From billiards to thermodynamics

Renato Feres

Washington University, St. Louis

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Acknowledgements

Collaborators:

Tim Chumley, Iowa State University

Scott Cook, Swarthmore College

Chris Cox, Washington University

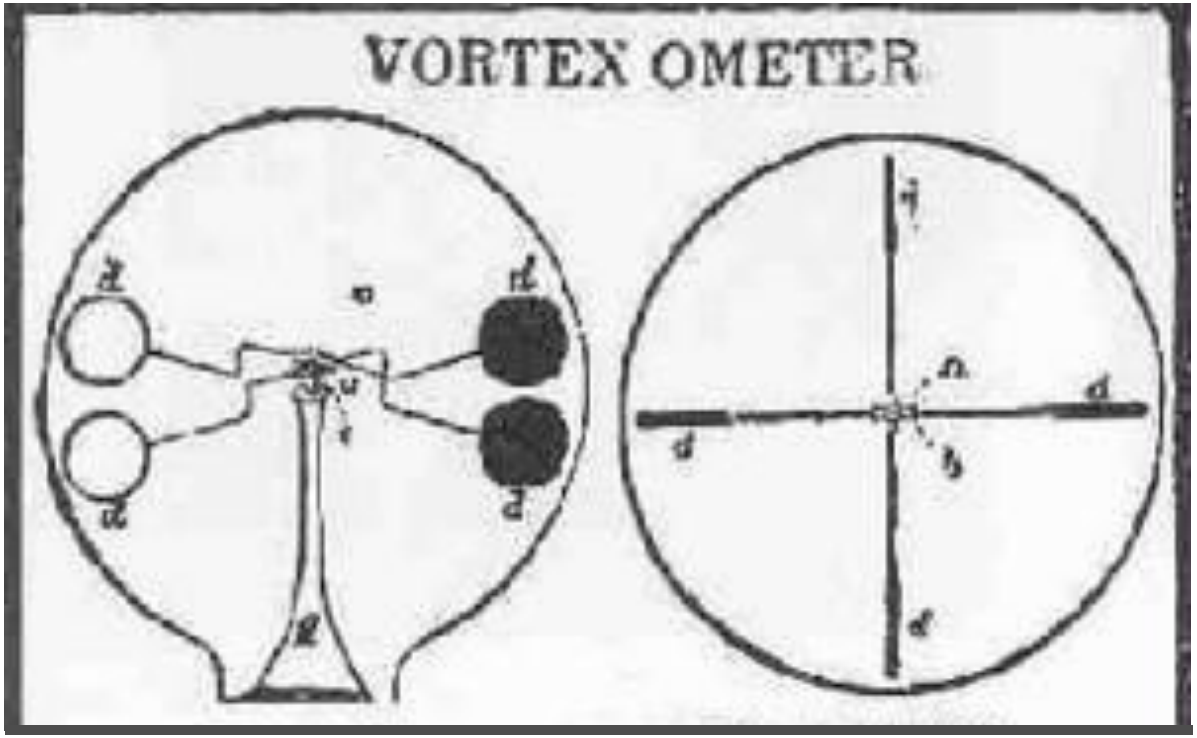
Hong-Kun Zhang, U. of Massachusetts, Amherst

Overview

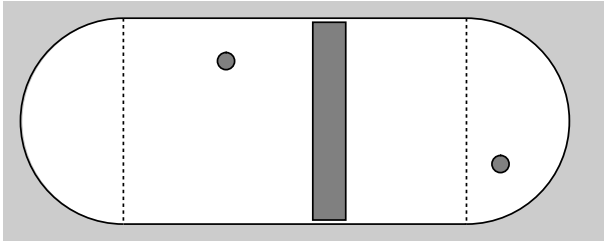
- Examples of billiard systems
- Markov chains from billiard systems
- Random billiards as models of thermodynamic systems
- A billiard heat engine
- Diffusion in position space and velocity space

Part I

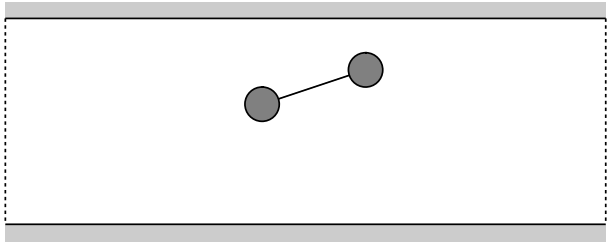
Thermodynamics of billiard engines



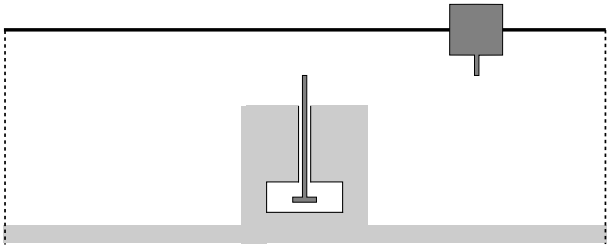
Billiards: systems of rigid masses with elastic collision interactions



Bunimovich stadium with piston

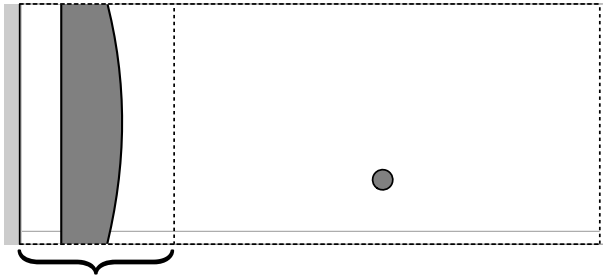


dumbbell

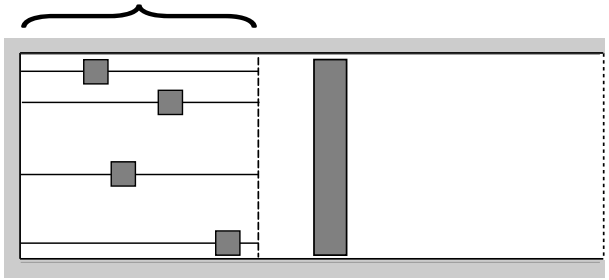


pin latch

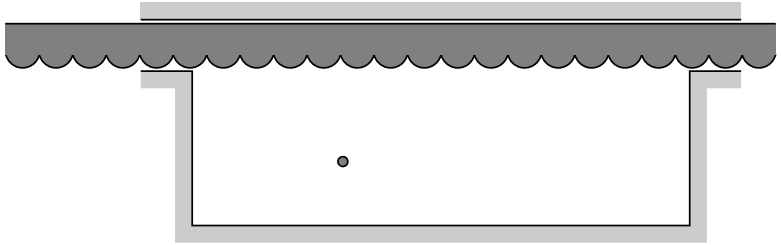
bouncing wall (thermostat)



range of motion of bound masses



heat bath

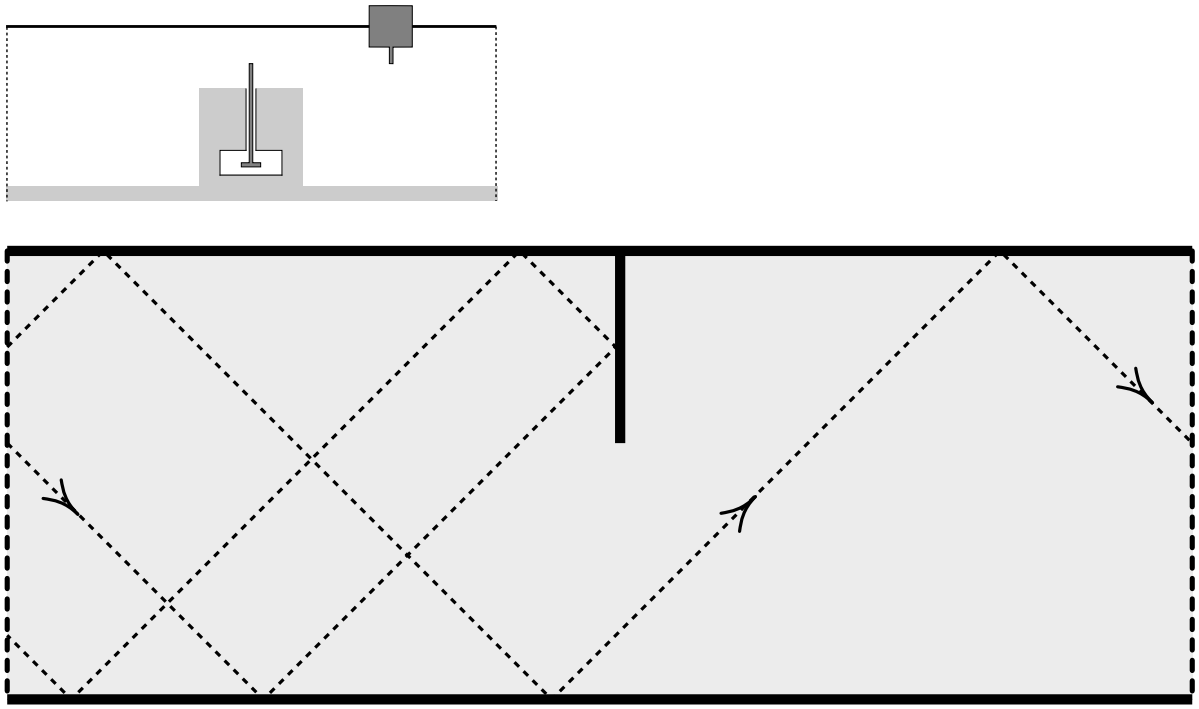


sliding wall

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).

