Random dynamical systems with microstructure

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- *Scott Cook* (Random billiards with Maxwellian limits)
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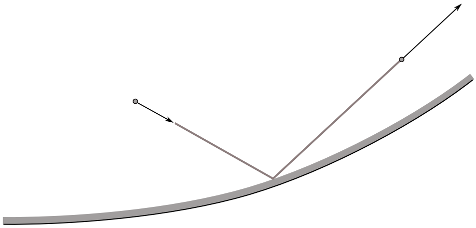
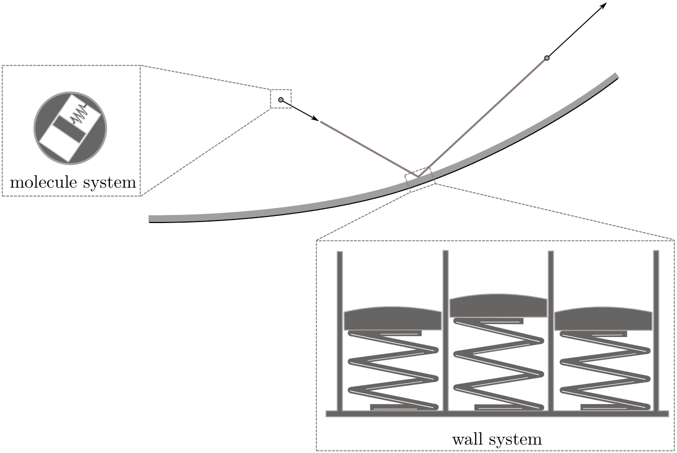
- *Hong-Kun Zhang* (Current work on most of these topics)

Plan of talk

- Billiards with random microstructure
  - Billiards: Hamiltonian flows on manifolds with boundary
  - Microstructure: geometric structure on the boundary
- The Markov operator
  - Derived from the random microstructure
  - Defines generalized billiard reflection
- Properties of the Markov operator
  - Stationary distributions
  - Spectral gap and moments of scattering
  - The billiard Laplacian
  - Conditioning
  - Case studies
- CLT and Diffusion



Random billiards with microstructure



Wall and molecule subsystems

- Configuration spaces: Riemannian manifolds with corners

$$M_{\text{wall}},\ M_{\text{mol}} := \overline{M}_{\text{mol}} \times \mathbb{R} \times \mathbb{T}^k$$

and potential functions:

  - $U_{\text{wall}} : M_{\text{wall}} \to \mathbb{R}$
  - $U_{\text{Mol}} : \overline{M}_{\text{mol}} \to \mathbb{R}$

- The total system has configuration space M and potential

$$U : M \to \mathbb{R}.$$

- When subsystems sufficiently far away, $M \cong M_{\text{wall}} \times M_{\text{mol}}$ and

$$U = U_{\text{wall}} + U_{\text{mol}}.$$

- Outside of product region = interaction zone. Motion:

$$\frac{\nabla c'(t)}{dt} = -\text{grad}_{c(t)} U$$

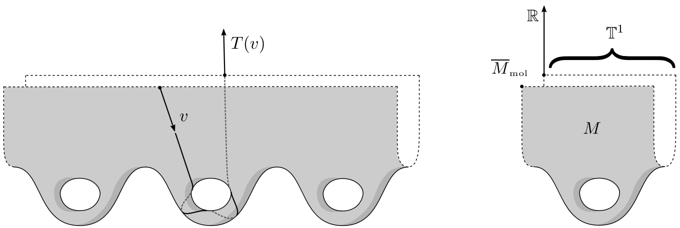
with specular collisions at boundary.

