# New horizons in multidimensional diffusion: The Lorentz gas and the Riemann Hypothesis

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# Preview

The Lorentz gas is a model in which a point particle diffuses in a periodic array of convex (eg spherical) scatterers.

- It is of interest in
  - Theory: Foundations of statistical mechanics, chaotic billiards
  - Applications: Crystal and optical lattices, nanopores, molecular dynamics

- Corridors provide timescale separation; their enumeration gives a logarithmic superdiffusion coefficient.

- New phenomena appear in dimensions $\geq 6$.

- The small scatterer limit is related to the Riemann Hypothesis.

See arxiv:1103.1225

# Deterministic diffusion

Consider dynamics $\Phi^t : M \to M$ with $M \subset \mathbb{R}^d \times \mathbb{S}^{d-1}$ periodic,

$$\Phi^t(\mathbf{x} + \mathbf{l}, \mathbf{v}) = (\Phi^t_x(\mathbf{x}, \mathbf{v}) + \mathbf{l}, \Phi^t_v(\mathbf{x}, \mathbf{v}))$$

for $\mathbf{l} \in \mathbb{Z}^d$ or more general.

Then we consider scaling properties of $\Delta(t) = \Phi^t_x(\mathbf{x}, \mathbf{v}) - \mathbf{x}$. In increasing order of strength, we can try to show:

- $\langle \Delta(t)^2 \rangle \sim 2dDt$ (Einstein formula). $\langle\rangle$ is average over unit cell.
- $\frac{\Delta(t)}{\sqrt{t}}$ converges (weakly) to a normal distribution.
- $\frac{\Delta(st)}{\sqrt{t}}$ converges (weakly) to a Wiener process on $s \in [0, 1]$.

# Correlations and (super)diffusion

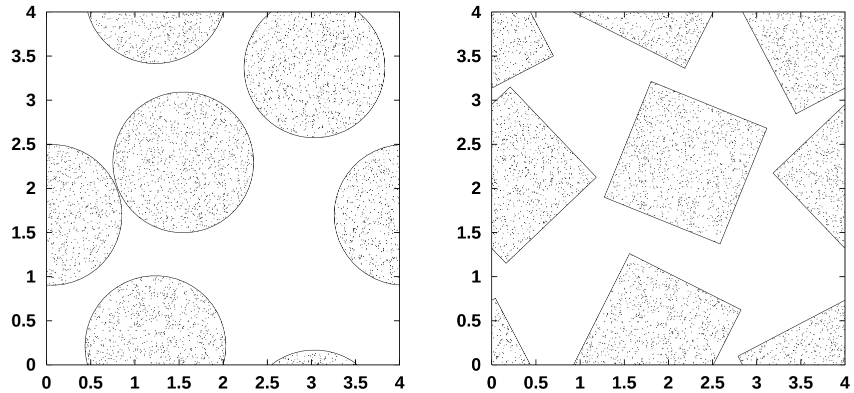
We denote $\mathbf{v}_t = \Phi_v^t(\mathbf{x}, \mathbf{v})$. Then

$$
\begin{aligned}
\langle \Delta(t)^2 \rangle &= \int_0^t ds \int_0^t ds' \langle \mathbf{v}_s \cdot \mathbf{v}_{s'} \rangle \\
&= 2 \int_0^t ds \int_0^s ds'' \langle \mathbf{v}_0 \cdot \mathbf{v}_{s''} \rangle \\
&= 2t \int_0^t \langle \mathbf{v}_0 \cdot \mathbf{v}_s \rangle ds - 2 \int_0^t s \langle \mathbf{v}_0 \cdot \mathbf{v}_s \rangle ds
\end{aligned}
$$

Normal diffusion: Correlation integral converges; $\langle \Delta(t)^2 \rangle \sim 2dDt$

Logarithmic superdiffusion: If $\langle \mathbf{v}_0 \cdot \mathbf{v}_s \rangle \sim \frac{d\mathcal{D}}{s}$ as $s \to \infty$ we get $\langle \Delta(t)^2 \rangle \sim 2d\mathcal{D}t \ln t$.

# Extended billiards: Lorentz and Ehrenfest




A point particle collides with nonoverlapping scatterers.

**Random** scatterer arrangements (Lorentz 1905, Ehrenfest 1912) arise naturally from statistical mechanics (limit of binary mixture), a few rigorous results for the Boltzmann-Grad scaling and for percolation style randomness.

**Periodic** scatterer arrangements (Galton, 1873) arise naturally from computer simulation methods and motion in periodic structures. Reducible to a finite domain and hence better understood.

