Emerging Issues in Nonequilibrium Statistical Physics

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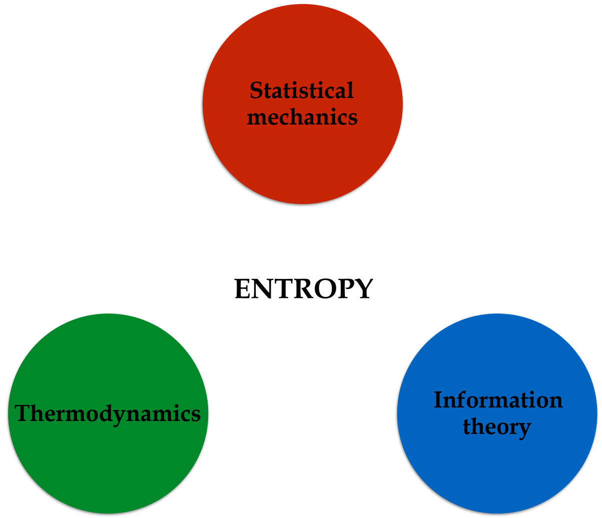
Physics Colloquium at POSTECH (DEC 06, 2017)



Classical thermodynamics

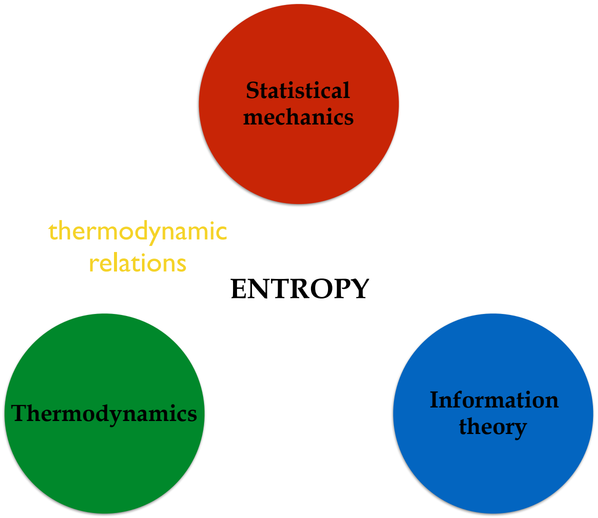
- Kelvin, Clausius, Carnot,…
- Entropy as a state function for thermal equilibrium systems

$$S(A) = \int_0^A \frac{dQ_{rev}}{T}$$

Statistical mechanics

- Boltzmann, Maxwell, Gibbs, …
- Entropy as a state function for thermal equilibrium systems

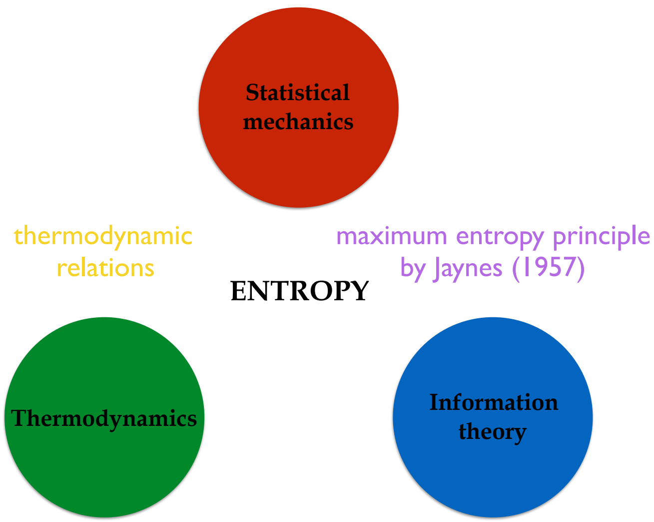
$$S(A) = k_B \ln \Omega(A)$$



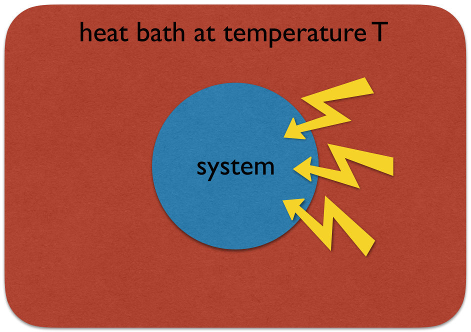
Information theory

- C. E. Shannon, "A Mathematical Theory of Communication", The Bell System Technical Journal **27**, 379 (1948)
- Information as a measure of how much choice is involved in the selection of the event or of how uncertain we are of the outcome
- Set {1,2,3,…,n} with occurrence probabilities $\{p_1,p_2,\ldots,p_n\}$.