Interaction region (microscopic): definitions

- $S := \overline{M}_{\text{mol}} \times \{0\} \times \mathbb{T}^k \times M_{\text{wall}}$ boundary of inter. zone;
- $E(q,v) := \frac{1}{2}\|v\|_q^2 + U(q)$ energy function on $N := TM$;
- $N_S := T_S M$, $N(\mathcal{E}) := E^{-1}(\mathcal{E})$, $N_S(\mathcal{E}) := N_S \cap N(\mathcal{E})$;
- $\theta_v(\xi) := \langle v, d\tau_v \xi \rangle$ contact form on N;
- $d\theta$ symplectic form on N;
- X^E Hamiltonian vector field: $X^E \lrcorner\, d\theta = -dE$;
- $\eta := (\text{grad } E)/\|\text{grad } E\|^2$ (in Sasaki metric on N);
- $\Omega := (d\theta)^m$ Liouville volume form on N;
- $\Omega^E := \eta \lrcorner\, \Omega$ flow invariant volume on energy surfaces;
- $T : N_S \to N_S$ the return (billiard) map to S.

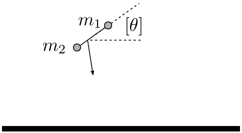
Geodesic flow example (M_{wall} trivial)

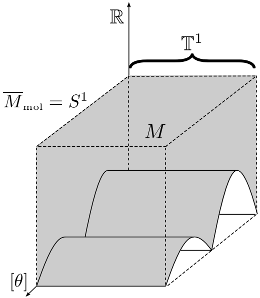
- M_{wall} = single point
- $\overline{M}_{\text{mol}} = \{0, 1\}$
- $M_{\text{mol}} := \{0, 1\} \times \mathbb{R} \times \mathbb{T}^1$
- $S = \{0, 1\} \times \{0\} \times \mathbb{T}^1$
- Potentials are constant



Example: a dumbbell molecule

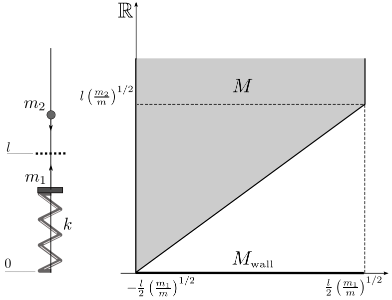
- M_{wall} = single point
- $\overline{M}_{\text{mol}} = SO(2)$
- $M_{\text{mol}} := SO(2) \times \mathbb{R} \times \mathbb{T}^1$
- $S = SO(2) \times \{0\} \times \mathbb{T}^1$
- Potentials are constant





Example with potential ($\overline{M}_{\text{mol}}$ trivial)

Coordinates: $x = \sqrt{m_1/m}\,(x_1 - l/2),\ y = \sqrt{m_2/m}\,x_2.$



$$E(x, y, \dot{x}, \dot{y}) = \frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \frac{k}{m_1}x^2\right).$$

- $B :=$ billiard table: Riemannian manifold with boundary;
- $F(\partial B)$ orthonormal frame bundle with group $O(k)$;
- $N_{\text{wall}} := TM_{\text{wall}}$ state space of wall system;
- $\mathcal{V} := \mathcal{P}(O(k) \times N_{\text{wall}})$ space of probability measures;
- $\mathcal{V}$ is naturally an $O(k)$-space.

Random microstructure on ∂B: $O(k)$-equivariant map

$$\mathcal{G} : F(\partial B) \to \mathcal{P}(O(k) \times N_{\text{wall}}).$$

Example: $\mathcal{G} = (\xi, \zeta)$ constant, where $\xi \in \mathcal{P}(O(k))$ is rotation invariant and ζ is Gibbs canonical distribution.

Gibbs canonical distribution at temperature T

An invariant volume form on N_{wall} of physical significance:

$$\zeta := \frac{e^{-\beta E}}{Z(\beta)} \Omega^E_{\text{wall}} \wedge dE$$

where $\beta = 1/\kappa T$. (κ = Boltzmann constant.) Density ρ is obtained by maximizing Boltzmann entropy:

$$\mathcal{H}(\rho) := -\int_{N_{\text{wall}}} \rho \log \rho \, \Omega_{\text{wall}}$$

under constraint $\int_{N_{\text{wall}}} E \rho \, \Omega_{\text{wall}} = \mathcal{E}_0$. ($\beta$ = Lagrange multiplier.)
Maximal uncertainty about state given mean value of E.