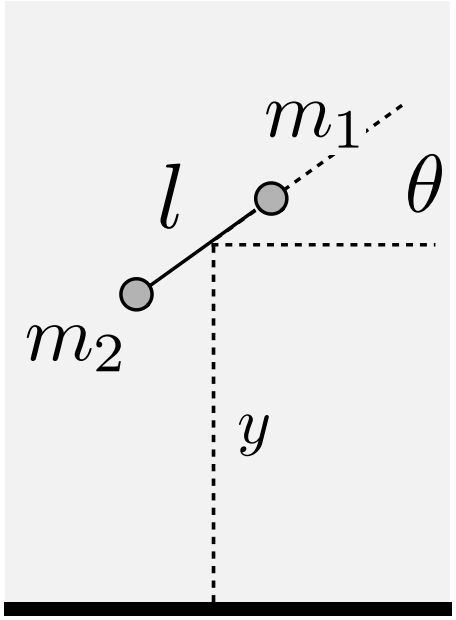


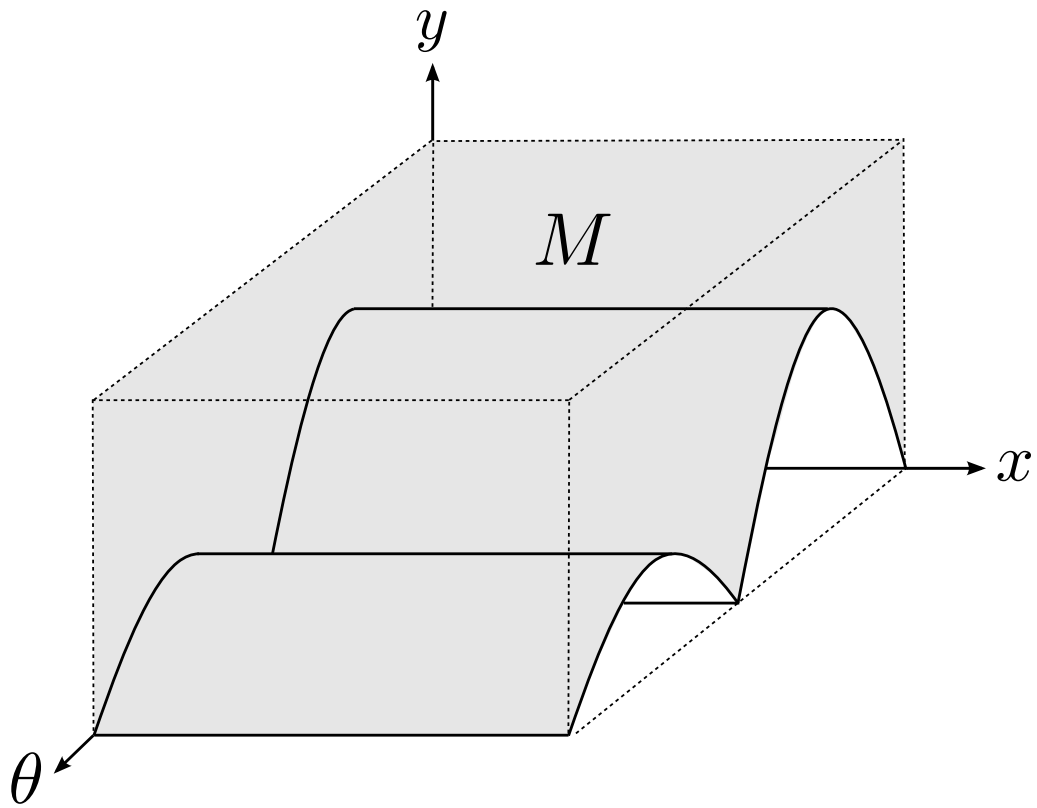
The dimension of M equals the number of degrees of freedom of the system.

The configuration manifold (dumbbell)

(x, y) = center of mass; θ = angle of rotation; $m = m_1 + m_2$.

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

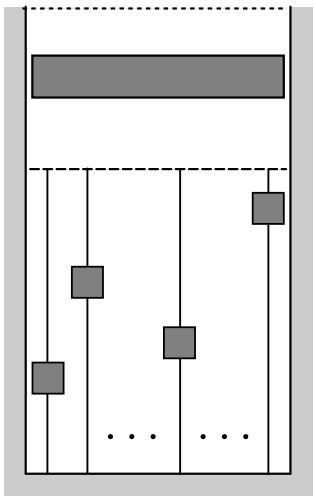


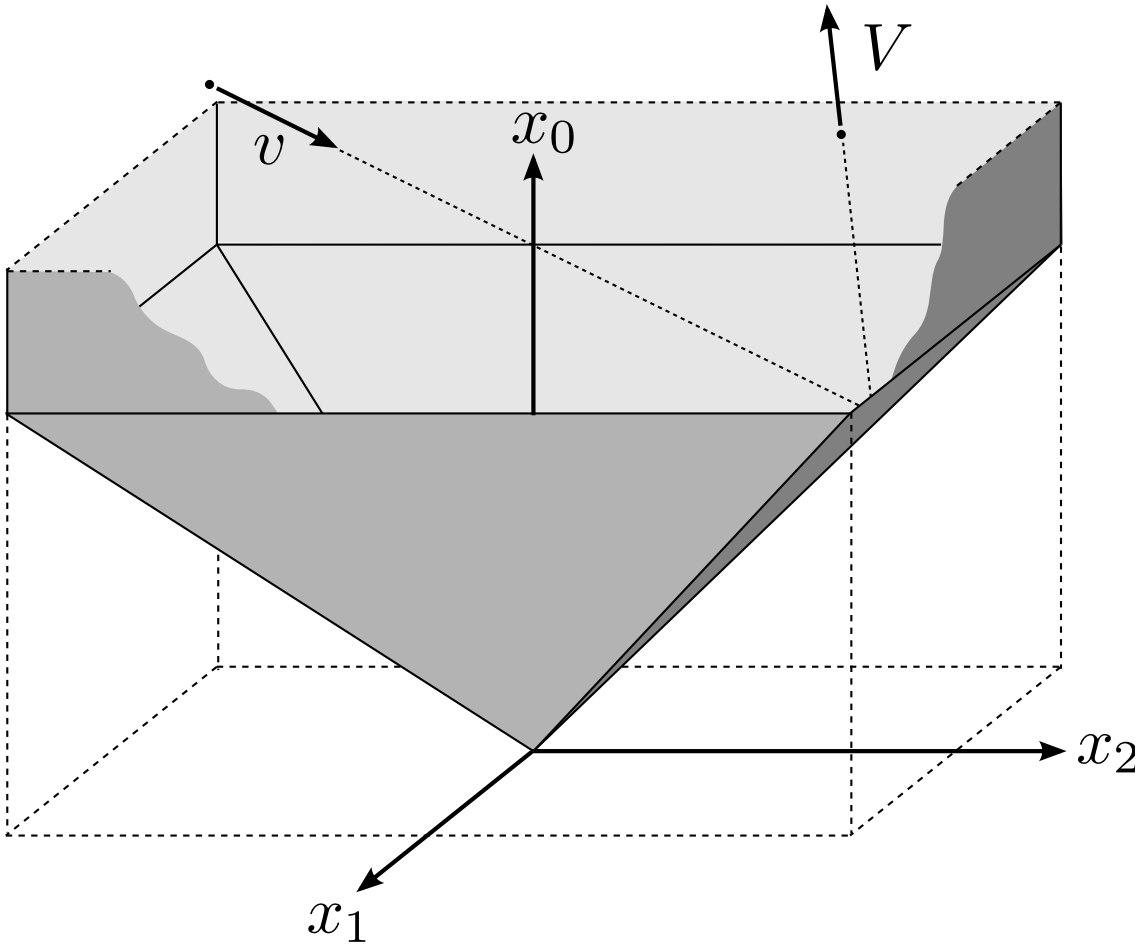


Set $z := \frac{\sqrt{m_1 m_2}}{m} l\theta$. Then the kinetic energy (Riemannian metric) is Euclidean:

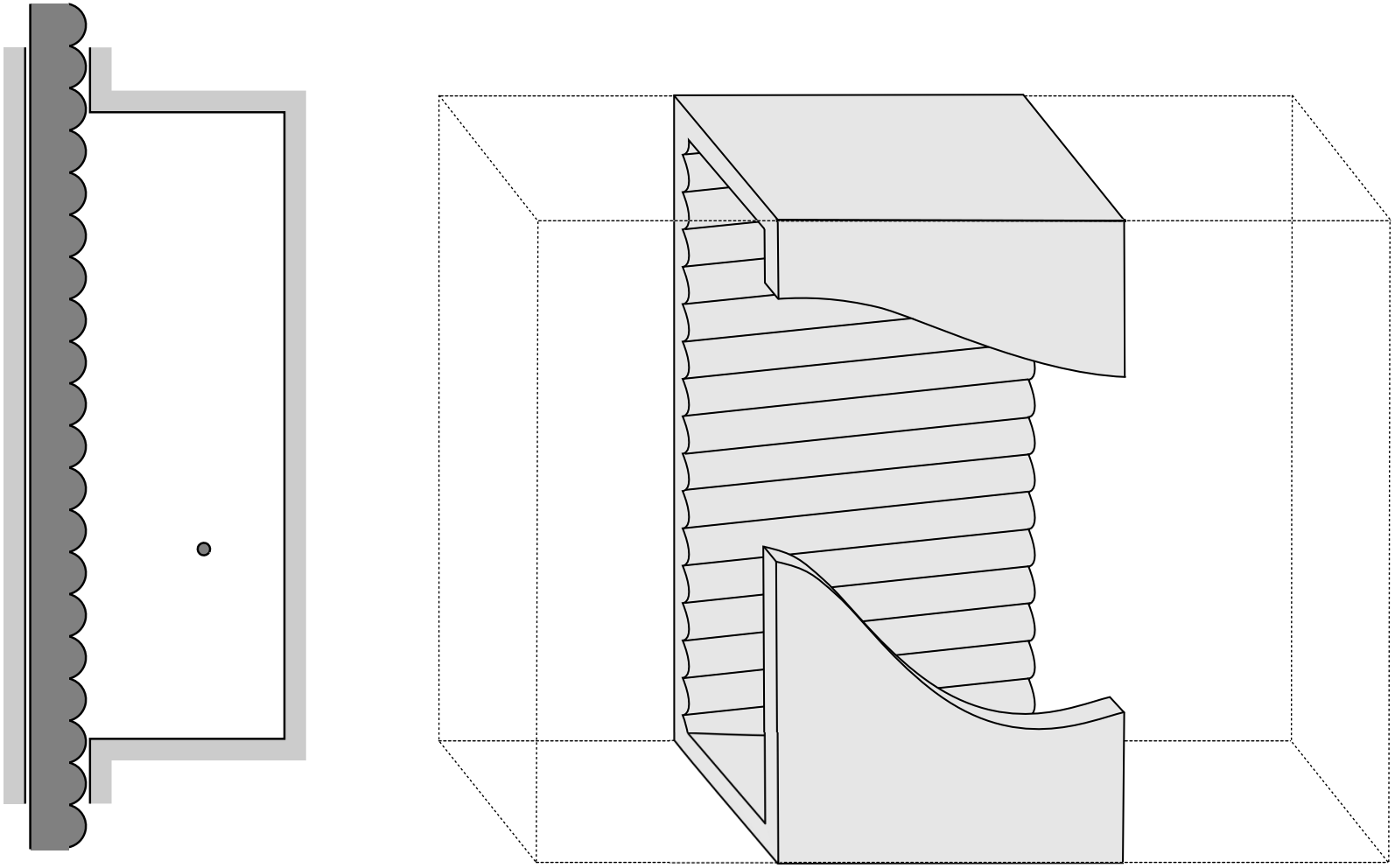
$$K(\dot{x}, \dot{y}, \dot{z}) = \frac{1}{2} m \left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2 \right)$$

The configuration manifold (heat bath)





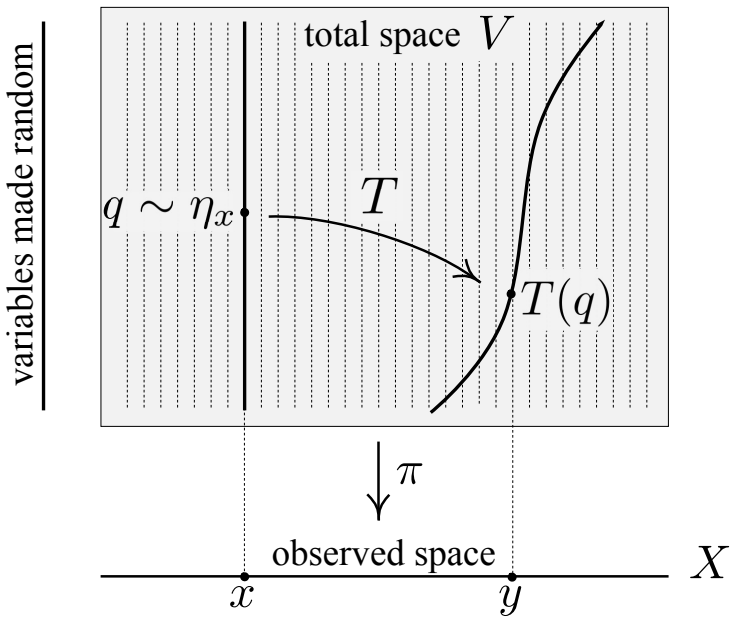
The configuration manifold (sliding wall)



