

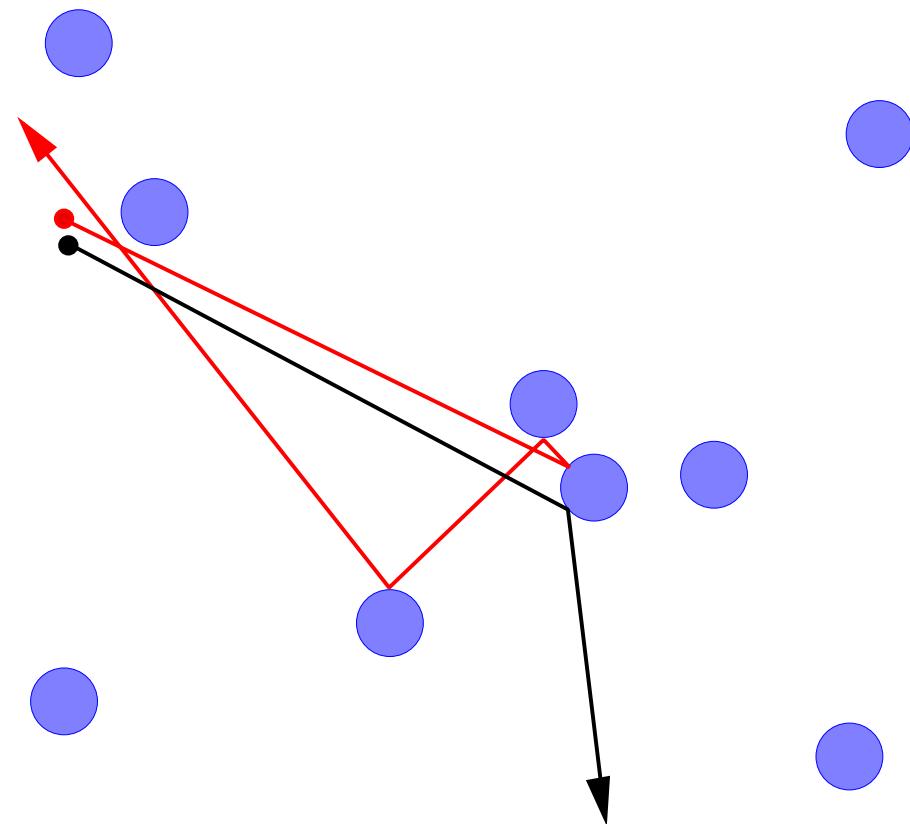
Kinetic transport in crystals

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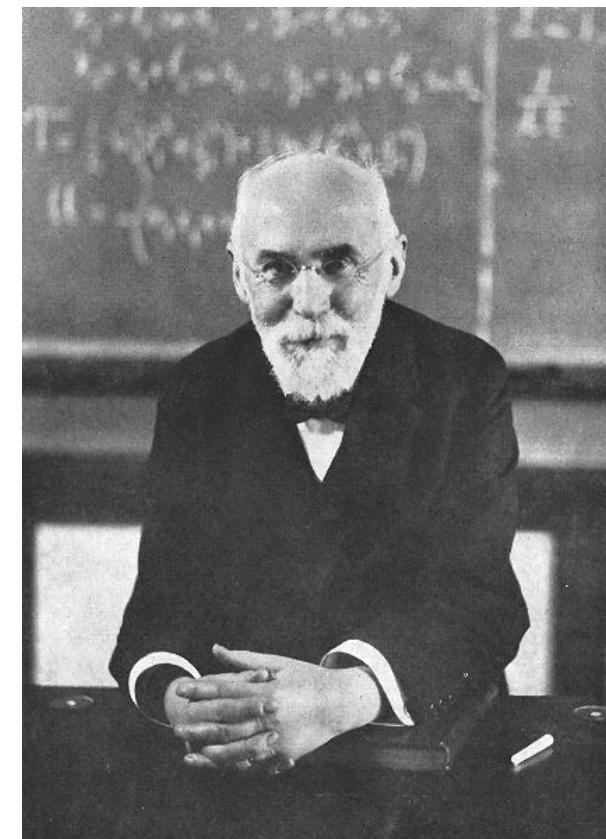
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based on joint work with Andreas Strömbergsson (Uppsala)

