Deterministic diffusion

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The big picture

We will apply cycle expansions to the analysis of **transport** properties of chaotic systems

Derive formulas for **diffusion coefficients** in 2-dimensional Lorentz gas

Then apply the theory to diffusion induced by 1-dimensional maps

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Diffusion in periodic arrays

Lorentz gas

Lorentz gas: diffusion of a light molecule in a gas of heavy scatterers

Modeled by point particle in a plane bouncing of an array of reflecting disks

One of simplest dynamical systems that exhibits deterministic diffusion

Periodic Lorentz gas

Quantities characterizing global dynamics can be computed from dynamics restricted to **elementary cell**

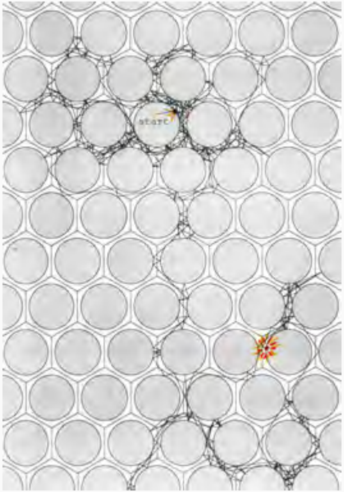
Applies to any hyperbolic dynamical system that is a periodic tiling

$$\hat{\mathcal{M}} = \bigcup_{\hat{n} \in T} \mathcal{M}_{\hat{n}} \tag{1}$$

T is abelian group of lattice translations, $\hat{\mathcal{M}}$ refers to the full state space; spatial coordinates and momenta

If scattering array has further discrete rotational and reflection symmetries, each cell can be built from a **fundamental domain** $\tilde{\mathcal{M}}$

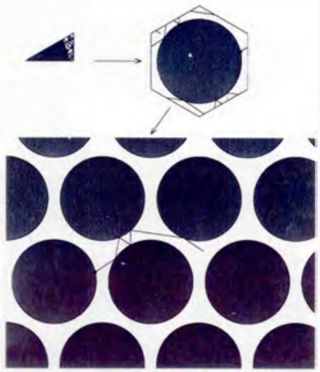
Sinai billiard Lorentz gas



Exercise: What are the fundamental domain, elementary cell, and full state space?

Three kinds of state spaces

- fundamental domain, triangle (denoted ˜)
- elementary cell, hexagon (denoted by nothing)
- full state space, lattice (denoted ˆ)



Types of diffusive behavior

Finite horizon: any free particle trajectory must hit a disk in finite time

Infinite horizon

Parameterized by

$$\frac{w}{r} < \frac{4}{\sqrt{3}} - 2 = 0.3094... \tag{2}$$

where r is the radius of the disk and w is the distance between

Exercise: Is the horizon finite or infinite when equation (2) is satisfied?

Exercise

Finite

We will restrict our consideration in this chapter to finite horizon case

In this case diffusion is normal: $\hat{x}(t)^2$ grows like t

Pop quiz: What does the ^ signify?

Evolution operator for each state space

$\hat{x}(t) = \hat{f}^t(\hat{x})$ denotes point in the global space $\hat{\mathcal{M}}$ reached by the flow in time t

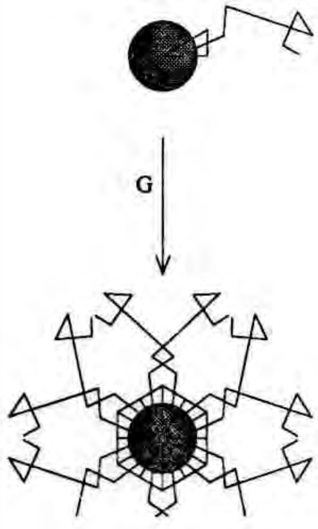
$x(t) = f^t(x_0)$ denotes corresponding flow in the elementary cell

$$\hat{n}_t(x_0) = \hat{f}^t(x_0) - f^t(x_0) \in T \tag{3}$$

$\tilde{x}(t) = \tilde{f}^t(\tilde{x})$ denotes the flow in the fundamental domain $\tilde{\mathcal{M}}$.