$$H = \sum_{i=1}^{n} p_i \log_2 \frac{1}{p_i} = -\sum_i p_i \log_2 p_i$$ [binary digit]



Thermodynamic systems out of equilibrium



relaxation

driving force

time-dependent process

feedback

multi heat baths

…

Nonequilibrium statistical mechanics

- Heat bath
  - ideal heat bath : thermal equilibrium always
  - its entropy is given by the Clausius relation
- Nonequilibrium physical system
  - ideal heat bath leads to stochastic dynamics
  - probability distribution P(q,t)
  - Shannon entropy $S[P] = -k_B \sum_q P(q,t) \ln P(q,t) = \langle -k_B \ln P(q,t) \rangle$

Stochastic thermodynamics

- Stochastic equations of motion (Langevin eq)

$$\frac{dx}{dt} = v$$

nonconservative driving force

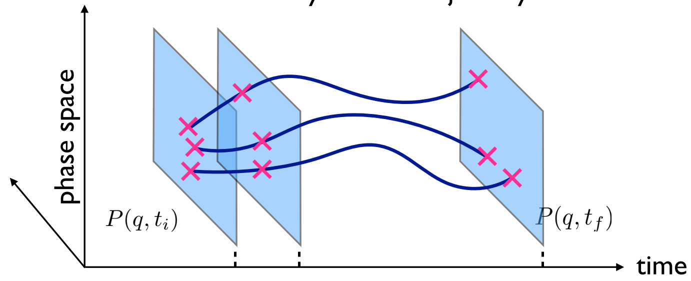
$$m\frac{dv}{dt} = \boxed{-\nabla U(x,\lambda(t))} \boxed{+ f_{nc}(x)} \boxed{- \gamma v + \sqrt{2\gamma T}\xi(t)}$$

white noise of unit variance

conservative force with t-dep. process

heat bath forces

- Statistical ensemble theory for the trajectory



Stochastic thermodynamics

$$m\frac{dv}{dt} = -\nabla U(x,\lambda(t)) + f_{nc}(x) - \gamma v + \sqrt{2\gamma T}\xi(t)$$

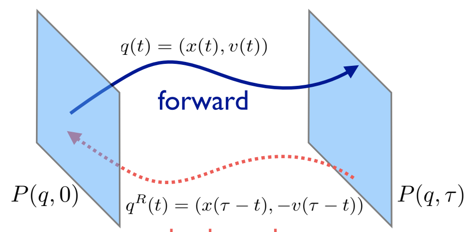
- Trajectory dependent fluctuating thermodynamic quantities
  - work $\Delta W = \int dt \left[f_{nc}(x) \circ v + \frac{\partial U}{\partial \lambda}\frac{d\lambda}{dt} \right]$
  - heat $\Delta Q = \int dt \left[\left(-\gamma v + \sqrt{2\gamma T}\xi(t) \right) \circ v \right]$
  - entropy $\Delta S_{tot} = -\frac{\Delta Q}{T} + [-\ln P(q_f,t_f) + \ln P(q_i,t_i)]$

1st law of thermodynamics

2nd law of thermodynamics?

Stochastic thermodynamics

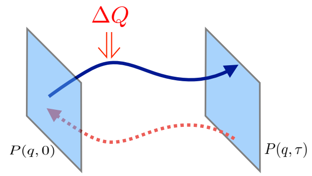
- Path probabilities



$$\mathrm{Prob}^F[q(t)] = W[q(t)|q(0)]P(q(0),0) \quad \text{(Forward)}$$

$$\mathrm{Prob}^R[q^R(t)] = W^R[q^R(t)|q^R(0)]P(q(\tau),\tau) \quad \text{(Backward)}$$

