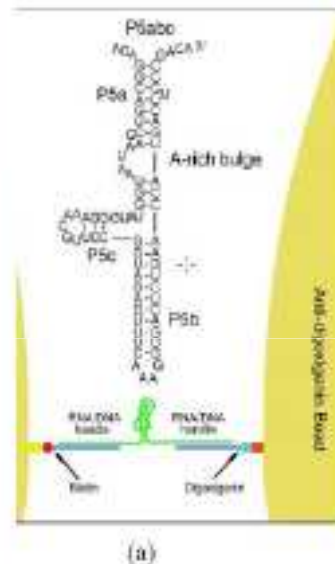


F. Ritort, J. Phys. (Cond. Matter) **18** R531 (2006))

## Non-equilibrium work can be measured in small systems and determines $\Delta F$ ...



...or at least  $\Delta\Delta F$ , the change in free energy when the RNA changes



Different pulling speeds give different force-elongation curves

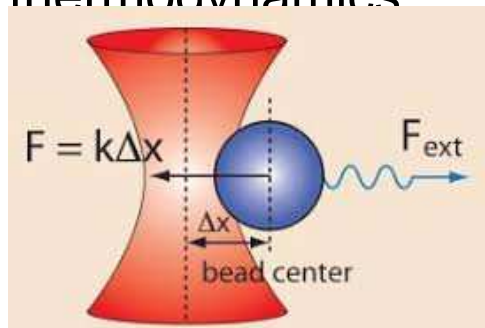
*Theory:* Jarzynski, Crooks, Evans, and others

*Experiments:* Bustamante, Ritort, and others

# The Nobel Prize in Physics 2018

Arthur Ashkin  
“Optical tweezer”

Key application:  
Study of  
Stochastic  
thermodynamics



Ill. Niklas Elmehed, © Nobel Media

Arthur Ashkin

Prize share: 1/2



Ill. Niklas Elmehed, © Nobel Media

Gérard Mourou

Prize share: 1/4



Ill. Niklas Elmehed, © Nobel Media

Donna Strickland

Prize share: 1/4



KUNGL.  
VETENSKAPS-  
AKADEMIEN

THE ROYAL SWEDISH ACADEMY OF SCIENCES

RNA molecules under mechanical force [36]. Force-extension curves for an RNA molecule were subsequently used for the first experimental test [37] of Jarzynski's equality in stochastic thermodynamics, which relates nonequilibrium work distributions to equilibrium free energy differences [38].

# Application of Stochastic Thermodynamics

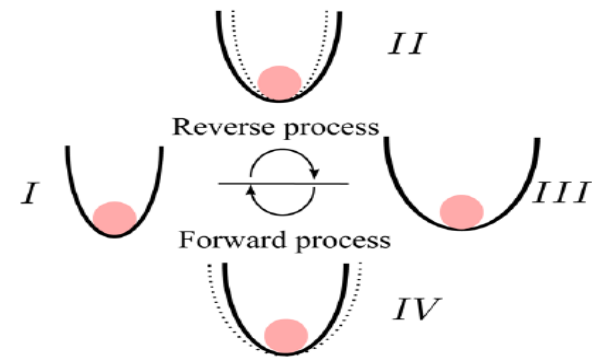
## QUICK STUDY

### A single-atom heat engine

Eric Lutz

The power of an engine scales with the number of particles that make up its working fluid, a generalization that has proven true down to a single atom.

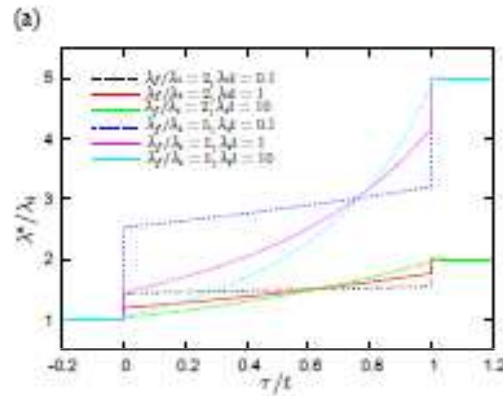
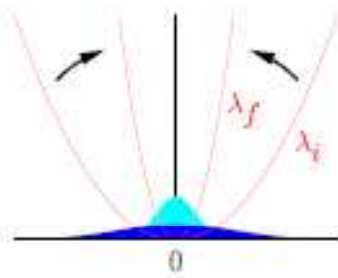
66 PHYSICS TODAY | MAY 2020





# Optimal Protocol in a Finite-Time Process

$$V(x, \lambda) = \lambda(\tau)x^2/2$$

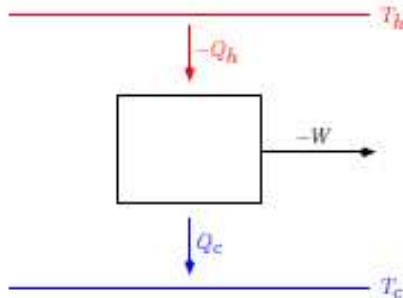


- jumps are generic
- should help to improve convergence of  $\langle \exp(-W) \rangle$
- generalization: underdamped dynamics  $\Rightarrow$  delta-peaks

[A. Gomez-Marin, T.Schmiedl , U.S., J. Chem. Phys., 129 : 024114, 2008]

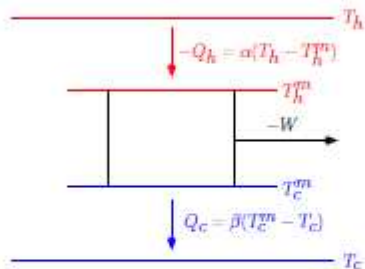
# Carnot Efficiency at the Maximum Power

- Carnot (1824)



- $\eta_c \equiv 1 - T_c/T_h$   
but zero power

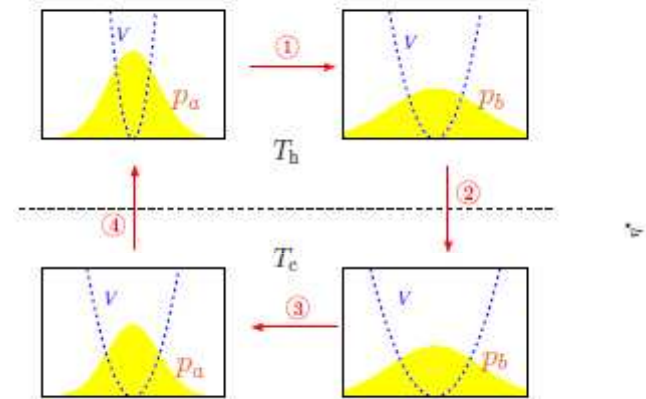
- Curzon-Ahlborn (1975)



- efficiency at maximum power  
 $\eta_{ca} \equiv 1 - \sqrt{T_c/T_h}$
- recent claims for universality(?)
- what about fluctuations?

