Entropy production in random billiards and the second law of thermodynamics

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Washington University, St. Louis

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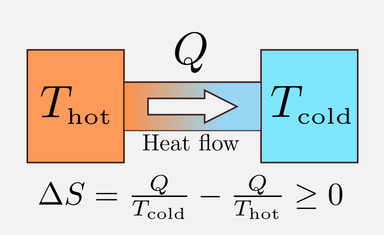


Plan of talk

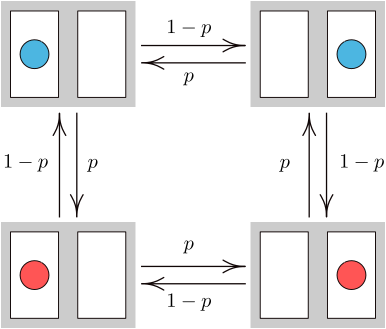
- Entropy production rate and irreversibility
- Random billiard dynamical systems
- Billiard systems with wall temperature
- Entropy production in random billiards
- The second law of thermodynamics
- Billiard heat engines

Entropy production rate in a simple Markov chain

A system consisting of a token and two chambers can be in 4 states:

$$\mathcal{S} = \{\text{Blue-Left}, \text{Blue-Right}, \text{Red-Left}, \text{Red-Right}\}.$$

It can transition between states with the following probabilities:



Transition matrix and stationary probabilities

- The transition probabilities matrix is:

$$P = \begin{array}{c} \\ \text{BL} \\ \text{BR} \\ \text{RL} \\ \text{RR} \end{array} \begin{array}{c} \begin{array}{cccc} \text{BL} & \text{BR} & \text{RL} & \text{RR} \end{array} \\ \begin{bmatrix} 0 & 1-p & p & 0 \\ p & 0 & 0 & 1-p \\ 1-p & 0 & 0 & p \\ 0 & p & 1-p & 0 \end{bmatrix} \end{array}$$

- The stationary probability vector $\pi = \pi P$, where

$$\pi = [\pi(\text{BL}), \pi(\text{RL}), \pi(\text{RL}), \pi(\text{RR})],$$

is given by

$$\pi = \left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$$

for all values of $p \neq 0, 1$.

Time irreversibility

- Suppose the Markov chain is stationary and defined by (π, P).
- We wish to compare the probabilities of forward chain segments

$$S_1, S_2, \ldots, S_{n-1}, S_n$$

  and backward chain segments

$$S_n, S_{n-1}, \ldots, S_1, S_0.$$

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- The probabilities of forward chains are

$$\mathbb{P}_n^+(s_1, \ldots, s_n) = \pi(s_1)P(s_1, s_2)\cdots P(s_{n-1}, s_n)$$

  and of backward chains are

$$\mathbb{P}_n^-(s_1, \ldots, s_n) = \pi(s_n)P(s_n, s_{n-1})\cdots P(s_2, s_1).$$

How to compare probability distributions?

- The Kullback-Leibler divergence (or relative entropy):

$$D_{KL}\left(\mathbb{P}_n^+ \| \mathbb{P}_n^-\right) = -\sum_{s} \mathbb{P}_n^+(s) \log \frac{\mathbb{P}_n^-(s)}{\mathbb{P}_n^+(s)}.$$

- This is a kind of (non-symmetric) distance between distributions.
- It is always non-negative and equals zero exactly when $\mathbb{P}_n^+ = \mathbb{P}_n^-$.

Definition (Entropy production rate)

$$e_p = \lim_{n\to\infty} \frac{1}{n} D_{KL}\left(\mathbb{P}_n^+ \| \mathbb{P}_n^-\right).$$

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- A calculation for Markov chains gives:

$$e_p = \frac{1}{2}\sum_{i,j} \left(\pi(s_i)P(s_i, s_j) - \pi(s_j)P(s_j, s_i)\right) \log \frac{\pi(s_i)P(s_i, s_j)}{\pi(s_j)P(s_j, s_i)} \geq 0.$$

Entropy production rate

- $e_p = 0 \Leftrightarrow$ chain satisfies the detailed balance property:

Definition (Detailed balance)

π and P are in detailed balance if $\pi(s_i)P(s_i, s_j) = \pi(s_j)P(s_j, s_i)$ for all s_i, s_j.

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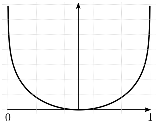
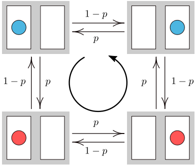
- For the example: $e_p = (2p - 1)\log \frac{p}{1-p}$.

