From billiards to thermodynamics

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AIM, June 2015
Acknowledgements

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Overview

- Examples of billiard systems
- Markov chains from billiard systems
- Random billiards as models of thermodynamic systems
- A billiard heat engine
- Diffusion in position space and velocity space
Part I

Thermodynamics of billiard engines
**Billiards**: systems of rigid masses with elastic collision interactions

- Bunimovich stadium with piston
- Bouncing wall (thermostat)
- Dumbbell heat bath
- Pin latch
- Sliding wall
- Range of motion of bound masses

No friction or potential forces; assume smooth contact between surfaces.
The configuration manifold (pin latch)

The configuration space of the system is a manifold $M$ with boundary (corners).

The dimension of $M$ equals the number of degrees of freedom of the system.
The configuration manifold \textit{(dumbbell)}

\[(x, y) = \text{center of mass}; \ \theta = \text{angle of rotation}; \ m = m_1 + m_2.\]

\[M = \left\{([\theta], x, y) : \min \left\{ y - \frac{m_2}{m} l \sin \theta, y + \frac{m_1}{m} l \sin \theta \right\} \geq 0 \right\}\]

Set \(z := \frac{\sqrt{m_1 m_2}}{m} l \theta.\) Then the kinetic energy (Riemannian metric) is Euclidean:

\[K(\dot{x}, \dot{y}, \dot{z}) = \frac{1}{2} m \left( \dot{x}^2 + \dot{y}^2 + \dot{z}^2 \right)\]
The configuration manifold (heat bath)
The configuration manifold (sliding wall)

Billiard motion in 3-D channel corresponds to Brownian motion of sliding wall.
Introducing randomness

Random dynamical system derived from a deterministic system:

The transition probabilities operator $P : \mathcal{P}(X) \rightarrow \mathcal{P}(X)$ is defined by

$$
\mu \mapsto \mu P := (\pi \circ T)_* \mu \circ \eta
$$

where $(\mu \circ \eta)(f) = \int_X \eta_x(f) \, d\mu(x)$ is a probability measure on $V$. 

Invariant measure for $T \Rightarrow$ stationary measure for $P$

A statistical state $\mu$ is stationary (or an equilibrium state) if $\mu P = \mu$.

**Proposition**

Let $\nu$ be a $T$-invariant probability measure on the total space $V$ of the random system and suppose that $\eta$ is the disintegration of $\nu$ with respect to $\mu := \pi_* \nu$. Then $\mu$ is stationary.
Example: **heat bath** system (large # of bound masses)

- **Observable**: position and velocity of the unbound mass.
- **Assume**: bound masses before each “scattering event” are random, uniform.

\[ x \sim \text{Unif} ([0, a]^n) \]

\[ v \sim \cos \theta \, dA_S \]

\[ \bar{v} \sim d\nu(s) = \frac{s}{\sigma} \exp \left( -\frac{1}{2} \frac{s^2}{\sigma^2} \right) ds \]

\[ \nu := \pi_*\mu \approx \text{surface Maxwellian.} \]
Example: 1-D billiard thermostat

Scattering event at the wall:

choose initial state of wall-bound mass from:

\[
x \sim \text{Unif}[0, l]
\]
\[
v \sim \text{Norm}(0, \sigma^2)
\]

let masses interact according to deterministic mechanical laws

register velocity of molecule and reset state of wall-bound mass.

This is very special case of following general construction:
Surface scattering operator and Markov chains

General procedure for constructing Markov chains from Hamiltonian systems:

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

Resulting $P$ has generally nice spectral properties (more later).
Scattering operator of 1-D billiard thermostat

Define $\gamma = m_2/m_1$. $P_\gamma$ is operator on $L^2((0, \infty), \mu)$.