The Markov operator P of a microstructure

- $\mathbb{H}$:= half-space in dimension $k+1$;
- $N^+_{\mathrm{mol}} := T\overline{M}_{\mathrm{mol}} \times \mathbb{H}$;
- $\pi : N^+_S := N^+_{\mathrm{mol}} \times \mathbb{T}^k \times M_{\mathrm{wall}} \to N^+_{\mathrm{mol}}$ projection to first factor;
- $\lambda \in \mathcal{P}(\mathbb{T}^k)$ Lebesgue;
- $\zeta \in \mathcal{P}(N_{\mathrm{wall}})$ a fixed probability (say, the Gibbs measure);
- $T : N^+_S \to N^+_S$ the return map.

Define the map $P : \mathcal{P}(N^+_{\mathrm{mol}}) \to \mathcal{P}(N^+_{\mathrm{mol}})$, by

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

Markov chains (dynamics under partial state info)

no knowledge of state along fiber

$$\begin{array}{ccc} M & \xrightarrow{T} & M \\ \pi\downarrow & & \downarrow\pi \\ V & \longrightarrow & V \end{array}$$

random map

states manifold

$v \mapsto \eta_v$

probability measure on $\pi^{-1}(v)$

observable states (probability measures on V)

Random dynamics on V:

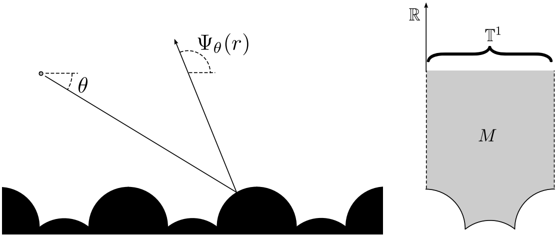
$$\mu \mapsto \mu P := (\pi \circ T)_* \mu \circ \eta$$

Standard finite state Markov chains with **detailed balance**: M is a groupoid, V is the set of units, T is the inverse operation, $v \mapsto \eta_v$ are the transition probabilities, and $\mu \circ \eta$ is T-invariant.

Example of P (constant speed)

Transition probabilities operator:

$$(Pf)(\theta) = \int_0^1 f(\Psi_\theta(r))\, dr.$$



Surface microstructure defined by a billiard table contour. The coordinate r is random (uniform between 0 and 1).

Stationary distributions

Definition: $\mu \in \mathcal{P}(N^+_{\text{mol}})$ is **stationary** if $\mu P = \mu$.

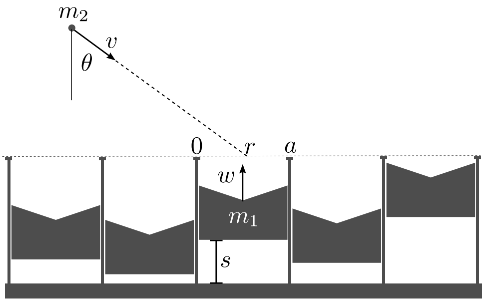
Theorem

Let $P : \mathcal{P}(N^+_{mol}) \to \mathcal{P}(N^+_{mol})$ be the Markov operator associated to the Gibbs canonical distribution on N_{wall} with temperature parameter β. Then the Gibbs canonical distribution on N^+_{mol} with the same parameter β is stationary.

Proof.

Use $e^{-\beta(E_{\text{mol}}+E_{\text{wall}})} = e^{-\beta E_{\text{mol}}} e^{-\beta E_{\text{wall}}}$ and invariance of the symplectic volume form on $N_S(\mathcal{E})$ under the return map T. □

Example: Let $Ce^{-\frac{\beta}{2}m_1 w^2}\,dw\,ds$ be fixed state of wall



- Equilibrium state of molecule: $d\mu(v) = C\cos\theta |v|^2 e^{-\frac{\beta}{2}m_2|v|^2}\,d\theta\,d|v|$
- If no moving parts (fixed speed $|v| = 1$): $d\mu(\theta) = \frac{1}{2}\cos\theta\,d\theta$.
- No dependence on shapes.