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
- $(\mathbf{q}(t), \mathbf{v}(t))$ = “microscopic” phase space coordinate at time t
- A dimensional argument shows that, in the limit $\rho \rightarrow 0$, 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

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

The linear Boltzmann equation

- Time evolution of initial data (Q, V) :

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

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

$$f_t = \mathcal{L}_\rho^t f, \quad [L_\rho^t f](Q, V) := f(\Phi_\rho^{-t}(Q, V))$$

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

$$\left[\frac{\partial}{\partial t} + V \cdot \nabla_Q \right] f_t(Q, V) = \int_{S_1^{d-1}} [f_t(Q, V_0) - f_t(Q, V)] \sigma(V_0, V) dV_0$$

where the collision kernel $\sigma(V_0, V)$ is the cross section of the individual scatterer. E.g.: $\sigma(V_0, V) = \frac{1}{4} \|V_0 - V\|^{3-d}$ for specular reflection at a hard sphere

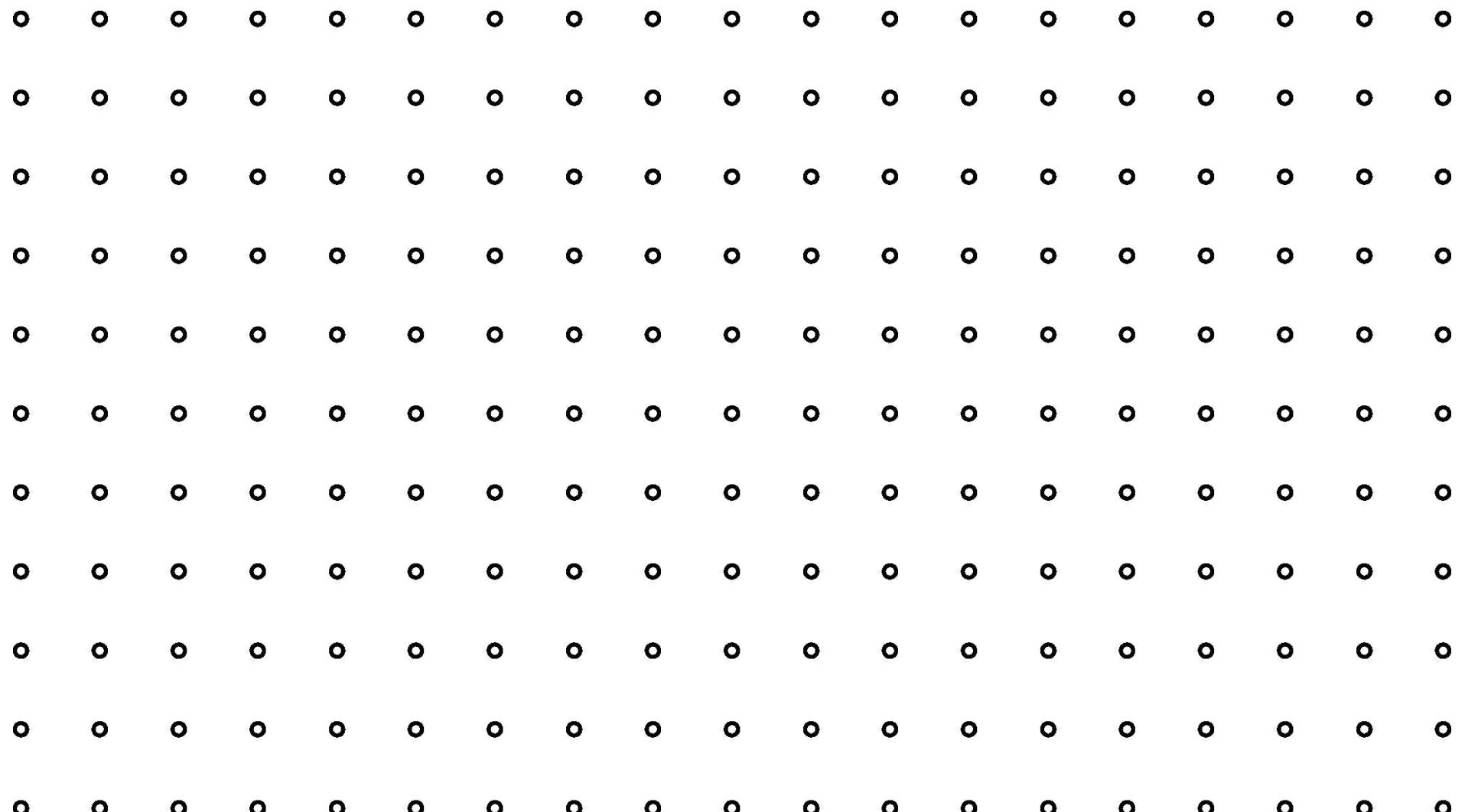
The linear Boltzmann equation—rigorous proofs