# Classification of extended 2D billiards

- **Periodic Ehrenfest gas**: Anomolous diffusion (Hardy-Weber 1980; Delecroix-Hubert-Lelievre, arxiv 2011)

- **Random Ehrenfest gas, locally finite horizon**: Numerics consistent with a Wiener process! (Dettmann-Cohen 2001)

- **Random Lorentz gas, locally finite horizon**: Kinetic theory gives normal diffusion, correlations $t^{-d/2-1}$ (Ernst-Weyland 1971)

- **Periodic Lorentz gas, finite horizon**: Convergence to a Wiener process (Bunimovich-Sinai 1981) exponential mixing in map (Young 1998), stretched exponential bound in flow (Chernov 2007).

- **Periodic Lorentz gas with infinite horizon**: Superdiffusion (Bleher 1992; Szasz-Varju 2007) with $\Delta(t)$ distributed normally when scaled by $\sqrt{t \ln t}$; also ergodicity of the infinite invariant measure.

# Normal diffusion in the periodic Lorentz gas

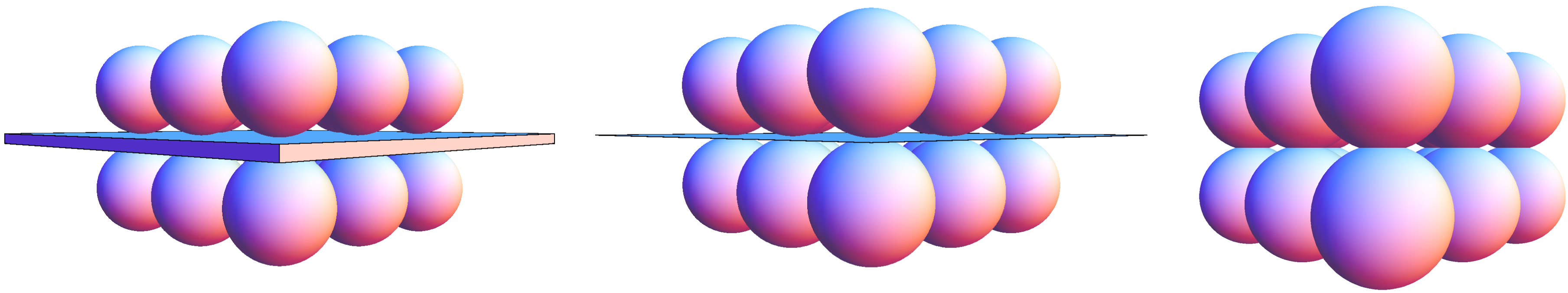
In 2D, finite horizon: finite Markov state model of Machta-Zwanzig (1983) gives

$$D \approx \frac{1-2r}{\pi(\sqrt{3}-2\pi r^2)}$$

In arbitrary dimension and finite horizon, Chernov (1994) shows (weak) convergence to a Wiener process, subject to a "complexity" bound.

In 3D, Sanders (2008) points out that both finite and "cylindrical" horizon are expected to have normal diffusion, while the "planar" horizon is superdiffusive. Gilbert, Nyugen and Sanders (2011) use a finite Markov model to estimate the diffusion coefficient in the normal diffusion case.

# Horizon terminology



**Horizon** Connected $H \subset M$ with infinite free path, of the form $H_x \times H_v$ and not extensible. It has dimension $1 \leq D_H \leq d - 1$.

**Maximal horizon** A horizon with the maximum dimension for the given billiard.

**Principal horizon** A horizon with $D = d - 1$

**Incipient horizon** A horizon with respect to the interior of the scatterers, but not their boundary.

# The $d$-dimensional cubic Lorentz gas

Let $P(t)$ be the probability of not colliding before time $t$. If there are non-incipient maximal horizons $H \in \mathcal{H}$, orbits that remain in $H_x$ for time $t$ provide a major — we assume leading — contribution to $P(t)$:

$$\textbf{Conjecture 1:} \quad P(t) \sim \sum_{H \in \mathcal{H}} P_H(t)$$

For the Lorentz gas, principal horizons $H_x$ are of infinite extent in $d-1$ directions, with width

$$w_L = \begin{cases} L^{-1} - 2r & L < (2r)^{-1} \\ 0 & \text{otherwise} \end{cases}$$

in the remaining direction, where $L$ is the length of the primitive lattice vector $\mathbf{l} \in \mathbb{Z}^d$ orthogonal to the horizon.