Brownian heat engine at maximal power

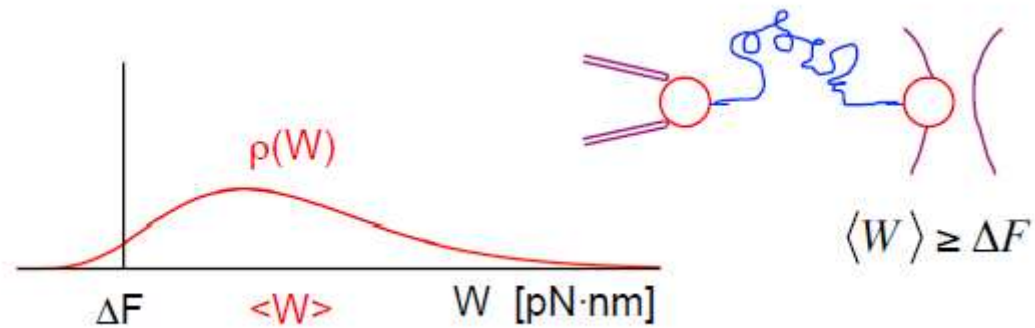
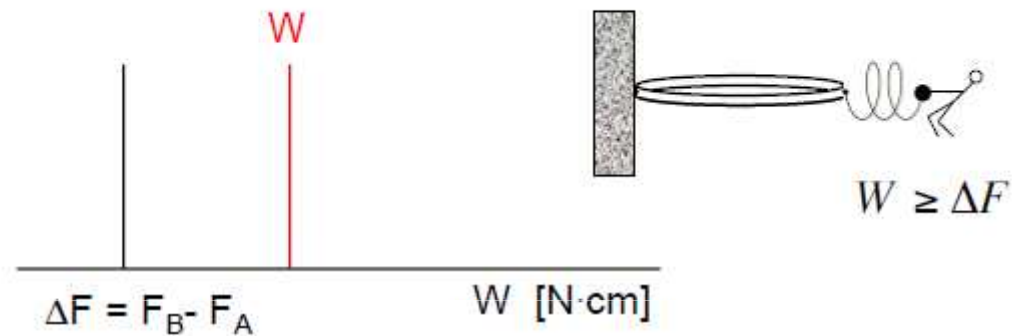
[T. Schmiedl and U.S., EPL 81, 20003, (2008)]



- Curzon-Ahlborn neither universal nor a bound

# “Violation” of the Second Law at the Nanoscale

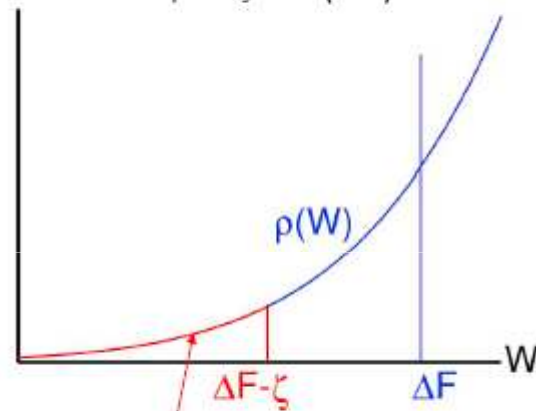
Clausius inequality, *macro & micro*



## Irreversibility in microscopic systems

$$\left. \begin{array}{l} \langle e^{-\beta W} \rangle = e^{-\beta \Delta F} \\ \text{Jensen's inequality } \langle e^x \rangle \geq e^{\langle x \rangle} \end{array} \right\} \longrightarrow \langle W \rangle \geq \Delta F$$

(Clausius inequality)



What is the probability that the 2nd law will be “violated” by at least  $\zeta$  units of energy?

$$\begin{aligned} P[W < \Delta F - \zeta] &= \int_{-\infty}^{\Delta F - \zeta} dW \rho(W) \leq \int_{-\infty}^{\Delta F - \zeta} dW \rho(W) e^{\beta(\Delta F - \zeta - W)} \\ &\leq e^{\beta(\Delta F - \zeta)} \int_{-\infty}^{+\infty} dW \rho(W) e^{-\beta W} = \exp(-\zeta / kT) \end{aligned}$$

The probability of observing the “violating” the second law decay exponentially with energy scale of the system, and becomes unobservable for any systems whose energy scale is a few times of  $kT$ .

# quantum Jarzynski equality

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

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

free energy difference

$$\langle e^{-W/k_B T} \rangle = \int dW e^{-W/k_B T} P(W)$$

average exponented work

$$P(W) = \sum_{m,n} \delta[W - (E_m^\tau - E_n^0)] P_{m,n}^\tau P_n^0$$

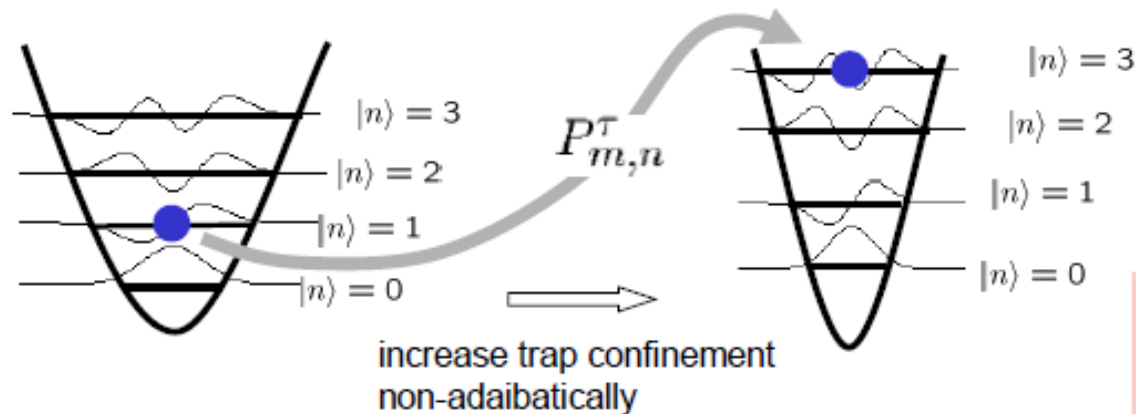
quantum work probability

no expectation value,  
but correlation function

Energy  
difference

Transition  
probabilities

Thermal  
occupation



P. Talkner et al.,  
Phys. Rev. E 75 R  
(2007) 050102

# Non-equilibrium phonon States in a Paul trap

quantum work probability

## Proposed exp. Scheme:

- 1) Start with thermal state  $n=0 \dots \sim 10$
- 2) Determine  $E^0$
- 3) Act (non-adiabatically) on trap potential
- 4) Determine  $E^t$