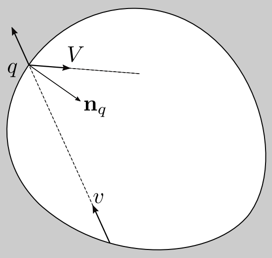


- For the example, if $p > 1/2$, there is overall rotation counterclockwise.

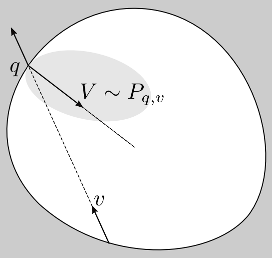


Random billiards

- In ordinary billiard, particle velocity at collision undergoes mirror-reflection.



standard billiard system



random billiard system

- In random billiard, velocity scatters randomly upon collision with wall.
- Post-collision velocity has probability distribution $P_{q,v} = P_q(\cdot|v)$.
- Given initial (q, v), we obtain a Markov chain

$$(Q_0, V_0), (Q_1, V_1), (Q_2, V_2), \ldots$$

Introducing boundary temperature

- Define the surface Maxwell-Boltzman distribution of velocities as

$$\mu_q(\mathcal{U}) = \int_{\mathcal{U}} C_q \langle \mathbb{n}_q, u \rangle \exp\left\{-\frac{1}{2}\frac{m|u|^2}{\kappa T_q}\right\} d\mathrm{Vol}(u).$$

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$$d\zeta_q(v, w) = d\mu_q(v) dP_{q,v}(w).$$

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$$d\zeta_q(v, w) = d\zeta_q(-w, -v).$$

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- Detailed balance:

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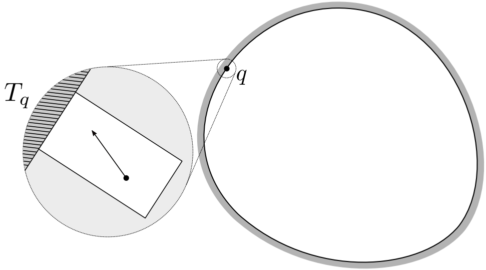
Definition (Boundary has temperature T_q at point q)

P_q and the Maxwell-Boltzmann distribution μ_q satisfy detailed balance.

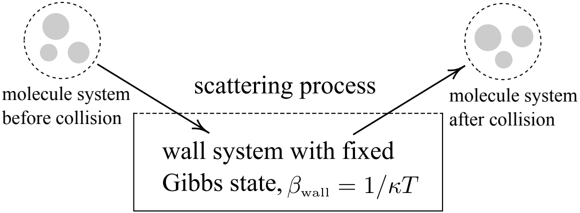
- P is said to satisfy reciprocity (in Boltzmann Equation literature.)

Physical definition of boundary temperature



- Enclose particle m in perfectly reflecting and rigid small cup open at q.
- Velocity distribution eventually becomes stationary.
- Stationary distribution is Maxwell-Boltzmann with temperature T_q.
- We also assume equilibrium is time-reversible.

Side remark: deriving P from microstructure



- Sample pre-collision condition of wall system from fixed Gibbs state
- Compute trajectory of deterministic Hamiltonian system
- Obtain post-collision state of molecule system.

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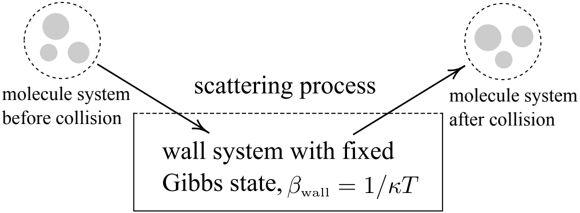

- Sample pre-collision condition of wall system from fixed Gibbs state
- Compute trajectory of deterministic Hamiltonian system
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Theorem (Cook-F)

Resulting P satisfies reciprocity. The stationary distribution is given by Gibbs state of molecule system with same parameter β as the wall system.

Example: One-dimensional billiard thermostat

- Mass m_1 is bound to wall. It moves freely within short interval.
- Mass m_2 can freely enter domain of m_1.