$\tilde{f}^t(\tilde{x})$ is related to $f^t(\tilde{x})$ by a discrete symmetry which maps $\tilde{x}(t) \in \tilde{\mathcal{M}}$ to $x(t) \in \mathcal{M}$

Discrete symmetry mapping



Calculating diffusion coefficient

$$s(\beta) = \lim_{t\to\infty} \frac{1}{t} \log \left\langle e^{\beta\cdot(\hat{x}(t)-x)} \right\rangle_{\mathcal{M}} \tag{4}$$

If all odd derivatives vanish by symmetry, there is no drift and the second derivatives yield a diffusion matrix

$$2dD_{ij} = \frac{\partial}{\partial\beta_i}\frac{\partial}{\partial\beta_j} s(\beta)\bigg|_{\beta=0} = \lim_{t\to\infty} \frac{1}{t} \langle(\hat{x}(t)-x)_i(\hat{x}(t)-x)_j\rangle_{\mathcal{M}} \tag{5}$$

Spatial diffusion constant:

$$D = \frac{1}{2d} \sum_i \frac{\partial^2}{\partial\beta_i^2} s(\beta)\bigg|_{\beta=0} = \lim_{t\to\infty} \frac{1}{2dt} \left\langle(\hat{q}(t)-q)^2\right\rangle_{\mathcal{M}} \tag{6}$$

Reduction from $\hat{\mathcal{M}}$ to $\mathcal{M}$

$$\left\langle e^{\beta\cdot(\hat{x}(t)-x)}\right\rangle_{\mathcal{M}} = \frac{1}{|\mathcal{M}|}\int_{x\in\mathcal{M},\hat{y}\in\hat{\mathcal{M}}} \mathrm{d}x\,\mathrm{d}\hat{y}\; e^{\beta\cdot(\hat{y}-x)}\delta(\hat{y}-\hat{f}^t(x)) \tag{7}$$

Translation invariance can be used to reduce this average to the elementary cell:

$$\left\langle e^{\beta\cdot(\hat{x}(t)-x)}\right\rangle_{\mathcal{M}} = \frac{1}{|\mathcal{M}|}\int_{x,y\in\mathcal{M}} \mathrm{d}x\,\mathrm{d}y\; e^{\beta\cdot(\hat{f}^t(x)-x)}\delta(y-f^t(x)) \tag{8}$$

$\hat{y} = y - \hat{n}$ so Jacobian equals unity

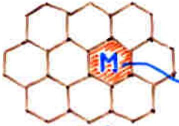
Question: Does this make sense?

Local v.s. global

diffusion constant:

$$D \equiv \lim_{t\to\infty} \frac{1}{2t} \langle (\vec{x}_t - x_0)^2 \rangle = \frac{1}{2} \frac{\partial^2}{\partial \vec{\beta}^2} Q(\beta) \Big|_{\vec{\beta}=0}$$

what is $\langle \cdots \rangle$? by symmetry, sufficient to average over a single tile M:



$$\langle \cdots \rangle_M = \langle \cdots \rangle$$

$$\left\langle e^{\vec{\beta}\cdot(\vec{x}_t - \vec{x})} \right\rangle_M = \frac{1}{|M|} \int_M dx\, dy\, \delta(\phi^t(x) - y)\, e^{\vec{\beta}\cdot(\vec{x}_t - x)}$$

volume of M ($|M|$); start (x); end (y)

THE IDEA: local dynamics ($\int_M dx\, dy\, \delta(\phi^t(x) - y)$), global diffusion ($e^{\vec{\beta}\cdot(\vec{x}_t - x)}$)

Evolution operator

$$\mathcal{L}^t(y,x) = e^{\beta\cdot(\hat{x}(t)-x)}\delta(y - f^t(x)) \tag{9}$$

This operator satisfies the semigroup property:

$$\mathcal{L}^{t_1+t_2}(y,x) = \int_{\mathcal{M}} \mathrm{d}z\, \mathcal{L}^{t_2}(y,z)\mathcal{L}^{t_1}(z,x) \tag{10}$$

For $\beta = 0$, Perron-Frobenius operator, $e^{s_0} = 1$ because there is no escape from this system