# Free flights in a principal horizon

Given a long time $t$, the fraction of $v$ remaining in the horizon is $S_{d-2}/(tS_{d-1})$, independent of $x$. The fraction of $x$ in the horizon is $Lw_L^2/(1-V_dr^d)$.

Thus the measure of initial conditions not colliding for time $t$ is given by

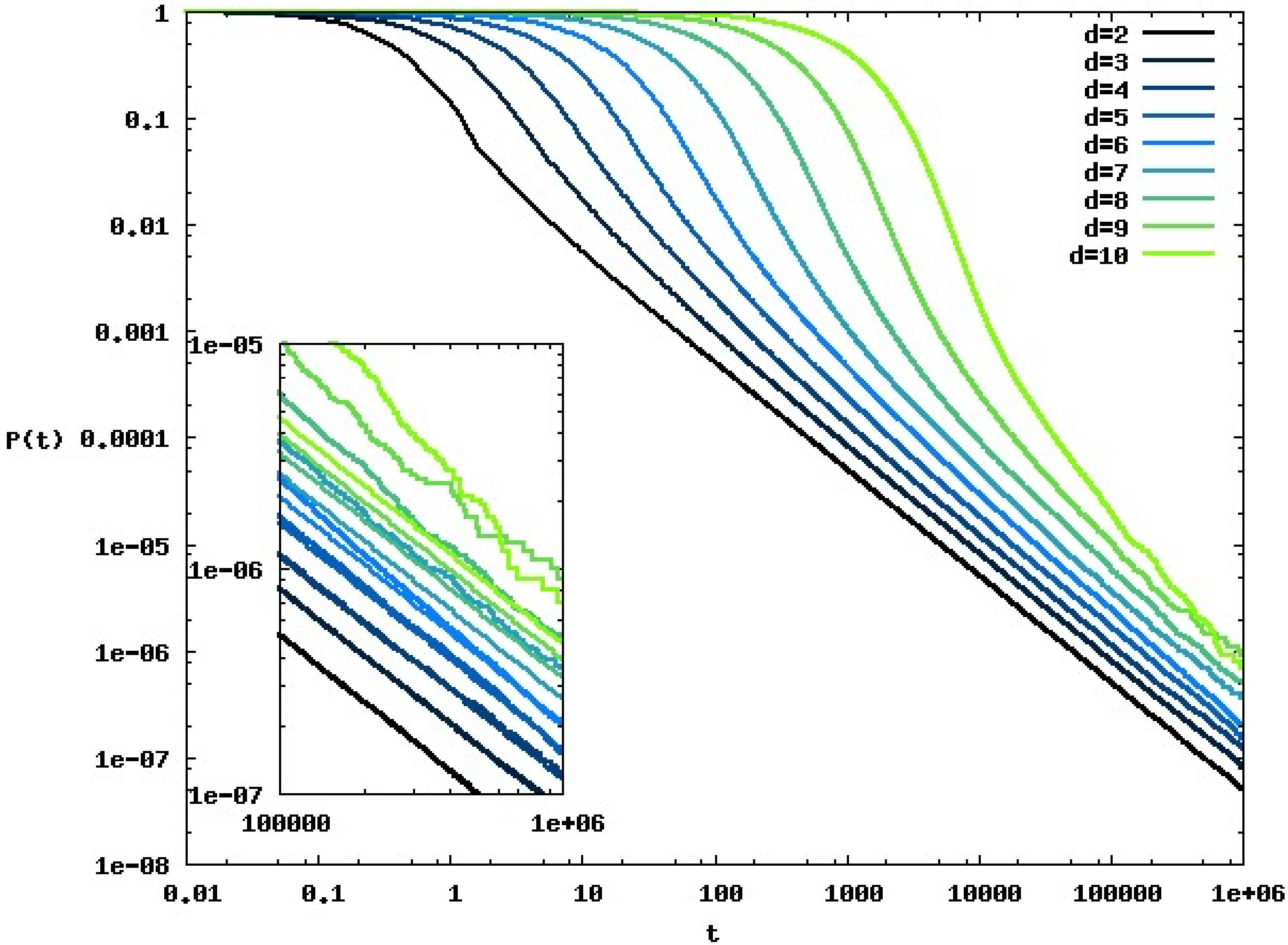
$$P(t) \sim \frac{S_{d-2}}{2S_{d-1}(1-V_dr^d)} \sum_{\mathbf{l}\text{ primitive}} \frac{Lw_L^2}{t}$$

**Theorem 1: This holds, subject to conjecture 1.**

Remove the primitivity condition using Möbius inversion:

$$P(t) \sim \frac{S_{d-2}}{2S_{d-1}(1-V_dr^d)} \sum_{C=1}^{\infty} \sum_{\mathbf{l}\neq\mathbf{0}} \mu(C) \frac{CLw_{CL}^2}{t}$$

This is a finite sum.