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 $P : \mathcal{P}(X) \to \mathcal{P}(X)$ 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

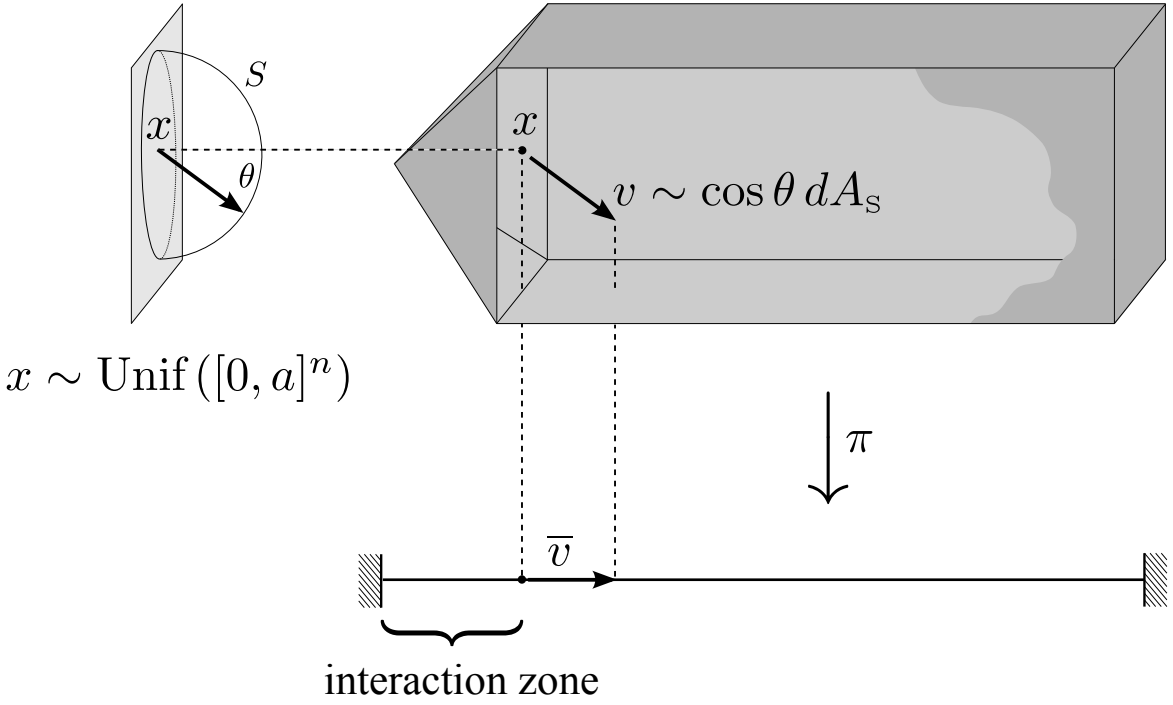
A statistical state μ is stationary (or an equilibrium state) if $\mu P = \mu$.

Proposition

Let ν be a T-invariant probability measure on the total space V of the random system and suppose that η is the disintegration of ν with respect to $\mu := \pi_* \nu$. Then μ is stationary.

Example: heat bath system (large # of bound masses)

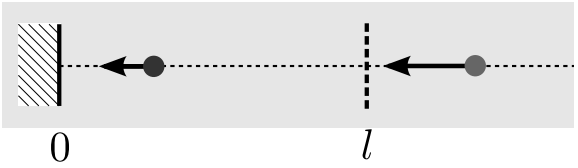
- Observable: position and velocity of the unbound mass.
- Assume: bound masses before each "scattering event" are random, uniform.



- v has stationary distribution $\boxed{d\mu(v) = \text{const.} \cos\theta \, dA_{\mathrm{S}}(v)}$
- $\boxed{\bar{v} \sim d\nu(s) = \frac{s}{\sigma} \exp\left(-\frac{1}{2} s^2/\sigma^2\right) ds}$ $\nu := \pi_* \mu \approx$ surface Maxwellian.

Example: 1-D billiard thermostat

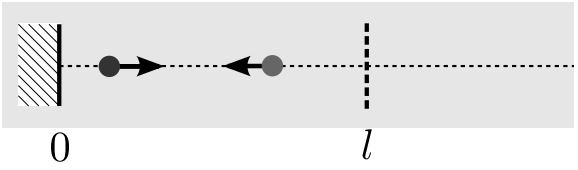
Scattering event at the wall:



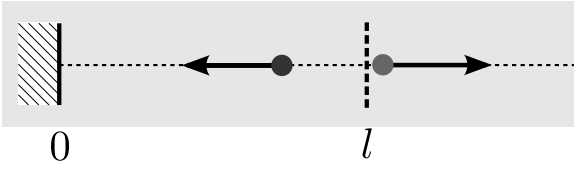
choose initial state of wall-bound mass from:

$x \sim \mathrm{Unif}[0, l]$

$v \sim \mathrm{Norm}(0, \sigma^2)$



let masses interact according to deterministic mechanical laws

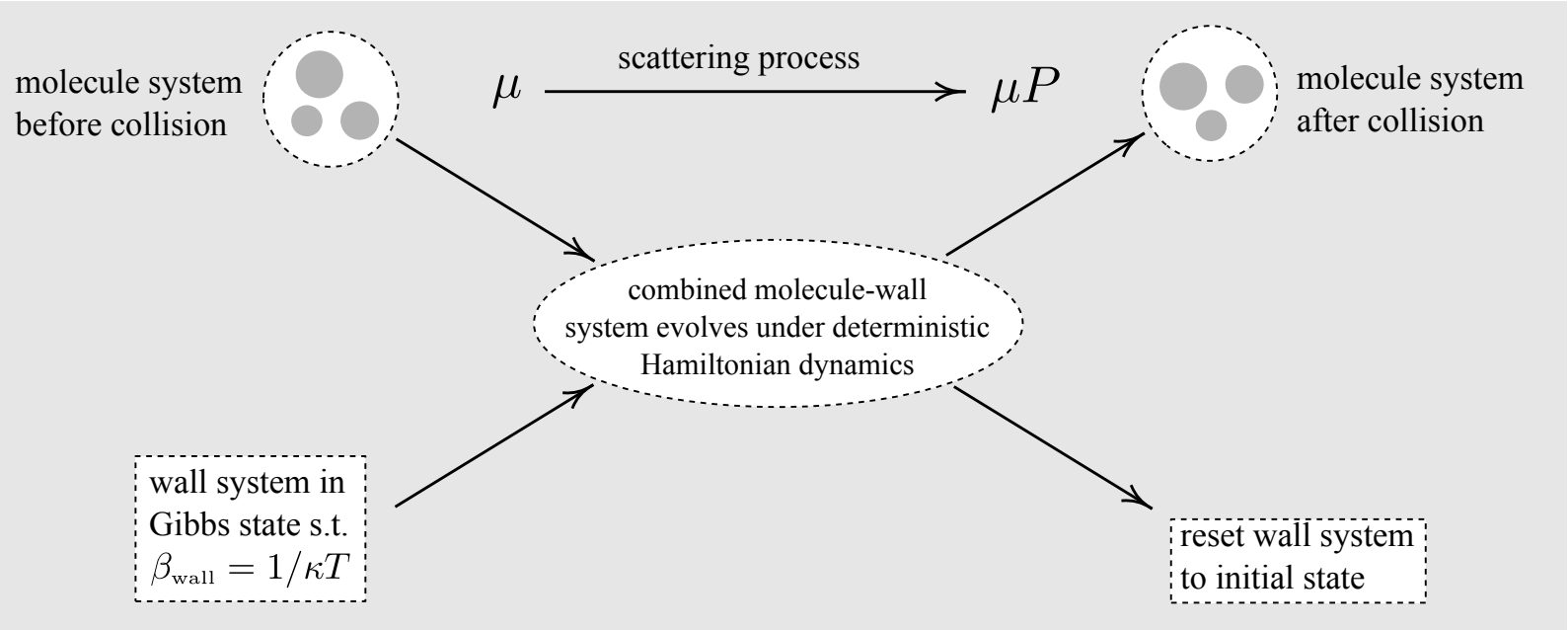


register velocity of molecule and reset state of wall-bound mass.

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_γ is operator on $L^2((0,\infty),\mu)$.

Theorem (Speed of convergence to thermal equilibrium)

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

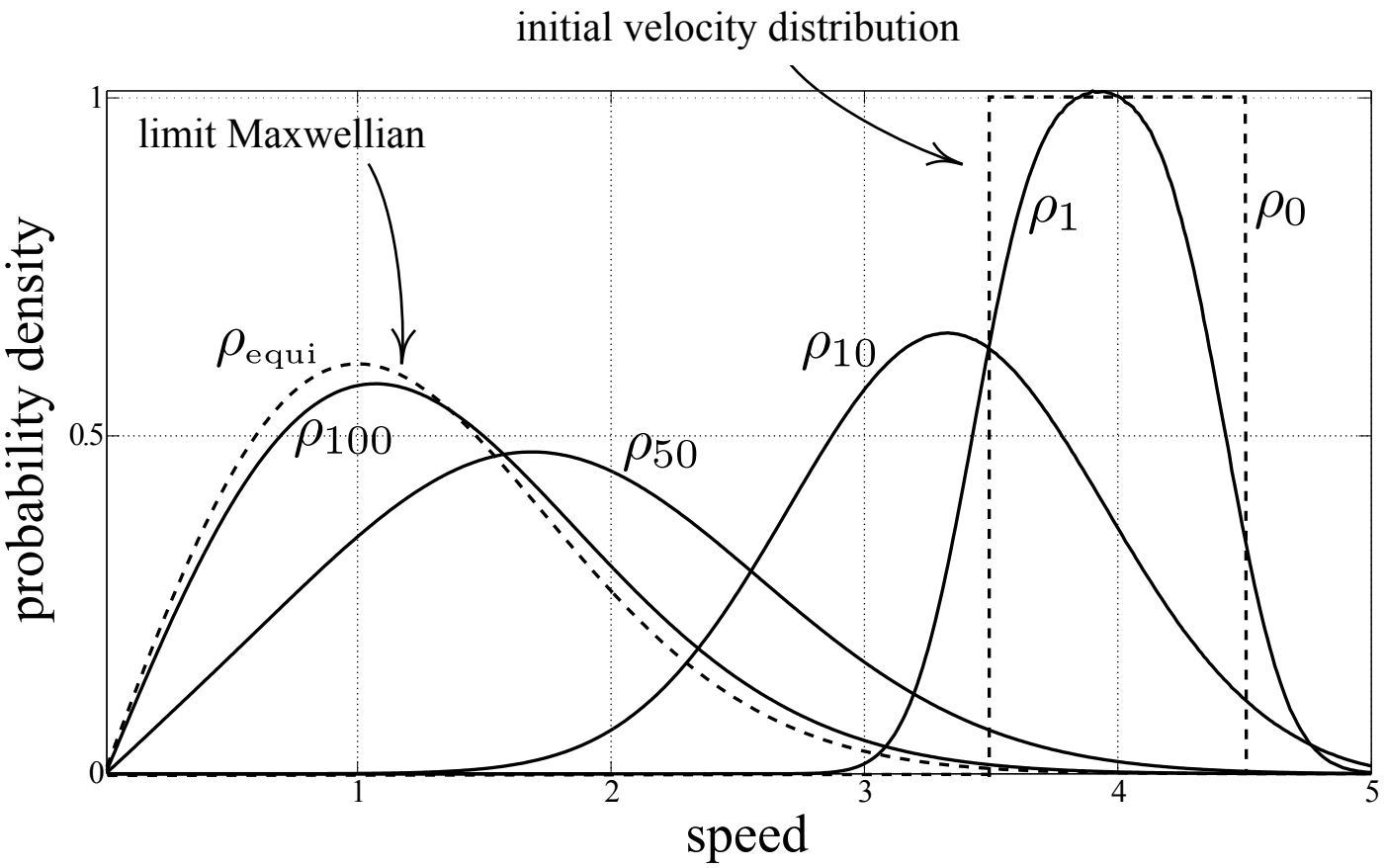
1. P_γ is a Hilbert-Schmidt; μ is the unique stationary distribution. Its density relative to Lebesgue measure on $(0,\infty)$ is