**Theorem (Speed of convergence to thermal equilibrium)**

The following assertions hold for $\gamma < 1/3$:

1. $P_\gamma$ is a Hilbert-Schmidt; $\mu$ is the unique stationary distribution. Its density relative to Lebesgue measure on $(0, \infty)$ is

   $$\rho(v) = \sigma^{-1} v \exp\left(-\frac{v^2}{2\sigma^2}\right).$$

2. For arbitrary initial $\mu_0$ and small $\gamma$

   $$\|\mu_0 P_\gamma^n - \mu\|_{TV} \leq C \left(1 - 4\gamma^2\right)^n \to 0.$$
Approach to thermal equilibrium

Initial velocity distribution

Limit Maxwellian

Probability density

Speed

$\rho_{\text{equi}}$

$\rho_{100}$

$\rho_{50}$

$\rho_1$

$\rho_0$
Molecule moves faster (on average) from hot to cold.
Heat flow and temperature difference

Expected energy transfer per collision = $c(\gamma)(T_{\text{hot}} - T_{\text{cold}})$

$\gamma$ is the mass ratio.
A billiard heat engine

$T_1 = T_2$ and 0 load $\implies$ Brownian motion.
$T_1 \neq T_2 \implies \text{Rotation (0 load)}$

Stochastic motion with steady drift (rotation). No load force yet.
Mean rotation **against** load for $T_1 > T_2$

If $T_1 - T_2$ great enough, obtain rotation against load, producing positive work.
Efficiency = heat flow from hot wall/rate of work produced
Part II

Diffusion in channels and transport coefficients
Engine motion: diffusion with drift in channels

Engine’s operation: motion in a 5-D configuration (channel) manifold.
Random billiards as microstructures

\[(Pf)(v) = \mathbb{E}_v [f(V)]\]
Microstructures with moving parts

- Random initial velocity of wall
- Random entrance point
- Random initial height
- Surface
- Velocity space (upper-half space)
- Random scattered velocity
- One step in Markov chain on velocity space

\[ \mathbb{H}^n \text{ velocity space (upper-half space)} \]

\[ \mathbf{u} \leftrightarrow \mathbf{V} \]

range of free motion of wall

\[ m_0 \]

\[ q \]
Requirements for a well-motivated \( P \):

1. \( \mu_\beta \) is a stationary distribution for the velocity Markov chain where

\[
d\mu_\beta(V) = 2\pi \left( \frac{\beta M}{2\pi} \right)^{\frac{n+1}{2}} \cos \theta \exp \left( -\frac{\beta M}{2} |V|^2 \right) d\text{Vol}(V)
\]

is the surface Maxwell-Boltzmann measure with parameter \( \beta = 1/\kappa T \).

2. The stationary process defined by \( P \) and \( \mu_\beta \) is time reversible:

\[
P(dV_2|V_1) d\mu_\beta(V_1) = P(dV_1|V_2) d\mu_\beta(V_2).
\]

Definition

\( P \) will be called natural if it satisfies these properties.

The previous two examples are natural.
Deriving $P$ from microstructure: general idea

Theorem (Cook-F, Nonlinearity 2012)

Resulting $P$ is natural. The stationary distribution is given by Gibbs state of molecule system with same parameter $\beta$ as the wall system.
Diffusion in (straight) channels
time-correlation and transport coefficients

Idealized diffusion experiment. Channel inner surface has micro-structure.

How does the micro-structure influence diffusivity?
Cylindrical channels

Define for the random flight of a particle starting in the middle of cylinder:

- $s_{\text{rms}}$ root-mean square velocity of gas molecules
- $\tau = \tau(L, r, s_{\text{rms}})$ expected exit time of random flight in channel

-Cylindrical channels

\[ n = 2, k = 1 \]
\[ n = 3, k = 1 \]
\[ n = 3, k = 2 \]
CLT and Diffusion in channels (anomalous diffusion)

Theorem (Chumley, F., Zhang, Transactions of AMS, 2014)

Let $P$ be quasi-compact (has spectral gap) natural operator. Then

$$
\tau(L, r, s_{\text{rms}}) \sim \begin{cases} 
\frac{1}{D} \frac{L^2}{k} & \text{if } n - k \geq 2 \\
\frac{1}{D} \frac{L^2}{k \ln(L/r)} & \text{if } n - k = 1
\end{cases}
$$

where $D = C(P)rs_{\text{rms}}$. Values of $C(P)$ are described next.