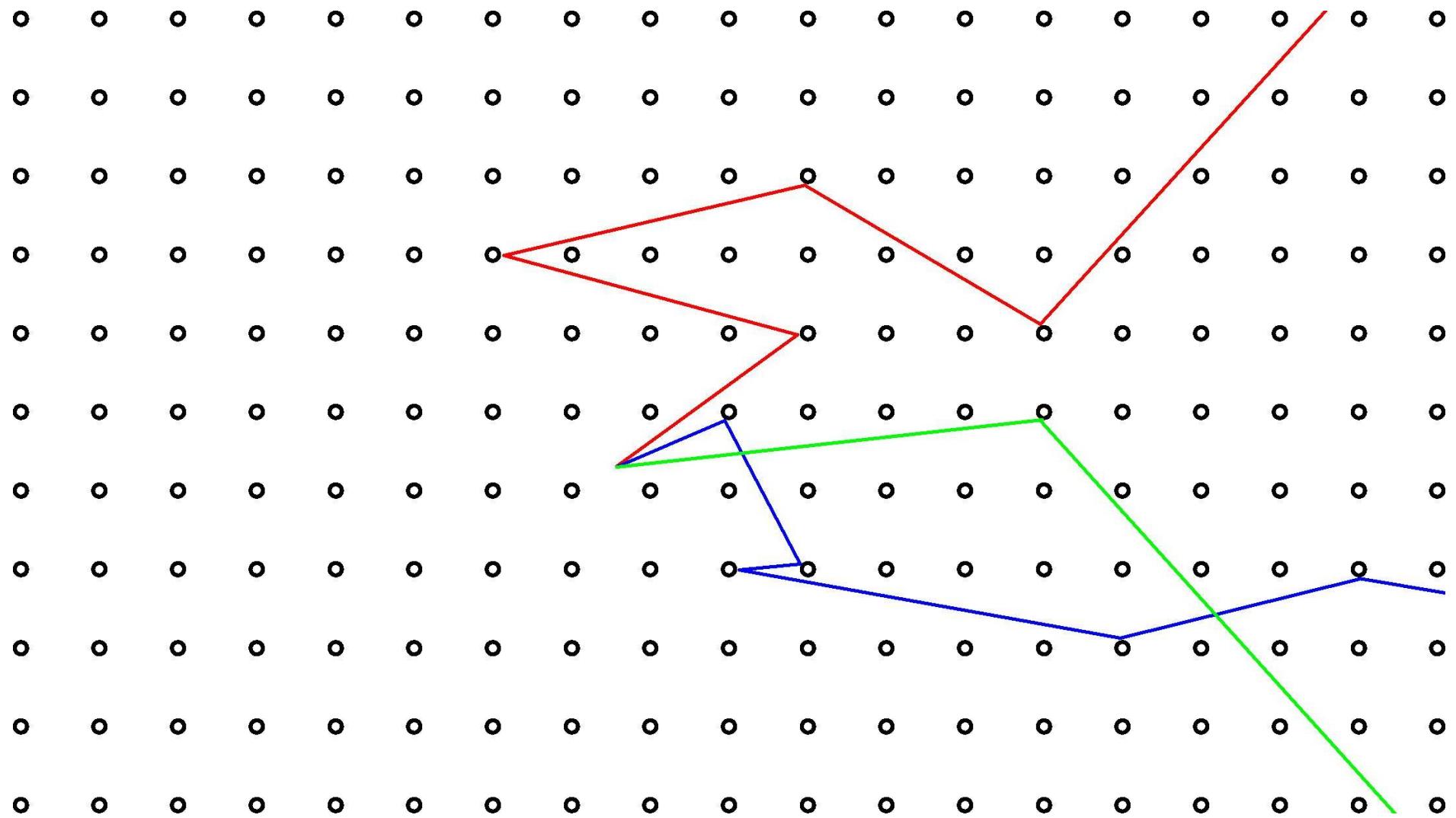
- Galavotti (Phys Rev 1969 & report 1972): Poisson distributed hard-sphere scatterers
- Spohn (Comm Math Phys 1978): extension to more general random scatterer configurations and potentials
- Boldrighini, Bunimovich and Sinai (J Stat Phys 1983): prove convergence for almost every scatterer configuration

