Statistical mechanics of random billiard systems

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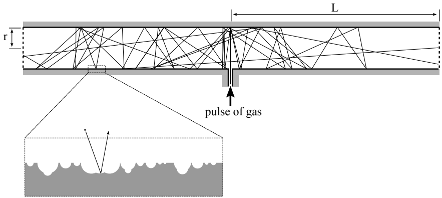
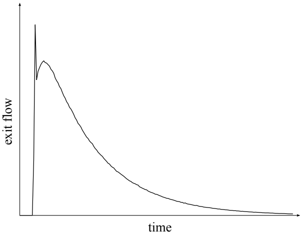
Diffusion in (straight) channels

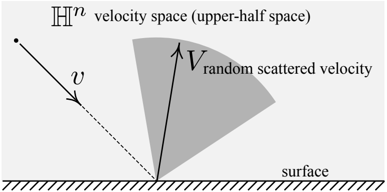
Idealized diffusion experiment. Channel inner surface has micro-structure.





How does the micro-structure influence diffusivity?

Surface scattering operators (definition of P)



Scattering characteristics of gas-surface interaction encoded in operator P.

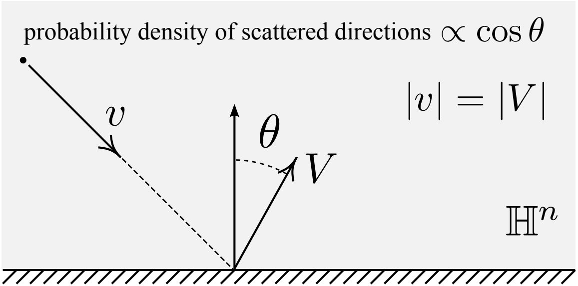
$$\boxed{(Pf)(v) = \mathbb{E}[f(V)|v]}$$

where f is any test function on $\mathbb{H}^n$ and $\mathbb{E}[\cdot|v]$ is conditional expectation given initial velocity v. If $f(V) = \begin{cases} 1 & \text{if } V \in \mathfrak{U} \\ 0 & \text{if } V \notin \mathfrak{U} \end{cases}$ then

$$\boxed{(Pf)(v) = \text{ probability that } V \text{ lies in } \mathfrak{U} \text{ given initial } v.}$$

Standard model I - Knudsen cosine law

$$\boxed{d\mu_\infty(V) = C_{n,s}\cos\theta\, d\mathrm{Vol}^s(V)} \quad C_{n,s} = \frac{1}{s^n \pi^{\frac{n-1}{2}}}\Gamma\left(\frac{n+1}{2}\right)$$

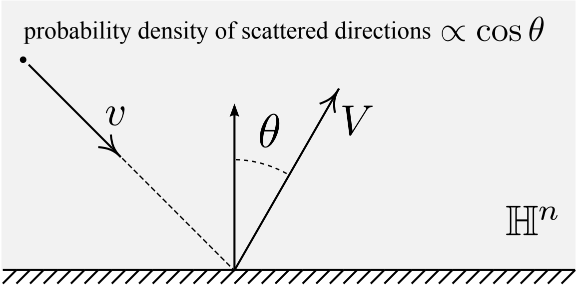


$$(Pf)(v) = \int_{\mathbb{H}^n} f(V)\, d\mu_\infty(V) \text{ independent of } v$$

Standard model II - Maxwellian at temperature T

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

where $\beta = 1/\kappa T$.



$$(Pf)(v) = \int_{\mathbb{H}^n} f(V)\, d\mu_\beta(V) \text{ independent of } v$$

Natural requirements on a general P

We say that P is natural if

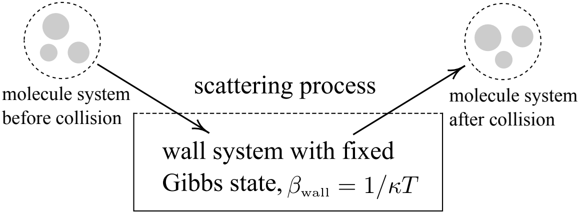
- $\boxed{\mu_\beta \text{ is a stationary probability distribution}}$ for the velocity Markov chain.
- The stationary process defined by P and μ_β is $\boxed{\text{time reversible.}}$

I.e., in the stationary regime, all V_j have the surface Maxwellian distribution μ_β and the process satisfies

$$\boxed{P(dV_2|V_1)d\mu_\beta(V_1) = P(dV_1|V_2)d\mu_\beta(V_2)}$$

Time reversibility a.k.a. reciprocity a.k.a. detailed balance.