Useful for comparison to obtain values of diffusion constant $D$ for the i.i.d. velocity process before looking at specific micro-structures. We call these reference values $D_0$. 
Values of $\mathcal{D}_0$ for reference (Trans. AMS, 2014)

For any direction $u$ in $\mathbb{R}^k$ diffusivities for the i.i.d. processes are:

$$\mathcal{D}_0 = \begin{cases} 
\frac{4}{\sqrt{2\pi(n+1)}} \frac{n-k}{(n-k)^2-1} rs_\beta & \text{when } n - k \geq 2 \text{ and } \nu = \mu_\beta \\
\frac{2}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)} \frac{n-k}{(n-k)^2-1} rs & \text{when } n - k \geq 2 \text{ and } \nu = \mu_\infty \\
\frac{4}{\sqrt{2\pi(n+1)}} rs_\beta & \text{when } n - k = 1 \text{ and } \nu = \mu_\beta \\
\frac{2}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)} rs & \text{when } n - k = 1 \text{ and } \nu = \mu_\infty
\end{cases}$$

where $s_\beta = (n + 1)/\beta M$ and $M$ is particle mass. We are, therefore, interested in

$$\eta^u(P) := \frac{\mathcal{D}^u_P}{\mathcal{D}_0} \quad \text{(coefficient of diffusivity in direction } u)$$

a signature of the surface’s scattering properties. ($u$ is a unit vector in $\mathbb{R}^k$.)
Top: $\mathcal{D}$ is smaller then in i.i.d. (perfectly diffusive) case.
Middle and bottom: $\mathcal{D}$ increases by adding flat top.

\[ \eta(0) = \frac{1 - \frac{1}{4} \log 3}{1 + \frac{1}{4} \log 3} \]

\[ \eta(h) = \frac{\eta(0) + h}{1 - h} \]

\[ h = \frac{l}{2r} \]
Examples in 2-D

Diffusivity can be discontinuous on geometric parameters:

\[
\eta(h) = \begin{cases} 
\frac{1 - \frac{1}{4} \log 3}{1 + \frac{1}{4} \log 3} & \text{if } h < \frac{1}{2} \\
\frac{1 + \frac{1}{4} \log 3}{1 - \frac{1}{4} \log 3} & \text{if } h = \frac{1}{2}
\end{cases}
\]

Peculiar effects when \( n - k = 1 \)

\[
\eta(h) = \frac{1 + \zeta_h}{1 - \zeta_h} \quad \zeta_h = -\frac{1+3h}{4} \frac{1-h}{1+h} \log \frac{3+h}{1-h}
\]
Diffusivity and the spectrum of $P$

Consider the Hilbert space $L^2(\mathbb{H}^n, \mu_\beta)$ of square-integrable functions on velocity space with respect to the stationary measure $\mu_\beta$ ($0 < \beta \leq \infty$).

**Proposition (F-Zhang, Comm. Math. Physics, 2012)**

The natural operator $P$ is a self-adjoint operator on $L^2(\mathbb{H}^n, \mu_\beta)$ with norm 1. In particular, it has real spectrum in the interval $[-1, 1]$. In many special cases we have computed, $P$ has discrete spectrum (eigenvalues) or at least a spectral gap.

Let $\Pi_u Z(d\lambda) := \|Z_u\|^{-2}\langle Z_u, \Pi(d\lambda)Z_u \rangle$, $\Pi$ the spectral measure of $P$. Then

$$\eta^u(P) = \int_{-1}^{1} \frac{1 + \lambda}{1 - \lambda} \Pi^u(d\lambda).$$

Example: Maxwell-Smolukowski model: $\eta = \frac{1 + \lambda}{1 - \lambda}$, $\lambda =$ prob. of specular reflec.
Related systems

- Billiard thermostat
- Charged particle
- Constant electric field
- Constant rotation speed
- Constant velocity of sliding wall
- Shear velocity profile
Remarks about diffusivity and spectrum

- From random flight determined by $P \Rightarrow \text{Brownian motion limit via C.L.T.}$

- $D$ determined by rate of decay of time correlations (Green-Kubo relation)

- All the information needed for $D$ is contained in the spectrum of $P$

- It is difficult to obtain detailed information about the spectrum of $P$; would like to find approximation more amenable to analysis.
Part III

Diffusion in velocity space
Weak scattering and diffusion in velocity space

Assume weakly scattering microstructure: $P$ is close to specular reflection. In example below small $h \Rightarrow$ small ratio $m/M$ and small surface curvature.