The quantum linear Boltzmann equation

- Spohn (J Stat Phys 1977): Gaussian random potentials, small times
- Erdős and Yau (Contemp Math 1998, Comm Pure Appl Math 2000): General random potentials, weak coupling limit
- Eng and Erdős (Rev Math Phys 2005): Low density limit

The periodic Lorentz gas





Chaotic diffusion for *fixed* scatterer radius ρ

- Bunimovich and Sinai (Comm Math Phys 1980/81): In the case of finite horizon* and in dimension $d = 2$, the dynamics is diffusive in the limit of large times t , and satisfies a central limit theorem with normalization \sqrt{t} .
- Melbourne and Nicol (Comm Math Phys 2005): Invariance principles for $d = 2$ and finite horizon.
- Bleher (J Stat Phys 1992), Szasz-Varju (2007): Central limit theorem for infinite horizon; the normalization is now $\sqrt{t \log t}$ (due to the free flight corridors).
- Central limit theorem still unproven in higher dimensions; cf. Chernov (J Stat Phys 1994), Balint-Toth (2007).

*“Finite horizon” means that the scatterers are configured so that the path length between consecutive collisions is bounded.

The Boltzmann-Grad limit

- *Recall:* We are interested in the dynamics in the limit of small scatterer radius
- $(\mathbf{q}(t), \mathbf{v}(t))$ = “microscopic” phase space coordinate at time t
- Re-define position and time and use the “macroscopic” coordinates

