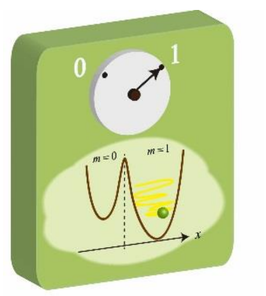
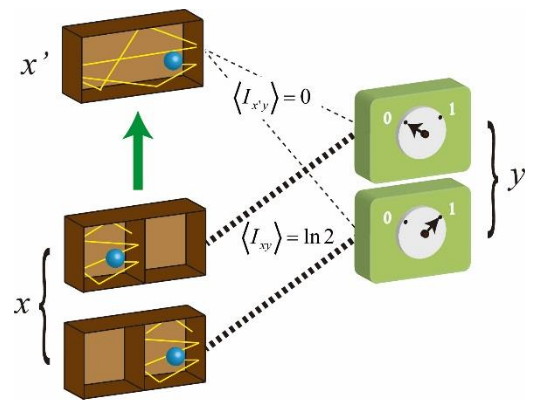
Quantum-Information Thermodynamics





Takahiro Sagawa

Department of Applied Physics, University of Tokyo

KIAS Workshop on Quantum Information and Thermodynamics

25-27 November 2015, Busan, Korea

Working on…

- Nonequilibrium statistical physics
- Quantum information theory

In particular, thermodynamics of information

Review: J. M. R. Parrondo, J. M. Horowitz, & T. Sagawa, *Nature Physics* 11, 131-139 (2015).

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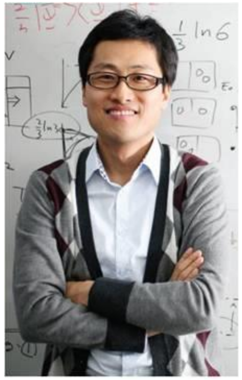


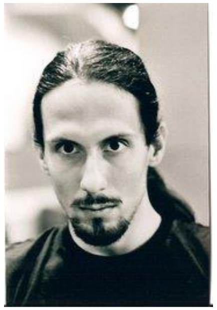
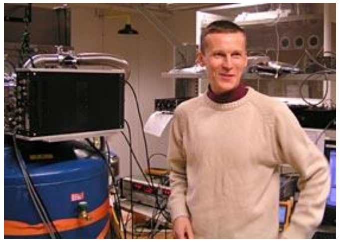

Plan of Lecture

- Part 0:
  General introduction
- Part 1:
  Fluctuation theorems
- Part 2:
  Classical/quantum measurement and information
- Part 3:
  Information thermodynamics

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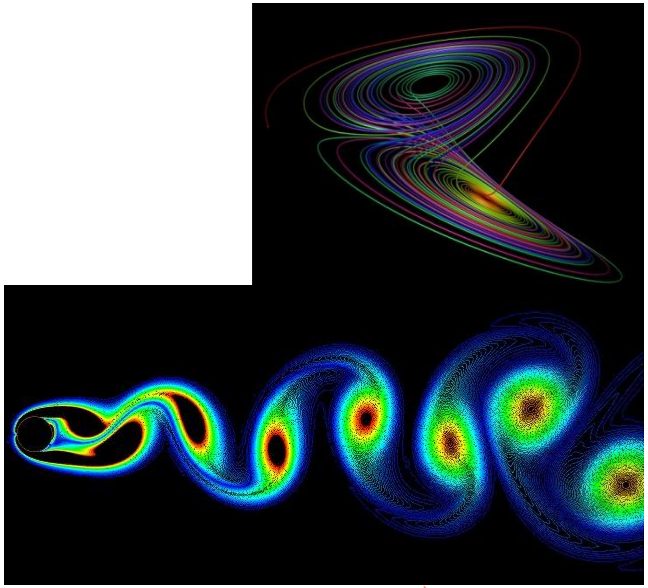
Nonequilibrium Statistical Mechanics