The operator P on functions

Define action of P on functions by $\nu(Pf) = (\nu P)(f)$.

Definition

The molecule-wall system is *symmetric* if there are volume preserving automorphisms $\widetilde{J}$ and $\widetilde{K}$ of N_S^+ that:

- respect the product $N_S^+ = N_{\mathrm{mol}}^+ \times N_{\mathrm{wall}}$;
- induce the same map J on N_{mol}^+;
- $\widetilde{J} \circ T = T^{-1} \circ \widetilde{J}$ (time reversibility)
- $\widetilde{K} \circ T = T \circ \widetilde{K}$ (symmetry).

Let μ be the stationary measure and $H := L^2(N_{\mathrm{mol}}^+, \mu)$.

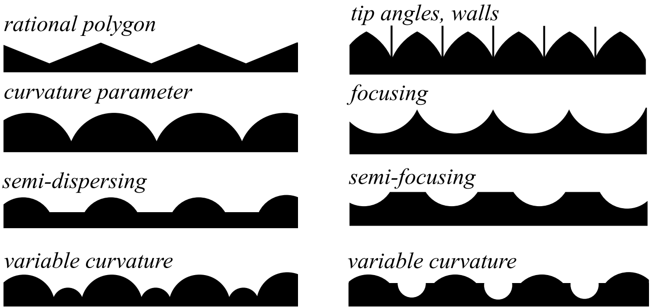
Theorem

If system is symmetric, P is a self-adjoint operator on H of norm 1.

The symmetry condition **essentially always holds.** Typically, we find in the examples that P is a **Hilbert-Schmidt operator.**

Problem: relate structural features and spectrum of P

For example, in purely geometric settings (no moving parts on the wall, no potentials) want to relate shape and spectrum.

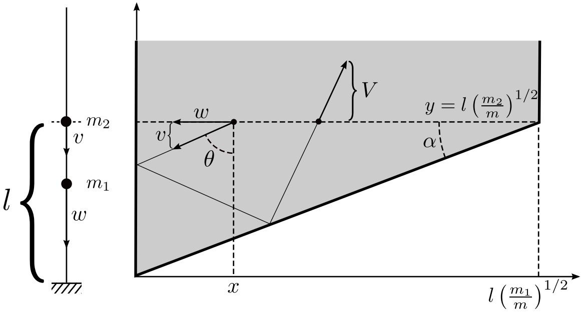


Of special interest: spectral gap.

Case studies (analytical and numerical)

- A simple two masses system;
- Adding a quadratic potential;
- Billiard systems with no energy exchange;
- The method of conditioning;
- Moments of scattering and spectral gap;
- Systems with weak scattering and the billiard Laplacian.

A simple two-masses system - I



Main system parameter: $\gamma := \sqrt{\frac{m_2}{m_1}} = \tan\alpha$.

A simple two-masses system - II

Define: $x = \sqrt{\frac{m_1}{m}}\,x_1$, $w := \sqrt{\frac{m_1}{m}}\,v_1$, $d\zeta(w) := C\exp\left(-\frac{1}{2}w^2/\sigma^2\right)dw\,dx$;

Theorem

- *P has a unique stationary distribution μ on $(0,\infty)$, given by*

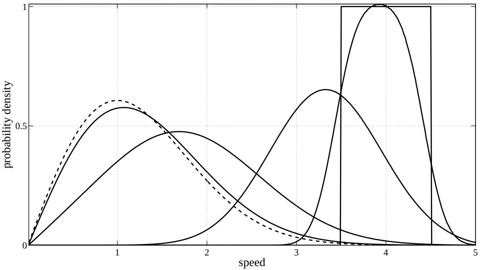
$$d\mu(v) = \sigma^{-2} v \exp\left(-\frac{v^2}{2\sigma^2}\right) dv.$$

