Kinetic transport in crystals

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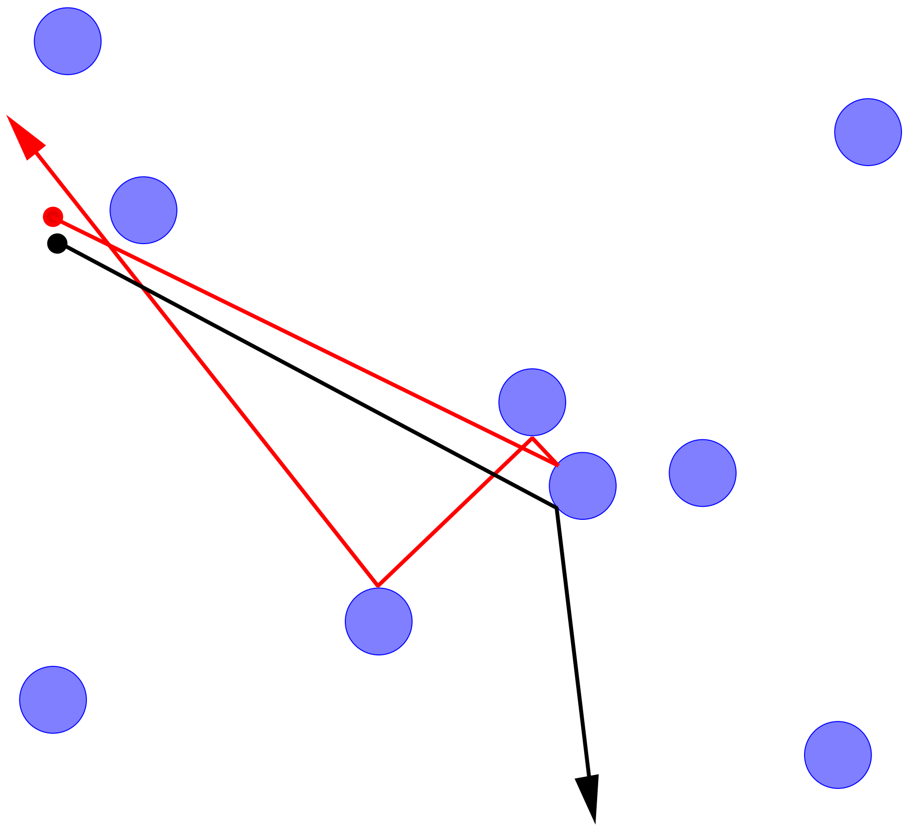
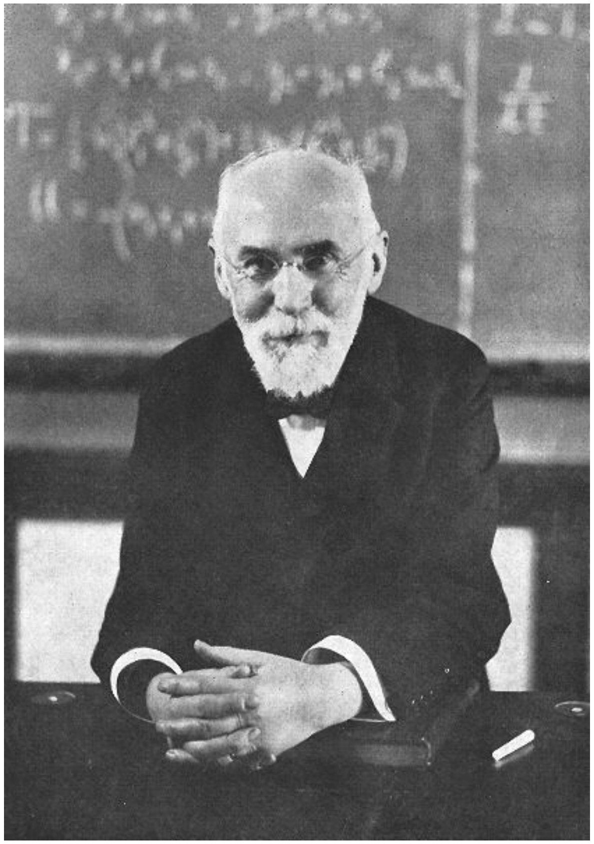
based on joint work with Andreas Strömbergsson (Uppsala)

The Lorentz gas



Arch. Neerl. (1905)



Hendrik Lorentz (1853-1928)

The Boltzmann-Grad limit

- Consider the dynamics in the limit of small scatterer radius ρ

- $\big(\boldsymbol{q}(t), \boldsymbol{v}(t)\big)$ = "microscopic" phase space coordinate at time t

- A dimensional argument shows that, in the limit $\rho \to 0$, the mean free path length (i.e., the average time between consecutive collisions) scales like $\rho^{-(d-1)}$ (= 1/total scattering cross section)

- We thus re-define position and time and use the "macroscopic" coordinates

$$\big(\boldsymbol{Q}(t), \boldsymbol{V}(t)\big) = \big(\rho^{d-1}\boldsymbol{q}(\rho^{-(d-1)}t), \boldsymbol{v}(\rho^{-(d-1)}t)\big)$$

The linear Boltzmann equation

- Time evolution of initial data $(\boldsymbol{Q}, \boldsymbol{V})$:

$$(\boldsymbol{Q}(t), \boldsymbol{V}(t)) = \Phi_\rho^t(\boldsymbol{Q}, \boldsymbol{V})$$

- Time evolution of a particle cloud with initial density $f \in \mathrm{L}^1$:

$$f_t = \mathrm{L}_\rho^t f, \qquad [L_\rho^t f](\boldsymbol{Q}, \boldsymbol{V}) := f\Big(\Phi_\rho^{-t}(\boldsymbol{Q}, \boldsymbol{V})\Big)$$

In his 1905 paper Lorentz suggested that f_t is governed, as $\rho \to 0$, by the linear Boltzmann equation:

$$\boxed{\left[\frac{\partial}{\partial t} + \boldsymbol{V} \cdot \nabla_{\boldsymbol{Q}}\right] f_t(\boldsymbol{Q}, \boldsymbol{V}) = \int_{\mathrm{S}_1^{d-1}} \Big[f_t(\boldsymbol{Q}, \boldsymbol{V}_0) - f_t(\boldsymbol{Q}, \boldsymbol{V})\Big] \sigma(\boldsymbol{V}_0, \boldsymbol{V}) \, d\boldsymbol{V}_0}$$

where the collision kernel $\sigma(\boldsymbol{V}_0, \boldsymbol{V})$ is the cross section of the individual scatterer. E.g.: $\sigma(\boldsymbol{V}_0, \boldsymbol{V}) = \frac{1}{4}\|\boldsymbol{V}_0 - \boldsymbol{V}\|^{3-d}$ for specular reflection at a hard sphere

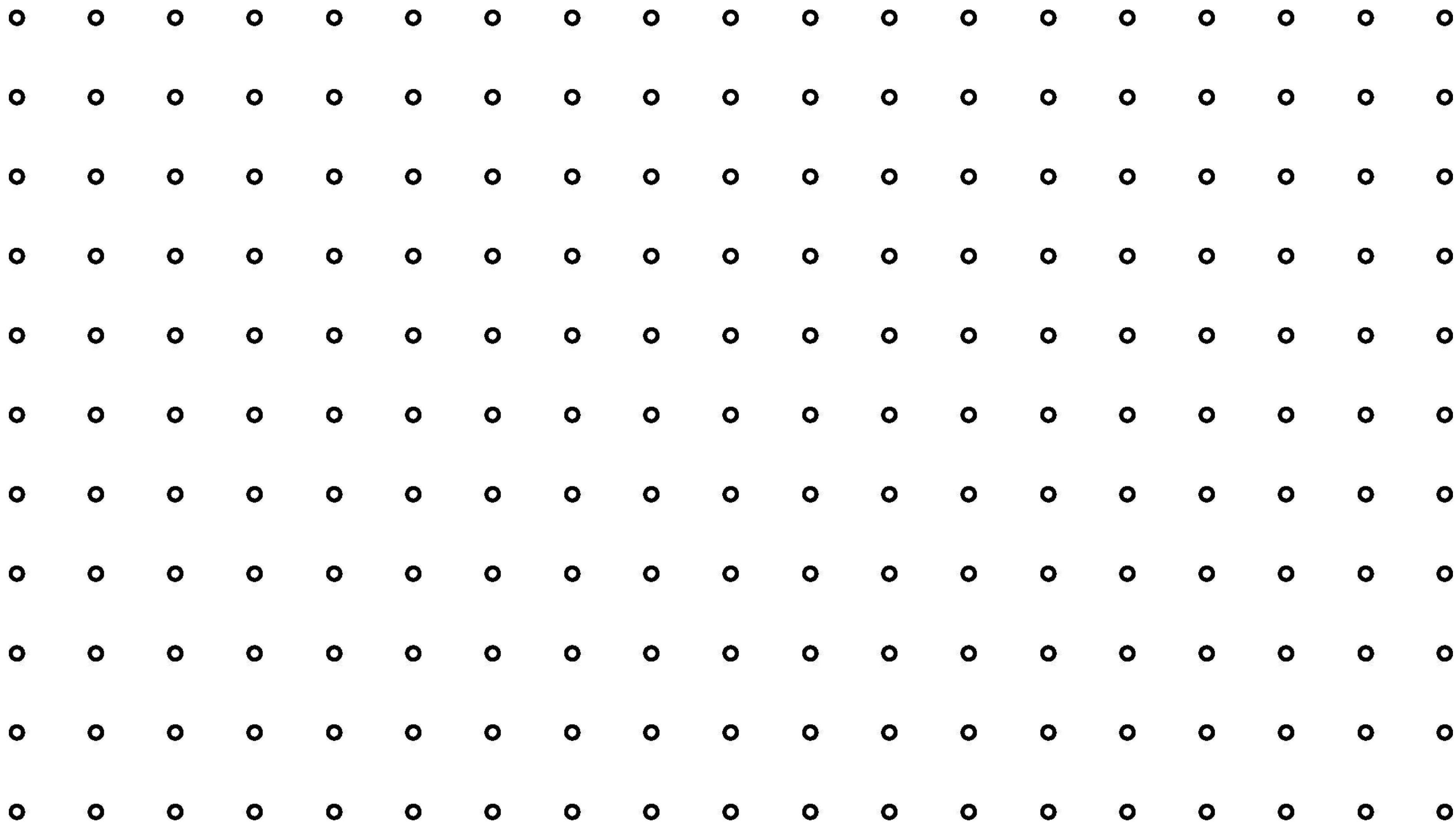
The linear Boltzmann equation—rigorous proofs