Lars Onsager

Ryogo Kubo



Linear response theory

Equilibrium

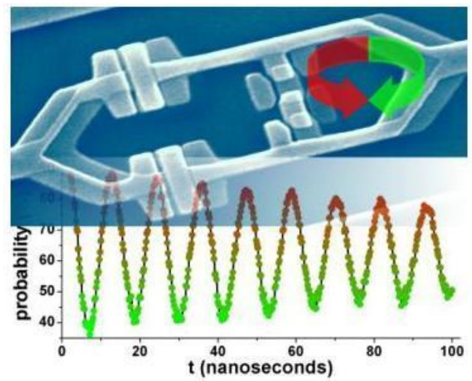
Nonequilibrium

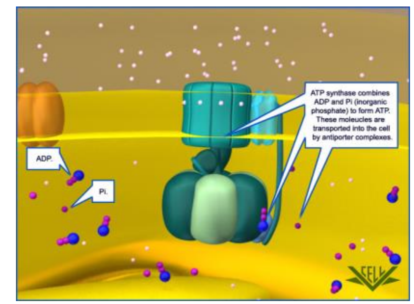
Universal thermodynamic law far from equilibrium?

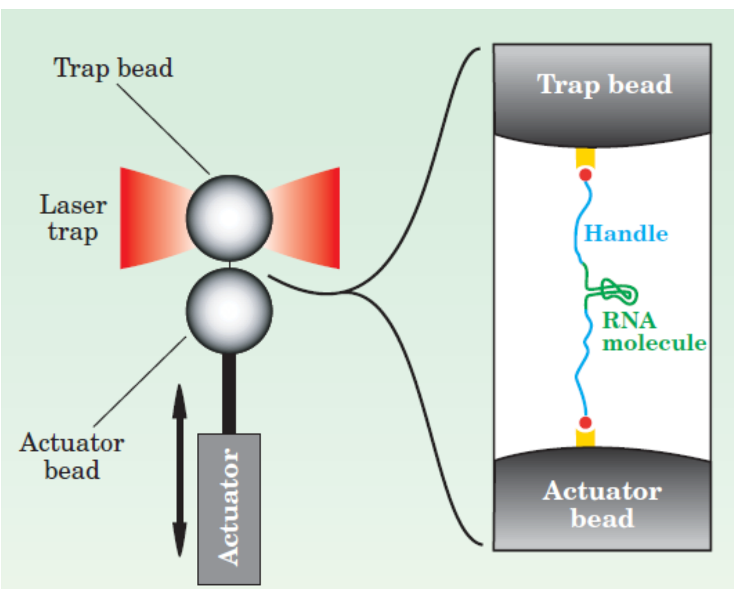
A New Field:
Thermodynamics in the Fluctuating World

Thermodynamics of small systems with large heat bath(s)

➡ Thermodynamic quantities are fluctuating!



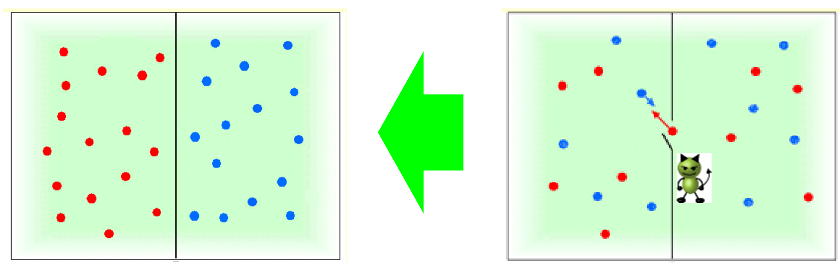


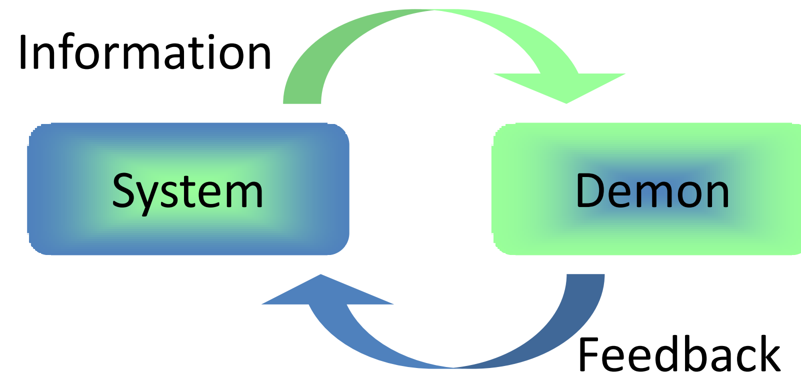


✓ **Second law** $\langle W \rangle \geq \Delta F$

✓ **Nonlinear & nonequilibrium relations**

Information Thermodynamics





Information processing at the level of thermal fluctuations

- ✓ Foundation of the second law of thermodynamics
- ✓ Application to nanomachines and nanodevices