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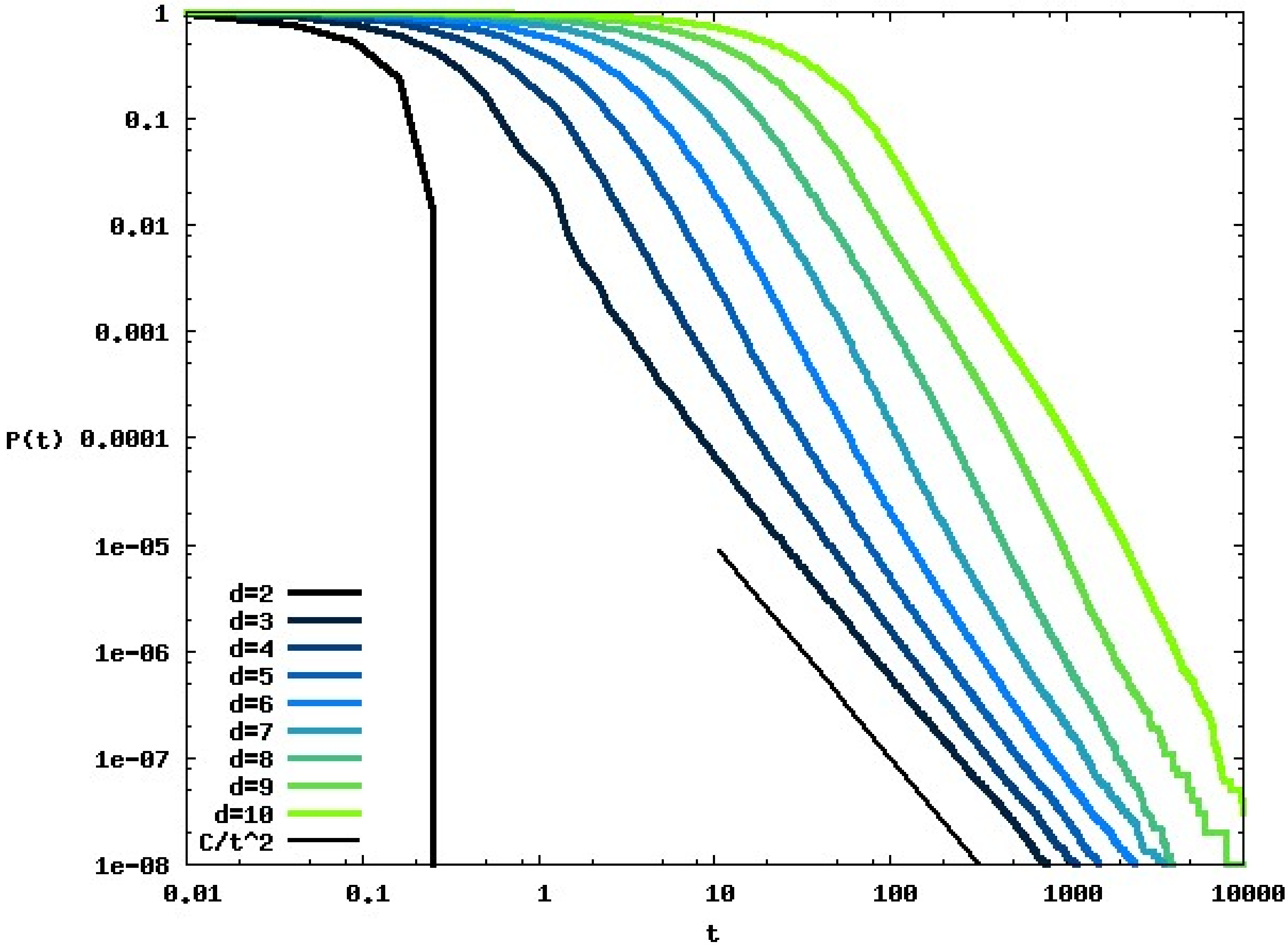