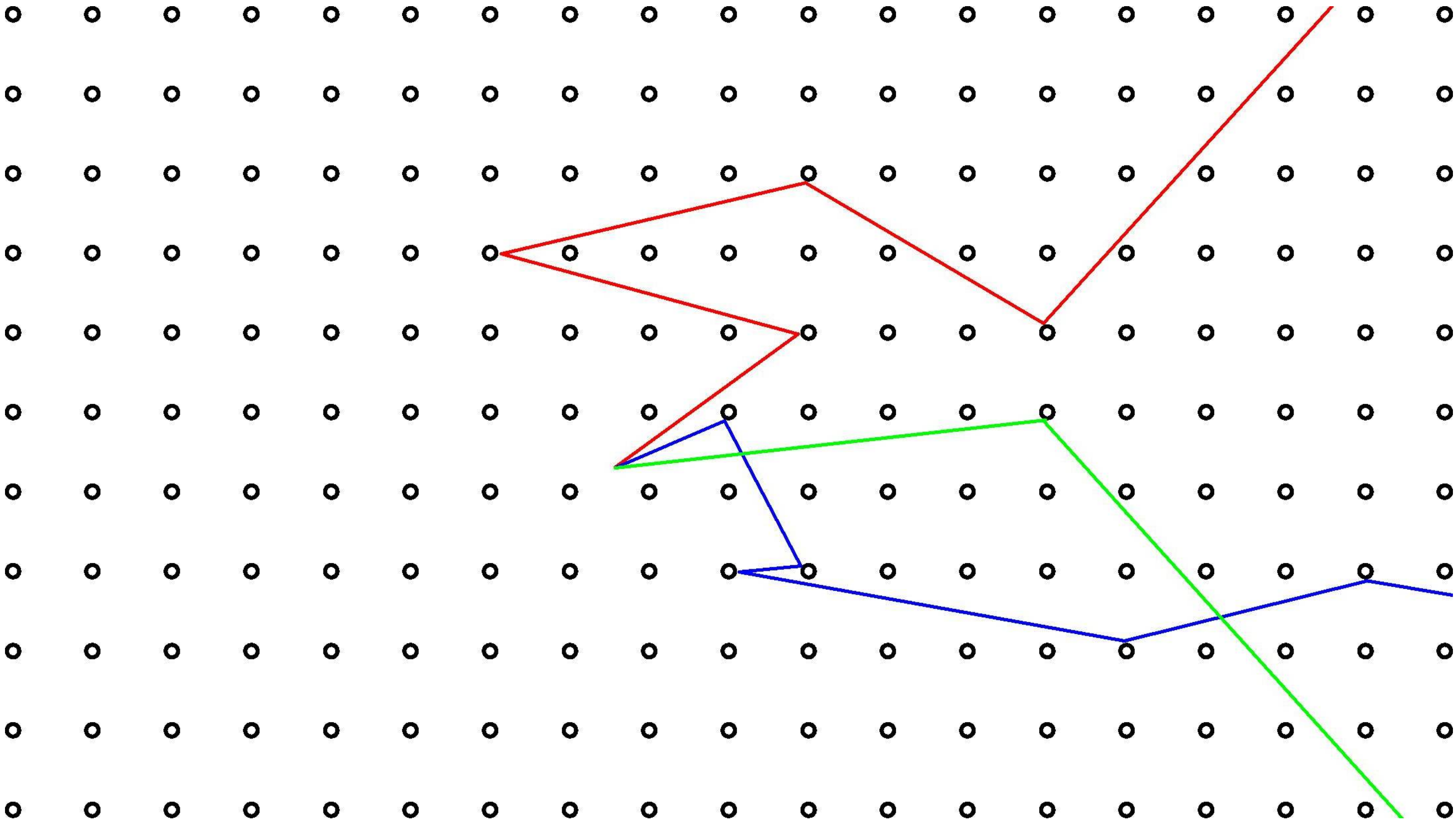
- Galavotti (Phys Rev 1969 & report 1972): Poisson distributed hard-sphere scatterers

- Spohn (Comm Math Phys 1978): extension to more general random scatterer configurations and potentials

- Boldrighini, Bunimovich and Sinai (J Stat Phys 1983): prove convergence for almost every scatterer configuration

The periodic Lorentz gas





The Boltzmann-Grad limit

- *Recall:* We are interested in the dynamics in the limit of small scatterer radius

- $(\boldsymbol{q}(t), \boldsymbol{v}(t))$ = "microscopic" phase space coordinate at time t

- Re-define position and time and use the "macroscopic" coordinates

$$(\boldsymbol{Q}(t), \boldsymbol{V}(t)) = (\rho^{d-1}\boldsymbol{q}(\rho^{-(d-1)}t), \boldsymbol{v}(\rho^{-(d-1)}t))$$

A limiting random process

A cloud of particles with initial density $f(\boldsymbol{Q},\boldsymbol{V})$ evolves in time t to

$$f_t(\boldsymbol{Q},\boldsymbol{V}) = [L_\rho^t f](\boldsymbol{Q},\boldsymbol{V}) = f\Big(\Phi_\rho^{-t}(\boldsymbol{Q},\boldsymbol{V})\Big).$$

Theorem A. For every $t > 0$ there exists a linear operator $L^t : \mathrm{L}^1(\mathrm{T}^1(\mathbb{R}^d)) \to \mathrm{L}^1(\mathrm{T}^1(\mathbb{R}^d))$, such that for every $f \in \mathrm{L}^1(\mathrm{T}^1(\mathbb{R}^d))$ and any set $\mathcal{A} \subset \mathrm{T}^1(\mathbb{R}^d)$ with boundary of Lebesgue measure zero,

$$\lim_{\rho\to 0} \int_{\mathcal{A}} [L_\rho^t f](\boldsymbol{Q},\boldsymbol{V})\, d\boldsymbol{Q}\, d\boldsymbol{V} = \int_{\mathcal{A}} [L^t f](\boldsymbol{Q},\boldsymbol{V})\, d\boldsymbol{Q}\, d\boldsymbol{V}.$$

The operator L^t thus describes the macroscopic diffusion of the Lorentz gas in the Boltzmann-Grad limit $\rho \to 0$.

Note: The family $\{L^t\}_{t\geq 0}$ does *not* form a semigroup.

A generalization of the linear Boltzmann equation

In the case of the periodic Lorentz gas L^t does not form a semigroup, and hence in particular the linear Boltzmann equation does not hold. This problem is resolved by considering extended phase space coordinates $(\boldsymbol{Q}, \boldsymbol{V}, \xi, \boldsymbol{V}_+)$ where

$(\boldsymbol{Q}, \boldsymbol{V}) \in \mathrm{T}^1(\mathbb{R}^d)$ — usual position and momentum
$\xi \in \mathbb{R}_+$ — flight time until the next scatterer
$\boldsymbol{V}_+ \in \mathrm{S}_1^{d-1}$ — velocity after the next hit

We prove the following generalization of the linear Boltzmann equation in the extended phase space:

$$\boxed{\begin{aligned}&\left[\frac{\partial}{\partial t} + \boldsymbol{V} \cdot \nabla_{\boldsymbol{Q}} - \frac{\partial}{\partial \xi}\right] f_t(\boldsymbol{Q}, \boldsymbol{V}, \xi, \boldsymbol{V}_+) \\ &\qquad\qquad = \int_{\mathrm{S}_1^{d-1}} f_t(\boldsymbol{Q}, \boldsymbol{V}_0, 0, \boldsymbol{V}) p_{\boldsymbol{0}}(\boldsymbol{V}_0, \boldsymbol{V}, \xi, \boldsymbol{V}_+) d\boldsymbol{V}_0\end{aligned}}$$

with a new collision kernel $p_{\boldsymbol{0}}(\boldsymbol{V}_0, \boldsymbol{V}, \xi, \boldsymbol{V}_+)$, given by ...