Plan of Lecture

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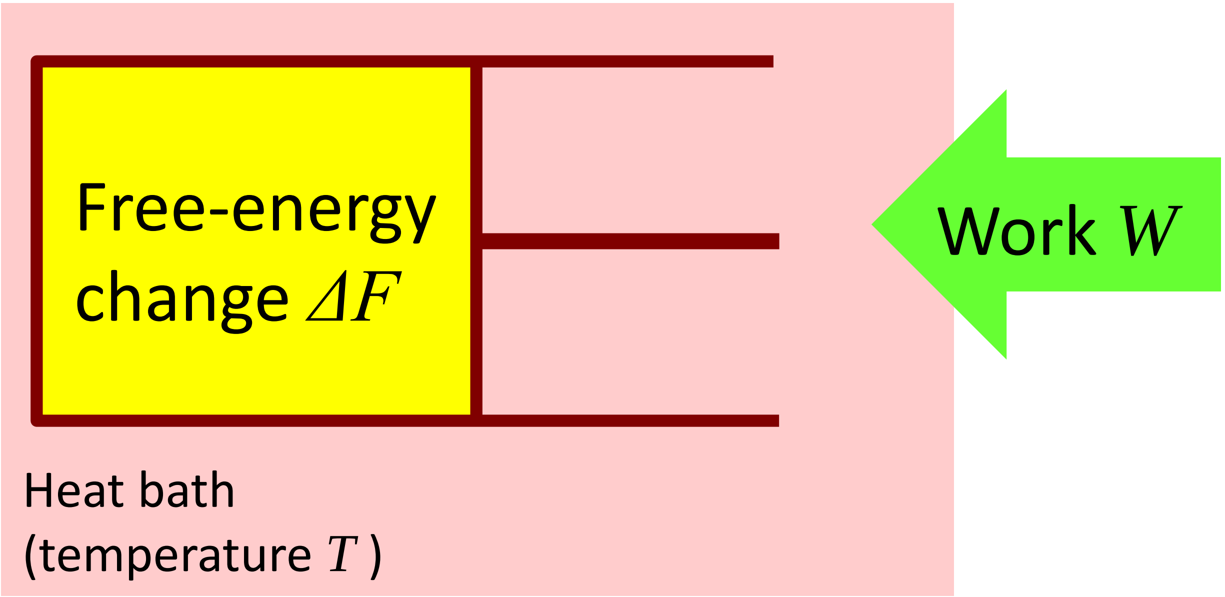
Conventional Second Law of Thermodynamics



$$W \geq \Delta F$$ (the equality is achieved in the quasi-static process)

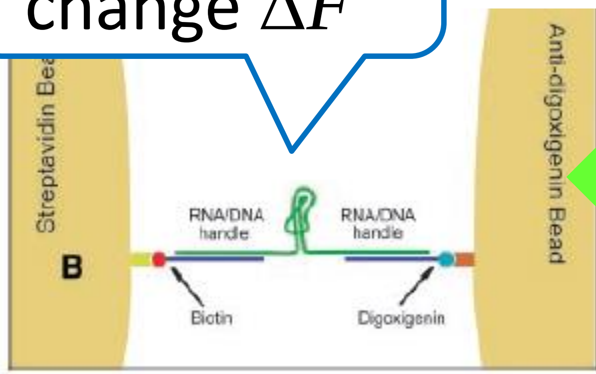
With a cycle, $\Delta F = 0$ holds, and therefore

$$W \geq 0$$ (impossibility of any perpetual motion of the second kind)

Second Law in Small Systems

Free-energy change ΔF

with a large heat bath

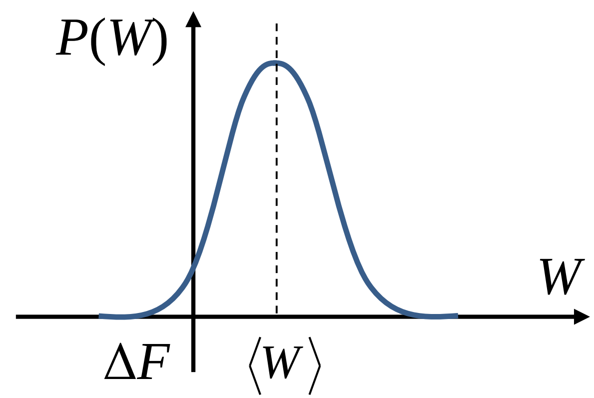


Work W

Drive the system from equilibrium

W becomes stochastic due to thermal fluctuations

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



$W < \Delta F$ can occur with a small probability
(stochastic violation of the second law)