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

A limiting random process

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

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

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

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

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

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 (Q, V, ξ, V_+) where

$(Q, V) \in \mathbb{T}^1(\mathbb{R}^d)$ — usual position and momentum

$\xi \in \mathbb{R}_+$ — flight time until the next scatterer

$V_+ \in S_1^{d-1}$ — velocity after the next hit

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

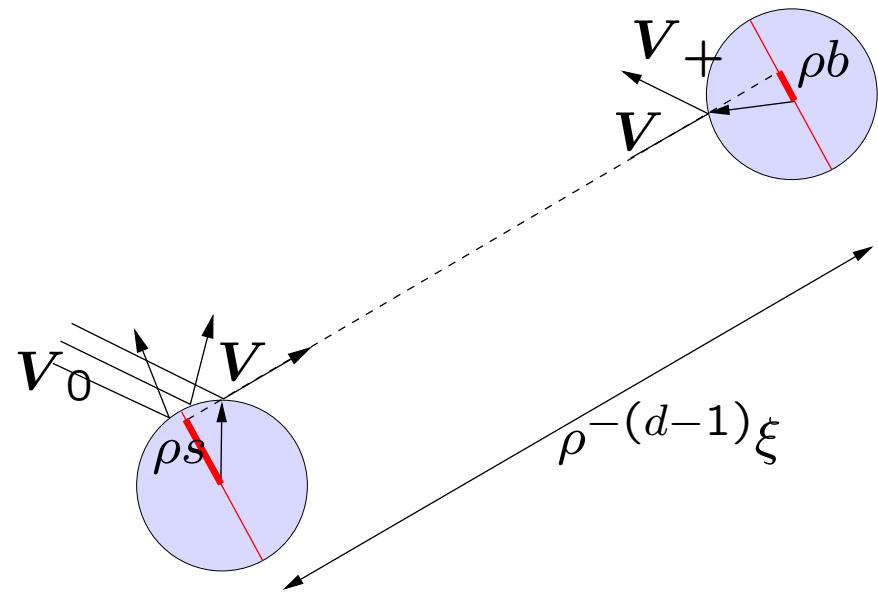
$$\begin{aligned} \left[\frac{\partial}{\partial t} + V \cdot \nabla_Q - \frac{\partial}{\partial \xi} \right] f_t(Q, V, \xi, V_+) \\ = \int_{S_1^{d-1}} f_t(Q, V_0, 0, V) p_0(V_0, V, \xi, V_+) dV_0 \end{aligned}$$

with a new collision kernel $p_0(V_0, V, \xi, V_+)$, given by ...

The collision kernel

$$p_0(V_0, V, \xi, V_+) = \sigma(V, V_+) \Phi_0(\xi, b(V, V_+), -s(V, V_0))$$

- $\sigma(V, V_+)$ the differential cross section
- $\Phi_0(\xi, b(V, V_+), -s(V, V_0))$ the transition probability to exit with parameter $s(V, V_0)$ and hit the next scatterer after time ξ with impact parameter $b(V, V_+)$



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 .

In dimension $d = 2$ (JM & Strömbergsson, Nonlinearity 2008):

$$\Phi_0(\xi, w, z) = \frac{6}{\pi^2} \Upsilon \left(1 + \frac{\xi^{-1} - \max(|w|, |z|) - 1}{|w + z|} \right)$$

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

cf. also Caglioti & Golse (C.R. Acad. Sci. 2008) and Ustinov (2008).

Our formulas for dimension $d > 2$ are not as explicit and substantially more involved.

The operators L^t in Theorem A can be defined by the relation

$$[L^t g](Q, V) := \int_0^\infty \int_{S_1^{d-1}} f_t(Q, V, \xi, V_+) dV_+ d\xi$$

where $f_t(Q, V, \xi, V_+)$ is a solution of the generalized linear Boltzmann equation subject to the initial condition

$$\lim_{t \rightarrow 0} f_t(Q, V, \xi, V_+) = g(Q, V) p(V, \xi, V_+)$$

with

$$p(V, \xi, V_+) := \int_\xi^\infty \int_{S_1^{d-1}} \sigma(V_0, V) p_0(V_0, V, \xi, V_+) dV_0 d\xi;$$

the latter is a stationary solution of the generalized linear Boltzmann equation.

Why “a generalization” of the linear Boltzmann equation?

$$\begin{aligned} \left[\frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla_{\mathbf{Q}} - \frac{\partial}{\partial \xi} \right] f_t(\mathbf{Q}, \mathbf{V}, \xi, \mathbf{V}_+) \\ = \int_{S_1^{d-1}} f_t(\mathbf{Q}, \mathbf{V}_0, 0, \mathbf{V}) p_0(\mathbf{V}_0, \mathbf{V}, \xi, \mathbf{V}_+) d\mathbf{V}_0 \end{aligned}$$