- *P is a Hilbert-Schmidt operator on $L^2((0,\infty),\mu)$ of norm 1;*
- *$\eta P^n \to \mu$ exponentially in TV-norm for all initial η.*
- *If ϕ is C^3 on $(0,\infty)$, then*

$$(\mathfrak{L}\phi)(z) := \lim_{\gamma\to 0}\frac{(P_\gamma\varphi)(z) - \varphi(z)}{2\gamma^2} = \left(\frac{1}{z} - z\right)\varphi'(z) + \varphi''(z)$$

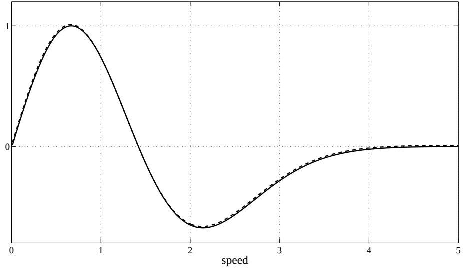
holds for all $z > 0$.

A simple two-masses system - III



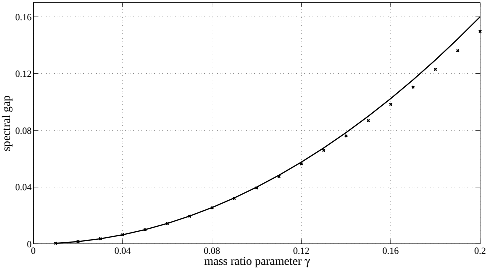
Evolution of an initial probability measure, μ_0, having a step function density. The graph in dashed line is the limit density $v \exp(-v^2/2)$ and the other graphs, from right to left, are the densities of $\mu_0 P^n$ at steps $n = 1, 10, 50, 100$. Here $m_1/m_2 = 100$.

A simple two-masses system - IV



Comparison of the second eigendensity of P (numerical) and the second eigendensity of the billiard Laplacian $\mathcal{L}$: $(1 - z^2/2)\rho(z)$. Used $\gamma = 0.1$; the numerical value for the second eigenvalue of P was found to be 0.9606, to be compared with $1 + 2\gamma^2(-2) = 0.9600$ derived from eigenvalue -2 of $\mathcal{L}$.

A simple two-masses system - V

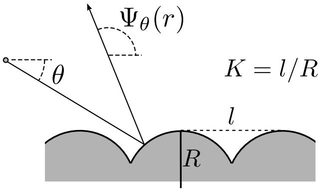


Asymptotics of the spectral gap of P for small values of the mass-ratio parameter γ. The discrete points are the values of the gap obtained numerically. The solid curve is the graph of $f(\gamma) = 4\gamma^2$, suggested by comparison with $\mathcal{L}$.

- $d\mu(\theta) = \frac{1}{2}\sin\theta\, d\theta$ and $H = L^2([0,\pi], \mu)$;
- P_K = the Markov operator for bumps with curvature K.

Theorem

- *P_K is a self-adjoint, compact operator on H of norm 1;*
- *For small K, the spectral gap of P_K is $g(K) = \frac{1}{3}K^2 + O(K^3)$;*



$$(P_K f)(\theta) = \frac{1}{l}\int_0^l f(\Psi_\theta(x))\, dx$$

The billiard Laplacian

The (reduced) billiard map is an area-preserving map

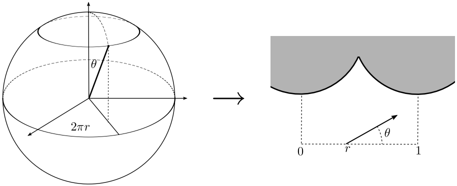
$$T : S^2 \to S^2.$$

Regard P_K as defined on $L^2(S^2, A)$. Let Δ be the spherical Laplacian.