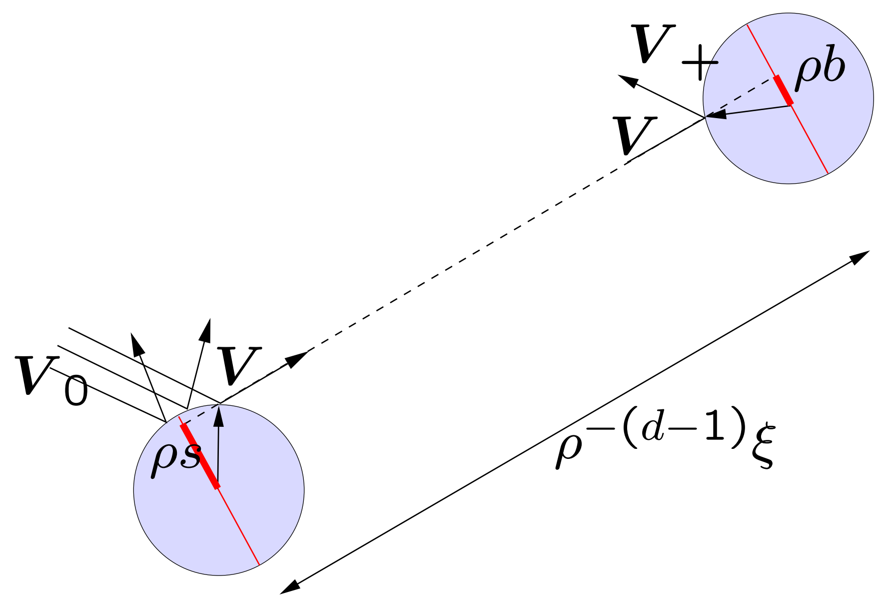
The collision kernel

$$p_{\mathbf{0}}(\boldsymbol{V}_0, \boldsymbol{V}, \xi, \boldsymbol{V}_+) = \sigma(\boldsymbol{V}, \boldsymbol{V}_+)\, \Phi_{\mathbf{0}}\Big(\xi, b(\boldsymbol{V}, \boldsymbol{V}_+), -s(\boldsymbol{V}, \boldsymbol{V}_0)\Big)$$

- $\sigma(\boldsymbol{V}, \boldsymbol{V}_+)$ the differential cross section
- $\Phi_{\mathbf{0}}\Big(\xi, b(\boldsymbol{V}, \boldsymbol{V}_+), -s(\boldsymbol{V}, \boldsymbol{V}_0)\Big)$ the transition probability to exit with parameter $s(\boldsymbol{V}, \boldsymbol{V}_0)$ and hit the next scatterer after time ξ with impact parameter $b(\boldsymbol{V}, \boldsymbol{V}_+)$

The function Φ_0

…yields the probability to exit a scatterer with parameter s and hit the next scatterer with impact parameter b after time ξ.



Why "a generalization" of the linear Boltzmann equation?

$$\left[\frac{\partial}{\partial t} + \boldsymbol{V} \cdot \nabla_{\boldsymbol{Q}} - \frac{\partial}{\partial \xi}\right] f_t(\boldsymbol{Q}, \boldsymbol{V}, \xi, \boldsymbol{V}_+)$$
$$= \int_{\mathrm{S}_1^{d-1}} f_t(\boldsymbol{Q}, \boldsymbol{V}_0, 0, \boldsymbol{V}) p_{\mathbf{0}}(\boldsymbol{V}_0, \boldsymbol{V}, \xi, \boldsymbol{V}_+) d\boldsymbol{V}_0$$

Substituting in the above the transition density for the random (rather than periodic) scatterer configuration

$$p_{\mathbf{0}}(\boldsymbol{V}_0, \boldsymbol{V}, \xi, \boldsymbol{V}_+) = \sigma(\boldsymbol{V}, \boldsymbol{V}_+) \mathrm{e}^{-\operatorname{vol}(\mathcal{B}_1^{d-1})\,\xi}$$

$$f_t(\boldsymbol{Q}, \boldsymbol{V}, \xi, \boldsymbol{V}_+) = g_t(\boldsymbol{Q}, \boldsymbol{V}) \sigma(\boldsymbol{V}, \boldsymbol{V}_+) \mathrm{e}^{-\operatorname{vol}(\mathcal{B}_1^{d-1})\,\xi}$$

yields the classical linear Boltzmann equation for $g_t(\boldsymbol{Q}, \boldsymbol{V})$.

The transition probability, $d = 2$

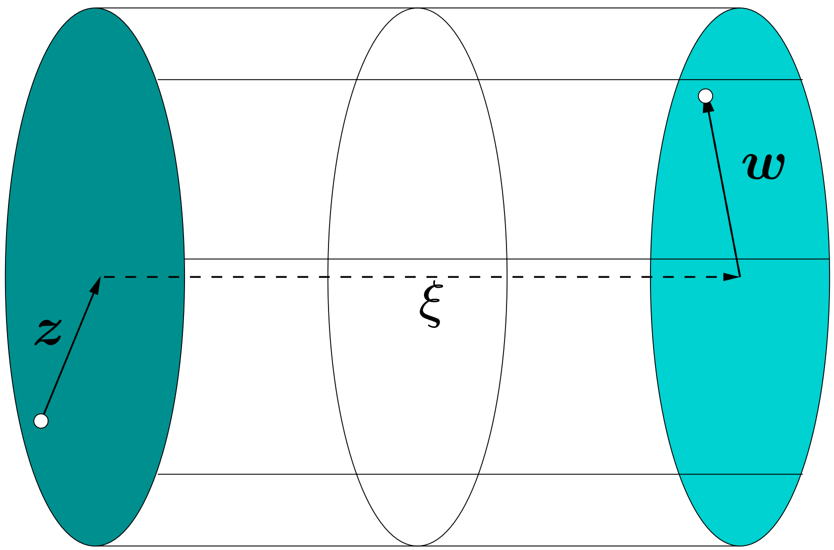
$$\Phi_{\mathbf{0}}(\xi, w, z) = \frac{6}{\pi^2} \Upsilon\left(1 + \frac{\xi^{-1} - \max(|w|, |z|) - 1}{|w+z|}\right)$$

$$\Upsilon(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } 0 < x < 1 \\ 1 & \text{if } 1 \leq x, \end{cases}$$

JM & Strömbergsson (Nonlinearity 2008), cf. also Caglioti & Golse (C.R. Acad. Sci. 2008) and Ustinov (Izv. Ran. Ser. Mat. 2009).

The transition probability, $d \geq 3$

...is given by the probability density that a "random d-dim euclidean lattice" has two lattice points at given locations, one one each cap of a cylinder of length ξ and radius 1, and no lattice point in the cylinder's interior.



The transition probability, $d \geq 3$, $\xi \to 0$

$$\Phi_{\mathbf{0}}(\xi, \boldsymbol{w}, \boldsymbol{z}) = \zeta(d)^{-1} + O(\xi)$$

The implied constant is independent of $\boldsymbol{w}, \boldsymbol{z}$ (JM & Strömbergsson, preprint 2010).

Compare with the case of a random scatterer configuration:

$$\Phi_{\mathbf{0}}(\xi, \boldsymbol{w}, \boldsymbol{z}) = \mathrm{e}^{-\operatorname{vol}(\mathcal{B}_1^{d-1})\,\xi}$$

The transition probability, $d \geq 3$, $\xi \to \infty$

There exists a continuous and uniformly bounded function

$$F : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \times \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$$

such that

$$\Phi_{\mathbf{0}}(\xi, \boldsymbol{w}, \boldsymbol{z}) = \xi^{-2+\frac{2}{d}} F\Big(\xi^{\frac{2}{d}}(1 - \|\boldsymbol{z}\|), \xi^{\frac{2}{d}}(1 - \|w\|), \xi^{\frac{1}{d}}\varphi\Big) + O(E),$$

with $\varphi := \angle(\boldsymbol{w}, \boldsymbol{z}) \in [0, \frac{\pi}{2})$, and the error term is

$$E = \begin{cases} \xi^{-2} & \text{if } \; d = 2, \\ \xi^{-2} \log(2 + \min(\xi, \varphi^{-1})) & \text{if } \; d = 3, \\ \min\Big(\xi^{-2}, \xi^{-3+\frac{2}{d-1}} \varphi^{2-d+\frac{2}{d-1}}\Big) & \text{if } \; d \geq 4. \end{cases}$$

See JM & Strömbergsson (preprint 2010).