The spectrum of $\mathcal{L}$ is evaluated by taking the trace

$$\mathrm{Tr}\,\mathcal{L}^t = \int_{\mathcal{M}} \mathrm{d}x\, e^{\beta\cdot\hat{n}_t(x)}\delta(x - x(t)) \tag{11}$$

Types of orbits

Two kinds of orbits periodic in $\mathcal{M}$ contribute:

Standing periodic orbit: also a periodic orbit of the infinite state space dynamics $\hat{f}^{T_p}(x) = x$

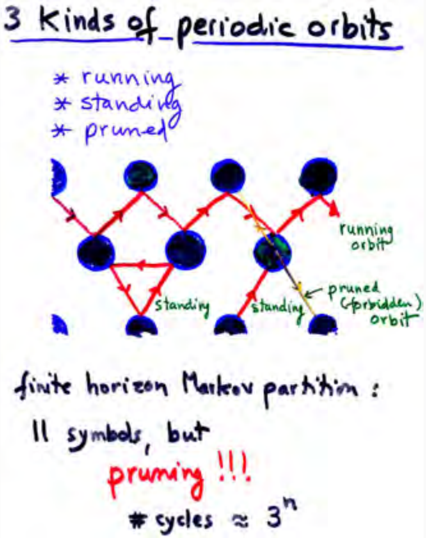
Running periodic orbit: corresponds to a lattice translation in dynamics on infinite state space $\hat{f}^{T_p}(x) = x + \hat{n}_p$

Shortest repeating segment of a running orbit is 'relative periodic orbit'

These orbits called **accelerator modes**: diffusion takes place along the momentum rather than position coordinate

Distance travelled $\hat{n}_p = \hat{n}_{T_p}(x_0)$ independent of x_0

Types of orbits



Spectral determinant:

$$\det(s(\beta) - \mathcal{A}) = \prod_p \exp\left(- \sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{(\beta \cdot \hat{n}_p - sT_p)r}}{\left|\det\left(1 - M_p^r\right)\right|} \right) \tag{12}$$

Question: What is M?

Corresponding dynamical zeta function:

$$1/\zeta(\beta, s) = \prod_p \left(1 - \frac{e^{(\beta \cdot \hat{n}_p - sT_p)}}{|\Lambda_p|}\right) \tag{13}$$

Diffusion constant

The dynamical zeta function cycle averaging formula for the diffusion constant, zero mean drift is given by

$$D = \frac{1}{2d} \frac{\left\langle \hat{x}^2 \right\rangle_\zeta}{\langle T \rangle_\zeta} = \frac{1}{2d} \frac{1}{\langle T \rangle_\zeta} \sum{}' \frac{(-1)^{k+1} (\hat{n}_{p_1} + \ldots + \hat{n}_{p_k})^2}{|\Lambda_{p_1} \ldots \Lambda_{p_k}|} \tag{14}$$

Sum over all distinct non-repeating combination of prime cycles

Globally periodic orbits have $\hat{x}_p^2 = 0$ and contribute only to time normalization, Mean square displacement gets contributions only from runaway trajectories $\hat{x}(t)^2 = (\hat{n}_p / T_p)^2 t^2$

So orbits that contribute exhibit either ballistic or no transport at all: diffusion arises as a balance between the two kinds of motion, weighted by $1/|\Lambda_p|$

Diffusion induced by chains of 1-dimensional maps

Diffusion constant

Refer to $\hat{n}_p \in \mathbb{Z}$ as the **jumping number**.

The cycle weight is

$$t_p = z^{n_p} e^{\beta \hat{n}_p} / |\Lambda_p| \tag{15}$$

Diffusion constant for 1-dimensional maps is

$$D = \frac{1}{2} \frac{\left\langle \hat{n}^2 \right\rangle_\zeta}{\langle n \rangle_\zeta} \tag{16}$$