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

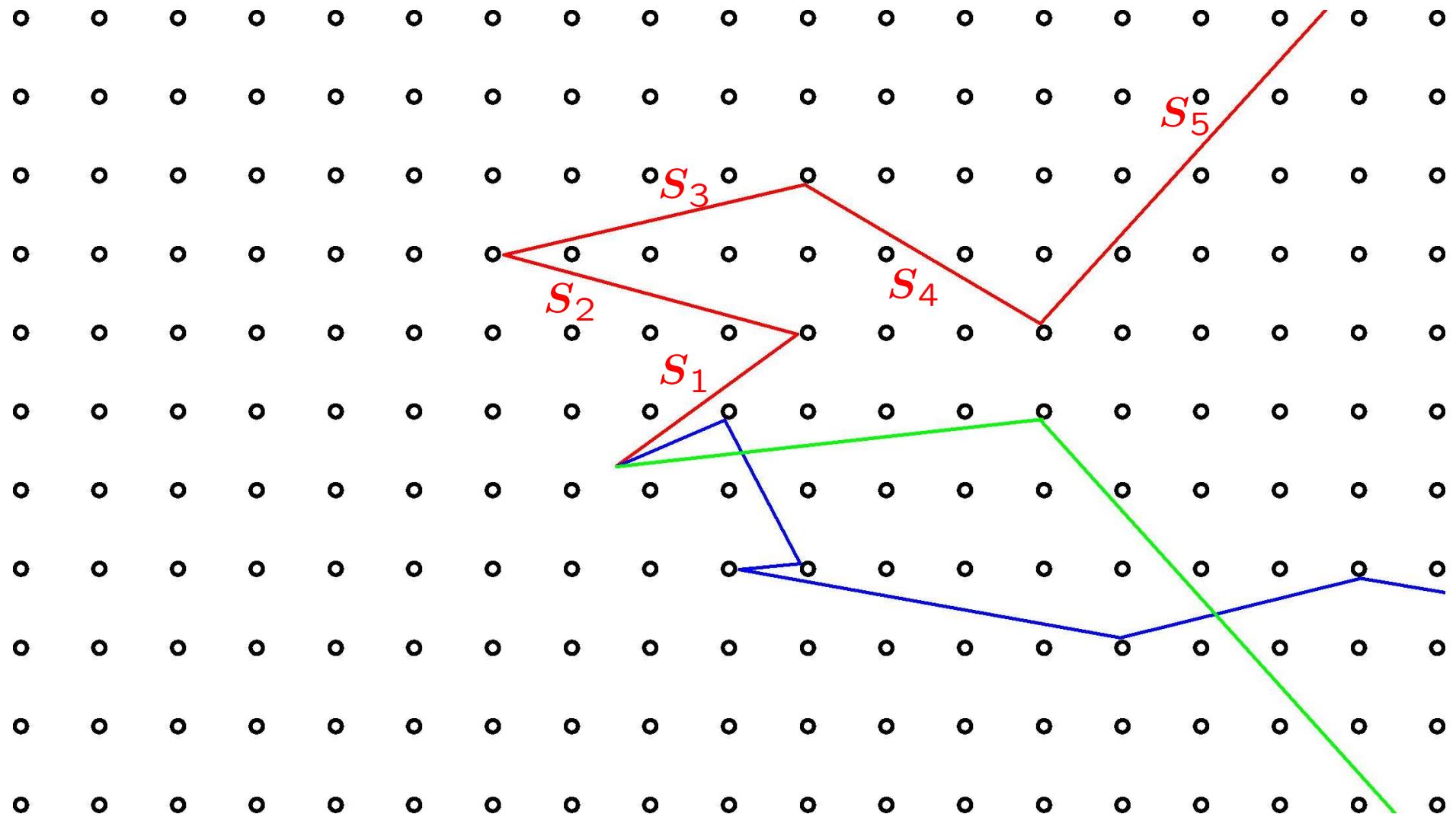
$$p_0(\mathbf{V}_0, \mathbf{V}, \xi, \mathbf{V}_+) = \sigma(\mathbf{V}, \mathbf{V}_+) e^{-\text{vol}(\mathcal{B}_1^{d-1}) \xi}$$