Choose velocity of $m_1 \sim \mathcal{N}(0, \sigma^2)$

Let masses interact deterministically

Reset velocity of m_1 from $\mathcal{N}(0, \sigma^2)$

Example: Maxwell-Smolukowski reflection model

- μ_q Maxwell-Boltzmann distribution of velocities with temperature $T(q)$.
- $\alpha(q)$ probability of diffuse reflection.
- Define

$$P_{q,v} = \begin{cases} \text{diffuse reflection } (\sim \mu_q) \text{ with probability } \alpha(q) \\ \text{specular reflection with probability } 1 - \alpha(q). \end{cases}$$

Time reversal in random billiard Markov chains

- States: (Q, V) specifies position and post-collision velocity.
- Forward chain segment:

$$(Q_0, V_0) \mapsto (Q_1, V_1) \mapsto \cdots \mapsto (Q_n, V_n)$$

- Time-reversal is a sequence of pre-collision states (velocities flipped):

$$(Q_n, -V_n) \mapsto (Q_{n-1}, -V_{n-1}) \mapsto \cdots \mapsto (Q_0, -V_0)$$

Irreversibility and entropy production

Given the random billiard map and stationary probability measure ν define

- $\mathbb{P}^{+}_{[0,n]}$ probability measure on space of chain segments
- $\mathbb{P}^{-}_{[0,n]}$ probability measure on space of reversed chain segments

Definition (Entropy production rate)

$e_p := \lim_{n\to\infty} \frac{1}{n} D_{KL}\left(\mathbb{P}^{+}_{[0,n]} \| \mathbb{P}^{-}_{[0,n]}\right)$ where the relative entropy D_{KL} is defined by

$$D_{KL}\left(\mathbb{P}^{+}_{[0,n]} \| \mathbb{P}^{-}_{[0,n]}\right) := \int_{\mathcal{D}} \log\left(\frac{d\mathbb{P}^{+}_{[0,n]}}{d\mathbb{P}^{-}_{[0,n]}}\right) d\mathbb{P}^{+}_{[0,n]}$$

Irreversibility and entropy production

- Define measure η on $\mathcal{D} = \{(Q, V), (Q', W) : Q' = Q + tV\}$ by

$$\boxed{d\eta(x, y) := d\nu(x) d\mathcal{B}_x(y)}$$

where $\mathcal{B}$ is the random billiard map, $x = (Q, V), y = (Q', W)$.

- Define $\eta^- := \mathcal{R}_* \eta$ where $\mathcal{R}$ is the proper reversal map (flip velocities!).

Proposition

The entropy production rate for the random billiard chain satisfies

$$e_p = \frac{1}{2} \int_{\mathcal{D}} \left[d\eta - d\eta^- \right] \log \left(\frac{d\eta}{d\eta^-} \right) \geq 0.$$

- This is the continuous state counterpart of

$$e_p = \frac{1}{2} \sum_{i,j} \left(\pi(s_i) P(s_i, s_j) - \pi(s_j) P(s_j, s_i) \right) \log \frac{\pi(s_i) P(s_i, s_j)}{\pi(s_j) P(s_j, s_i)}$$

for countable states Markov chains.

Bringing in temperature. Recall:

Definition (Maxwellian at temperature T)

The *Maxwell-Boltzmann distribution* at $q \in \partial M$ at temperature $T(q)$ is the probability measure $\mu_q^\pm \in \mathcal{P}(N_q^\pm)$ having density

$$\rho_q(v) = 2\pi \left(\frac{\beta(q)m}{2\pi}\right)^{\frac{n+1}{2}} |\langle v, \mathbb{n}_q\rangle| \exp\left\{-\beta(q)\frac{m|v|_q^2}{2}\right\}$$

with respect to the volume measure $dV_q(v)$, where $\beta(q) = 1/\kappa T(q)$.

- Define $\zeta_q \in \mathcal{P}\left(N_q^- \times N_q^+\right)$ by

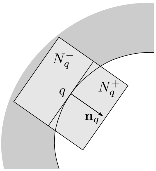
$$d\zeta_q(u,v) := d\mu_q^-(u)\, dP_{(q,u)}(v).$$

Definition (Reciprocity)

The reflection operator P has the property of reciprocity if at each $q \in \partial M$ the probability measure ζ_q is invariant under the proper time-reversal map.

Main result

- Given stationary $\nu \in \mathcal{P}(N^+)$ define $m := \pi_* \nu \in \mathcal{P}(\partial M)$.



- Let $\nu_q \in \mathcal{P}(N_q^+)$ be obtained by disintegrating ν along π, so that

$$\nu(\cdot) = \int_{\partial M} \nu_q(\cdot)\, dm(q).$$

- Let V_q be the Riemannian volume measure on N_q.
- Let $\mathcal{T} : N^+ \to N^-$ be the free-motion part of billiard map.
- Let $\nu^- := \mathcal{T}_* \nu$ and $\nu^+ := \nu$ pre- and post-collision velocity distributions.
- $E(q, v) := \frac{1}{2} m \|v\|_q^2$ particle kinetic energy.