Theorem

Let Φ be a compactly supported smooth function on $S^2 \setminus \{N, S\}$ invariant under rotations about the z-axis in $\mathbb{R}^3$. Then

$$P_K \Phi - \Phi = \frac{K^2}{6} \Delta \Phi + \mathcal{O}(K^3).$$



Moments of scattering for bumps family

- Define the *jth moment of scattering*

$$\mathcal{E}_j(\theta) = E_\theta\left[(\Theta - \theta)^j\right]$$

where Θ is the random post-collision angle given θ.

- and $P\Phi - \Phi = \sum_{j=1}^{n} \frac{\Phi^{(n)}}{n!}\mathcal{E}_j + \mathcal{O}(\mathcal{E}_{n+1})$ if Φ smooth.

Proposition

If $\sin\theta > 3K/2$ *(middle range of angles), the moments satisfy:*

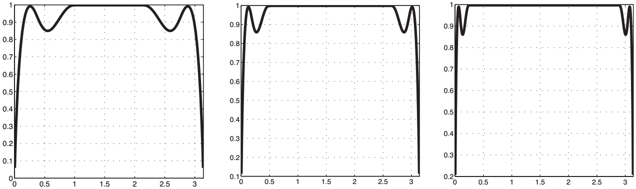
- *If* n *is odd,* $\mathcal{E}_n(\theta) = \frac{K^{n+1}}{2(n+2)}\cot\theta + \mathcal{O}(K^{n+3})$;
- *If* n *is even,* $\mathcal{E}_n(\theta) = \frac{K^n}{n+1} + \mathcal{O}(K^{n+2})$.

It follows that

$$\frac{P_K\Phi - \Phi}{\frac{1}{3}K^2} = \frac{1}{2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Phi}{d\theta}\right) + \mathcal{O}(K)$$

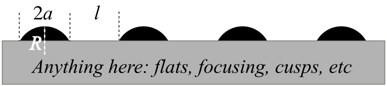
$\mathcal{E}_2(\theta)/\gamma_K$ for $K = 2/3, 1/3, 1/6$

$E(\Theta_K - \theta)^2/(\text{spectral gap}) \to 1$ (constant function)



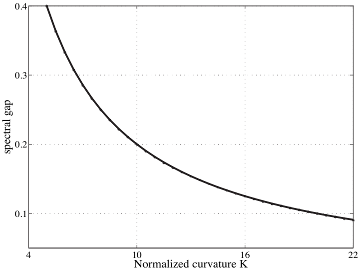
This gives an asymptotic interpretation of the spectral gap as the **mean square deviation from specularity.**

General bumps family, big K

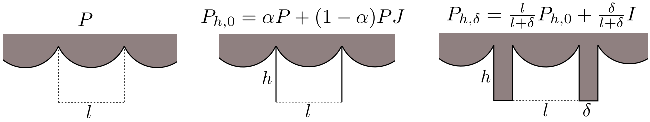


Theorem

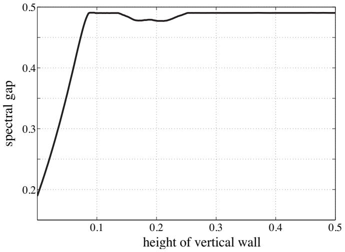
For the general bumps family P is quasi-compact.



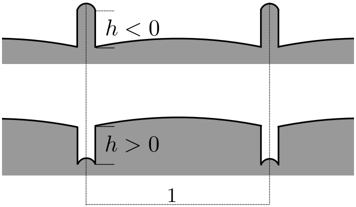
The solid line is the graph of $2/K$ and the values marked with an asterisk are numerically obtained.

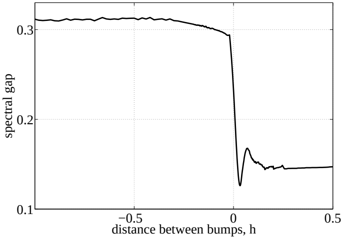


Wall does not affect J-even eigenvalues, but brings J-odd eigenvalues closer to 0.