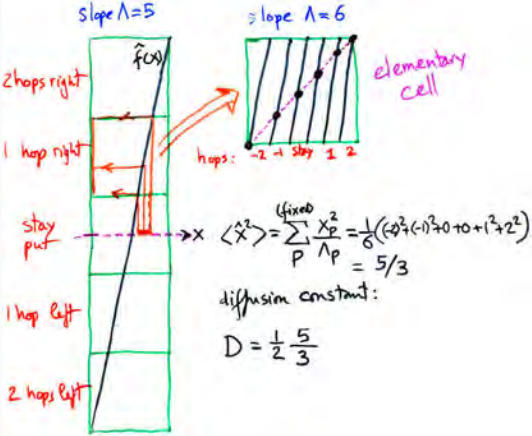
Calculating diffusion constant

The "mean cycle time" is given by

$$\langle n \rangle_\zeta = z \frac{\partial}{\partial z} \frac{1}{\zeta(0,z)}\bigg|_{z=1} = -\sum{}' (-1)^k \frac{n_{p_1} + \ldots + n_{p_k}}{|\Lambda_{p_1} \ldots \Lambda_{p_k}|} \tag{17}$$

and the "mean cycle displacement squared" is given by

$$\left\langle \hat{n}^2 \right\rangle_\zeta = \frac{\partial^n}{\partial \beta^n} \frac{1}{\zeta(\beta,1)}\bigg|_{\beta=0} = -\sum{}' (-1)^k \frac{(\hat{n}_{p_1} + \ldots + \hat{n}_{p_k})^2}{|\Lambda_{p_1} \ldots \Lambda_{p_k}|} \tag{18}$$



Drift: $\langle v \rangle = 0$ by symmetry

Diff.: $\langle \hat{x}^2 \rangle = \sum_p^{fixed} \frac{x_p^2}{\Lambda_p} = \frac{0+1^2+2^2+(-2)^2+(-1)^2+0}{6}$

$= 5/3$

Mean cycle

$\langle T \rangle = \sum_p^{fixed} \frac{T_p}{\Lambda_p} = \frac{1+1+1+1+1+1}{6} = 1$

Diffusion const:

$D = \frac{1}{2}\frac{5}{3}$

Higher order transport coefficients

Same approach

$$\mathcal{B}_k = \frac{1}{k!}\frac{\mathrm{d}^k}{\mathrm{d}\beta^k}s(\beta)\bigg|_{\beta=0}, \qquad \mathcal{B}_2 = D \tag{19}$$

for $k > 2$ known as the Burnett coefficients

Non-vanishing higher order coefficients signal deviations of deterministic diffusion from a Gaussian stochastic process

Exercise: Do we think deterministic diffusion is a Gaussian stochastic process?

deterministic diffusion **NOT** gaussian

$$B_4 = \frac{1}{4!}\frac{\partial^4}{\partial \beta^4} s(\beta)\Big|_{\beta=0}$$

$$= -\frac{1}{4!\,60}(m-1)(2m-1)(4m^2-9m+7) \neq 0$$

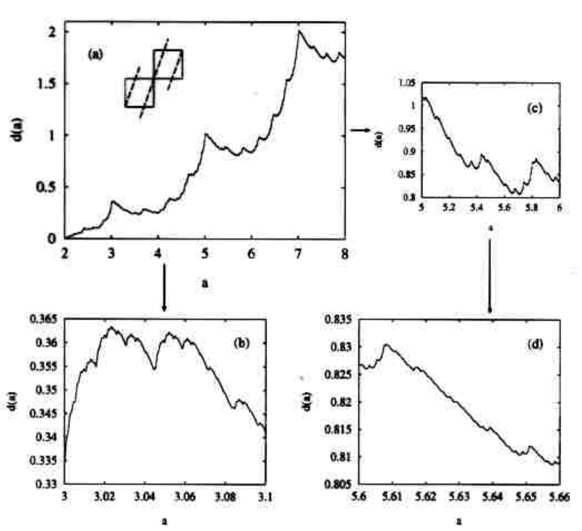
(here $m=3$)

Finite Markov partitions

Markov partition with intervals mapped onto unions of intervals

Map the critical value $f(1/2)$ into the fixed point at the origin $f^n(1/2) = 0$ in finite n. Taking higher and higher values of n - constructs a dense set of Markov parameters

Dependence of D on Λ



Marginal stability and anomalous diffusion

Marginal stability

Marginal fixed point affects the balance between running and standing orbits, thus generating a mechanism that may result in anomalous diffusion

When $\alpha = 1/s \leq 1$, $z''(\beta)|_{\beta=1} = 0$, so D vanishes by the implicit function theorem

Typical orbit will stick for long times near the $\bar{0}$ marginal fixed point

For 1-dimensional diffusion, where $'$ is a derivative with respect to s, inverse Laplace transform:

$$D = \lim_{t\to\infty} \frac{\mathrm{d}^2}{\mathrm{d}\beta^2} \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} \mathrm{d}s\, e^{st} \left. \frac{\zeta'(\beta, s)}{\zeta(\beta, s)} \right|_{\beta=0} \tag{20}$$

Exercise: Is the above equation for a flow or for a map?