Fluctuation-Dissipation Theorem (FDT)

In the linear response (or Gaussian) regime

$$\langle W \rangle - \Delta F = \frac{\beta}{2}\left(\langle W^2 \rangle - \langle W \rangle^2\right)$$

Dissipative work **Work fluctuation**

Right-hand side is obviously nonnegative ➡ **Second law**

Beyond the linear response theory?

Jarzynski Equality (1997)

$$\left\langle e^{-\beta(W-\Delta F)} \right\rangle = 1$$

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

Second law can be expressed by an **equality** by including the higher-order fluctuations!

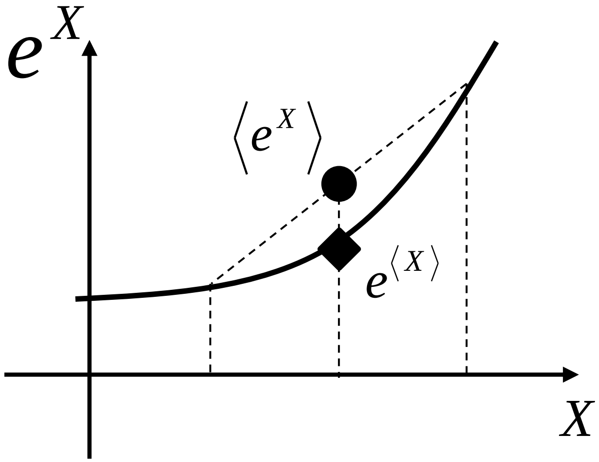
Reproduce Second Law and FDT

Second Law from Jarzynski Equality

Concavity of exponential function (Jensen's inequality)

$$\left\langle e^{X} \right\rangle \geq e^{\langle X \rangle}$$

for arbitrary X



$$\Rightarrow \quad \underbrace{\left\langle e^{-\beta(W-\Delta F)} \right\rangle}_{=1} \geq e^{-\beta(\langle W \rangle - \Delta F)}$$

$=1$ (Jarzynski equality)

$$\Rightarrow \quad \langle W \rangle - \Delta F \geq 0$$

Second law

FDT from Jarzynski Equality

Cumulant expansion:

$$\ln\left\langle e^{-\beta(W-\Delta F)}\right\rangle \cong -\beta(\langle W\rangle - \Delta F) + \frac{\beta^2}{2}(\langle W^2\rangle - \langle W\rangle^2)$$

(Exact if the work distribution is Gaussian)

$$= 0$$

(Jarzynski equality)

$$\Rightarrow \quad \langle W\rangle - \Delta F = \frac{\beta}{2}(\langle W^2\rangle - \langle W\rangle^2)$$

Free-energy Estimation by the Jarzynski Equality

Quasi-static process: $\Delta F = W_{\mathrm{rev}}$

Finite time process: Jarzynski equality $\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$

$$\Rightarrow \quad \Delta F = -\beta^{-1} \ln \left\langle e^{-\beta W} \right\rangle$$

Three estimators of the free-energy difference

$$W_{\mathrm{JE}} := -\beta^{-1} \ln \left\langle e^{-\beta W} \right\rangle$$

: expected to be exact

$$W_{\mathrm{FD}} := \langle W \rangle - \frac{\beta}{2} \left(\langle W^2 \rangle - \langle W \rangle^2 \right)$$