Stochastic thermodynamics



- Irreversibility
  - log ratio of path probabilities

$$\ln \frac{\mathrm{Prob}^F[q]}{\mathrm{Prob}^R[q^R]} = \boxed{\ln \frac{W[q(t)|q(0)]}{W^R[q^R(t)|q^R(0)]}} + \boxed{\ln \frac{P(q(0),0)}{P(q(\tau),\tau)}}$$

$$= -\frac{\Delta Q}{T} = \Delta S_{bath} \qquad = \Delta S_{sys}$$

$$\Delta S_{tot}[q(t)] = \ln \frac{\mathrm{Prob}^F[q(t)]}{\mathrm{Prob}^R[q^R(t)]}$$

[Schnackenberg, RMP (1976)]
[Lebowitz&Spohn, JSP (1999)]
[Seifert, PRL (2005)]
[Hinrichsen, Maes&Netocny, JSP (2003)]
[Chun&Noh, (2017)]

Fluctuation Theorem

- Integral FT for the total entropy production $\langle e^{-\Delta S_{tot}} \rangle = 1$
  - implication : the second law of thermodynamics

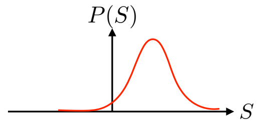
$$1 = \langle e^{-\Delta S_{tot}} \rangle \geq \langle 1 - \Delta S_{tot} \rangle \implies \langle \Delta S_{tot} \rangle \geq 0$$

(proof) $\langle e^{-\Delta S_{tot}} \rangle = \int [Dq] \mathrm{Prob}^F[q(t)] e^{-\Delta S_{tot}}$

$$= \int [Dq] \mathrm{Prob}^F[q(t)] \frac{\mathrm{Prob}^R[q^R(t)]}{\mathrm{Prob}^F[q(t)]} = 1$$

- Detailed FT
  - probability distribution $P(S) = \langle \delta(\Delta S_{tot} - S) \rangle$
  - in the steady state

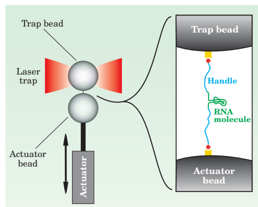
$$\frac{P(S)}{P(-S)} = e^S$$

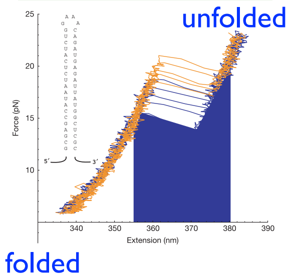


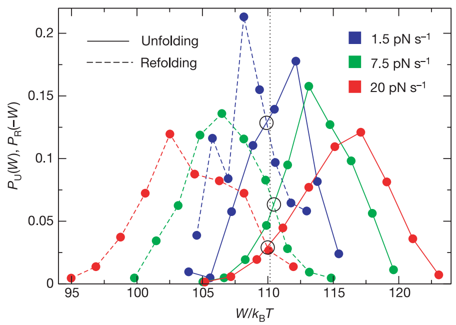
Fluctuation theorems

- Work
  - Jarzynski equality or IFT $\langle e^{-\beta W} \rangle = e^{-\beta \Delta F} \implies W \geq \Delta F$
    [Jarzynski, PRL(1997)]
  - Crooks relation or DFT $\frac{P_F(W)}{P_R(-W)} = e^{\beta(W-\Delta F)}$
    [Crooks, PRE (1999)]
- Heat
  - modified DFT $\frac{P_F(Q)}{P_R(-Q)} = e^{\beta(-Q-\Delta F)}/\Psi(Q)$ [Noh and Park, PRL (2012)]
- And many others…

Experiments



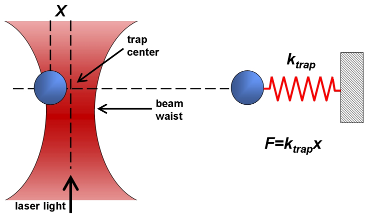




[Collin et al, Nature **437**, 231 (2005)]

Experiments

Colloidal particle trapped by the optical trap (≈harmonic potential)



moving trap

$$-\gamma\dot{x} = -k(x - vt) + \sqrt{2\gamma T}\xi(t)$$

[Wang et al, PRL (2002)]
[vanZon&Cohen, PRL (2003)]