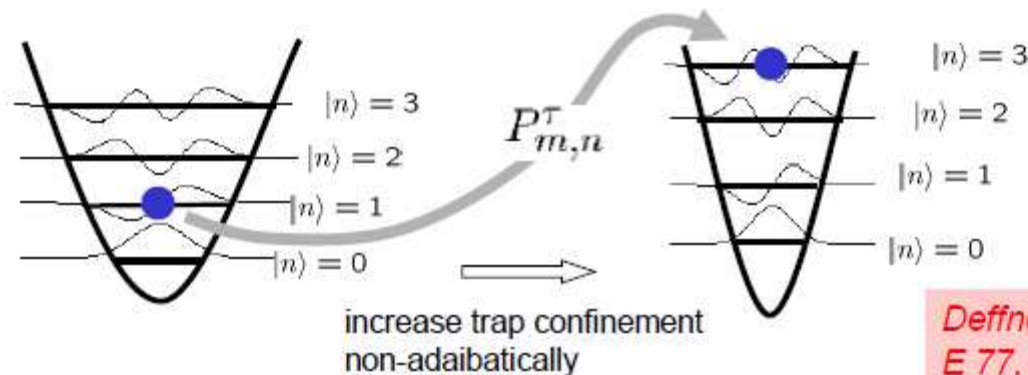
$$P(W) = \sum_{m,n} \delta[W - (E_m^\tau - E_n^0)] P_{m,n}^\tau P_n^0$$

no **expectation** value,  
but **correlation function**

Energy  
difference

Transition  
probabilities

Thermal  
occupation



*Huber et al.,  
PRL 101,  
070403 (2008)*

*Definer, Lutz, Phys. Rev.  
E 77, 021128 (2008)*

# Proof of Jarzynski equality in quantum systems

$$\langle e^{-\beta W} \rangle = \sum_{m,n} \frac{1}{Z_A} e^{-\beta E_n^A} \left| \langle E_m^B | U | E_n^A \rangle \right|^2 e^{-\beta(E_m^B - E_n^A)}$$

$$= \sum_{m,n} \frac{1}{Z_A} e^{-\beta E_m^B} \left| \langle E_m^B | U | E_n^A \rangle \right|^2$$

$$= \sum_m \frac{1}{Z_A} e^{-\beta E_m^B} \left( \sum_n \left| \langle E_m^B | U | E_n^A \rangle \right|^2 \right)$$

=1, Unitary evolution

$$= \sum_m \frac{1}{Z_A} e^{-\beta E_m^B}$$

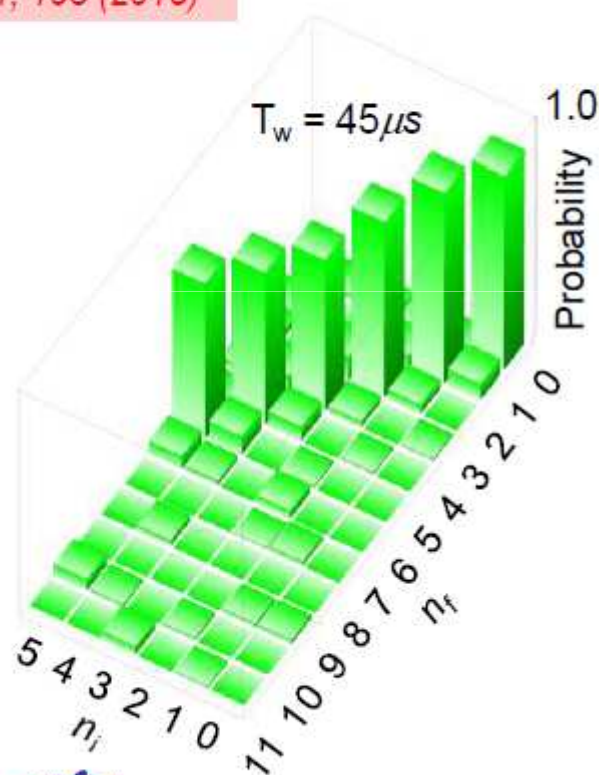
$$= \frac{Z_B}{Z_A} = e^{-\beta \Delta F}$$



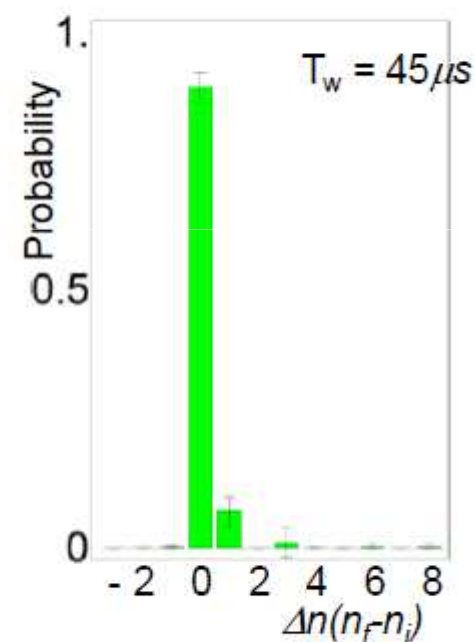
# Experiment test of quantum Jarzynski equality

## Final State Measurements – Intermediate Work

An et al., Nat.  
Phys. 11, 193 (2015)