In such cases, the sequence $V_0, V_1, V_2, \ldots$ of post-collision velocities can be approximated by a diffusion process in velocity space. If $\rho(v, t)$ is the probability density of velocity distribution

$$\frac{\partial \rho}{\partial t} = \text{Div}^{\text{MB}} \text{Grad}^{\text{MB}} \rho$$

where MB stands for “Maxwell-Boltzmann.”
Weak scattering and diffusion in velocity space

- $\Lambda$ square matrix of (first derivatives in perturbation parameter of) mass-ratios and curvatures.
- $C$ is a covariance matrix of velocity distributions of wall-system.

**Definition (MB-grad, MB-div, MB-Laplacian)**

- On $\Phi \in C^\infty_0(\mathbb{H}^m) \cap L^2(\mathbb{H}^m, \mu_\beta)$ (smooth, comp. supported) define

\[
(\text{Grad}^{\text{MB}} \Phi)(v) := \sqrt{2} \left[ \Lambda^{1/2} (v_m \text{grad}_v \Phi - \Phi_m(v) v) + \text{Tr}(C\Lambda)^{1/2} \Phi_m e_m \right]
\]

where $e_m = (0, \ldots, 0, 1)$ and $\Phi_m$ is derivative in direction $e_m$.

- On the pre-Hilbert space of smooth, compactly supported square-integrable vector fields on $\mathbb{H}^m$ with inner product $\langle \xi_1, \xi_2 \rangle := \int_{\mathbb{H}^m} \xi_1 \cdot \xi_2 \, d\mu_\beta$, define $\text{Div}^{\text{MB}}$ as the negative of the formal adjoint of $\text{Grad}^{\text{MB}}$.

- Maxwell-Boltzmann Laplacian: $\mathcal{L}_{\text{MB}} \Phi = \text{Div}^{\text{MB}} \text{Grad}^{\text{MB}} \Phi$. 

Let $\mu$ be a probability measure on $\mathbb{R}^k$ with mean 0, covariant matrix $C$ and finite 2nd and 3rd moments. Let $P_h$ be the collision operator of a family of microstructures parametrized by flatness parameter $h$. Then

- $\mathcal{L}_{MB}$ is second order, essent. self-adjoint, elliptic on $C_0(\mathbb{H}^m) \cap L^2(\mathbb{H}^m, \mu_\beta)$.
- The limit $\mathcal{L}_{MB} \Phi = \lim_{h \to 0} P_h \frac{\Phi - \Phi}{h}$ holds uniformly for each $\Phi \in C_0^\infty(\mathbb{H}^m)$.
- The Markov chain defined by $(P_h, \mu_\beta)$ converges to an Itô diffusion with diffusion PDE
  \[
  \frac{\partial \rho}{\partial t} = \mathcal{L}_{MB} \rho
  \]
Example1: 1-D billiard thermostat

Proposition
For $\gamma := m_2/m_1 < 1/3$, if $\varphi$ is a function of class $C^3$ on $(0, \infty)$, the MB-billiard Laplacian has the form

$$\left(\mathcal{L}\varphi\right)(v) = \lim_{\gamma \to 0} \frac{(P_\gamma \varphi)(v) - \varphi(v)}{2\gamma} := \left(\frac{1}{v} - v\right) \varphi'(v) + \varphi''(v).$$

Equivalently, $\mathcal{L}$ can be written in Sturm-Liouville form as

$$\mathcal{L}\varphi = \rho^{-1} \frac{d}{dv} \left( \rho \frac{d\varphi}{dv} \right),$$

which is a densely defined self-adjoint operator on $L^2((0, \infty), \mu)$.

$\mathcal{L}$ is Laguerre differential operator.
Example 2: no moving parts

Projecting orthogonally from spherical shell to unit disc, cosine law becomes the uniform probability on the disc. Choose a basis of $\mathbb{R}^n$ that diagonalizes $\Lambda$.

Proposition (Generalized Legendre operator in dim $n$)

When $k = 0$, the MB-Laplacian on the unit disc in $\mathbb{R}^n$ is

$$\begin{align*}
(\mathcal{L}_{MB} \Phi)(v) &= 2 \sum_{i=1}^{n} \lambda_i \left( (1 - |v|^2) \Phi_i \right)_i 
\end{align*}$$
Sample path of Legendre diffusion

What does the spectrum of MB-Laplacians say about the spectrum of $P$?