(Hardy–Littlewood) tauberian theorem

Take

$$\omega(\lambda) = \int_0^\infty \mathrm{d}x\, e^{-\lambda x} u(x) \tag{21}$$

with $u(x)$ monotone as $x \to \infty$; then as $\lambda \to 0$ and $x \to \infty$ respectively (and $\rho \in (0, \infty)$)

$$\omega(\lambda) \sim \frac{1}{\lambda^\rho} L\left(\frac{1}{\lambda}\right) \tag{22}$$

if and only if

$$u(x) \sim \frac{1}{\Gamma(\rho)} x^{\rho-1} L(x) \tag{23}$$

where L denotes any slowly varying function with $\lim_{t\to\infty} L(ty)/L(t) = 1$

Anomalous diffusion

We now have

$$\frac{1/\zeta_0'(e^{-s},\beta)}{1/\zeta_0(e^{-s},\beta)} = \frac{\left(\frac{4}{\Lambda} + \frac{\Lambda-4}{\Lambda\zeta(1+\alpha)}(J(e^{-s},\alpha+1) + J(e^{-s},\alpha))\right)\cosh\beta}{1 - \frac{4}{\Lambda}e^{-s}\cosh\beta - \frac{\Lambda-4}{\Lambda\zeta(1+\alpha)}e^{-s}J(e^{-s},\alpha+1)\cosh\beta J} \tag{24}$$

Questions: What is J?

Taking the second derivative with respect to β

$$\begin{aligned}&\frac{\mathrm{d}^2}{\mathrm{d}\beta^2}\left(1/\zeta_0'(e^{-s},\beta)/\zeta^{-1}(e^{-s},\beta)\right)_{\beta=0}\\ &= \frac{\frac{4}{\Lambda} + \frac{\Lambda-4}{\Lambda\zeta(1+\alpha)}(J(e^{-s},\alpha+1) + J(e^{-s},\alpha))}{\left(1 - \frac{4}{\Lambda}e^{-s} - \frac{\Lambda-4}{\Lambda\zeta(1+\alpha)}e^{-s}J(e^{-s},\alpha+1)\right)^2} = g_\alpha(s)\end{aligned} \tag{25}$$

Anomalous diffusion exponents

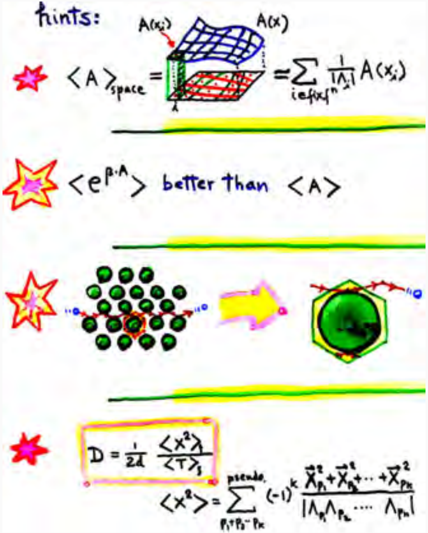
After some math...

$$g_\alpha(s) \sim \begin{cases} s^{-2} & \text{for } \alpha > 1 \\ s^{-(\alpha+1)} & \text{for } \alpha \in (0,1) \\ 1/(s^2 \ln s) & \text{for } \alpha = 1 \end{cases} \tag{26}$$

The anomalous diffusion exponents follow:

$$\left\langle (x - x_0)^2 \right\rangle_t \sim \begin{cases} t^\alpha & \text{for } \alpha \in (0,1) \\ t/\ln t & \text{for } \alpha = 1 \\ t & \text{for } \alpha > 1 \end{cases} \tag{27}$$

Summary



Questions?