Dissipated Work Distribution



$$\langle e^{-\beta W - \beta \Delta F} \rangle = 0.989 \pm 0.072$$

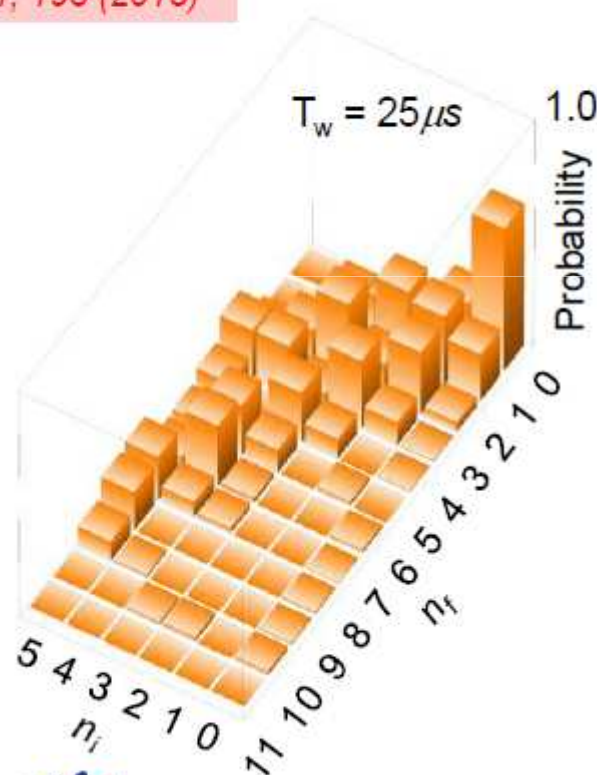




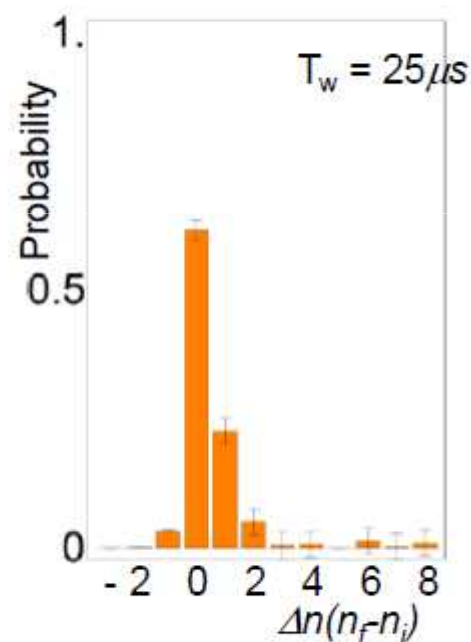
# Experiment test of quantum Jarzynski equality

## Final State Measurements – Intermediate Work

An et al., Nat.  
Phys. 11, 193 (2015)



Dissipated Work Distribution



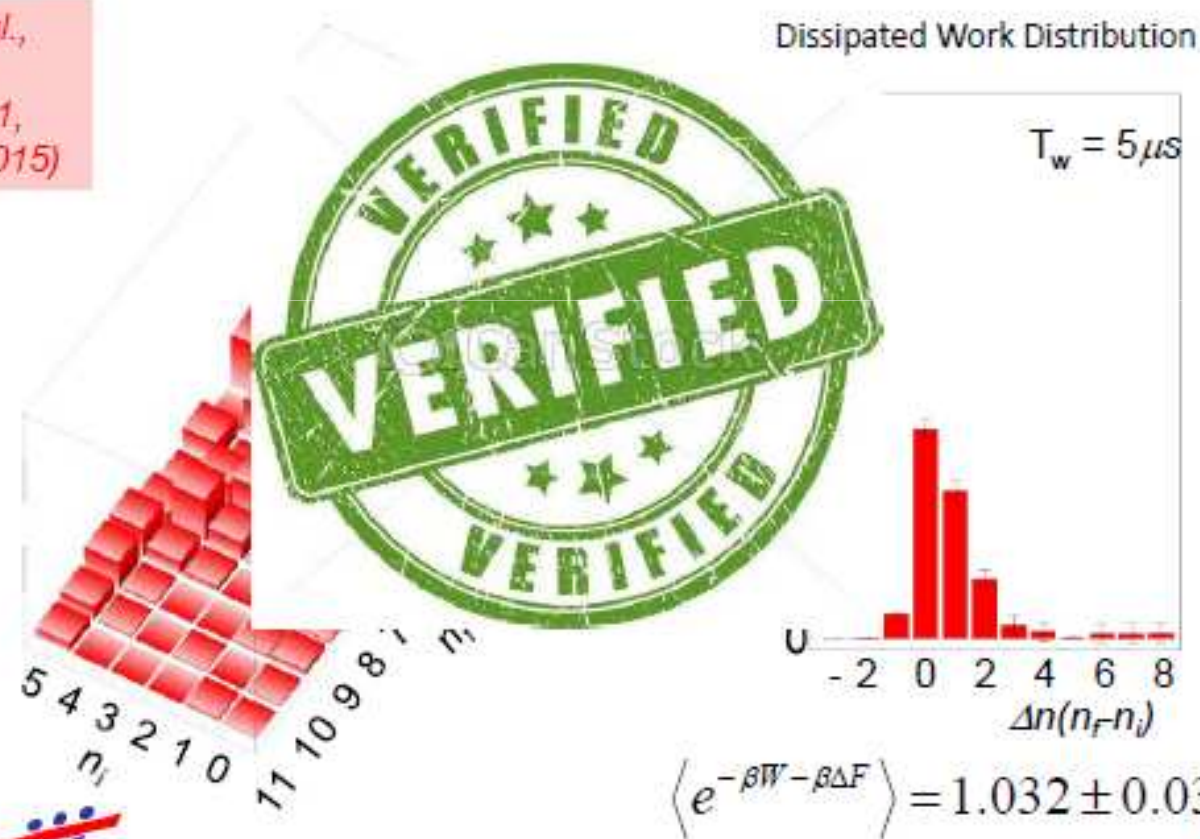
$$\langle e^{-\beta W - \beta \Delta F} \rangle = 0.995 \pm 0.045$$



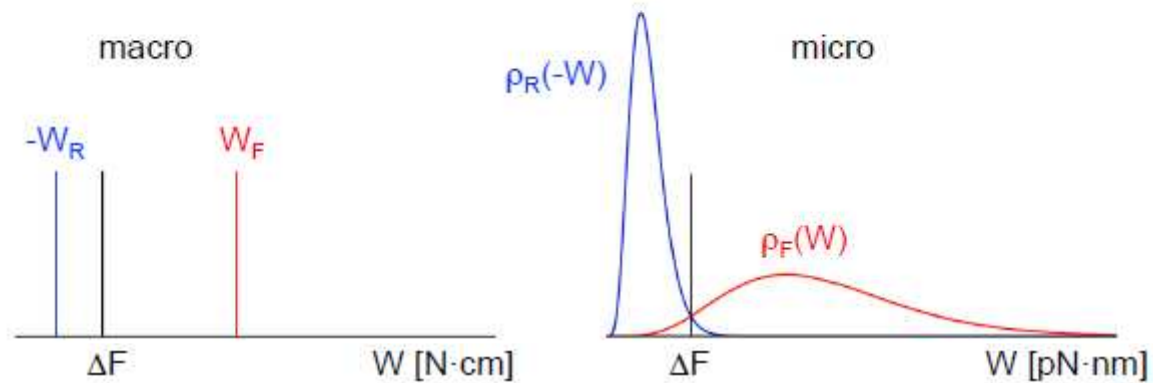
# Experiment test of quantum Jarzynski equality