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C/t^2

# Limit of small $r$

Extract small $r$ asymptotics using a Mellin transform

$$P(t) = \frac{S_{d-2}}{2tS_{d-1}(1-V_d r^d)} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{4r^{-s} E_d(\frac{s+1}{2}) ds}{2^{s+1} s(s+1)(s+2)\zeta(s+1)}$$

where $E_d(z)$ is the Epstein zeta function for the $d$-dimensional cubic lattice,

$$E_d(z) = \sum_{\mathbf{l} \neq \mathbf{0}} L^{-2z}$$

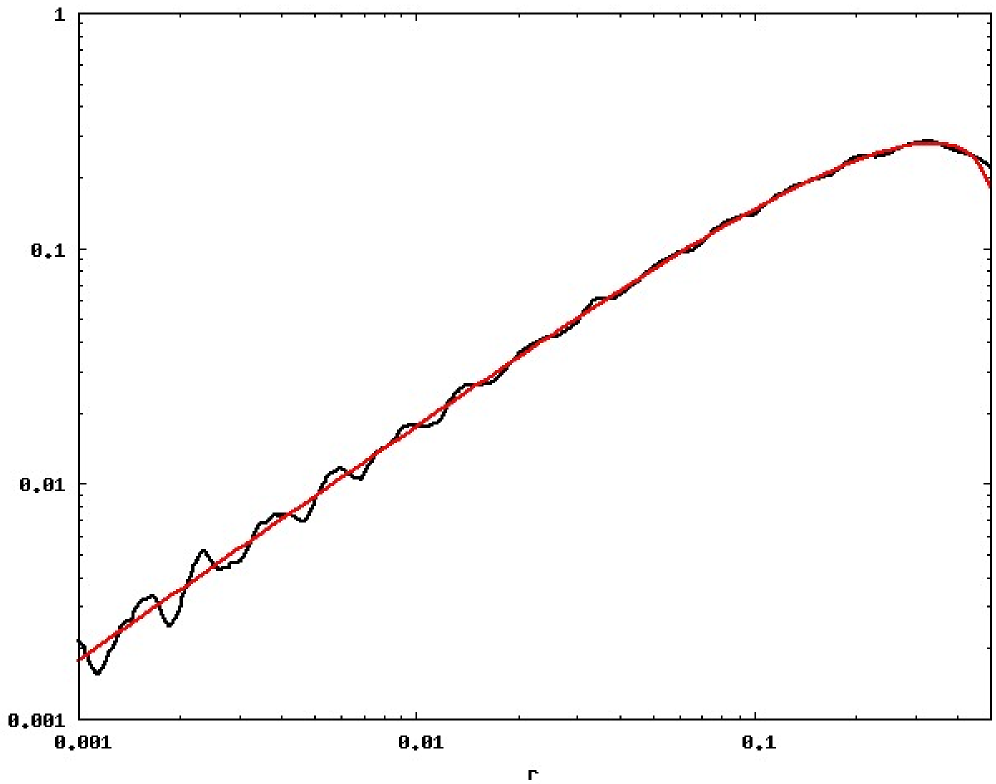
$\zeta(z) = E_1(\frac{z}{2})/2$ is the Riemann zeta function. The leading pole at $s = d-1$ gives (cf Marklof-Strömbergsson, arxiv 2010)

$$tP(t) \sim \frac{\sqrt{\pi^{d-1}}}{2^d d \Gamma(\frac{d+3}{2}) \zeta(d) r^{d-1}} + O(r^{1/2-\delta})$$

for $\delta > 0$ assuming the Riemann Hypothesis and convergence of a sequence of contour integrals.

# Subleading $P(t)$ contributions

After subtracting the leading pole, the trivial poles (smooth curve) give a good approximation for moderate $r$; irregular behaviour from the RH-type poles dominates at very small $r$.