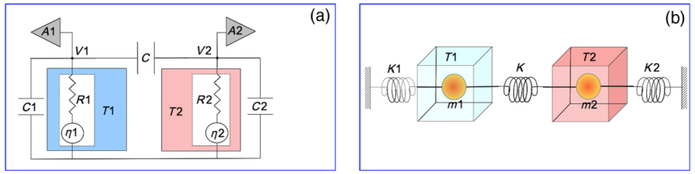
breathing trap

$$-\gamma\dot{x} = -k(t)x + \sqrt{2\gamma T}\xi(t)$$

[Lee&Kwon&Pak, PRL (2015)]

Experiments

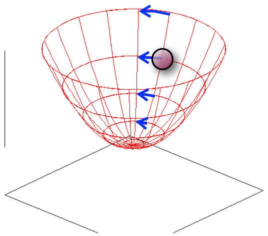
RC circuits



[Ciliberto et al, PRL (2013)]

Analytic works

Linear system



P(W) or P(Q) directly
to test the various FTs

[Kwon&Noh&Park, PRE (2011)]
[Noh&Park, PRL (2012)]
[Noh&Kwon&Park, PRL (2013)]
[Kwon&Noh&Park, PRE (2013)]

particle trapped in a harmonic potential and
driven by a nonconservative rotation force

Szilard Engine

(1898-1964)

Single gas particle in a single heat bath of temperature T

$W = Q = T\ln 2$
extracting work
from a single bath

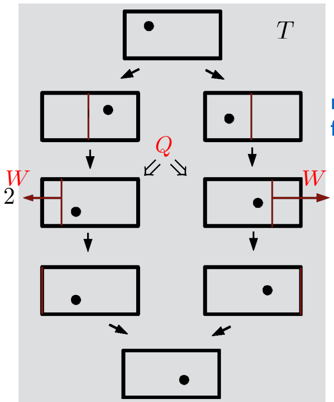
$\Delta S_{gas} = 0$

$\Delta S_{bath} = -\dfrac{Q}{T} = -\ln 2$

$\Delta S_{bath} + \Delta S_{gas} < 0$

second law?

Brillouin (1951)
Landauer (1961)
...

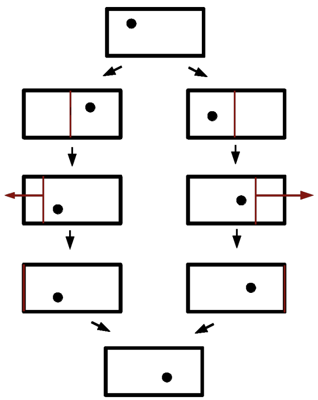


measurement and
feedback control by

isothermal expansion

= cousin of
Maxwell's demon

Szilard Engine



probability table for Gas and Demon

i) before m and fc

ii) after m and fc

iii) after process

G \ D	L	R
L	[illegible]	[illegible]
R	[illegible]	[illegible]

entropy changes

	S_G	S_D	$S_{G,D}$	S_{bath}	S_{tot}
i)	$\ln 2$	0	$\ln 2$	$+0$	$+0$
ii)	$\ln 2$	$\ln 2$	$\ln 2$	$+0$	$+0$
iii)	$\ln 2$	$\ln 2$	$\ln 4$	$-\ln 2$	$+0$

2nd law!

Information thermodynamics

[Sagawa&Ueda, PRL (2008, 2010, 2012)]

- In the presence of Maxwell's demon

$$S_{tot} = S_{sys,demon} + S_{bath}$$
$$= S_{sys} + S_{demon} - \boxed{I(sys;demon)} + S_{bath}$$

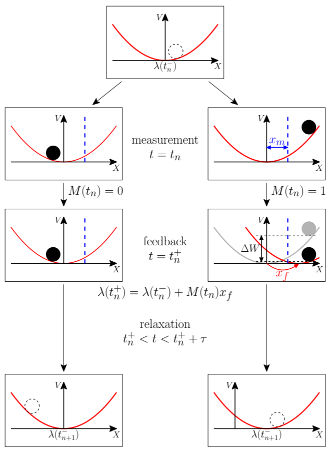
mutual information

- Extended second law

$$\Delta(S_{sys} + S_{demon} + S_{bath}) \geq \Delta I(sys;demon)$$

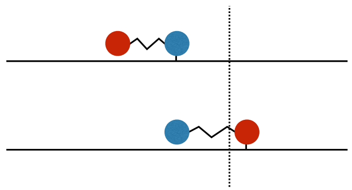
Information device

information heat engine



[Park&Lee&Noh, PRE (2016)]