## Final State Measurements – Non equilibrium Work

An et al.,  
Nat.  
Phys. 11,  
193 (2015)



## Summary



$$\langle W \rangle \geq \Delta F$$

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

$$-\langle W \rangle_R \leq \Delta F \leq \langle W \rangle_F$$

$$\frac{\rho_F(+W)}{\rho_R(-W)} = \exp[\beta(W - \Delta F)]$$

$$\langle \delta(x - x_t) \rangle \neq p^{eq}(x, \lambda_t)$$

$$\langle \delta(x - x_t) \exp(-\beta w_t) \rangle \propto p^{eq}(x, \lambda_t)$$

# Summary of Part I

- A MICROSCOPIC theory of nonequilibrium thermodynamics of small systems is being established (delayed by one century!!!)
- The theory of stochastic processes provides the mathematical foundation
- The second law of thermodynamics is sharpened, which has many applications in bio physics and chemical physics
- Quantum extension of the stochastic thermodynamics is not completed yet

# Outline

- Thermodynamics in the 19<sup>th</sup> and the 21<sup>st</sup> century
- Stochastic thermodynamics
- Fluctuation Theorems
- **Maxwell's demon**
- Summary

# Introduction to information

Is there any relation between information and heat?

Or is there any relation between the **computer** and the **refrigerator**?



What is information?

What is one bit of information?



- Information is related to probability, once you know the probability distribution, you know the information amount from one measurement

- Obtaining information  $\iff$  Reducing uncertainty

- Shannon Information amount:  $I = -\sum_i p_i \log_2 p_i$

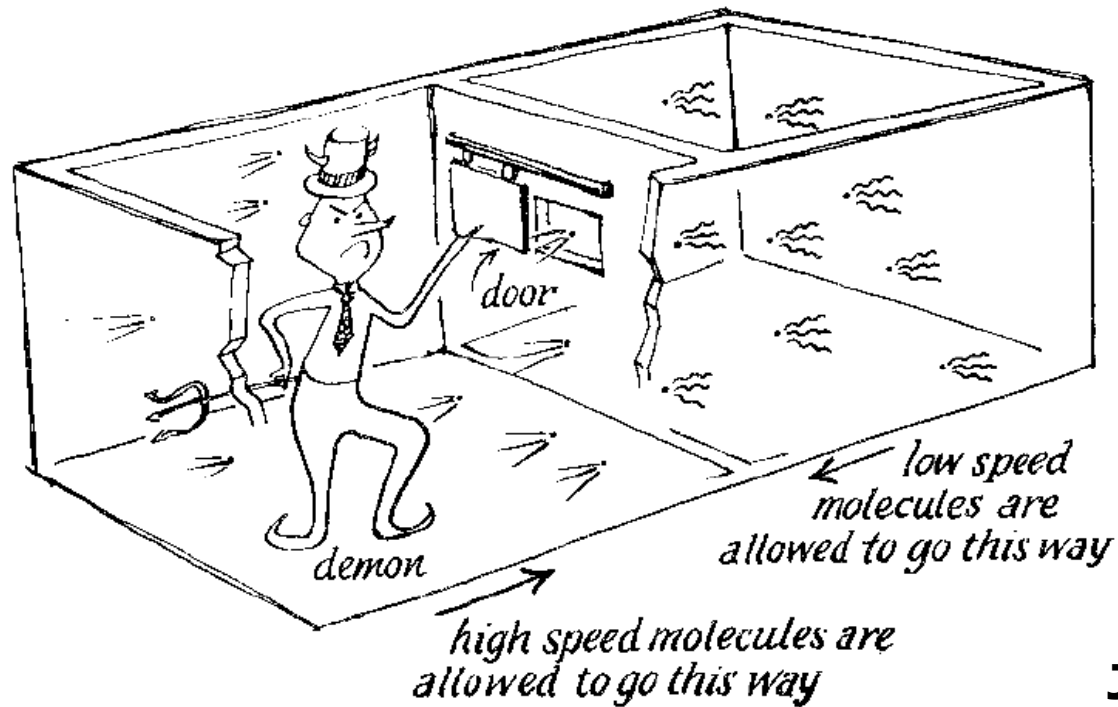


$$I = -\frac{1}{2} \log_2 \frac{1}{2} - \frac{1}{2} \log_2 \frac{1}{2} = 1 \text{ (bit)}$$

$$p_{up} = \frac{1}{2} \quad p_{down} = \frac{1}{2}$$



## Maxwell's demon thought experiment



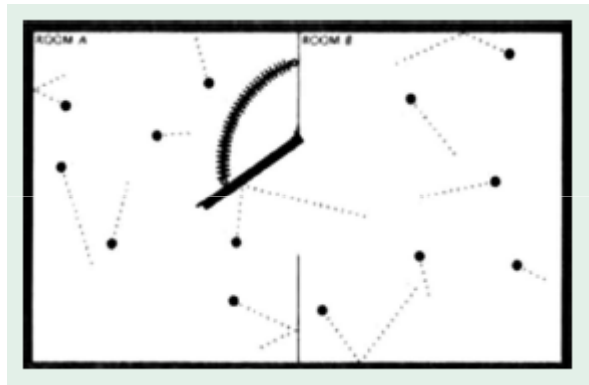
**James Clerk Maxwell**

*Theory of Heat* (Longmans, London, 1871)