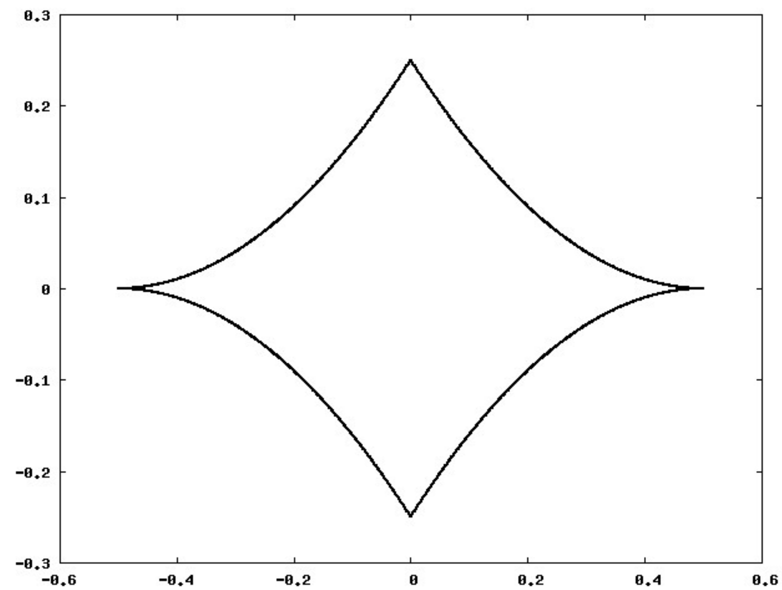


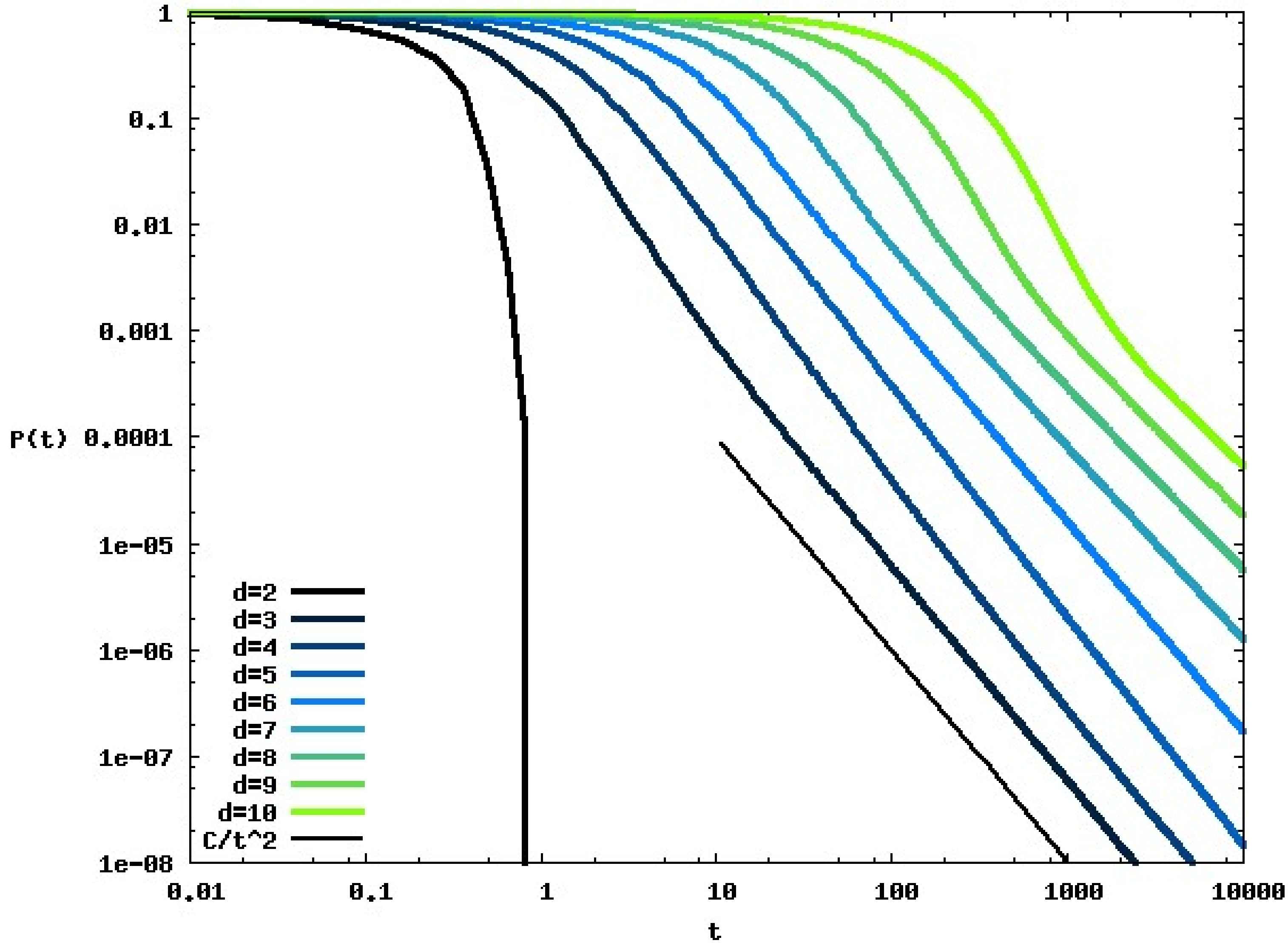
# Incipient horizons

Suppose the only principal horizons are incipient, for example the Lorentz gas with radius 0.5. The incipient horizon is connected to an infinite number of horizons of dimension $d-2$, in which the perpendicular subspace approaches a shape bounded by parabolas and of area proportional to $L^{-3}$, leading to

$$P_H(t) \sim \frac{C_d}{t^2 L^5}$$

The sum of this over lattice vectors converges only when $d < 6$.