Main result

Theorem (Chumley-F.)

Let $\nu \in \mathcal{P}(N^+)$ be the stationary measure for the random billiard map. Suppose the associated measures η and η^- on $\mathcal{D}$ are equivalent. Then

$$e_p = -\frac{1}{m(\partial M)} \int_{\partial M} \frac{1}{\kappa T(q)} \left[\nu_q^+(E) - \nu_q^-(E)\right] dm(q) \geq 0$$

where $m := \pi_* \nu$.

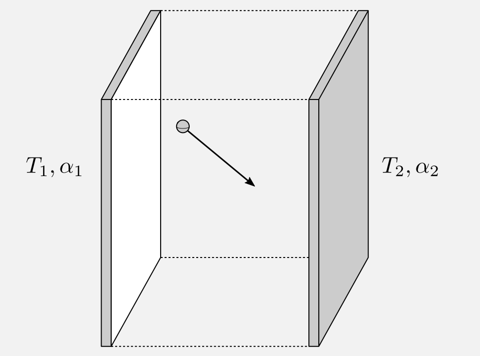
- That is, e_p is the average over boundary of M of

$$\frac{\nu_q\text{-mean heat transferred to wall at a collision point } q}{\text{wall temperature at } q}.$$

- Core problem: given a random billiard system, obtain ν.

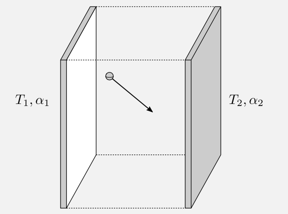
Example: Two plates

- $M = \mathbb{T}^2 \times [0, 1]$; boundary given Maxwell-Smolukowski thermostat.



Example: Two plates

- Q: the heat flow (mean energy tranfer per collision) from plate 1 to 2.
- Then $e_p = Q\left(\frac{1}{\kappa T_2} - \frac{1}{\kappa T_1}\right) > 0$.
- We recover Clausius form of second law: Heat flows from hot to cold.



- $Q = C(\kappa T_1 - \kappa T_2)$ where $C := \frac{\alpha_1\alpha_2}{2[1-(1-\alpha_1)(1-\alpha_2)]}$ = thermal conductivity.

Carnot's theory of heat engines

Need good examples to study entropy production, heat flow, work, efficiency, . . .

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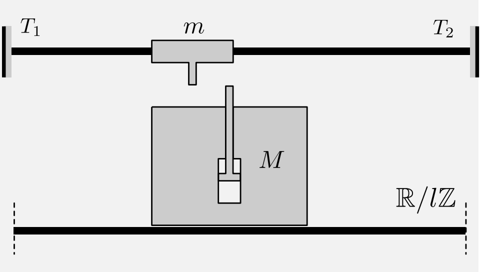

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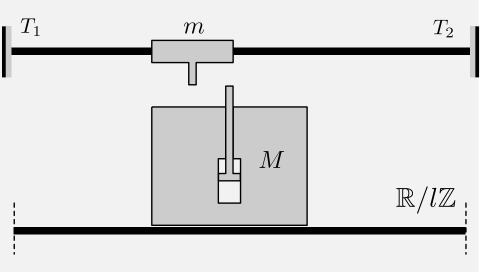

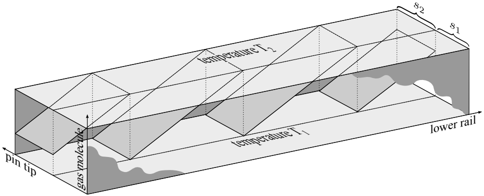

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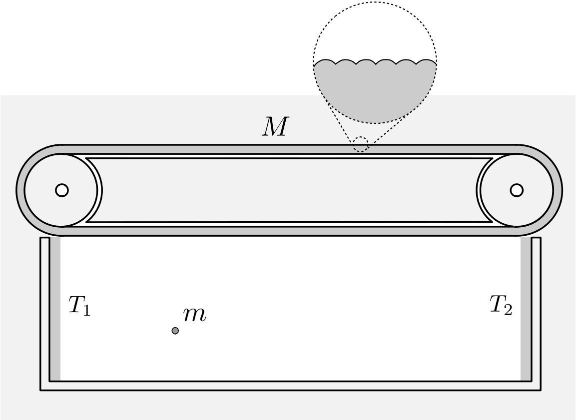
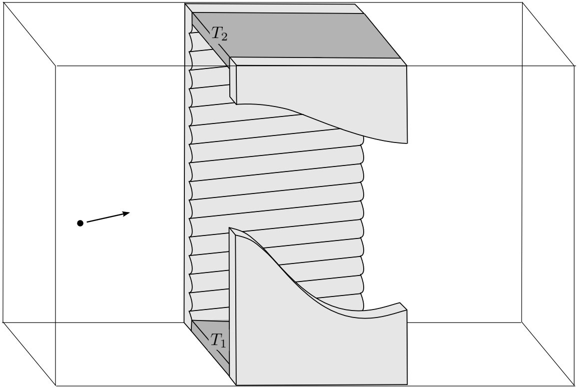