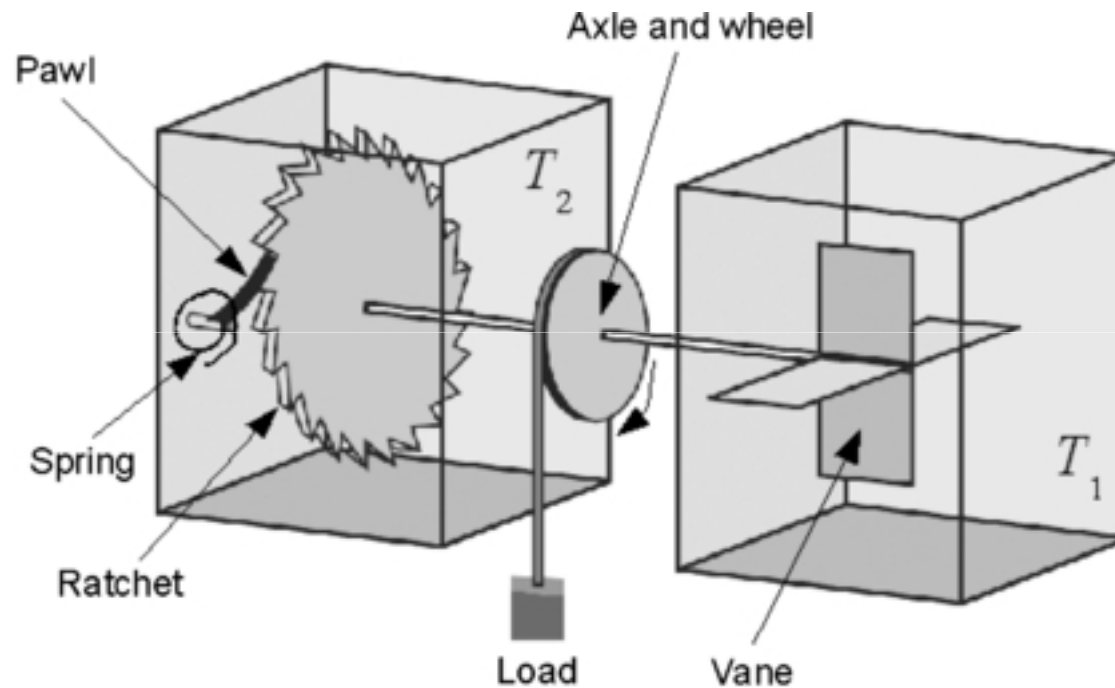
**1831 - 1879**

A perpetual motion machine?

## Smoluchowski trapped door (1912)



## Feynman's Ratchet (1963)



C. Jarzynski, et al PRE, 59, 6448 (1999); Z. C. Tu, J. Phys. A, 41, 312003 (2008)

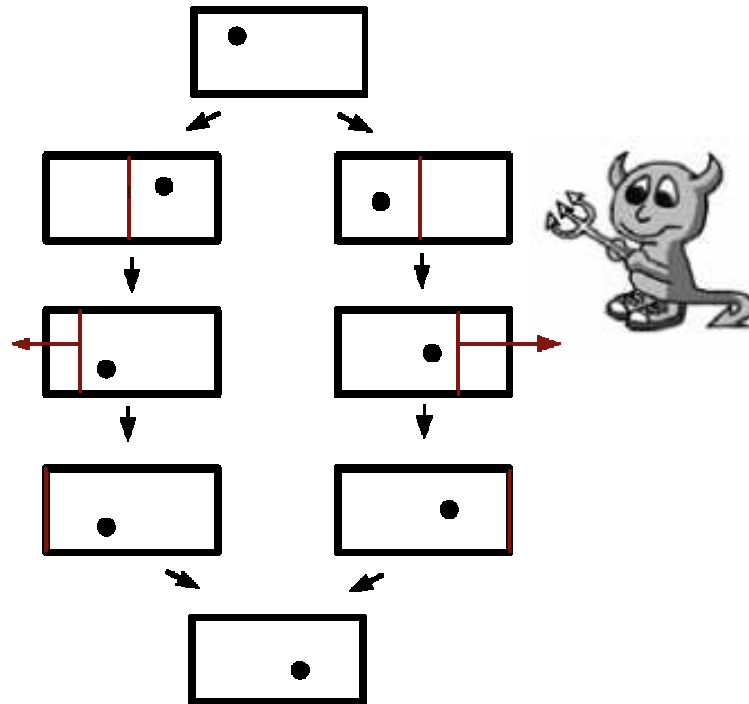
Sekimoto introduced the concept of trajectory work/heat in 1997 when he studied Feynman's ratchet, and thus initiated the whole field of stochastic thermodynamics

## Szilard's engine

(establish connection between information and entropy)



Leo Szilard  
1898-1964



Szilard's Single Molecule  
Engine (1929)



Leon Brillouin  
1889-1969

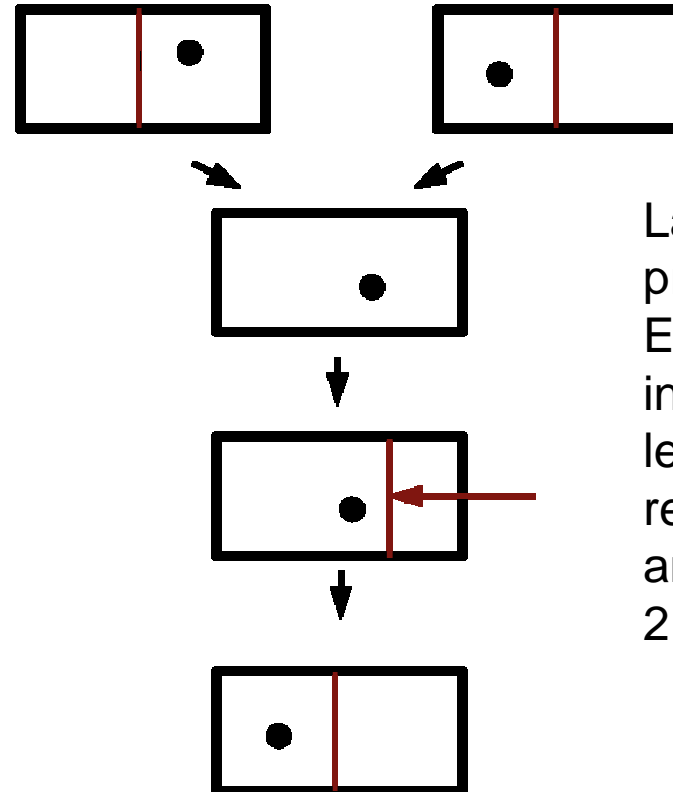
Leon Brillouin: Measurement process will cost energy and leads to entropy increase



...100101101  $\Rightarrow$  0000000...