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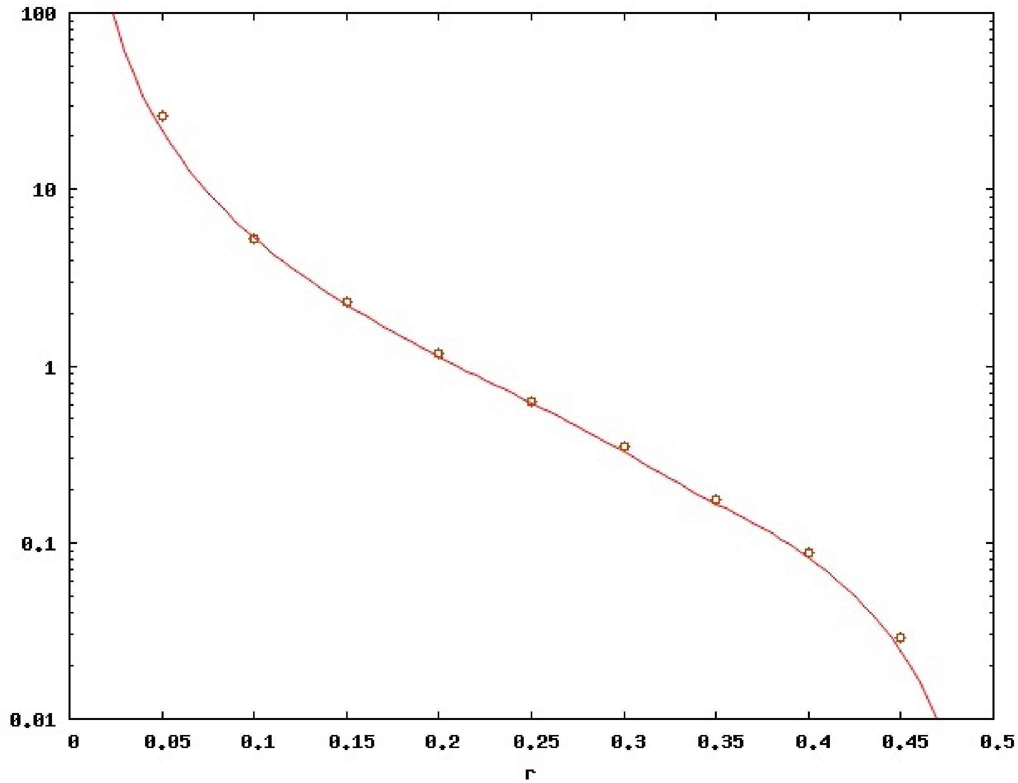
C/t^2

# Correlation conjecture

We now need **Conjecture 2**: Correlation decay is $o(P(t))$ for orbits that collide. In this numerical test, points are fits to the velocity autocorrelations, line is the sum over horizons, $d = 3$.



# Diffusion

Assuming that correlations are dominated by free paths, as above, we can calculate the superdiffusion coefficient in terms of a sum over horizons involving the normal vector to the hyperplane $\mathbf{n}$:

$$D_{ij} = \frac{1}{1-\mathcal{P}} \frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{d+1}{2}) 2\sqrt{\pi}} \sum_H \mathcal{V}_H w_H^2 (\delta_{ij} - n_i(H) n_j(H))$$