Deriving P from microstructure: general idea



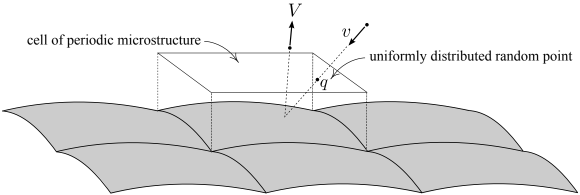
- Sample pre-collision condition of wall system from fixed Gibbs state
- Compute trajectory of deterministic Hamiltonian system
- Obtain post-collision state of molecule system.

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.

Purely geometric microstructures

V is billiard scattering of initial v with random initial point q over period cell.



Theorem (F-Yablonsky, CES 2004)

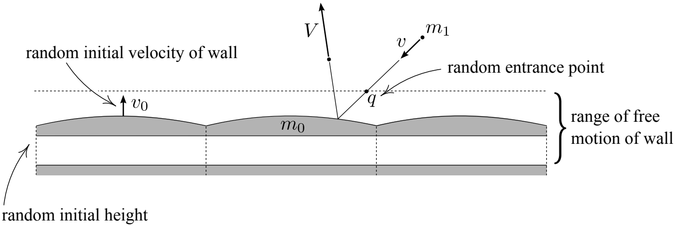
The resulting scattering operator is natural with stationary distribution μ_∞.

- The stationary probability distribution is Knudsen cosine law

$$\boxed{d\mu_\infty(V) = C_n \cos\theta \, dV_{\text{sphere}}(V)}, \quad C_n = \frac{\Gamma\left(\frac{n+1}{2}\right)}{\pi^{\frac{n-1}{2}}} \frac{1}{|V|^n}$$

- No energy exchange: $|v| = |V|$

Microstructures with moving parts



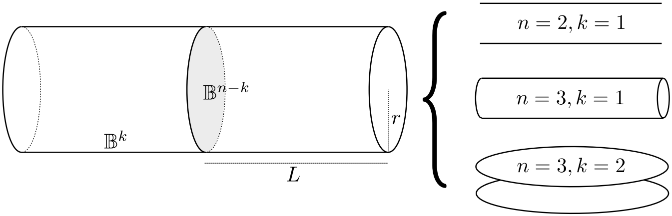
Assumptions:

- Hidden variables are initialized prior to each scattering event so that:
  - random displacements are uniformly distributed in their range;
  - initial hidden velocities are Gaussian satisfying energy equipartition.
- Statistical state of wall is kept constant.

Theorem (Thermal equilibrium. Cook-F, Nonlinearity 2012)

Resulting operator P is natural. The stationary probability distribution is μ_β, where $\beta = 1/\kappa T$ and T is the mean kinetic energy of each moving part.

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:

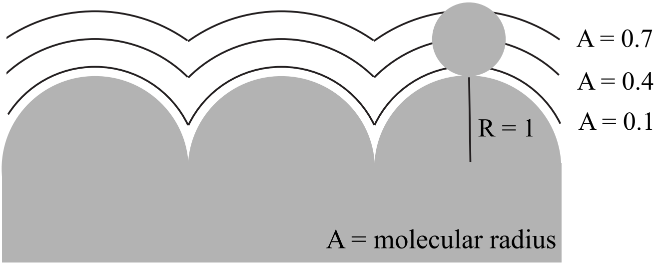
$$\mathcal{D}_0 = \begin{cases} \frac{4}{\sqrt{2\pi(n+1)}} \frac{n-k}{(n-k)^2-1} r s_\beta & \text{when } n-k \geq 2 \text{ and } \nu = \mu_\beta \\ \frac{2}{\sqrt{\pi}} \frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)} \frac{n-k}{(n-k)^2-1} r s & \text{when } n-k \geq 2 \text{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

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 $\mathbb{R}^k$.)

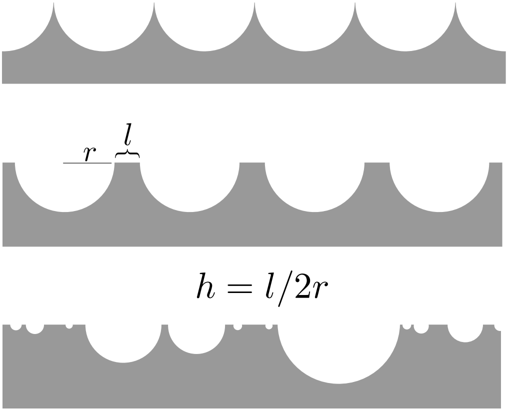
Numerical example (F-Yablonsky, CES 2006)



$$\frac{\mathcal{D}_P}{\mathcal{D}_0} \approx 1.3\left(1 + \frac{A}{R}\right)$$

Diffusivity increases with the radius of probing molecule.