Rolf Landauer  
1927-1999



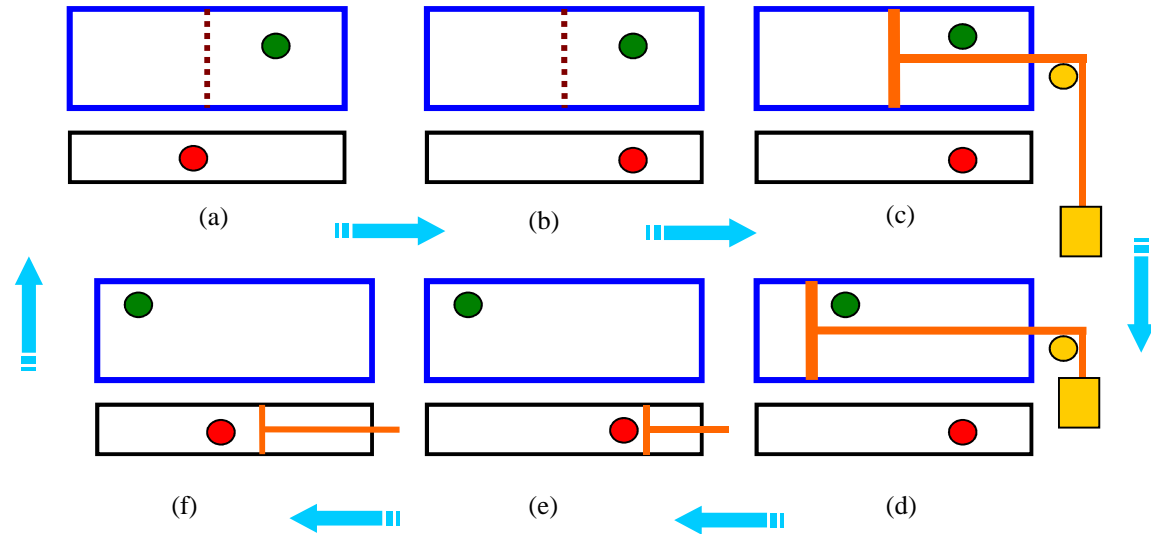
Landauer's  
principle (1961):  
Each bit of lost  
information will  
lead to an  
release of  
amount of  $KT \ln 2$   
heat

$$W = \int_V^{V/2} P dV = \int_V^{V/2} \frac{KT}{V} dV = -KT \ln 2$$

There is a lower bound of heat a computer must dissipate to process a given amount of information.

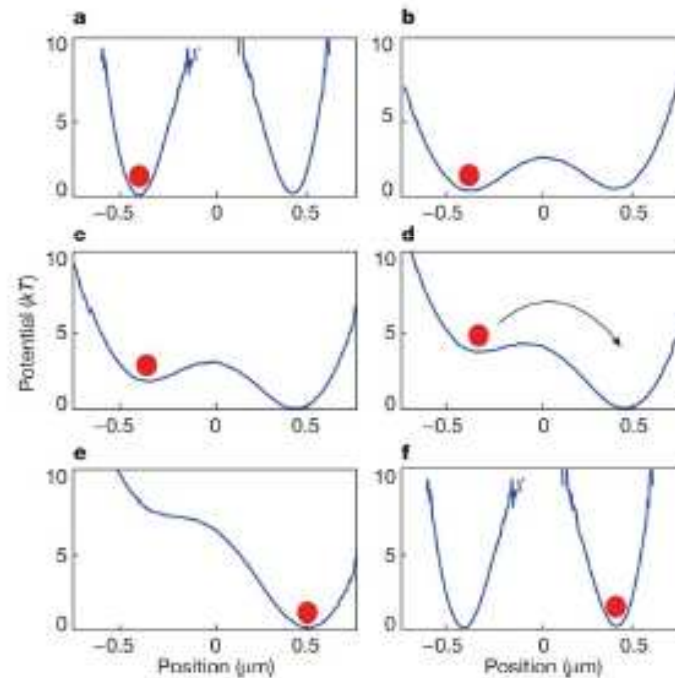


Charles H. Bennett  
1943-

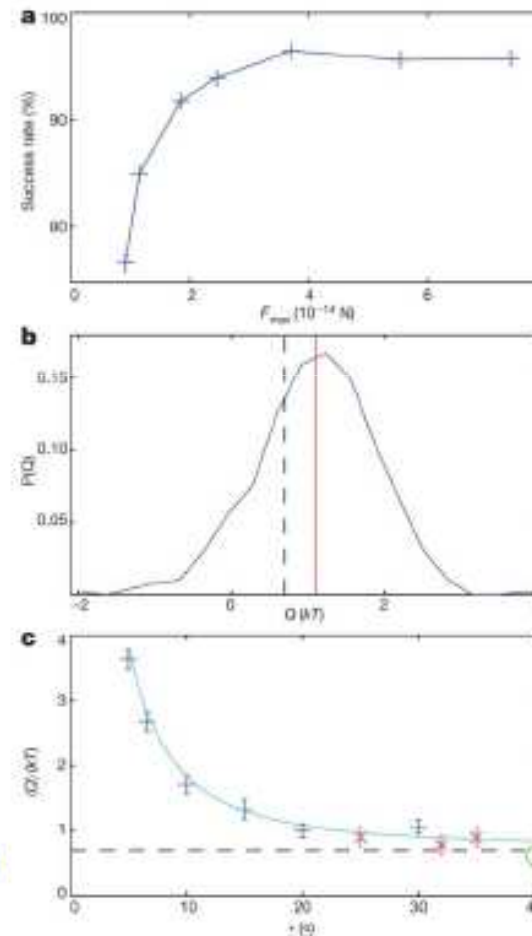


“The erasure of the memory of the demon compensates the entropy decreases and thus save the second law.”