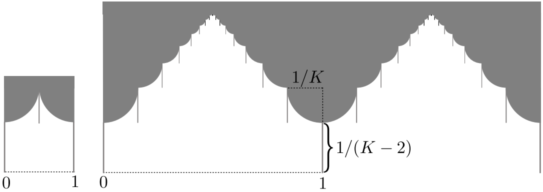
More complicated shapes





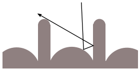
P does not specify shape (up to homothety)

Two billiard cells with the same Markov operator:

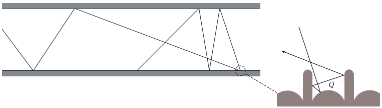


Gas transport in channels - 3 levels of description

- Microscopic model (deterministic motion)



- Random flight in channel (Markov process on set of directions)



- Diffusion limit: gas concentration $u(x,t)$ along $\mathbb{R}$ should satisfy

$$\frac{\partial u}{\partial t} = \mathcal{D}\frac{\partial^2 u}{\partial x^2}$$

Relate: (1) microstructure, (2) spectrum of P, (3) diffusion constant.

Transition to diffusion—the Central Limit Theorem

Consider the following experiment. Let

- r = radius of channel;
- v = constant particle speed;
- L = half channel length;

Release the particle from middle point with distribution ν. Measure the **expected exit time**, $\tau(aL, r, v)$ as $a \to \infty$.

Proposition

Suppose P on $L^2([0, \pi], \mu)$ has positive spectral gap and μ is ergodic for P. Then

$$\tau(aL, r, v) \sim \frac{1}{\mathcal{D}} \frac{a^2}{\ln a}$$

where $\mathcal{D} = \frac{4rv}{\pi}\xi(P)$.

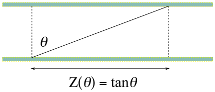
We wish to understand how $\mathcal{D}$ depends on P.

$\mathcal{D}$ and the spectrum of P

Let Π be the (projection-valued) spectral measure of P on $[-1,1]$:

$$P = \int_{-1}^{1} \lambda \, d\Pi(\lambda).$$

Fix $\beta > 1$ and let $Z|_a = Z\chi_{\{|Z| \le a/\ln^\beta a\}}$.



Spectral measure of Z on $[-1,1]$: $\Pi_Z(\cdot) = \lim_{a\to\infty} \frac{1}{\ln a} \langle Z|_a, \Pi(\cdot) Z|_a \rangle$.

Theorem

$\mathcal{D}_0$:= diffusion const. for i.i.d. process with angle distribution μ. Then

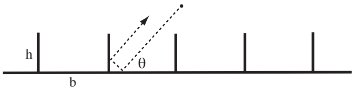
$$\mathcal{D} = \mathcal{D}_0 \int_{-1}^{1} \frac{1+\lambda}{1-\lambda} \, d\Pi_Z(\lambda).$$

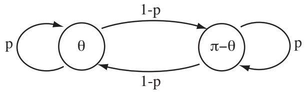
If P has discrete spectrum, $\Pi_Z(\lambda_i) := \lim_{a\to\infty} \frac{1}{\ln a} |\langle Z|_a, \phi_i \rangle|^2$.

An elementary example

θ = initial angle, define integer k, $s \in [0,1)$, and probability p:

$$\frac{2h}{b\tan\theta} = k + s, \qquad p = \begin{cases} s & \text{if } k \text{ is odd} \\ 1-s & \text{if } k \text{ is even} \end{cases}$$





Special case: $\theta = \pi/4$, $b > 2h$. Then $k = 0, s = 2h/b$. For a long channel of diameter $2r$ and particle speed v, the random flight tends to Brownian motion with

$$\sigma^2 = \sqrt{2}rv\left(\frac{b}{2h} - 1\right).$$

An application of the central limit theorem for Markov chains.