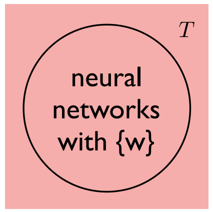
information motor



Thermodynamic bounds

- Stochastic learning in neural networks without feedback

$$\{(\xi^\mu, \sigma_T^\mu)\} \Longrightarrow$$



$$\Longrightarrow \{\sigma^\mu\}$$

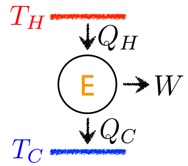
- Learning efficiency is bounded by the thermodynamic cost

$$I(\sigma_T;\sigma) \leq \Delta S(w) + \Delta Q/T$$ [Goldt&Seifert, PRL (2017)]

- Efficiency bound for a machine learning with feedback

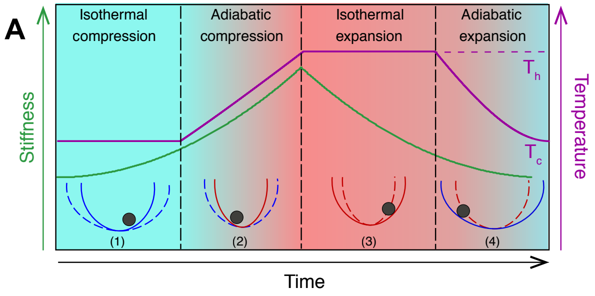
Microscopic heat engines

Heat engine



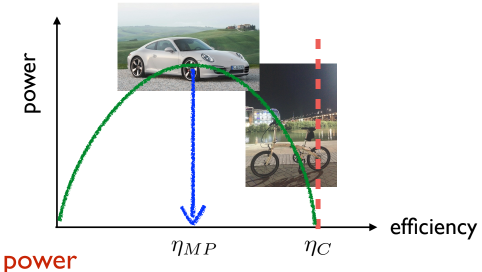
$$\eta = \frac{W}{Q_H} = 1 - \frac{Q_C}{Q_H} \le \eta_C \equiv 1 - \frac{T_C}{T_H}$$

Brownian heat engine [Martinez et al, NatPhys (2016)]



Microscopic heat engines

- Efficiency vs Power



- Efficiency at maximum power
- Trade-Off relation between power and efficiency

$$\frac{W}{\tau} \le \bar{\Theta}\beta_L \eta(\eta_C - \eta)$$ [Shiraishi&Saito&Tasaki, PRL (2016)]

Thermodynamic uncertainty relation

- Nonequilibrium system driven by external field,

fluctuating time-integrated current X = J t
heat dissipation with rate q

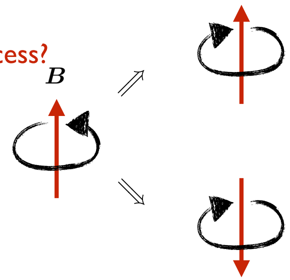
- Thermodynamic uncertainty relation

$$\mathcal{Q} \equiv \frac{\langle X^2\rangle - \langle X\rangle^2}{\langle X\rangle^2} \times \frac{qt}{T} = \frac{(\delta J)^2}{J^2} \times q \ge 2$$ [Barato&Seifert, PRL (2015)]

uncertainty $\epsilon = \delta J/J$ requires at least a cost of $2/\epsilon^2$

Velocity-dependent forces

- Charged particles with B field, active particles, …
- Entropy as Irreversibility $\Delta S_{tot}[q(t)] = \ln \dfrac{\mathrm{Prob}^F[q(t)]}{\mathrm{Prob}^R[q^R(t)]}$
- Reverse process to a given forward process?
- Fluctuation-dissipation relations,…



[Chun&Noh, arXiv (2017)]
[Lee&Lahiri&Park, PRE (2017)]
[Yeo&Kwon&Lee&Park, JSTAT (2016)]
[Lee&Kwon&Park, PRL (2013)]

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