: up to the second cumulant
(exact for the Gaussian distribution)

$$W_{\mathrm{A}} := \langle W \rangle$$

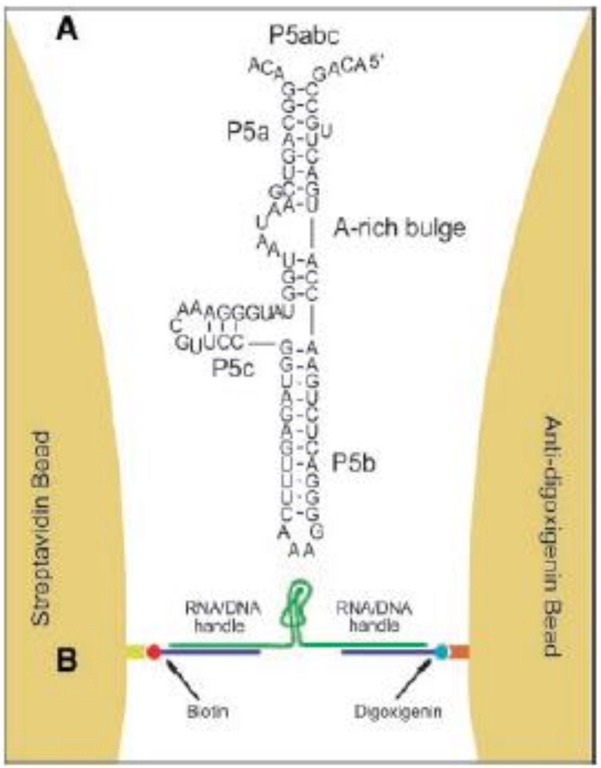
: not good in general

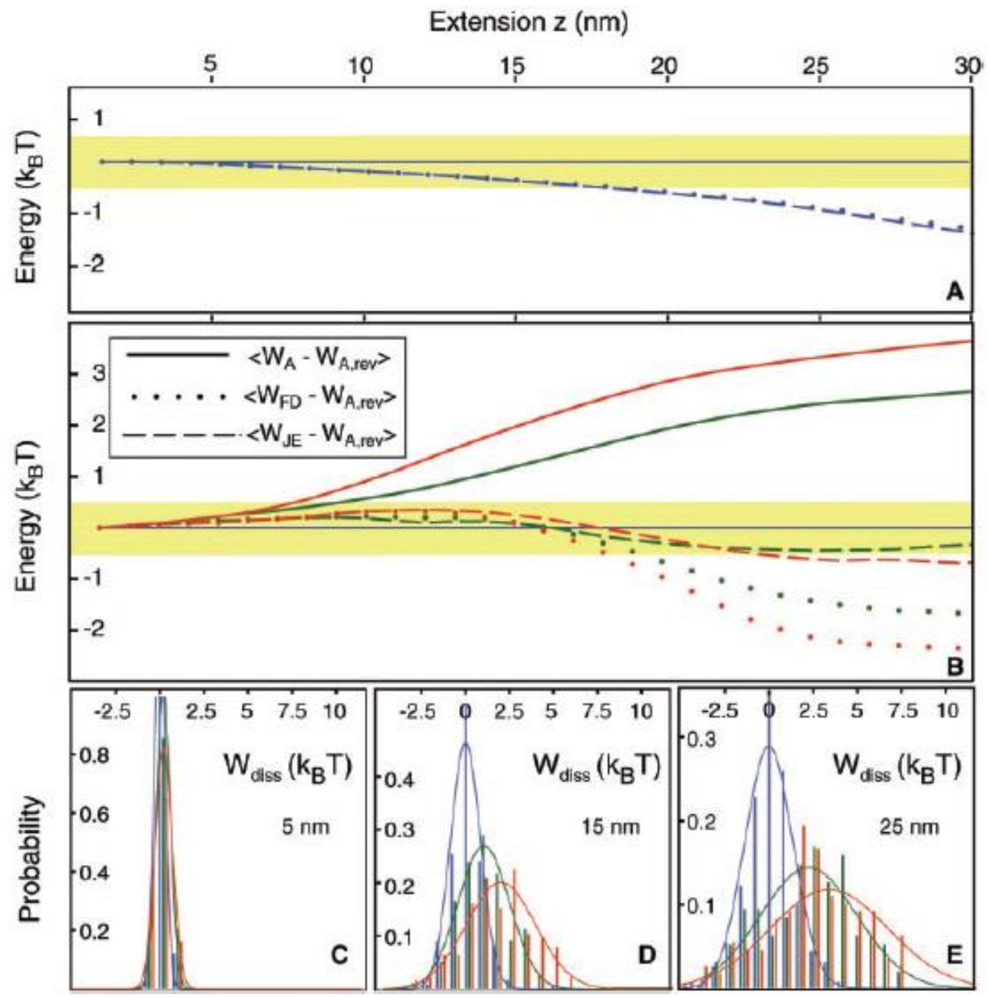
Experiment

Equilibrium Information from Nonequilibrium Measurements in an Experimental Test of Jarzynski's Equality