The distribution of the free path length ($\xi \to 0$)

free path length between consecutive collisions:

$$\overline{\Phi}_{\mathbf{0}}(\xi) = \frac{1}{\mathrm{vol}(\mathcal{B}_1^{d-1})} \int_{\mathcal{B}_1^{d-1}} \int_{\mathcal{B}_1^{d-1}} \Phi_{\mathbf{0}}(\xi, \boldsymbol{w}, \boldsymbol{z})\, d\boldsymbol{w}\, d\boldsymbol{z}$$

$$\overline{\Phi}_{\mathbf{0}}(\xi) = \frac{\mathrm{vol}(\mathcal{B}_1^{d-1})}{\zeta(d)} + O(\xi)$$

free path length from a generic initial point:

$$\Phi(\xi) = \mathrm{vol}(\mathcal{B}_1^{d-1}) \int_\xi^\infty \overline{\Phi}_{\mathbf{0}}(\eta)\, d\eta$$

$$\Phi(\xi) = \mathrm{vol}(\mathcal{B}_1^{d-1}) - \frac{\mathrm{vol}(\mathcal{B}_1^{d-1})^2}{\zeta(d)} \xi + O(\xi^2)$$

(compare with random scatterer configuration)

The distribution of the free path length ($\xi \to \infty$)

free path length between consecutive collisions:

$$\overline{\Phi}_{\mathbf{0}}(\xi) = \frac{1}{\mathrm{vol}(\mathcal{B}_1^{d-1})} \int_{\mathcal{B}_1^{d-1}} \int_{\mathcal{B}_1^{d-1}} \Phi_{\mathbf{0}}(\xi, \boldsymbol{w}, \boldsymbol{z}) \, d\boldsymbol{w} \, d\boldsymbol{z}$$

$$\overline{\Phi}_{\mathbf{0}}(\xi) = \frac{2^{2-d}}{d(d+1)\zeta(d)} \xi^{-3} + O\Big(\xi^{-3-\frac{2}{d}}\Big) \begin{cases} 1 & \text{if } d = 2 \\ \log \xi & \text{if } d = 3 \\ 1 & \text{if } d \geq 4 \end{cases}$$

free path length from a generic initial point:

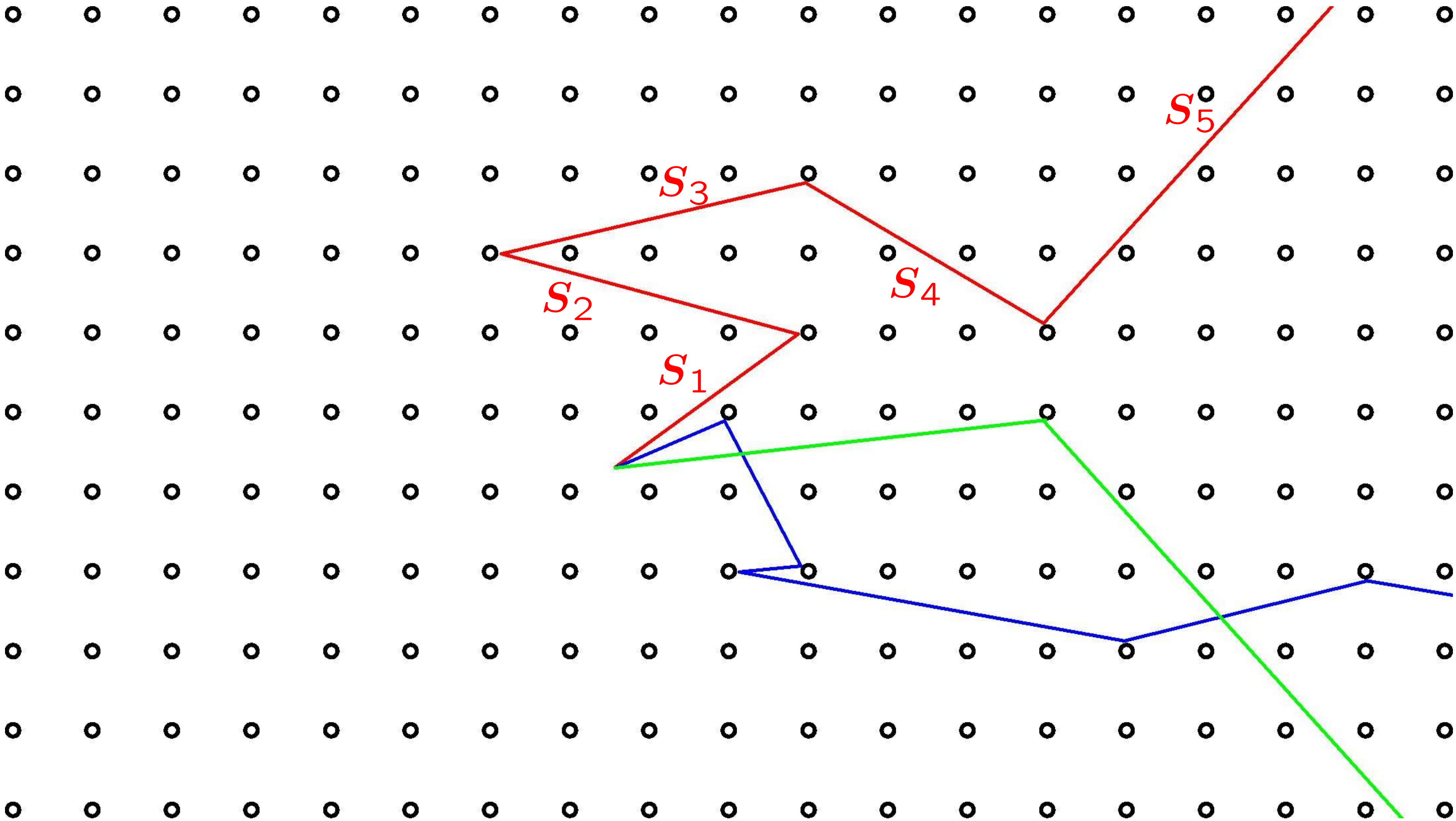
$$\Phi(\xi) = \mathrm{vol}(\mathcal{B}_1^{d-1}) \int_{\xi}^{\infty} \overline{\Phi}_{\mathbf{0}}(\eta) \, d\eta$$

$$\Phi(\xi) = \frac{\pi^{\frac{d-1}{2}}}{2^d d \, \Gamma(\frac{d+3}{2}) \, \zeta(d)} \xi^{-2} + O\Big(\xi^{-2-\frac{2}{d}}\Big)$$

This sharpens upper and lower bounds of Bourgain, Golse, Wennberg (CMP 1998) and Golse, Wennberg (CMP 2000).

The key theorem:

Joint distribution of path segments



Joint distribution for path segments

The following theorem proves the existence of a Markov process that describes the dynamics of the Lorentz gas in the Boltzmann-Grad limit.

Theorem B. Fix an a.c. Borel probability measure Λ on $\mathrm{T}^1(\mathbb{R}^d)$. Then, for each $n \in \mathbb{N}$ there exists a probability density $\Psi_{n,\Lambda}$ on $\mathbb{R}^{nd}$ such that, for any set $\mathcal{A} \subset \mathbb{R}^{nd}$ with boundary of Lebesgue measure zero,

$$\lim_{\rho \to 0} \Lambda\Big(\Big\{(\boldsymbol{Q}_0, \boldsymbol{V}_0) \in \mathrm{T}^1(\mathbb{R}^d) : (\boldsymbol{S}_1, \ldots, \boldsymbol{S}_n) \in \mathcal{A}\Big\}\Big) = \int_{\mathcal{A}} \Psi_{n,\Lambda}(\boldsymbol{S}_1', \ldots, \boldsymbol{S}_n') \, d\boldsymbol{S}_1' \cdots d\boldsymbol{S}_n',$$

and, for $n \geq 3$,

$$\Psi_{n,\Lambda}(\boldsymbol{S}_1, \ldots, \boldsymbol{S}_n) = \Psi_{2,\Lambda}(\boldsymbol{S}_1, \boldsymbol{S}_2) \prod_{j=3}^{n} \Psi(\boldsymbol{S}_{j-2}, \boldsymbol{S}_{j-1}, \boldsymbol{S}_j),$$

where Ψ is a continuous probability density independent of Λ (and the lattice).

Theorem A follows from Theorem B by standard probabilistic arguments.

First step: The distribution of free path lengths ($= S_1$)

Previous studies:

- Polya (Arch Math Phys 1918): "Visibility in a forest" ($d = 2$)

- Dahlquist (Nonlinearity 1997); Boca, Cobeli, Zaharescu (CMP 2000); Caglioti, Golse (CMP 2003); Boca, Gologan, Zaharescu (CMP 2003); Boca, Zaharescu (CMP 2007): Limit distributions for the free path lengths for various sets of initial data ($d = 2$)

- Dumas, Dumas, Golse (J Stat Phys 1997): Asymptotics of mean free path lengths ($d \geq 2$)