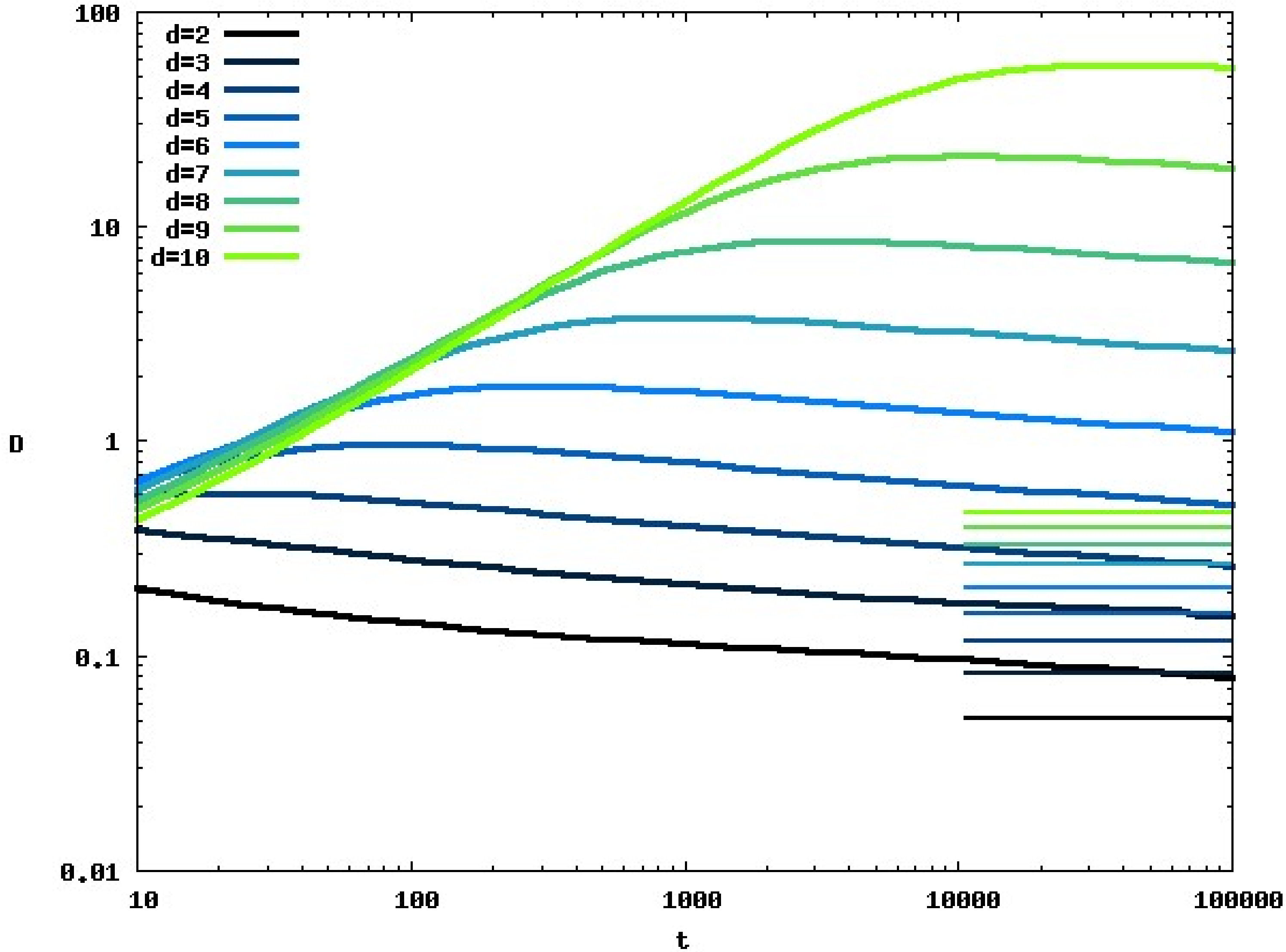
for example at $\frac{1}{2\sqrt{2}} < r < \frac{1}{2}$ in the cubic Lorentz gas we have

$$D_{ij} = \frac{(1-2r)^2}{1 - V_d r^d} \frac{\Gamma(\frac{d}{2}) \delta_{ij}}{\Gamma(\frac{d-1}{2})\sqrt{\pi}}$$

**Theorem 2: This holds, subject to conjectures 1 and 2.**

For small $r$ we find another connection with the Riemann Hypothesis:

$$\mathrm{tr} D_{ij} = \frac{\pi^d \Gamma(\frac{d}{2})}{2^{d-1} d \Gamma(\frac{d+1}{2}) \Gamma(\frac{d+3}{2}) \zeta(d) r^{d-1}} + O(r^{1/2-\delta})$$



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# Outlook

In more general lattices (including N hard balls)...

- We get anisotropic diffusion matrices $D_{ij}$
- Horizons of different dimension can coexist. Maximal dimension $D_H$ leads to correlations of $t^{D_H-d}$.
- The coefficient involves a double integral over a $d-D_H$ space, with a line of sight condition.
- For non-principal horizons, $D$ is normal and difficult, but $B$ may be anomolous (and easy?).

More open problems: Explicit finite horizon LG for $d > 2$; complexity conditions for $d > 2$; the Riemann Hypothesis.