Jan Liphardt,[1,4] Sophie Dumont,[2] Steven B. Smith,[3]
Ignacio Tinoco Jr.,[1,4] Carlos Bustamante[1,2,3,4]*

Science **296**, 1832-1835 (2002)



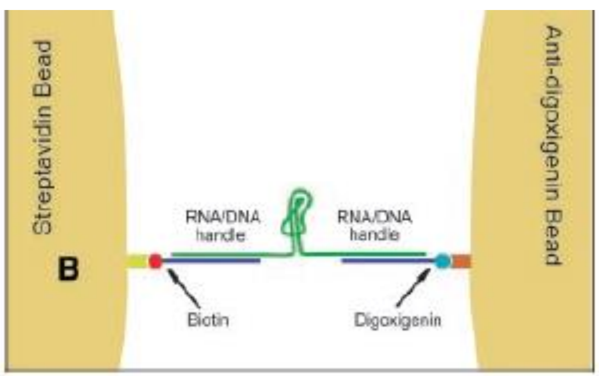


Crooks' Fluctuation Theorem (FT) (1)

Characterize the work distribution more quantitatively

Consider "forward experiment" VS "backward experiment"

For example…



Forward: push (folding)

Backward: stretch (unfolding)

Crooks' Fluctuation Theorem (FT) (2)

Work distribution in backward experiment

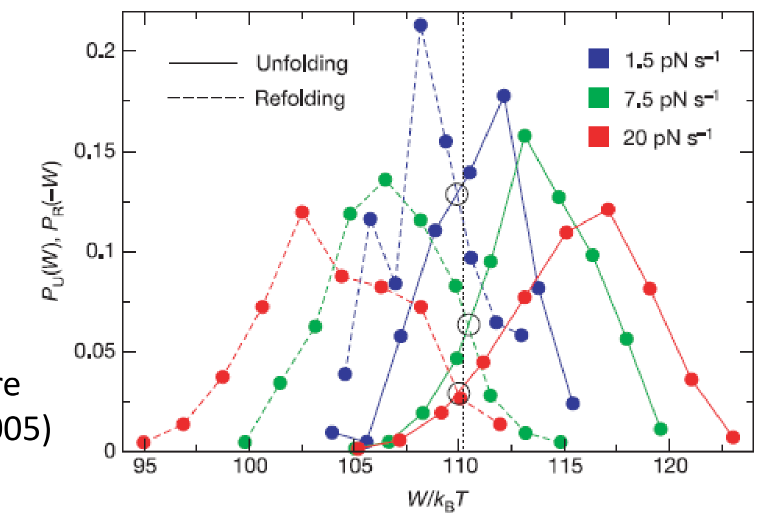
Dissipative work in forward experiment

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

Work distribution in forward experiment

G. E. Crooks, Phys. Rev. E **60**, 2721 (1999)

Collin et al, Nature **437**, 231–234 (2005)



The probability of the second-law violation is exponentially small

But observable in small systems

Jarzynski equality from Crooks' FT

$$\left\langle e^{-\beta(W-\Delta F)} \right\rangle \equiv \int dW P_F[W] e^{-\beta(W-\Delta F)}$$

$$= \int dW P_F[W] \frac{P_B[-W]}{P_F[W]}$$

Crooks' FT

$$= \int dW P_B[-W]$$

$$= 1$$

Summary: Hierarchy of Nonequilibrium Relations

Crooks' fluctuation theorem

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

Jarzynski equality

$$\left\langle e^{-\beta(W-\Delta F)} \right\rangle = 1$$

Second law

$$\langle W \rangle - \Delta F \geq 0$$

Torward Quantum

- Fundamental structure of nonequilibrium relations is very similar to the classical case;
  But some difficulties to introduce the concept of work

Classical: Work can be measured by continuously monitoring the system

Quantum: Such continuous monitoring will make the wave function collapse, and the dynamics of the system will be drastically changed.

How to observe the work in the quantum regime without changing the dynamics of the system?