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

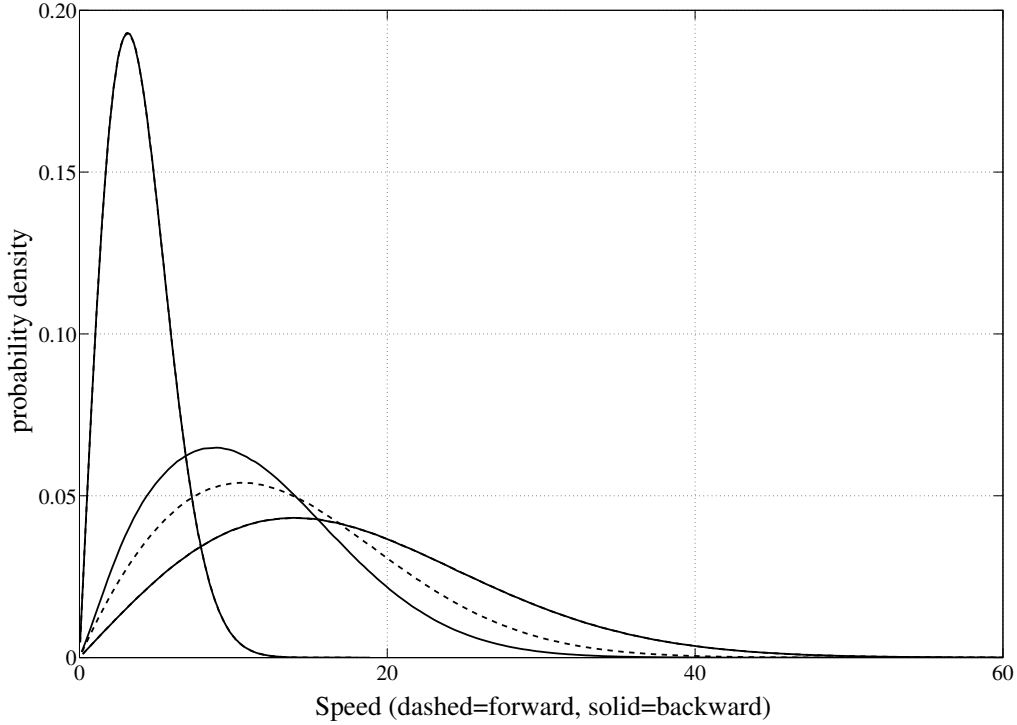
2. For arbitrary initial μ_0 and small γ

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

Approach to thermal equilibrium

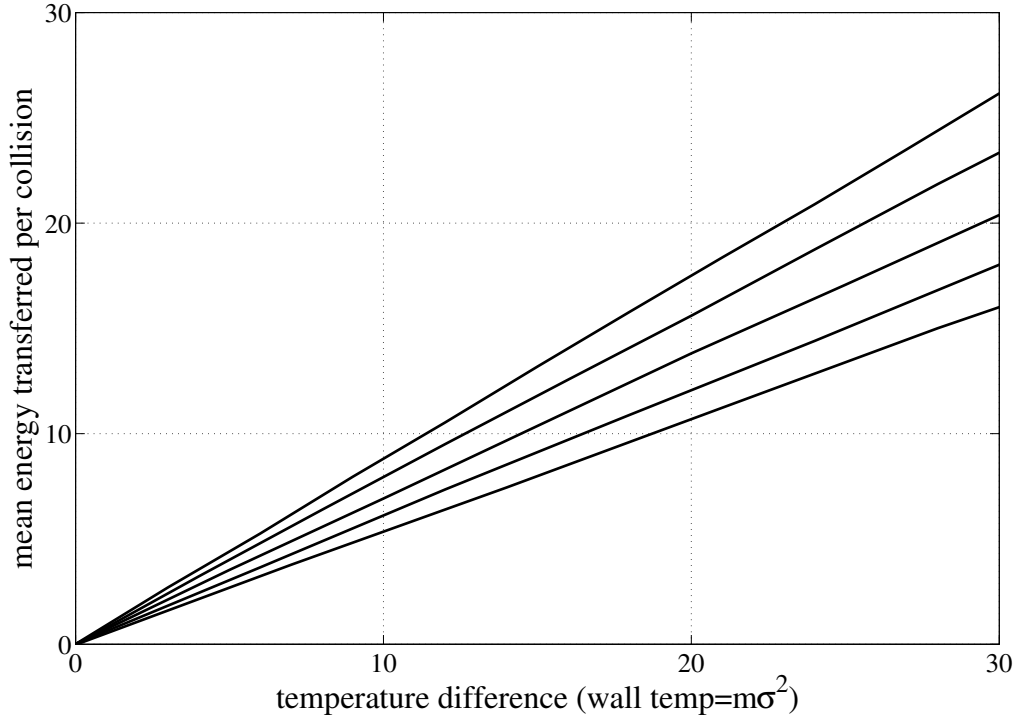


Heat flow



Molecule moves faster (on average) from hot to cold.

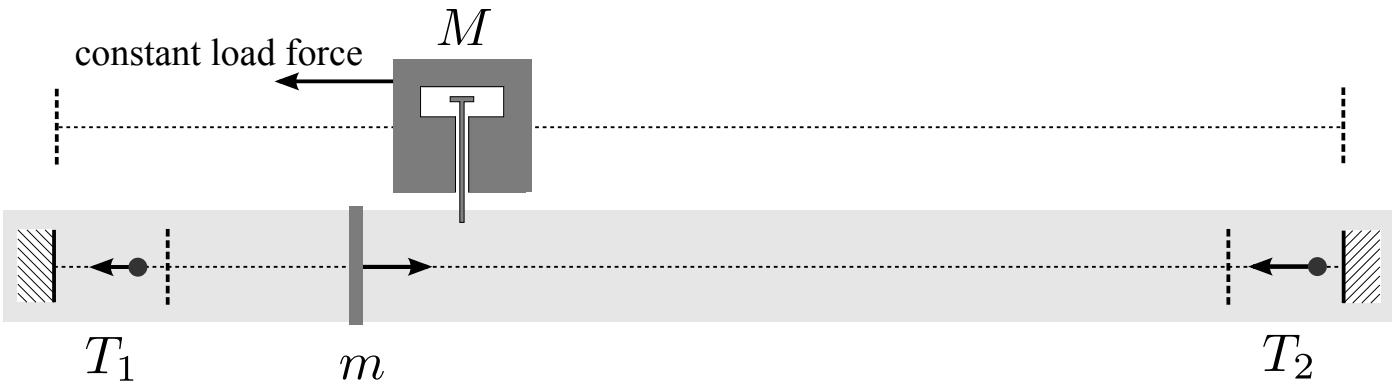
Heat flow and temperature difference



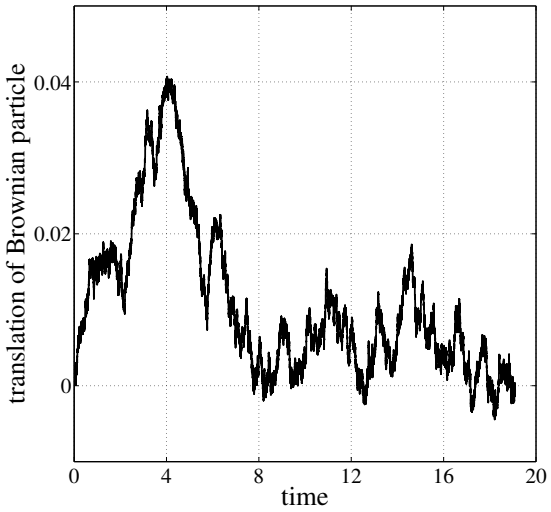
$$\text{Expected energy transfer per collision} = c(\gamma)(T_{\text{hot}} - T_{\text{cold}})$$

γ is the mass ratio.

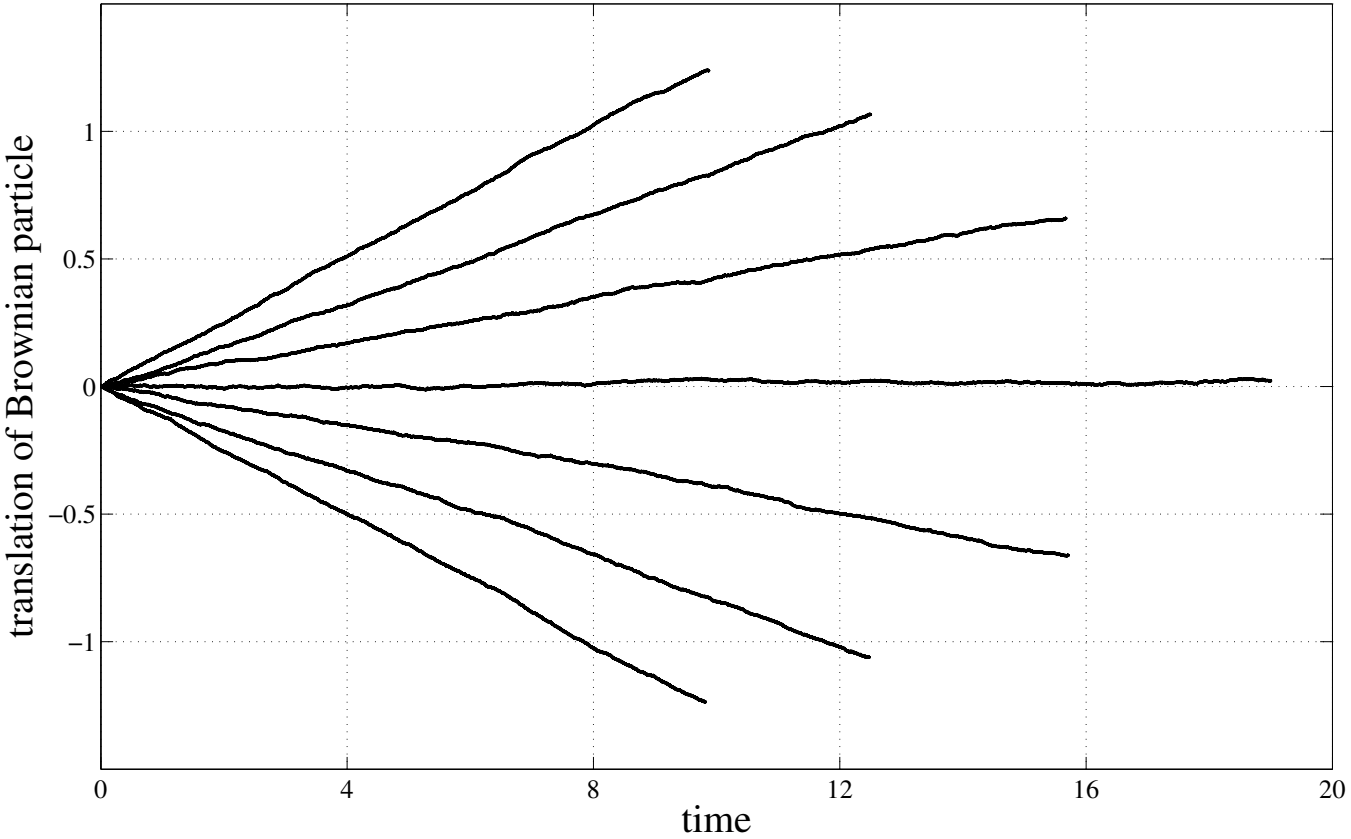
A billiard heat engine



$T_1 = T_2$ and 0 load $\Longrightarrow$ Brownian motion.