So moving a particle between wells in a measurable fashion is now feasible



Bérut et al, *Nature* (2012) 483:187–189



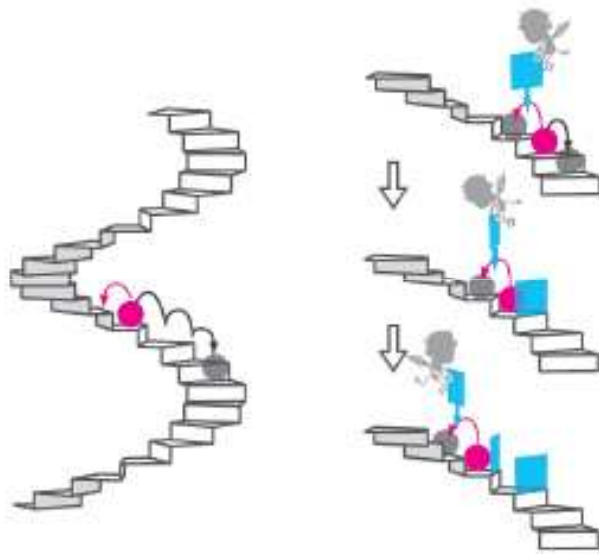
Fluctuating released heat

Released heat vs time duration & Landauer



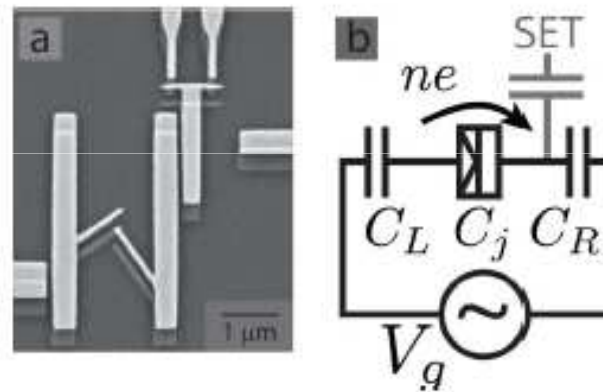
...there are also recent concrete proposals for Maxwell demons and Szilard engines...

...which have been realized in single-electron traps



**Figure 1 | Schematic illustration of the experiment.** **a**, A microscopic particle on a spiral-staircase-like potential with a step height comparable to  $k_B T$ . The particle stochastically jumps between steps owing to thermal fluctuations. As the downward jumps along the gradient are more frequent than the upward ones, the particle falls down the stairs, on average. **b**, Feedback control. When an upward jump is observed, a block is placed behind the particle to prevent downward jumps. By repeating this cycle, the particle is expected to climb up the stairs without direct energy injection.

Toyabe *et al.*, *Nature Physics* 2010



Jukka Pekola group, Aalto University

Saira *et al Phys Rev Lett* **109**, 180601 (2012)

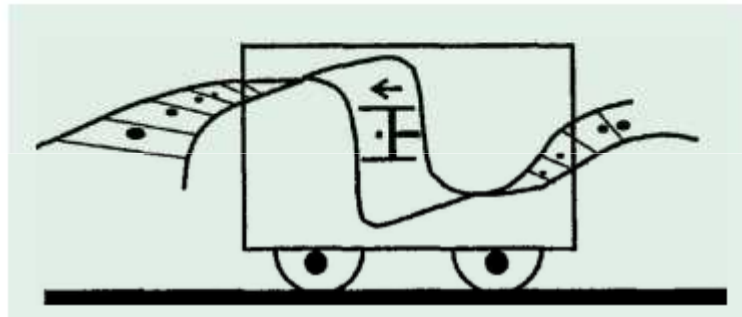
Averin *et al Phys Rev B* **84**, 245448 (2011)

Koski *et al Phys Rev Lett* **113**, 030601 (2014)

Koski *et al, PNAS* **111**, 13786 (2014)

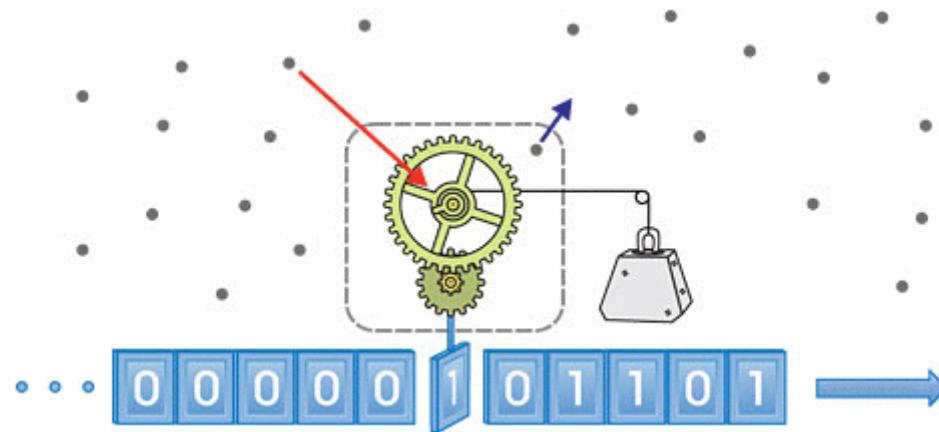
Can one use information as “energy” to drive a car?

In principle yes, but how?



R. Feynman, Feynman Lecture on Computation

# An autonomous information engine proposal

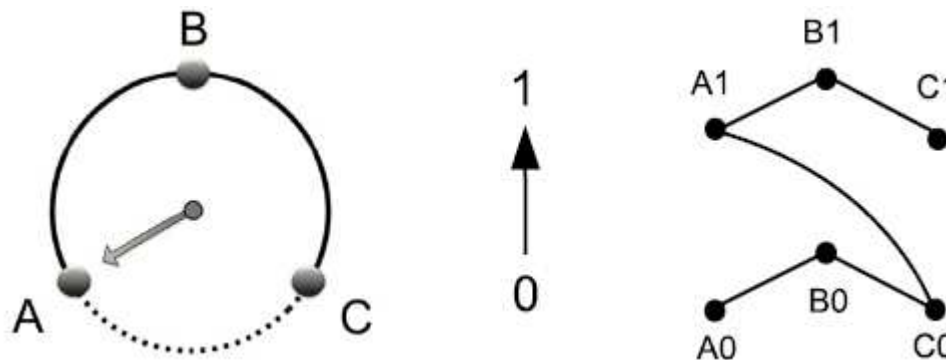


Two competing  
Driving forces

- Information  
(entropy force)

- Mechanical  
work

Information Engine  
/Eraser



D. Mandal, C. Jarzynski, PNAS, 109, 11641, (2012)

## Summary of Part II

- Maxwell's demon paradox was proposed by Maxwell in 1871
- Smoluchowski proposed a mechanical demon in 1912; Similarly in 1963 by Feynman. Both did not violate the second law of thermodynamics
- Szilard simplified Maxwell's model to a single-molecular engine in 1929
- Brillouin proposed a tentative "solution" in 1949, but was later invalidated
- Landauer proposed the Landauer's principle in 1961
- Bennett exorcised Maxwell's demon by using Landauer's principle in 1982
- Sekimoto introduced the concept of trajectory work/heat when studying Feynman's ratchet in 1997
- Landuaer's principle was first experimented tested by Ciliberto's group in 2012
- Jarzynski proposed a model of autonomous information engine in 2012

# Thank you!

Some materials from the internet. Acknowledgements to all authors!