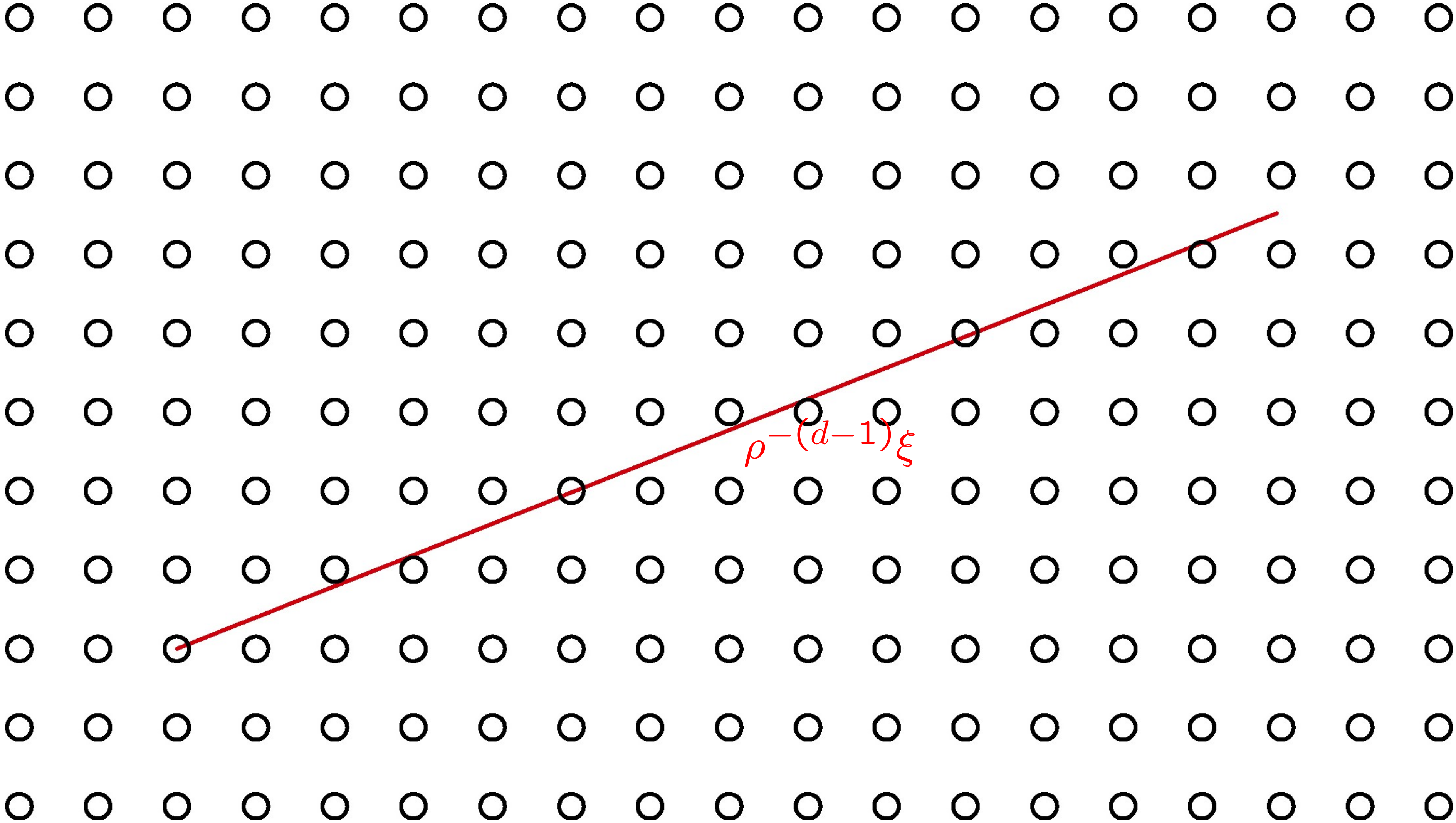
- Bourgain, Golse, Wennberg (CMP 1998); Golse, Wennberg (CMP 2000): bounds on possible weak limits ($d \geq 2$)

See also Golse's ICM review (Madrid 2006).

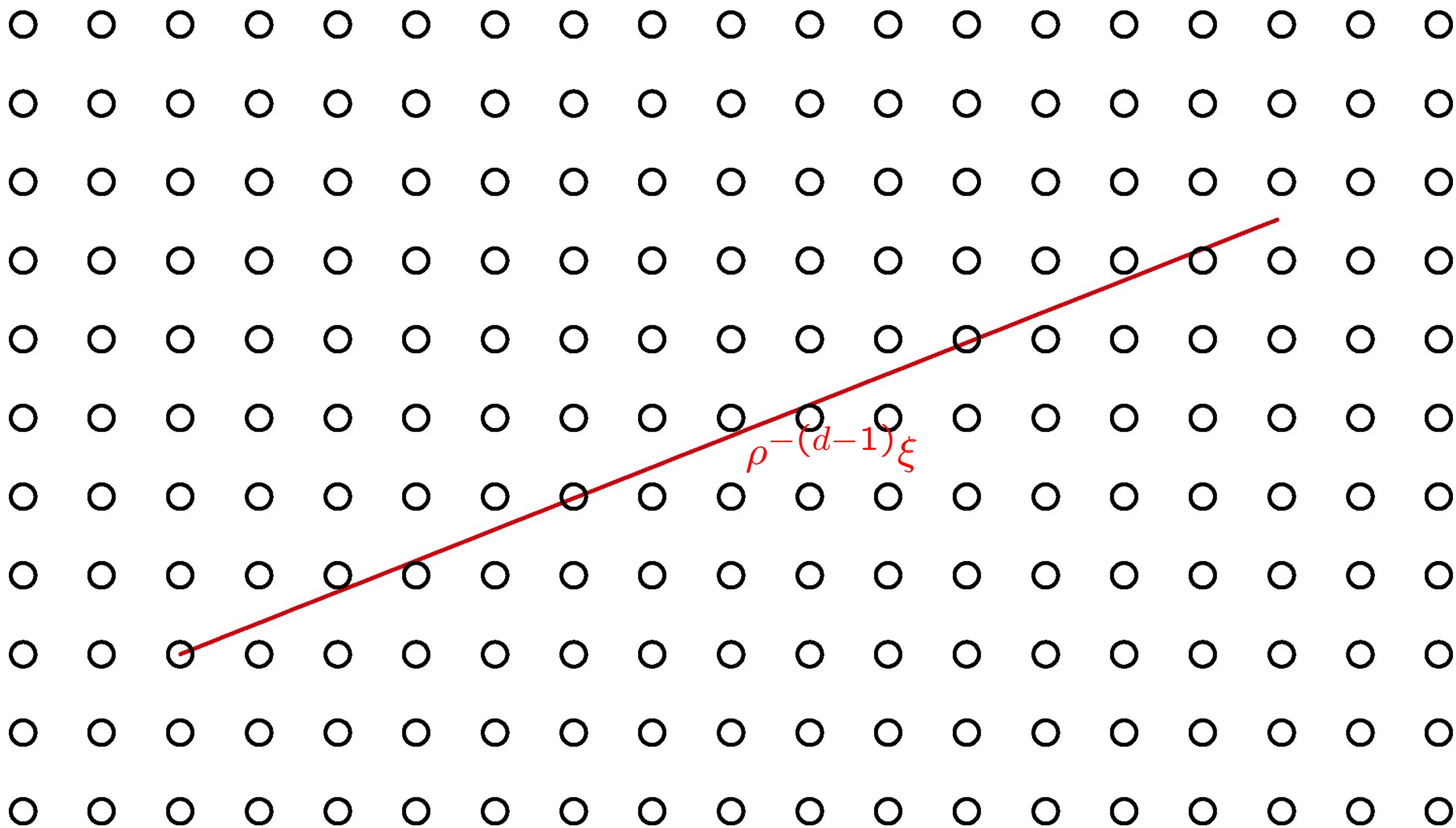
Polya's forest

The distribution of free path lengths ($= S_1$)

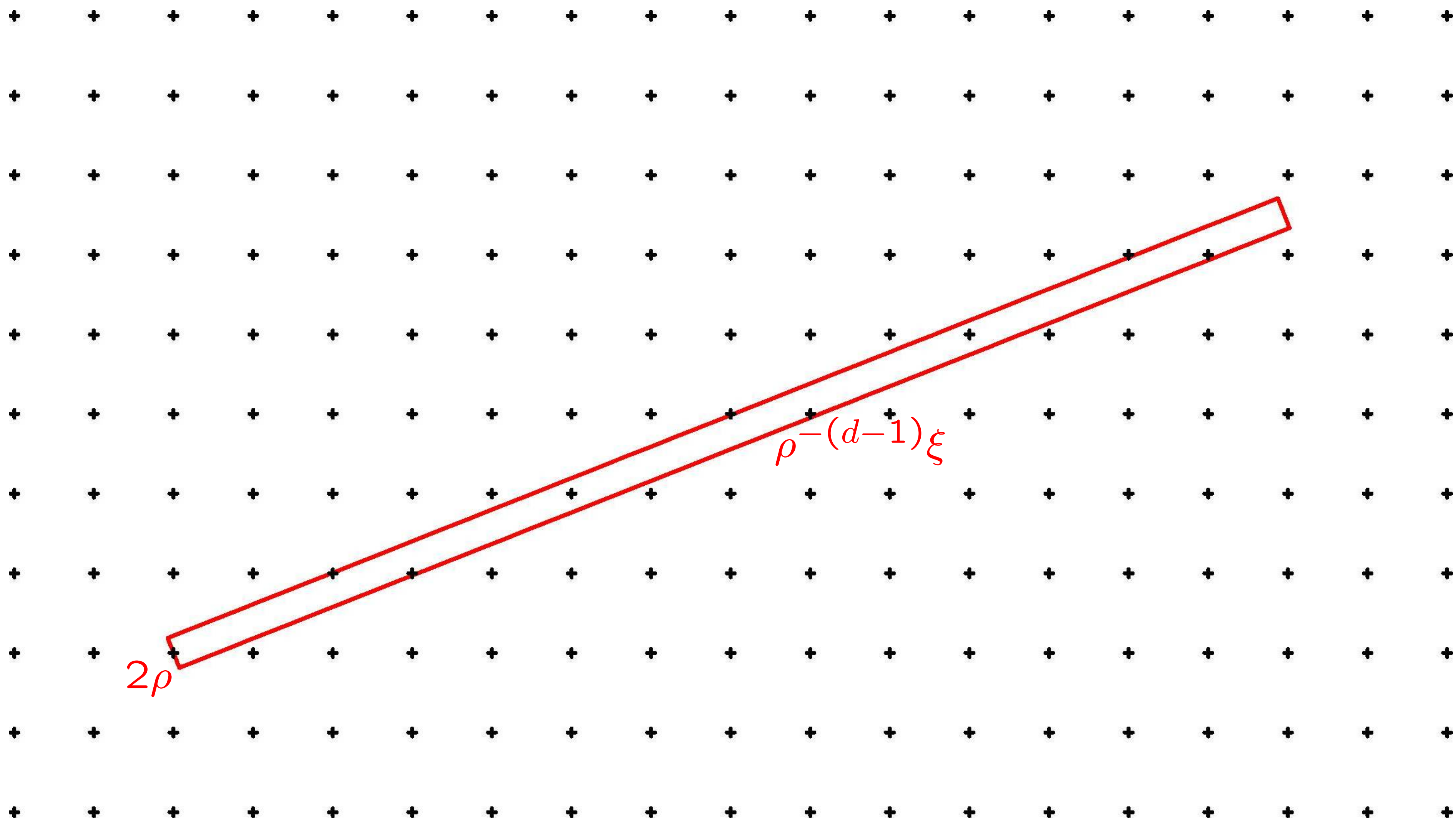
For simplcity assume $\boldsymbol{Q}_0 = \boldsymbol{0}$ and $\boldsymbol{V}_0 = \boldsymbol{v}$ random w.r.t. some a.c. prob. measure λ on S_1^{d-1}.