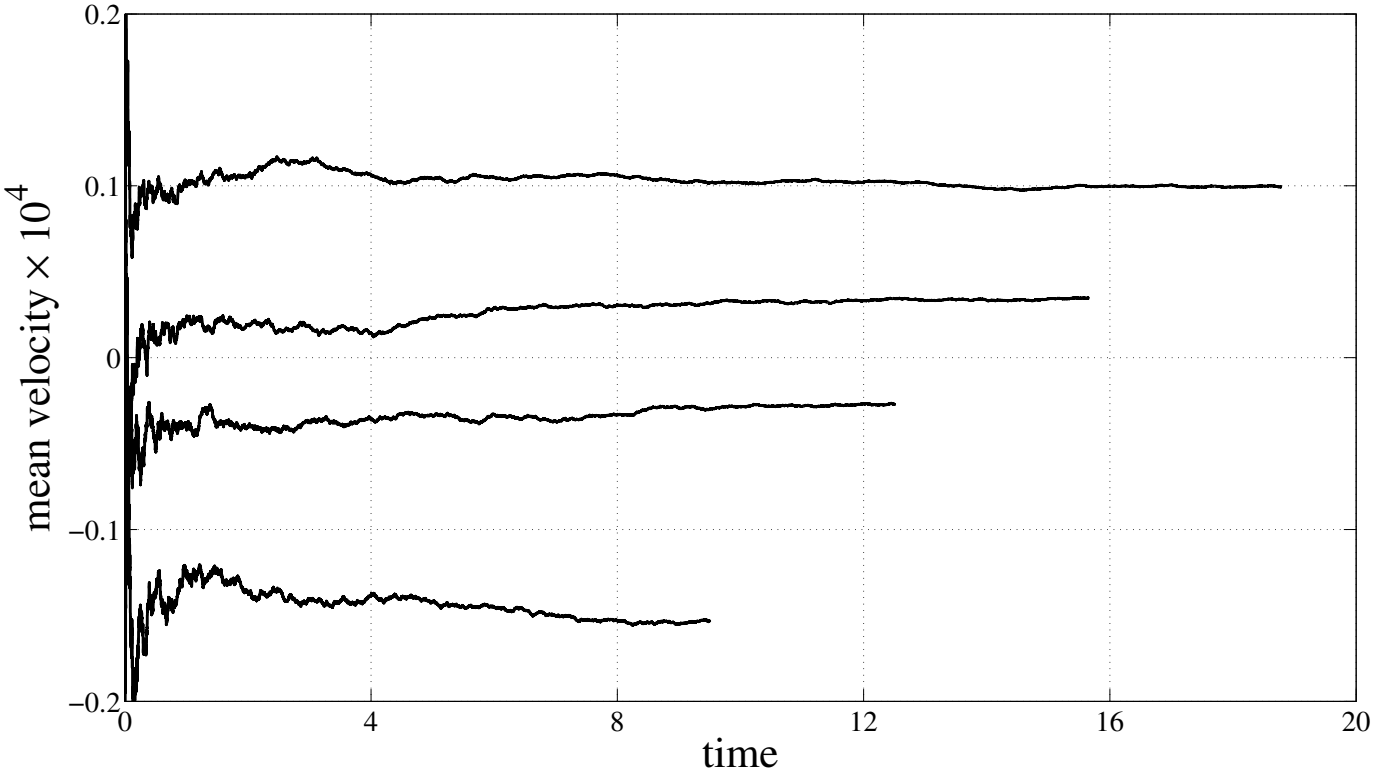


$T_1 \neq T_2 \Longrightarrow$ Rotation (0 load)



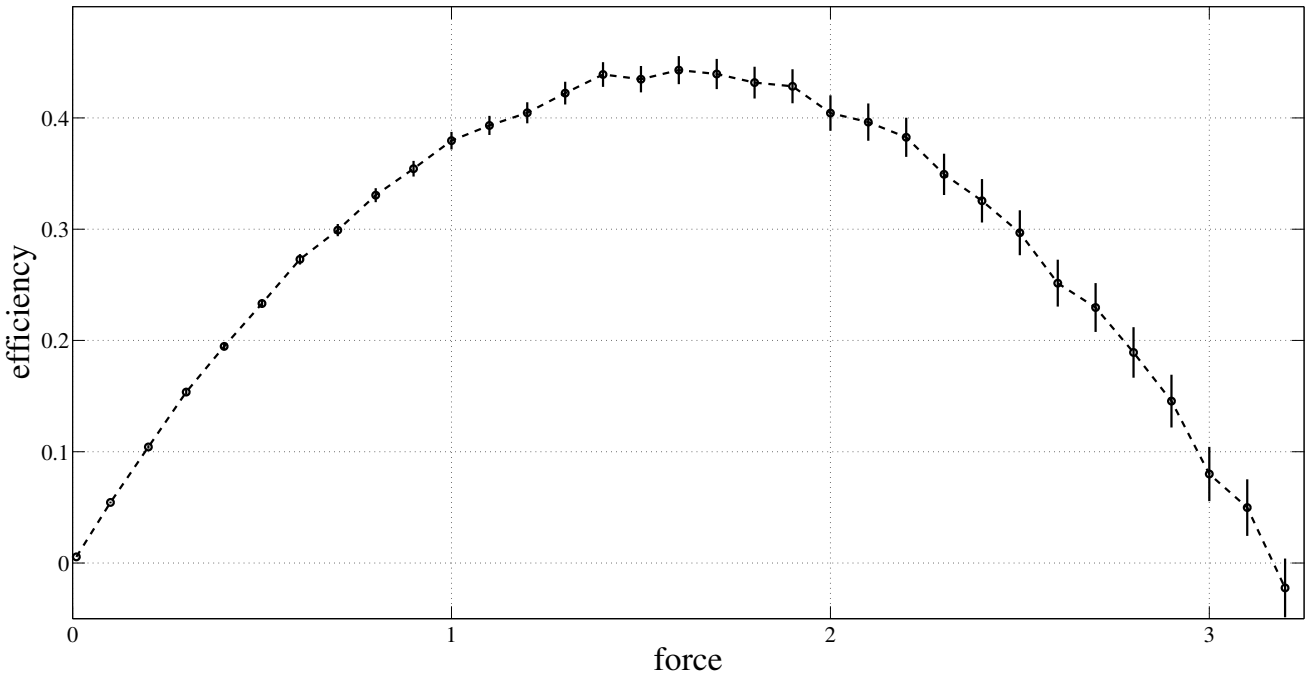
Stochastic motion with steady drift (rotation). No load force yet.

Mean rotation against load for $T_1 > T_2$



If $T_1 - T_2$ great enough, obtain rotation against load, producing positive work.