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



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

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

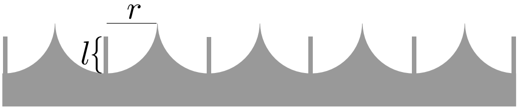
Top: $\mathcal{D}$ is smaller then in i.i.d. (perfectly diffusive) case.

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

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

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 $n - k = 1$

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

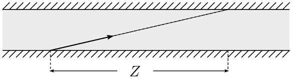
$$\eta(h) = \frac{1+\zeta_h}{1-\zeta_h} \qquad \zeta_h = -\frac{1+3h}{4}\,\frac{1-h}{1+h}\log\frac{3+h}{1-h}$$

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.



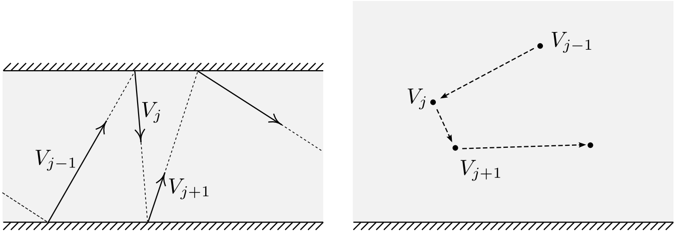
Let $\boxed{\Pi^u_Z(d\lambda) := \|Z^u\|^{-2}\langle Z^u, \Pi(d\lambda)Z^u\rangle}$, Π the spectral measure of P. Then

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

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

Remarks about diffusivity and spectrum

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



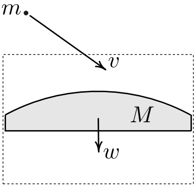
Random flight in channel

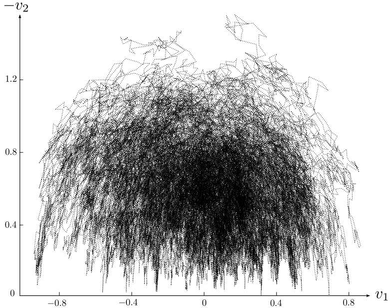
Random walk in velocity space $\mathbb{H}^n$

- $\mathcal{D}$ 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.

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. self-adjoint, elliptic on $C_0(\mathbb{H}^m) \cap L^2(\mathbb{H}^m, \mu_\beta)$.
- The limit $\mathcal{L}_{MB}\Phi = \lim_{h\to 0} \frac{P_h\Phi - \Phi}{h}$ 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
$$\frac{\partial \rho}{\partial t} = \mathcal{L}_{\mathrm{MB}}\rho$$

Example: 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 $\gamma < 1/3$:

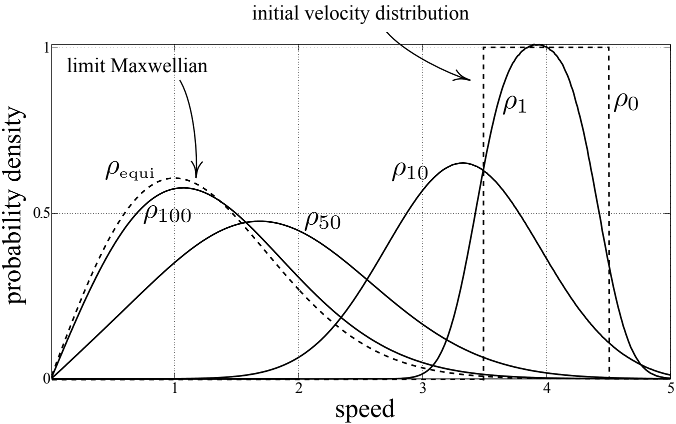
1. P_γ is a Hilbert-Schmidt; μ is the unique stationary distribution. Its density relative to Lebesgue measure on $(0,\infty)$ is

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

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



Velocity diffusion for 1-dim 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

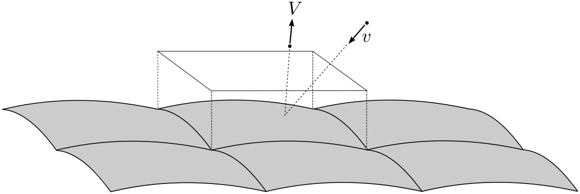
$$\mathcal{L}\varphi = \rho^{-1} \frac{d}{dv} \left(\rho \frac{d\varphi}{dv}\right),$$

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.