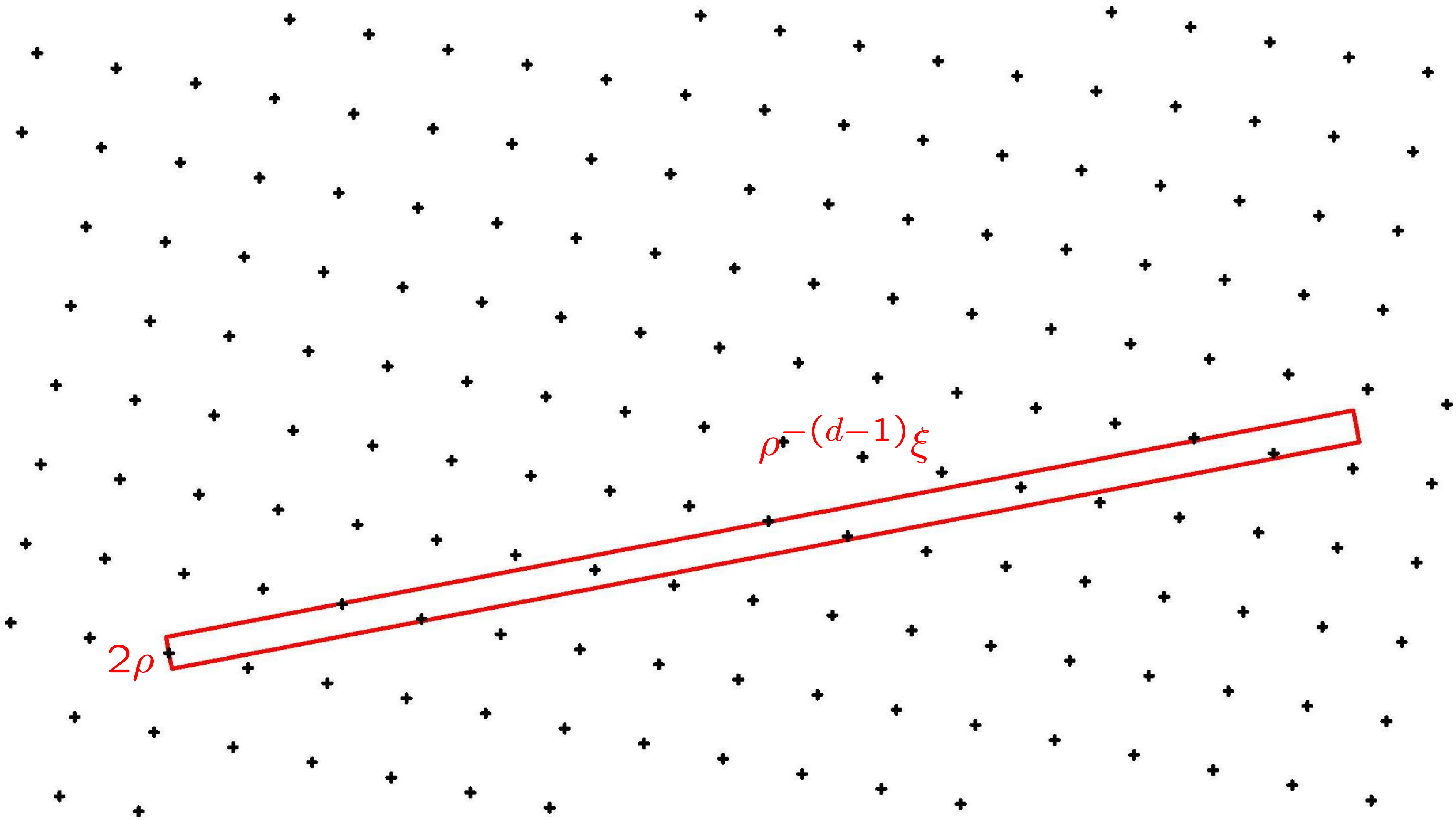
$$\lambda\Big(\Big\{\boldsymbol{v} \in \mathsf{S}_1^{d-1} : \rho^{d-1}\tau_1 \leq \xi\Big\}\Big) = \ldots$$



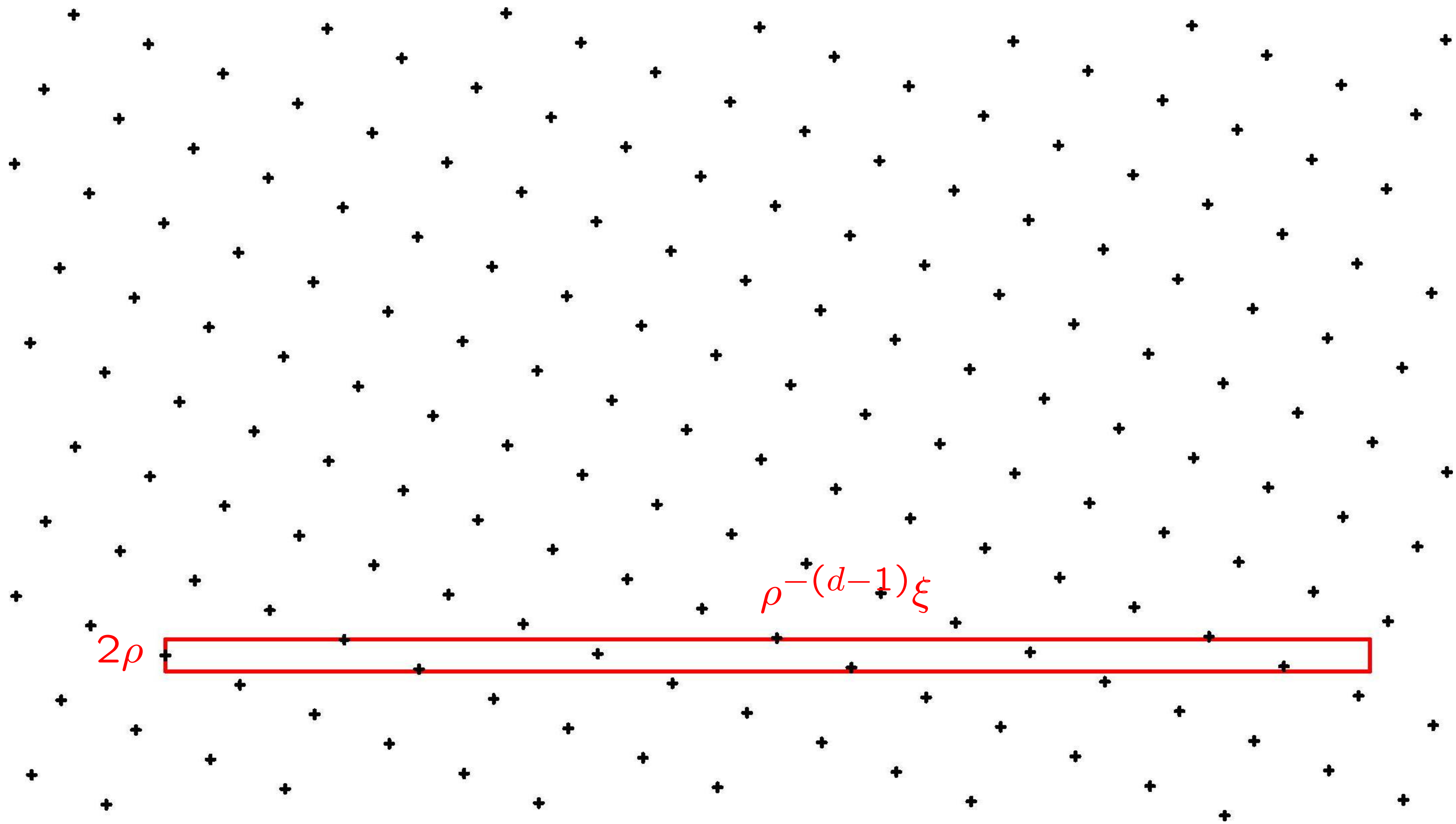
$$= \lambda\Big(\Big\{\boldsymbol{v} \in \mathsf{S}_1^{d-1} : \text{ at least one scatterer intersects } \mathsf{ray}(\boldsymbol{v}, \rho^{-(d-1)}\xi)\Big\}\Big)$$