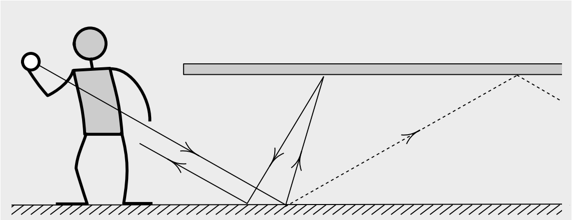
A thermophoretic motor.

Carnot's theory of heat engines

Billiard system for the thermophoretic motor.

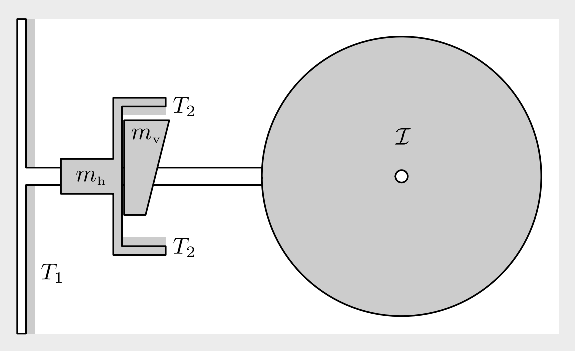


No-slip billiards



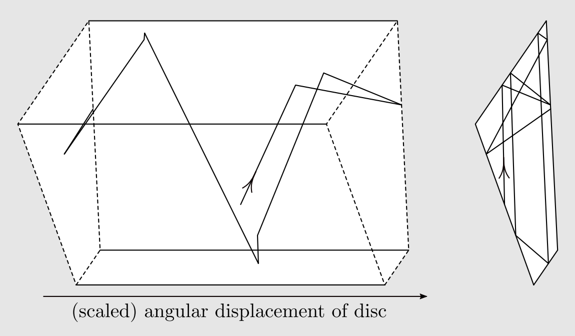
- Richard L. Garwin's 1969 paper *Kinematics of an Ultraelastic Rough Ball.*
- No-slip condition was used to explain bouncing of a Wham-O Super Ball®
- Further work by Wojtkowski and Broomhead-Gutkin 1993.
- No-slip dynamics being developed with Hongkun Zhang and Chris Cox.
- Conservative, reversible planar billiards: only the standard and no-slip.

A billiard heat engine with no-slip contact

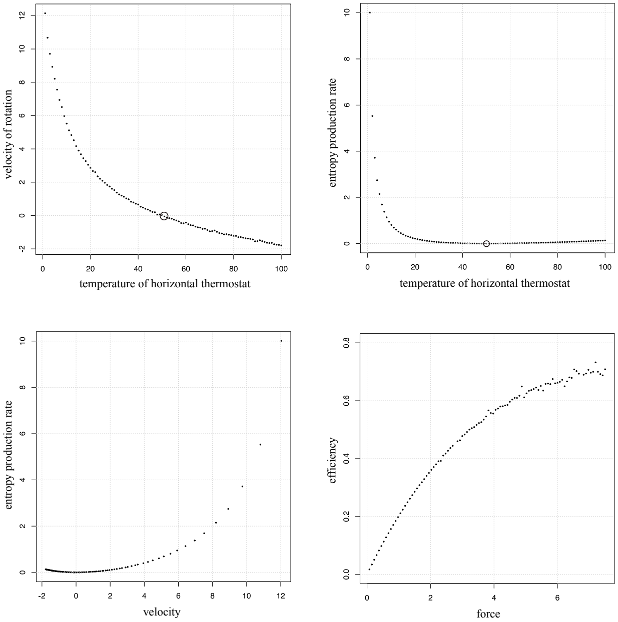


- We assume contact between disc and moving wedge is <u>no-slip</u> (rubbery).

The corresponding billiard system



Numerical results



Thank you!