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

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

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 $T^1(\mathbb{R}^d)$. 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,

$$\begin{aligned} \lim_{\rho \rightarrow 0} \Lambda\left(\left\{(\mathbf{Q}_0, \mathbf{V}_0) \in T^1(\mathbb{R}^d) : (\mathbf{S}_1, \dots, \mathbf{S}_n) \in \mathcal{A}\right\}\right) \\ = \int_{\mathcal{A}} \Psi_{n,\Lambda}(\mathbf{S}'_1, \dots, \mathbf{S}'_n) d\mathbf{S}'_1 \cdots d\mathbf{S}'_n, \end{aligned}$$

and, for $n \geq 3$,

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

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

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



Lattices

- $\mathcal{L} \subset \mathbb{R}^d$ —euclidean lattice of covolume one
- recall $\mathcal{L} = \mathbb{Z}^d M$ for some $M \in \text{SL}(d, \mathbb{R})$, therefore the homogeneous space $X_1 = \text{SL}(d, \mathbb{Z}) \backslash \text{SL}(d, \mathbb{R})$ parametrizes the space of lattices of covolume one
- μ_1 —right- $\text{SL}(d, \mathbb{R})$ invariant prob measure on X_1 (Haar)

Affine lattices

- $\text{ASL}(d, \mathbb{R}) = \text{SL}(d, \mathbb{R}) \ltimes \mathbb{R}^d$ —the semidirect product group with multiplication law

$$(M, x)(M', x') = (MM', xM' + x').$$

An action of $\text{ASL}(d, \mathbb{R})$ on \mathbb{R}^d can be defined as

$$y \mapsto y(M, x) := yM + x.$$

- the space of affine lattices is then represented by $X = \text{ASL}(d, \mathbb{Z}) \backslash \text{ASL}(d, \mathbb{R})$ where $\text{ASL}(d, \mathbb{Z}) = \text{SL}(d, \mathbb{Z}) \ltimes \mathbb{Z}^d$, i.e.,

$$\mathcal{L}_\alpha := (\mathbb{Z}^d + \alpha)M = \mathbb{Z}^d(1, \alpha)(M, 0)$$

- μ —right- $\text{ASL}(d, \mathbb{R})$ invariant prob measure on X

Let us denote by $\tau_1 = \tau(\mathbf{q}, \mathbf{v})$ the free path length corresponding to the initial condition (\mathbf{q}, \mathbf{v}) . Recall that $\rho^{d-1}\tau_1 = \|S_1\|$.

Theorem C. Fix a lattice \mathcal{L} and the initial position \mathbf{q} . Let λ be any a.c. Borel probability measure on S_1^{d-1} . Then, for every $\xi > 0$, the limit

$$F_{\mathcal{L}, \mathbf{q}}(\xi) := \lim_{\rho \rightarrow 0} \lambda(\{\mathbf{v} \in S_1^{d-1} : \rho^{d-1}\tau_1 \leq \xi\})$$

exists, is continuous in ξ and independent of λ . Furthermore

$$F_{\mathcal{L}, \mathbf{q}}(\xi) = \begin{cases} \mu_1(\{M \in X_1 : \mathbb{Z}^d M \cap \mathcal{Z}(\xi) \neq \emptyset\}) & \text{if } \mathbf{q} \in \mathcal{L} \\ \mu(\{(M, x) \in X : (\mathbb{Z}^d M + x) \cap \mathcal{Z}(\xi) \neq \emptyset\}) & \text{if } \mathbf{q} \notin \mathbb{Q}\mathcal{L}. \end{cases}$$