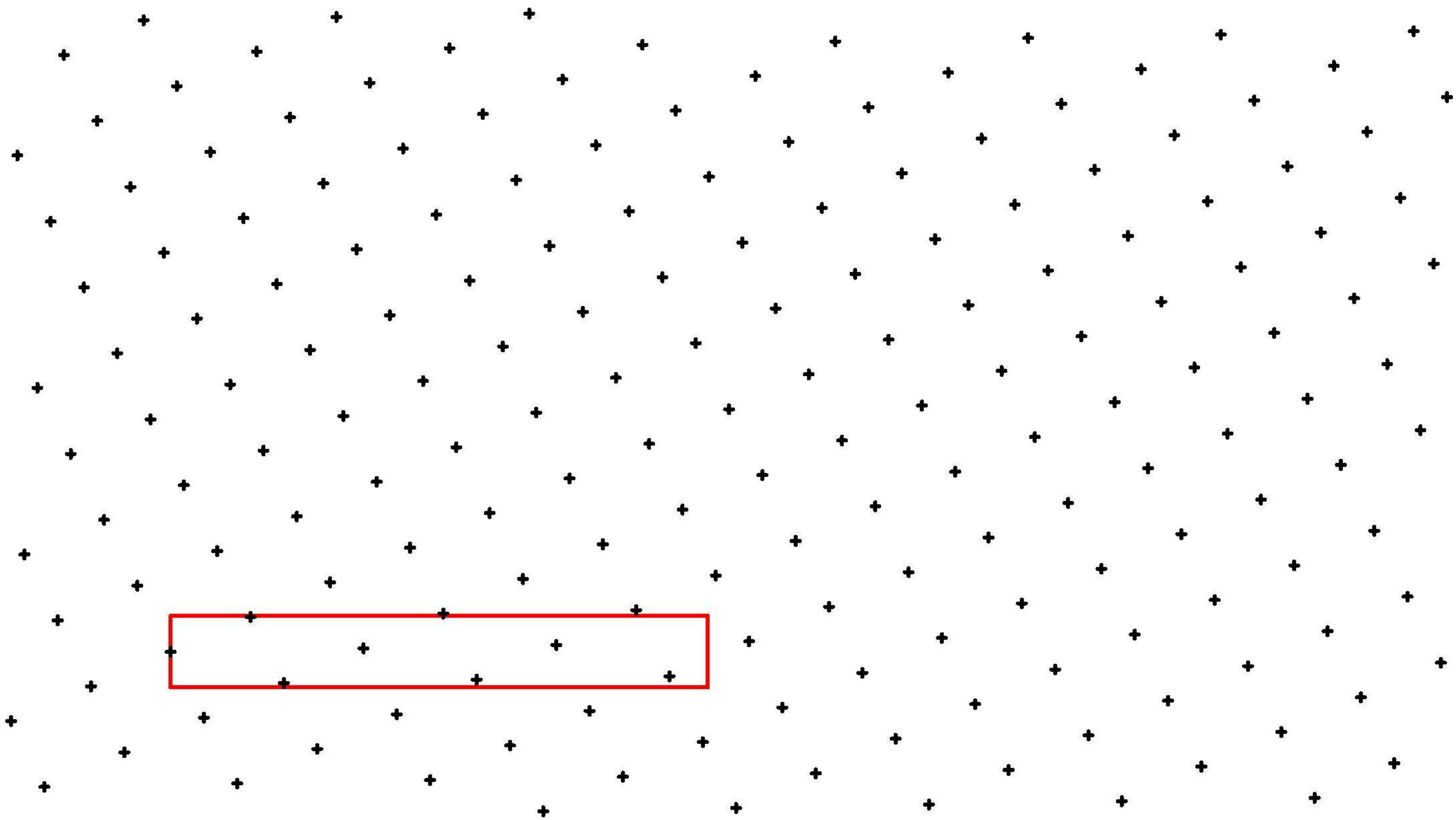
$$\approx \lambda\Big(\Big\{\boldsymbol{v} \in \mathsf{S}_1^{d-1} : \mathbb{Z}^d \cap \mathcal{Z}(\boldsymbol{v}, \rho^{-(d-1)}\xi, \rho) \neq \emptyset\Big\}\Big)$$



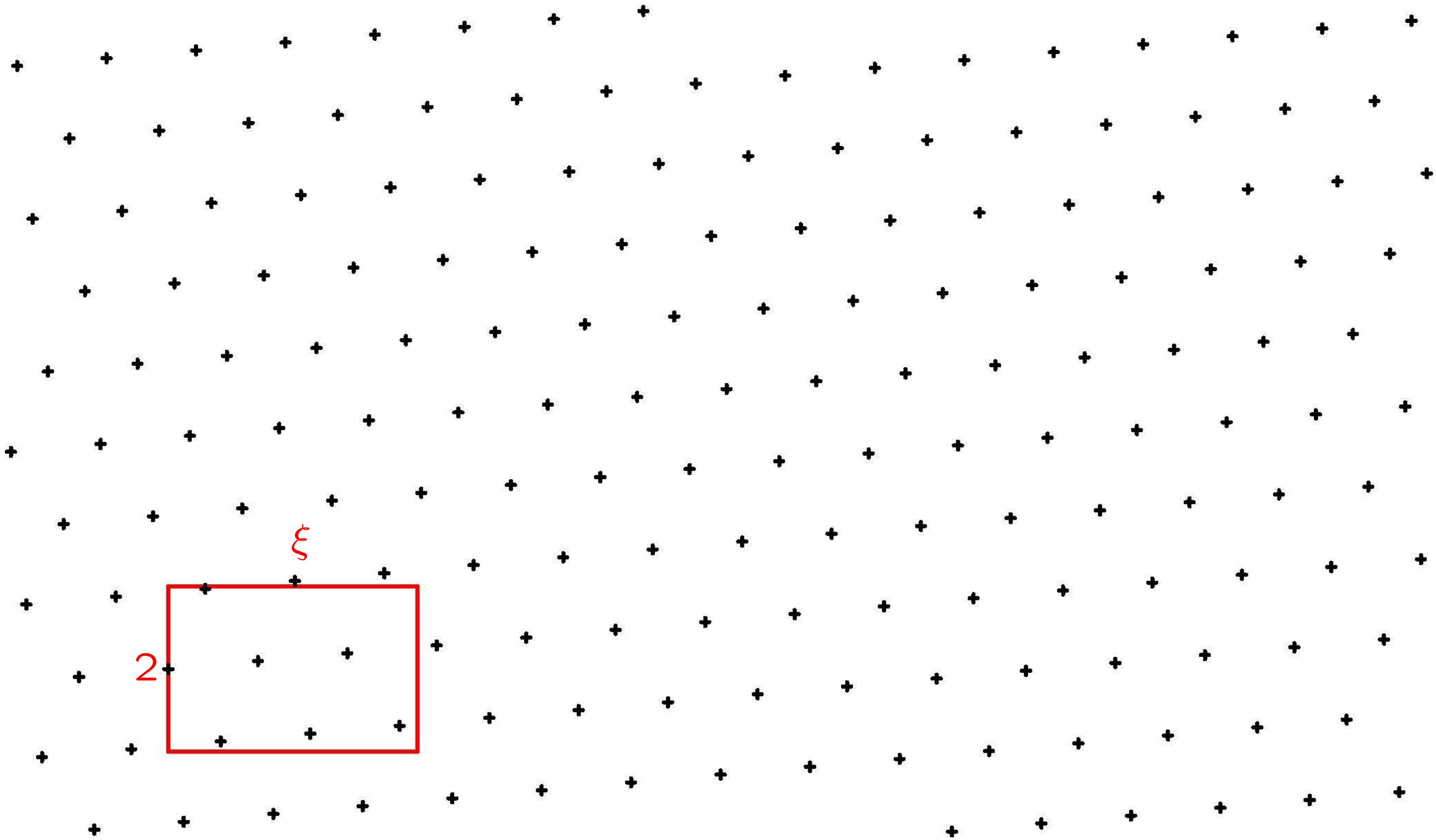
$\big($Rotate by $K(\boldsymbol{v}) \in \mathsf{SO}(d)$ such that $\boldsymbol{v} \mapsto \boldsymbol{e}_1\big)$



$$\lambda\Big(\Big\{\boldsymbol{v} \in \mathsf{S}_1^{d-1} : \mathbb{Z}^d K(\boldsymbol{v}) \cap \mathcal{Z}(\boldsymbol{e}_1, \rho^{-(d-1)}\xi, \rho) \neq \emptyset\Big\}\Big)$$



$$\Big(\text{Apply } D_\rho = \mathsf{diag}(\rho^{d-1}, \rho^{-1}, \ldots, \rho^{-1}) \in \mathsf{SL}(d, \mathbb{R})\Big)$$



$$\lambda\Big(\Big\{\boldsymbol{v} \in \mathsf{S}_1^{d-1} : \mathbb{Z}^d K(\boldsymbol{v}) D_\rho \cap \mathcal{Z}(\boldsymbol{e}_1, \xi, 1) \neq \emptyset\Big\}\Big)$$

The following Theorem shows that in the limit $\rho \to 0$ the lattice

$$\mathbb{Z}^d K(\boldsymbol{v}) \begin{pmatrix} \rho^{d-1} & \mathbf{0} \\ {}^t\mathbf{0} & \rho^{-1}1 \end{pmatrix}$$

behaves like a random lattice with respect to Haar measure μ_1.