Several Approaches

- **Unitary formalism: "Tasaki-Crooks" fluctuation theorem**
    - Hal Tasaki, arXiv:cond-mat/0009244
    - J. Kurchan, arXiv:cond-mat/0007360
    - M. Esposito, U. Harbola & S. Mukamel, Rev. Mod. Phys. **81**, 1665 (2009)
  - Two projection method
    - Experiment: S. An *et al.,* arXiv:1409.4485
  - Interferometer method
    - Theory: R. Dorner *et al.*, Phys. Rev. Lett. **110**, 230601 (2013)
    - Experiment: T. B. Batalhao *et al.*, Phys. Rev. Lett. **113**, 140601 (2014)
- **Quantum trajectory formalism**
    - J. M. Horowitz & J. M. R. Parrondo, New J. Phys. **15**, 085028 (2013)
    - F. W. J. Hekking & J. P. Pekola, Phys. Rev. Lett. **111**, 093602 (2013)

Two Projection Method

Main idea:

Consider a unitary system (without any heat bath)

Projection measurements of the energy in the initial and final steps

Work is just the energy difference $W \equiv E^f_{\mathrm{fin}} - E^i_{\mathrm{ini}}$

Stochastic due to thermal and quantum fluctuations

Simplest Setup (1)

Initial state: Canonical distribution

$$\rho_{\text{ini}} = e^{\beta(F_{\text{ini}} - H_{\text{ini}})}$$

ρ_{ini}: initial density operator H_{ini}: initial Hamiltonian

Spectrum decomposition: $$H_{\text{ini}} = \sum_i E_{\text{ini}}^i |\varphi_i\rangle\langle\varphi_i|$$

Projection measurement of the initial Hamiltonian

(without destroying the initial state)

Outcome: E_{ini}^i (one of the eigenvalues of H_{ini})

Simplest Setup (2)

Unitary evolution with external driving

$$U = \mathrm{T}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^\tau H(t)dt\right)$$

(Hamiltonian is time-dependent)

$$H_{\mathrm{ini}} = H(0) \quad H_{\mathrm{fin}} = H(\tau)$$

$$\Rightarrow \quad \rho_{\mathrm{fin}} = U\rho_{\mathrm{ini}}U^\dagger$$

Projection measurement of the final Hamiltonian

Spectrum decomposition: $H_{\mathrm{fin}} = \sum_f E_{\mathrm{fin}}^f \left|\psi_f\right\rangle\left\langle\psi_f\right|$

Outcome: E_{fin}^f (one of the eigenvalues of H_{fin})

Quantum Jarzynski Equality

Work: $$W \equiv E^{f}_{\text{fin}} - E^{i}_{\text{ini}}$$

Just the energy conservation:
no heat bath outside

Free energy:

$$F_{\text{ini}} \equiv -\beta^{-1} \ln \operatorname{tr}[e^{-\beta H_{\text{ini}}}]$$

$$F_{\text{fin}} \equiv -\beta^{-1} \ln \operatorname{tr}[e^{-\beta H_{\text{fin}}}]$$

$$\Delta F \equiv F_{\text{fin}} - F_{\text{ini}}$$

$$\left\langle e^{-\beta(W-\Delta F)} \right\rangle = 1$$

Quantum Jarzynski Equality: Proof

$$\left\langle e^{-\beta(W-\Delta F)}\right\rangle \equiv \sum_{if} e^{-\beta(W-\Delta F)} \left|\left\langle \psi_f \left| U \right| \varphi_i\right\rangle\right|^2 e^{\beta(F_{\mathrm{ini}}-E^i_{\mathrm{ini}})}$$

$$= \sum_{if} e^{-\beta(E^f_{\mathrm{fin}}-E^i_{\mathrm{ini}}-F_{\mathrm{fin}}+F_{\mathrm{ini}})} \left|\left\langle \psi_f \left| U \right| \varphi_i\right\rangle\right|^2 e^{\beta(F_{\mathrm{ini}}-E^i_{\mathrm{ini}})}$$

$$= \sum_{if} e^{-\beta(E^f_{\mathrm{fin}}-F_{\mathrm{fin}})} \left|\left\langle \psi_f \left| U \right| \varphi_i\right\rangle\right|^2$$

$$= \sum_{f} e^{-\beta(E^f_{\mathrm{fin}}-F_{\mathrm{fin}})} \qquad \sum_{i} \left|\left\langle \psi_f \left| U \right| \varphi_i\right\rangle\right|^2 = 1$$

$$= 1$$

Sum of a probability distribution