Efficiency

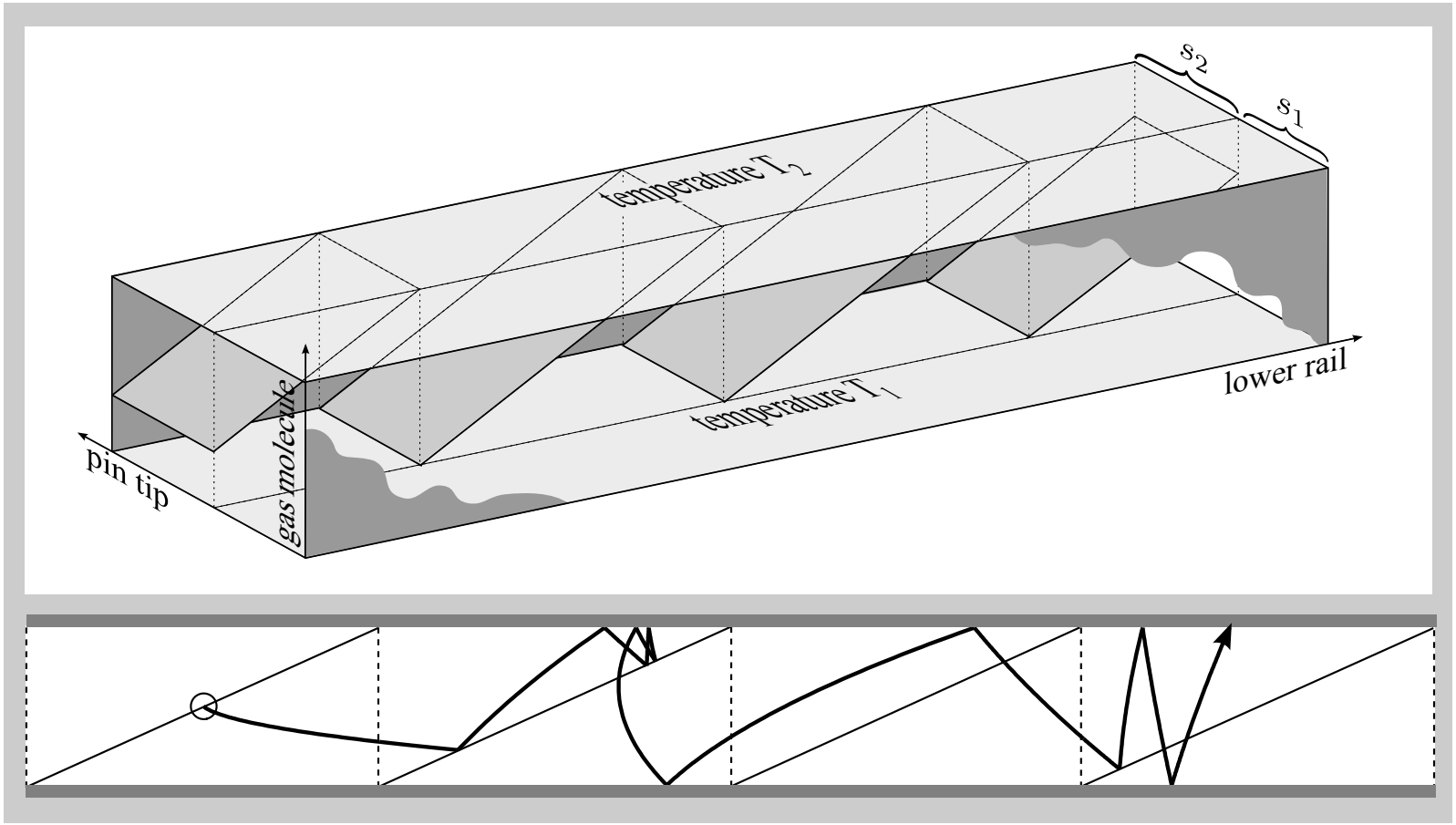


Efficiency = heat flow from hot wall/rate of work produced

Part II

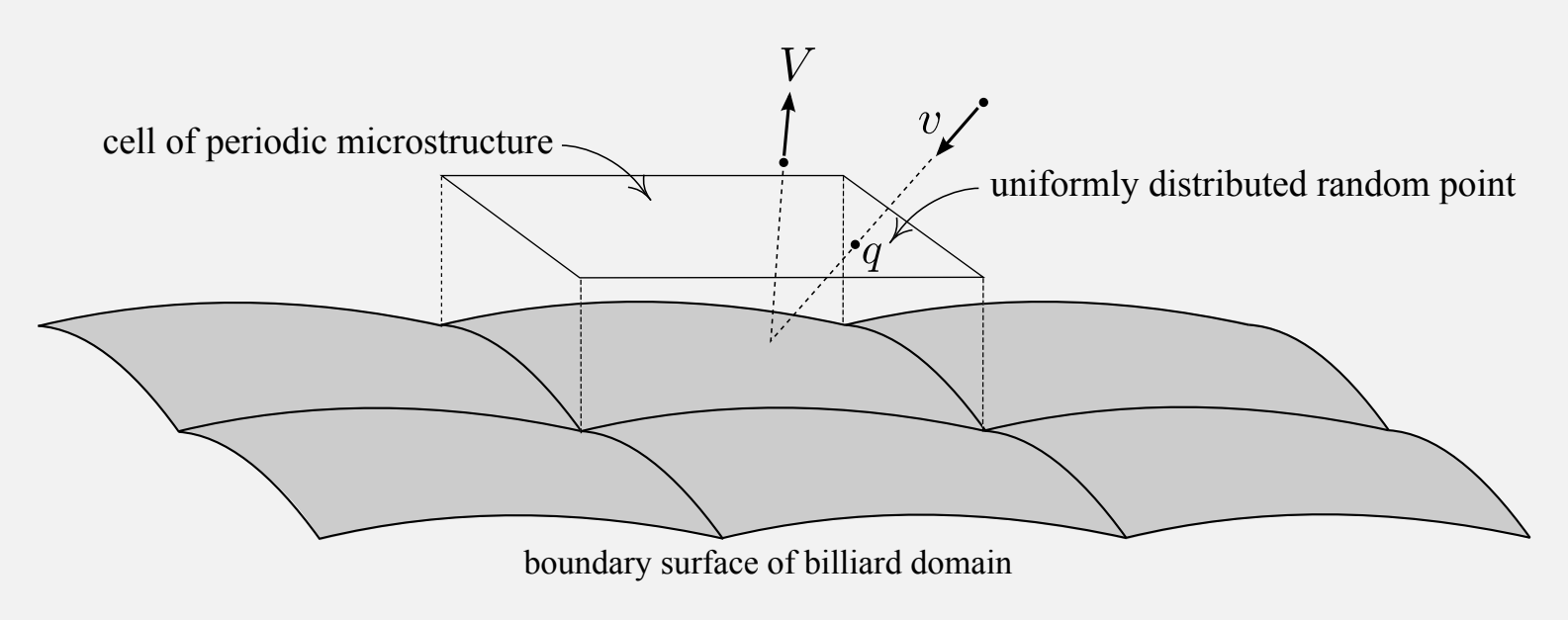
Diffusion in channels and transport coefficients

Engine motion: diffusion with drift in channels



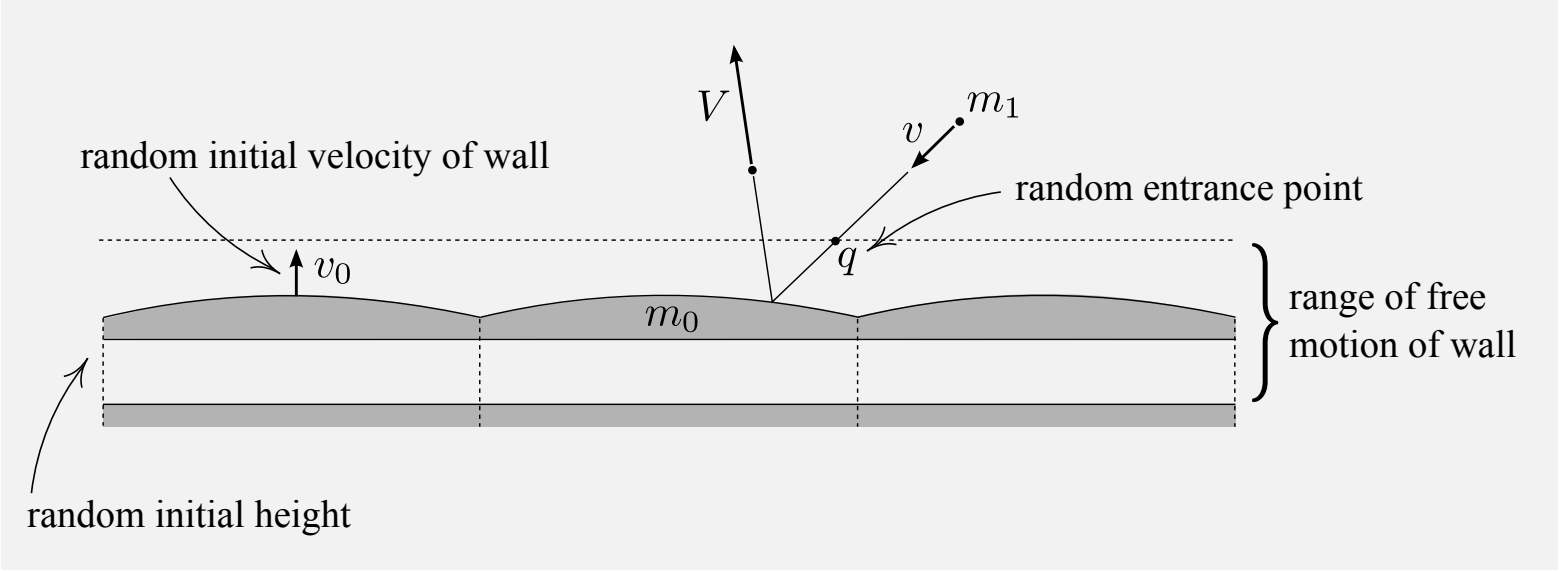
Engine's operation: motion in a 5-D configuration (channel) manifold.

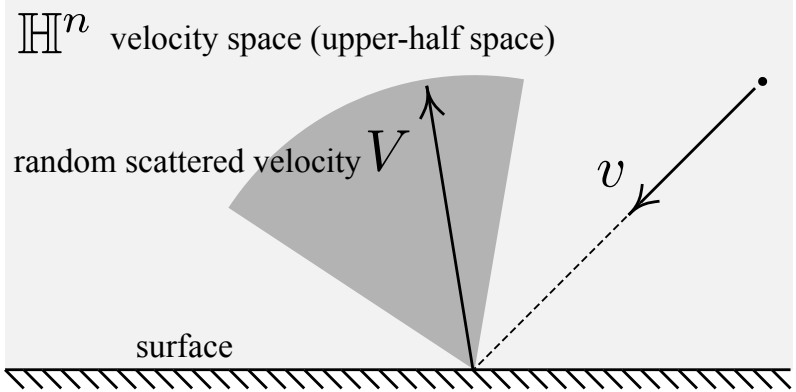
Random billiards as microstructures



$$(Pf)(v) = \mathbb{E}_v\left[f(V)\right]$$

Microstructures with moving parts





$$v \mapsto V$$

one step in Markov chain on velocity space

Requirements for a well-motivated P:

1. μ_β is a <u>stationary</u> distribution for the velocity Markov chain where

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

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

2. The stationary process defined by P and μ_β is <u>time reversible</u>:

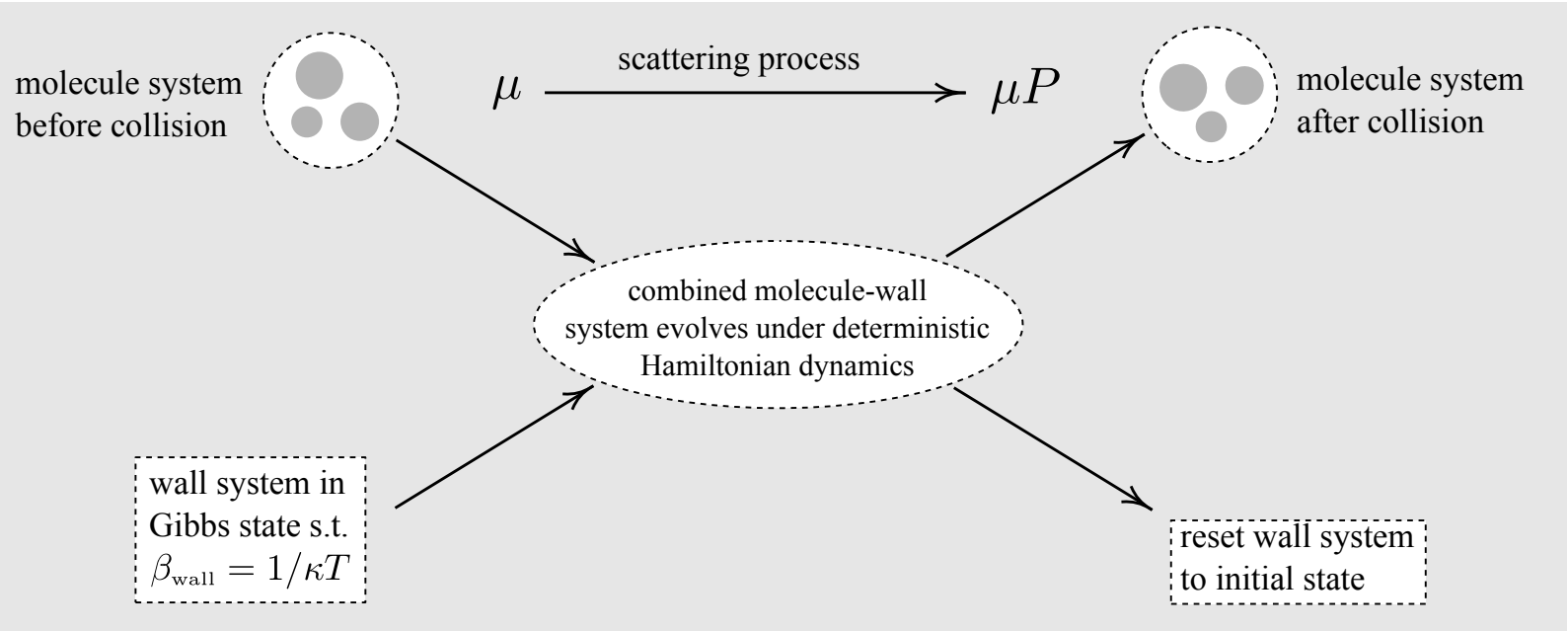
$$P(dV_2|V_1)d\mu_\beta(V_1) = P(dV_1|V_2)d\mu_\beta(V_2).$$

Definition

P will be called <u>natural</u> if it satisfies these properties.

The previous two examples are natural.