Define a flow on $X_1 = \mathrm{SL}(d,\mathbb{Z})\backslash\,\mathrm{SL}(d,\mathbb{R})$ via right translation by

$$\Phi^t = \begin{pmatrix} \mathrm{e}^{-(d-1)t} & \mathbf{0} \\ {}^t\mathbf{0} & \mathrm{e}^t 1 \end{pmatrix}, \qquad t = \log 1/\rho.$$

Theorem C. Fix any $M_0 \in \mathrm{SL}(d,\mathbb{R})$. Let λ be an a.c. Borel probability measure on S_1^{d-1}. Then, for every bounded continuous function $f : X_1 \to \mathbb{R}$,

$$\lim_{t\to\infty} \int_{\mathrm{S}_1^{d-1}} f(M_0 K(\boldsymbol{v})\Phi^t)\, d\lambda(\boldsymbol{v}) = \int_{X_1} f(M)\, d\mu_1(M).$$

Theorem C is a direct consequence of the mixing property for the flow Φ^t.

The generalization of Theorem C required for the full proof of Theorem C uses Ratner's classification of ergodic measures invariant under a unipotent flow. We exploit a close variant of a theorem by N. Shah (Proc. Ind. Acad. Sci. 1996) on the uniform distribution of translates of unipotent orbits.

The central argument in the proof of Theorem B (joint distribution of path segments) follows a similar route, but is significantly more involved.

Conclusions

- We have seen that the dynamics of the periodic Lorentz gas converges, in the Boltzmann-Grad limit, to a random flight process that is Markov with memory two.

- The distribution of the free path lengths has polynomial tails, in stark contrast to the random scatterer configuration, where the distribution is exponential.

- The corresponding evolution equation is a generalized Boltzmann equation with a collision kernel that is independent of the choice of lattice.

- The proof exploits the dynamics on the space of (affine) lattices, and the transition probabilities of the limit process are related to natural measures on these homogeneous spaces.

Outlook

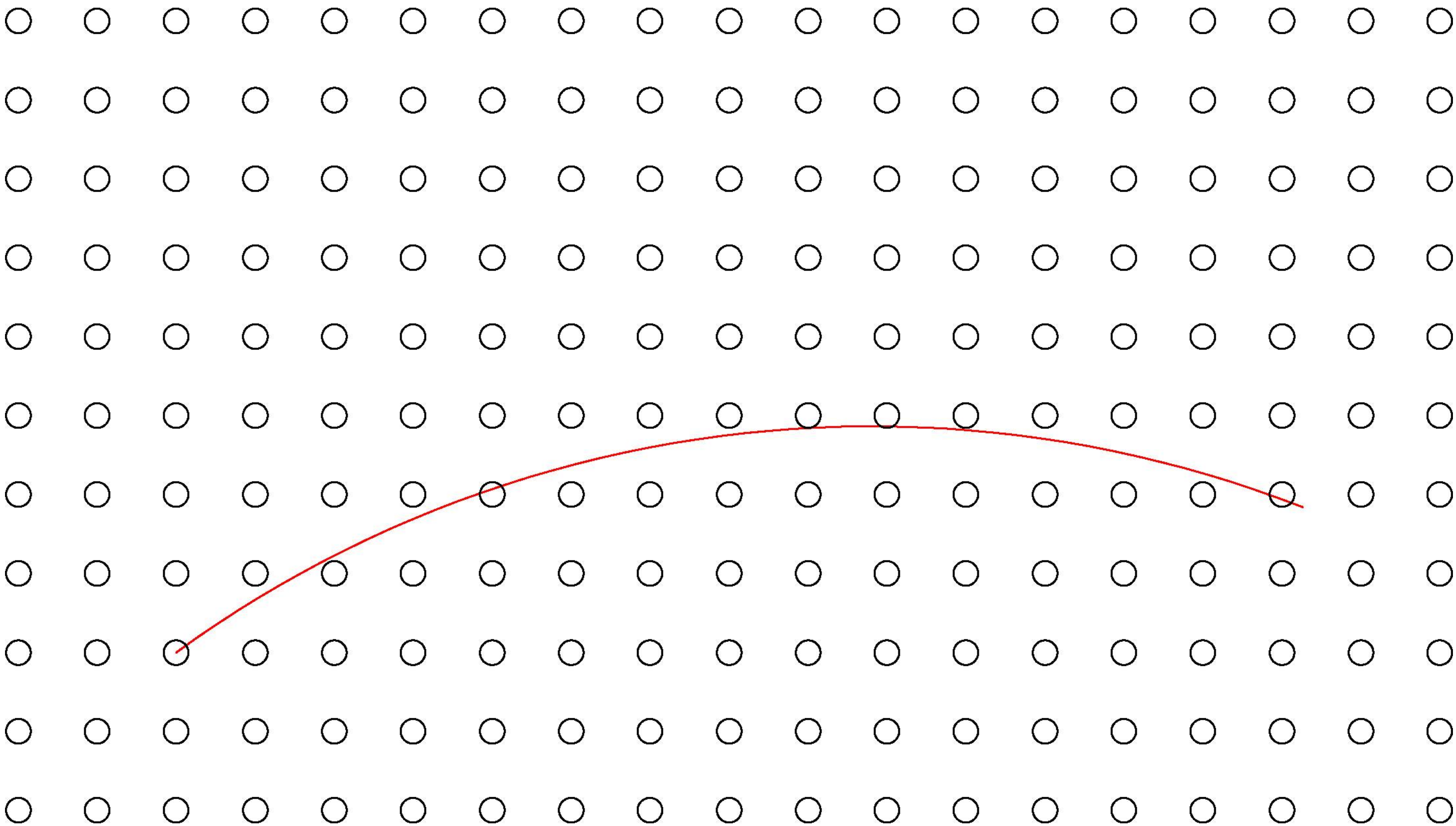
- Long-time dynamics of the limit process? Intermediate scaling limits?

- Other scatterer configurations: Random defects, quasicrystals, electron-phonon interactions?

- Long-range potentials? Electro-magnetic fields?

- Quantum analogue of the generalized linear Boltzmann equation?

The Lorentz gas in external fields



$\Big($work in progress . . . $\Big)$

The Lorentz gas in external fields

Rescaled Lagrangian:

$$L_\epsilon(\boldsymbol{q}, \boldsymbol{v}) = L(\epsilon \boldsymbol{q}, \boldsymbol{v}),$$

where $L(\boldsymbol{q}, \boldsymbol{v})$ is a fixed macroscopic Lagrangian, and $\epsilon > 0$ a small scaling parameter. A classical example is

$$L(\boldsymbol{q}, \boldsymbol{v}) = \frac{1}{2}\|\boldsymbol{v}\|^2 + \boldsymbol{A}(\boldsymbol{q}) \cdot \boldsymbol{v} - \varphi(\boldsymbol{q}),$$

where $(\varphi(\boldsymbol{q}), \boldsymbol{A}(\boldsymbol{q}))$ is the electro-magnetic potential.

Example

In dimension $d = 3$ this leads to the evolution equation

$$\dot{\boldsymbol{v}} = \boldsymbol{E}(\boldsymbol{q}) + \boldsymbol{v} \times \boldsymbol{B}(\boldsymbol{q})$$

with electric and magnetic field defined by

$$\boldsymbol{E} = -\nabla \varphi, \qquad \boldsymbol{B} = \nabla \times \boldsymbol{A}.$$

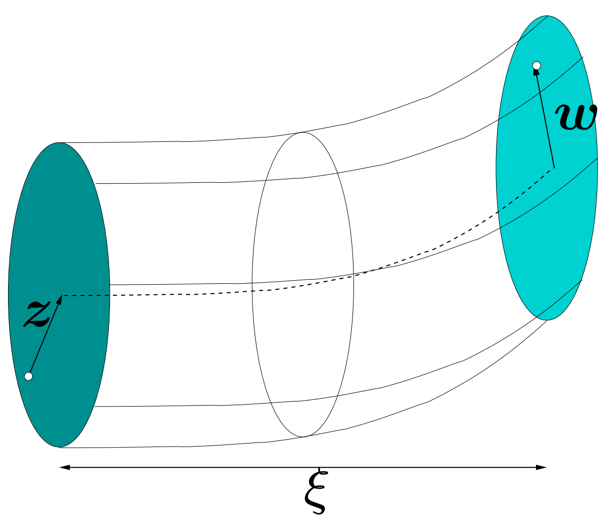
A simple calculation shows that the corresponding equation for the scaled Lagragian reads

$$\dot{\boldsymbol{v}} = \epsilon \boldsymbol{E}(\epsilon \boldsymbol{q}) + \boldsymbol{v} \times \epsilon \boldsymbol{B}(\epsilon \boldsymbol{q}).$$

Hence the effective fields are *weak* (of order ϵ) and *external* (slowly varying on a scale of $1/\epsilon$).

Interesting scaling limits

- $\epsilon \asymp \rho^{d-1}$ (inverse free path length): This leads to the problem of counting lattice points in long and thin *curved* strips, similar to those discussed by Sinai, Major, Cheng-Lebowitz-Major in connection with problems in quantum chaos. For typical fields I conjecture the classical linear Boltzmann equation to hold (or one of its standard generalizations).
- $\rho^{2d-1} \lll \epsilon \lll \rho^{d-1}$: Again we can expect the classical linear Boltzmann equation to hold.
- $\epsilon \asymp \rho^{2d-1}$: Here we can prove the analogs of the above results for zero external fields, where the in the transition probability the cylinder is replaced by a "parabolic tube".



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