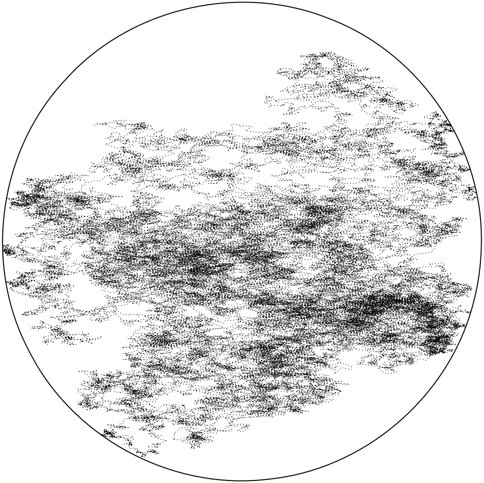


Proposition (Generalized Legendre operator in dim n)

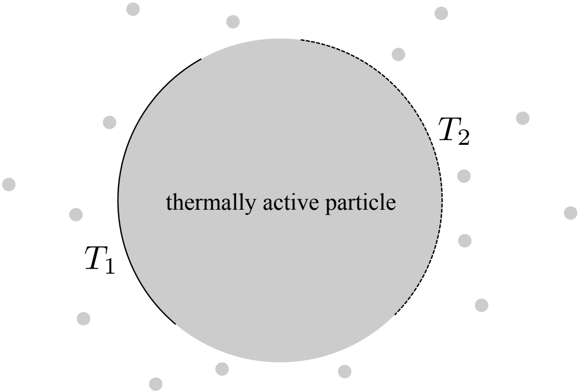
When $k = 0$, the MB-Laplacian on the unit disc in $\mathbb{R}^n$ is

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

Sample path of Legendre diffusion

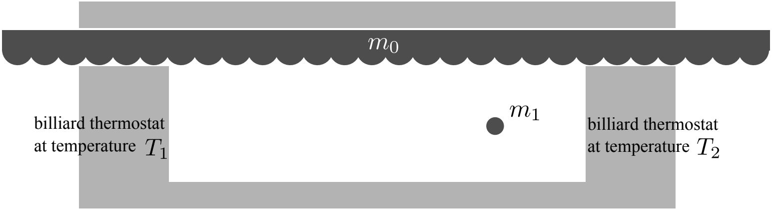


Ongoing work: Knudsen stochastic thermodynamics



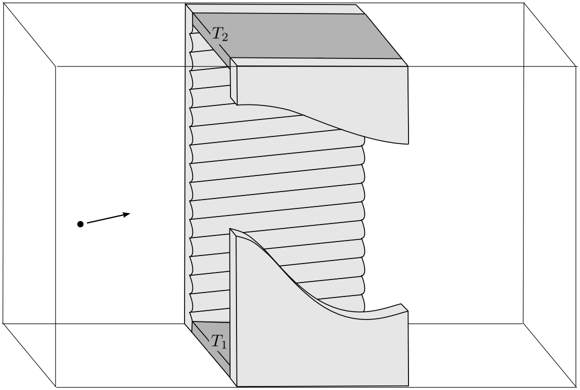
Diffusion in the Euclidian group $SE(n)$ of Brownian particle with non-uniform temperature distribution.

A linear billiard heat engine

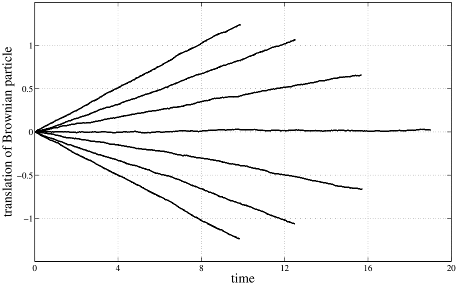


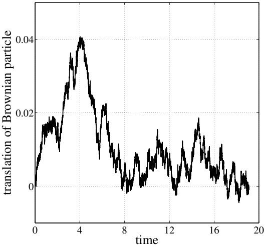
Back to transport in channels

Study of the random dynamics of such billiard heat engines reduces to study of <u>Knudsen diffusion in channels</u> (but in higher dimensions).



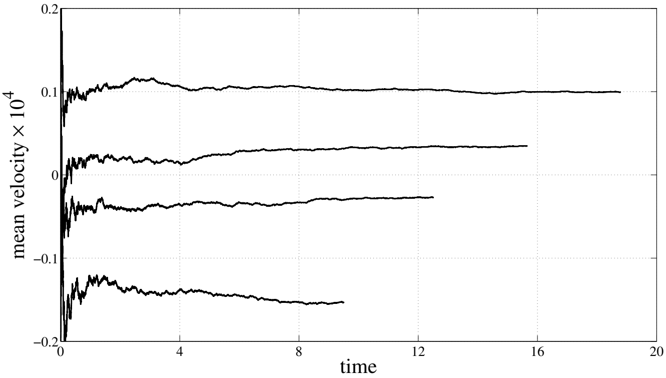
Drift velocity





Velocity drift against load if temperature differential is great enough.

Mean speed against load



Efficiency