Deriving P from microstructure: general idea



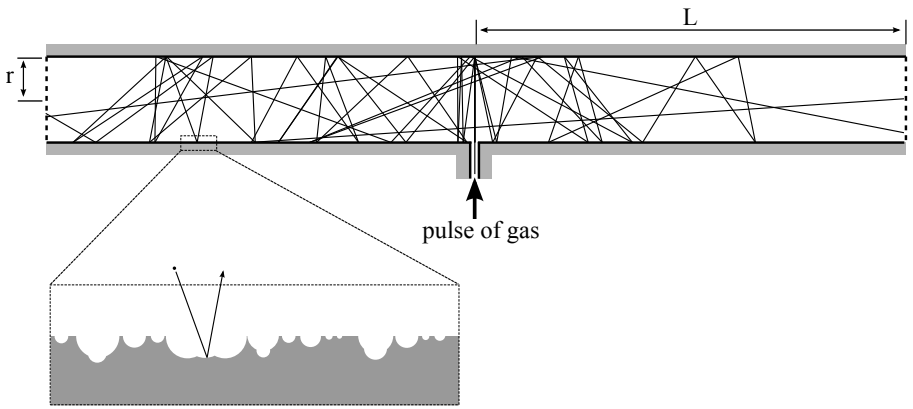
Theorem (Cook-F, Nonlinearity 2012)

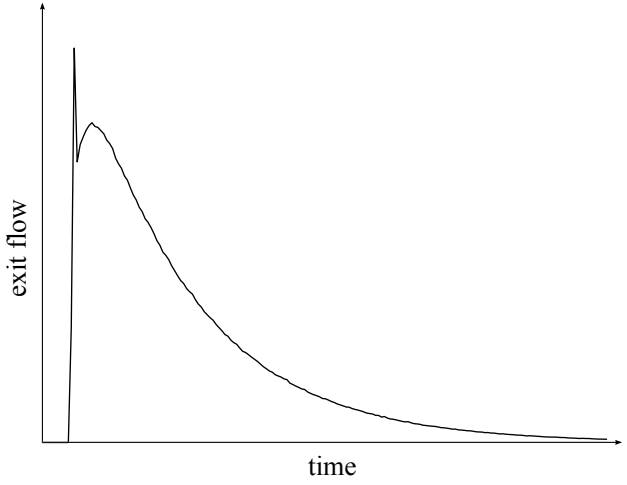
Resulting P is natural. The stationary distribution is given by Gibbs state of molecule system with same parameter β as the wall system.

Diffusion in (straight) channels

time-corrrelation and transport coefficients

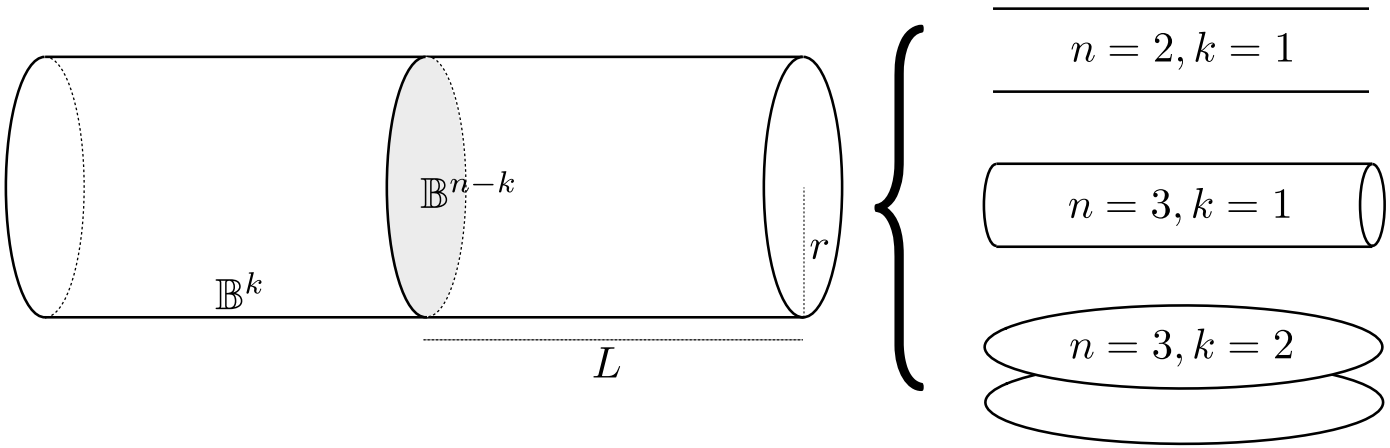
Idealized diffusion experiment. Channel inner surface has micro-structure.





How does the micro-structure influence diffusivity?

Cylindrical channels



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

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

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

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

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

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

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:

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

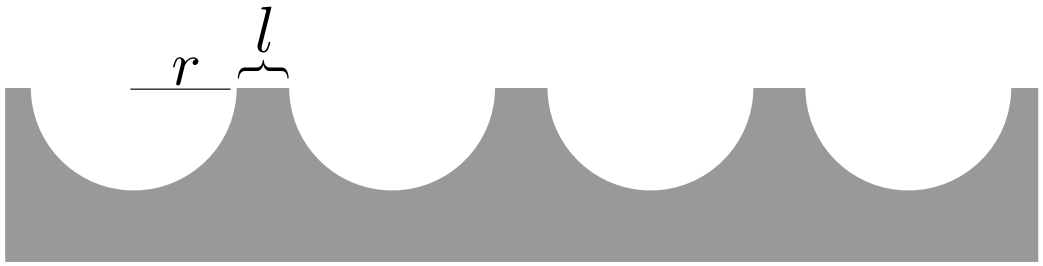
where $s_\beta = (n+1)/\beta M$ and M is particle mass. We are, therefore, interested in

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

a signature of the surface's scattering properties. (u is a unit vector in $\mathbb{R}^k$.)

Examples in 2-D (C. F. Z., Trans. AMS, 2014)

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



$$h = l/2r$$

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

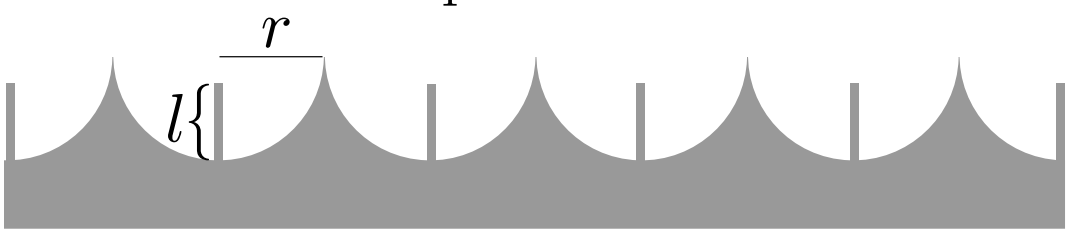
Top: $\mathcal{D}$ is <u>smaller</u> then in i.i.d. (perfectly diffusive) case.

Middle and bottom: $\mathcal{D}$ <u>increases</u> by adding flat top.

Examples in 2-D

Diffusivity can be discontinuous on geometric parameters:

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



Peculiar effects when $n - k = 1$

$$h = l/(l + 2r)$$

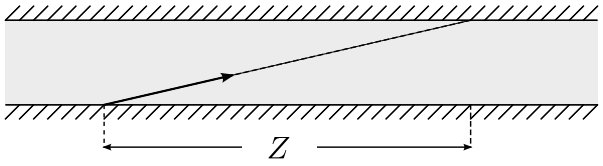
$$\eta(h) = \frac{1+\zeta_h}{1-\zeta_h} \qquad \zeta_h = -\frac{1+3h}{4}\,\frac{1-h}{1+h}\log\frac{3+h}{1-h}$$

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 μ_β $(0 < \beta \leq \infty)$.

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.

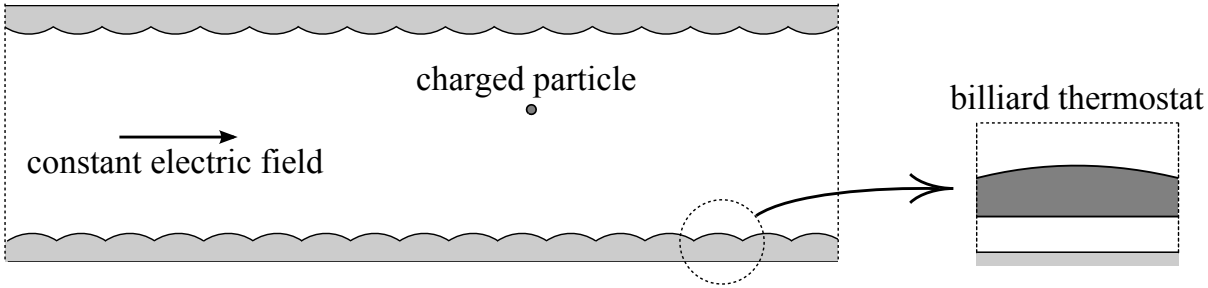


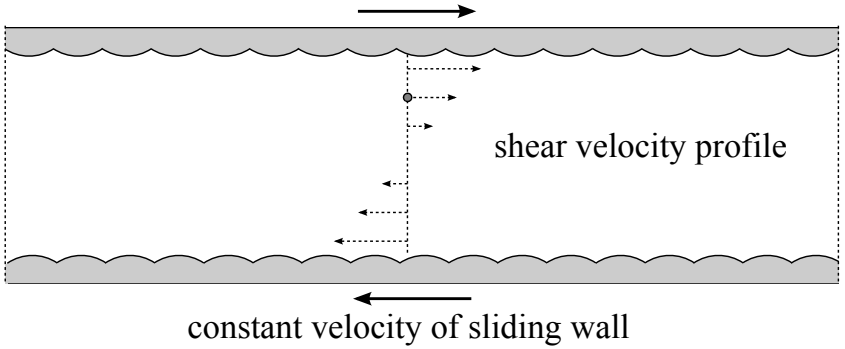
Let $\boxed{\Pi^u_Z(d\lambda) := \|Z^u\|^{-2}\langle Z^u, \Pi(d\lambda)Z^u\rangle}$, Π the spectral measure of P. Then

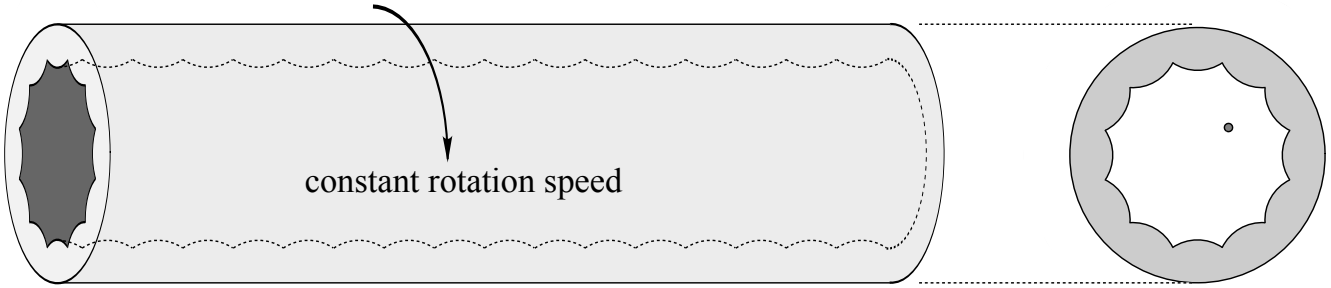
$$\boxed{\eta^u(P) = \int_{-1}^{1} \frac{1+\lambda}{1-\lambda}\Pi^u(d\lambda).}$$

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

Related systems

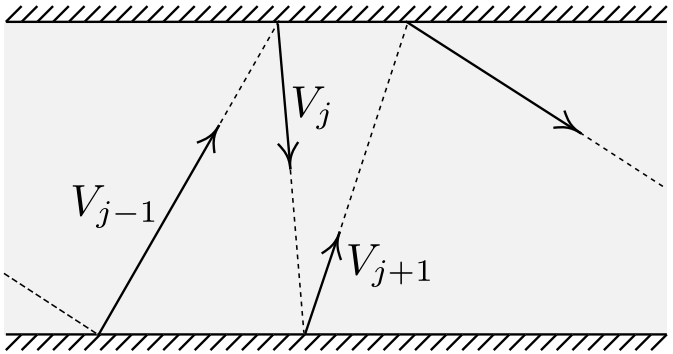




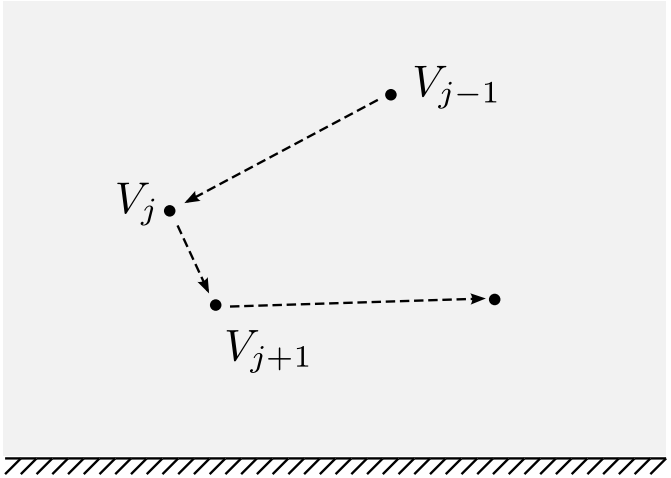


Remarks about diffusivity and spectrum

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



Random flight in channel



Random walk in velocity space $\mathbb{H}^n$

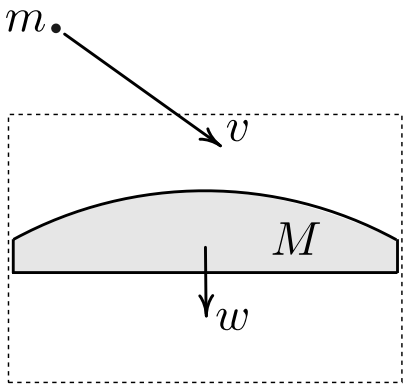
- $\mathcal{D}$ determined by rate of decay of time correlations (Green-Kubo relation)
- All the information needed for $\mathcal{D}$ is contained in the spectrum of P
- It is difficult to obtain detailed information about the spectrum of P; would like to find approximation more amenable to analysis.

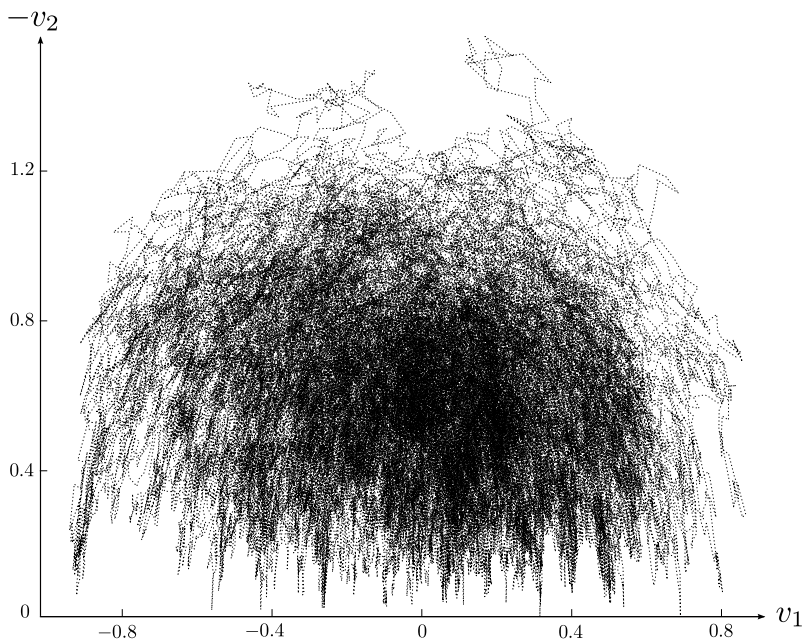
Part III

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

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

where MB stands for "Maxwell-Boltzmann."

Weak scattering and diffusion in velocity space

- Λ 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 $\Phi \in C_0^\infty(\mathbb{H}^m) \cap L^2(\mathbb{H}^m, \mu_\beta)$ (smooth, comp. supported) define

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

  where $e_m = (0, \ldots, 0, 1)$ and Φ_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 $\mathrm{Div}^{\mathrm{MB}}$ as the negative of the formal adjoint of $\mathrm{Grad}^{\mathrm{MB}}$.
- Maxwell-Boltzmann Laplacian: $\boxed{\mathcal{L}_{MB}\Phi = \mathrm{Div}^{\mathrm{MB}}\mathrm{Grad}^{\mathrm{MB}}\ \Phi}$.

Weak scattering limit

Theorem (F.-Ng-Zhang, Comm. Math. Phys. 2013)

Let μ 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. <u>self-adjoint</u>, <u>elliptic</u> on $C_0(\mathbb{H}^m) \cap L^2(\mathbb{H}^m, \mu_\beta)$.
- The limit $\mathcal{L}_{MB}\Phi = \lim_{h\to 0} \frac{P_h\Phi - \Phi}{h}$ holds uniformly for each $\Phi \in C_0^\infty(\mathbb{H}^m)$.
- The Markov chain defined by (P_h, μ_β) converges to an Itô diffusion with diffusion PDE

$$\frac{\partial \rho}{\partial t} = \mathcal{L}_{\mathrm{MB}}\rho$$

Example1: 1-D billiard thermostat

Proposition

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

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

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

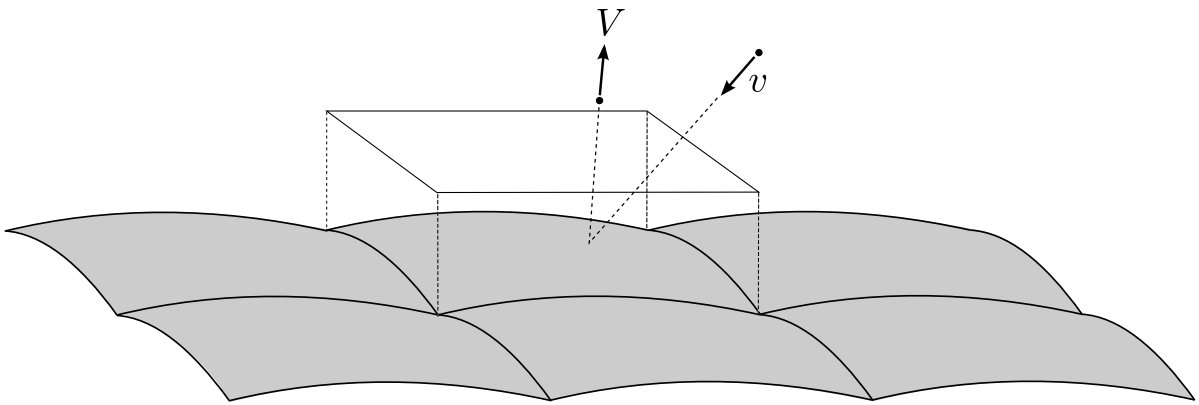
$$\mathcal{L}\varphi = \rho^{-1}\frac{d}{dv}\left(\rho\frac{d\varphi}{dv}\right),$$

which is a densily 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 Λ.

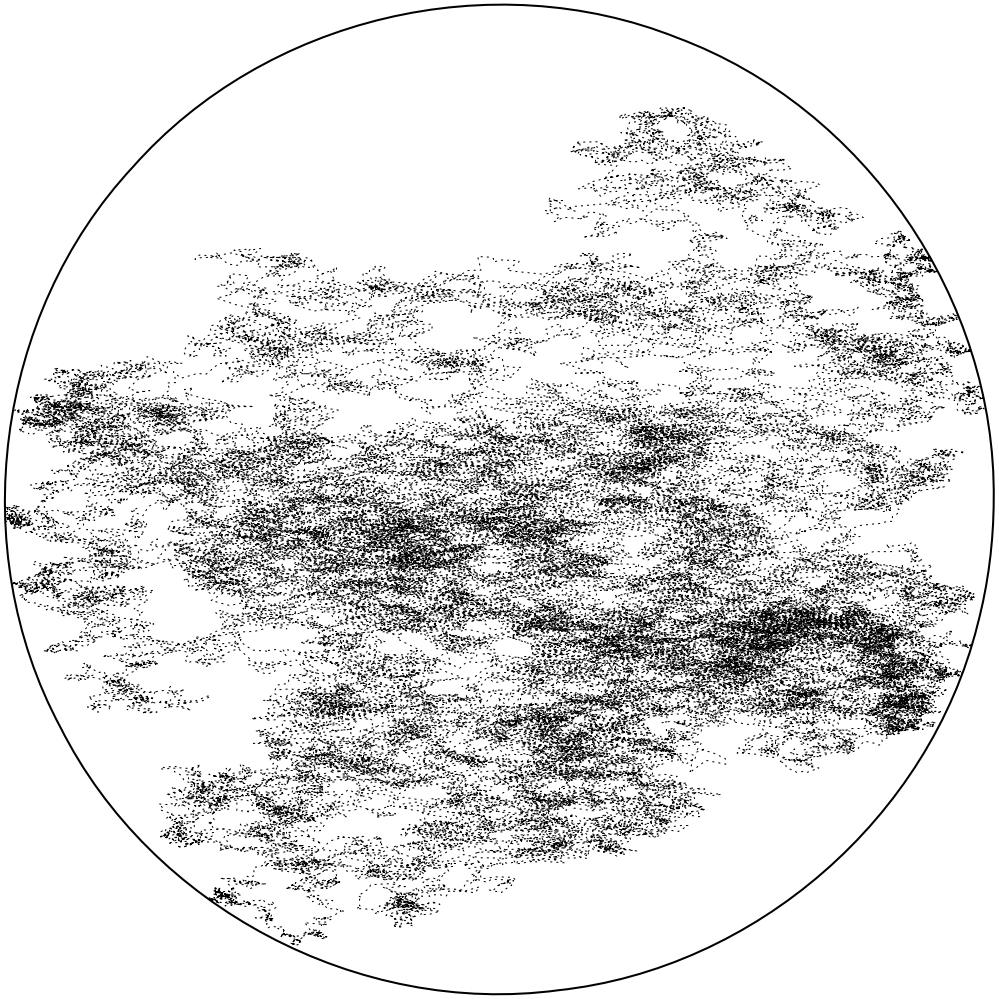


Proposition (Generalized Legendre operator in dim n)

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

$$(\mathcal{L}_{MB}\Phi)(v) = 2\sum_{i=1}^{n} \lambda_i \left(\left(1 - |v|^2\right)\Phi_i\right)_i$$

Sample path of Legendre diffusion



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