with the cylinder

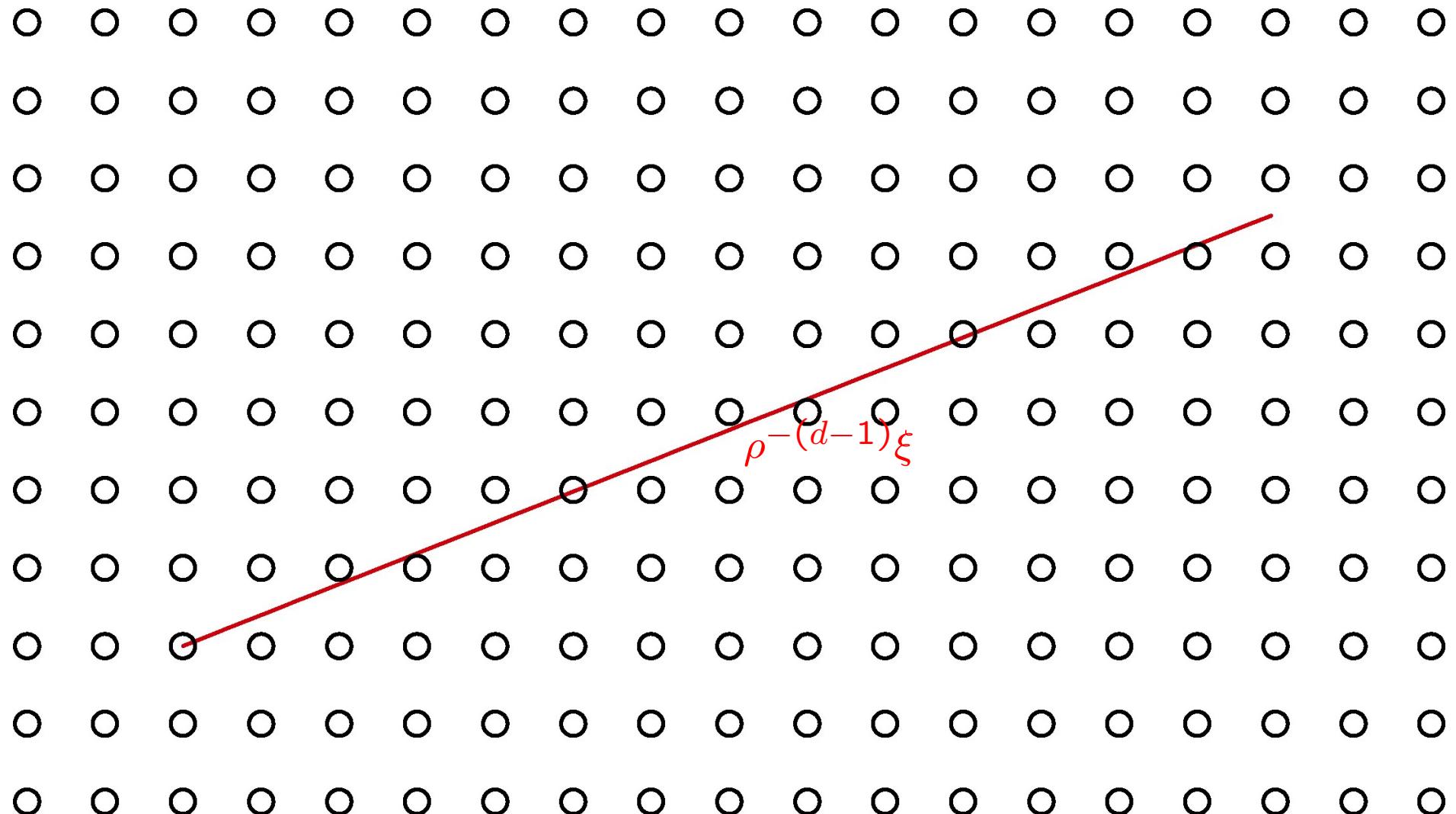
$$\mathcal{Z}(\xi) = \{(x_1, \dots, x_d) \in \mathbb{R}^d : 0 < x_1 < \xi, \|(x_2, \dots, x_d)\| < 1\}.$$

Remarks

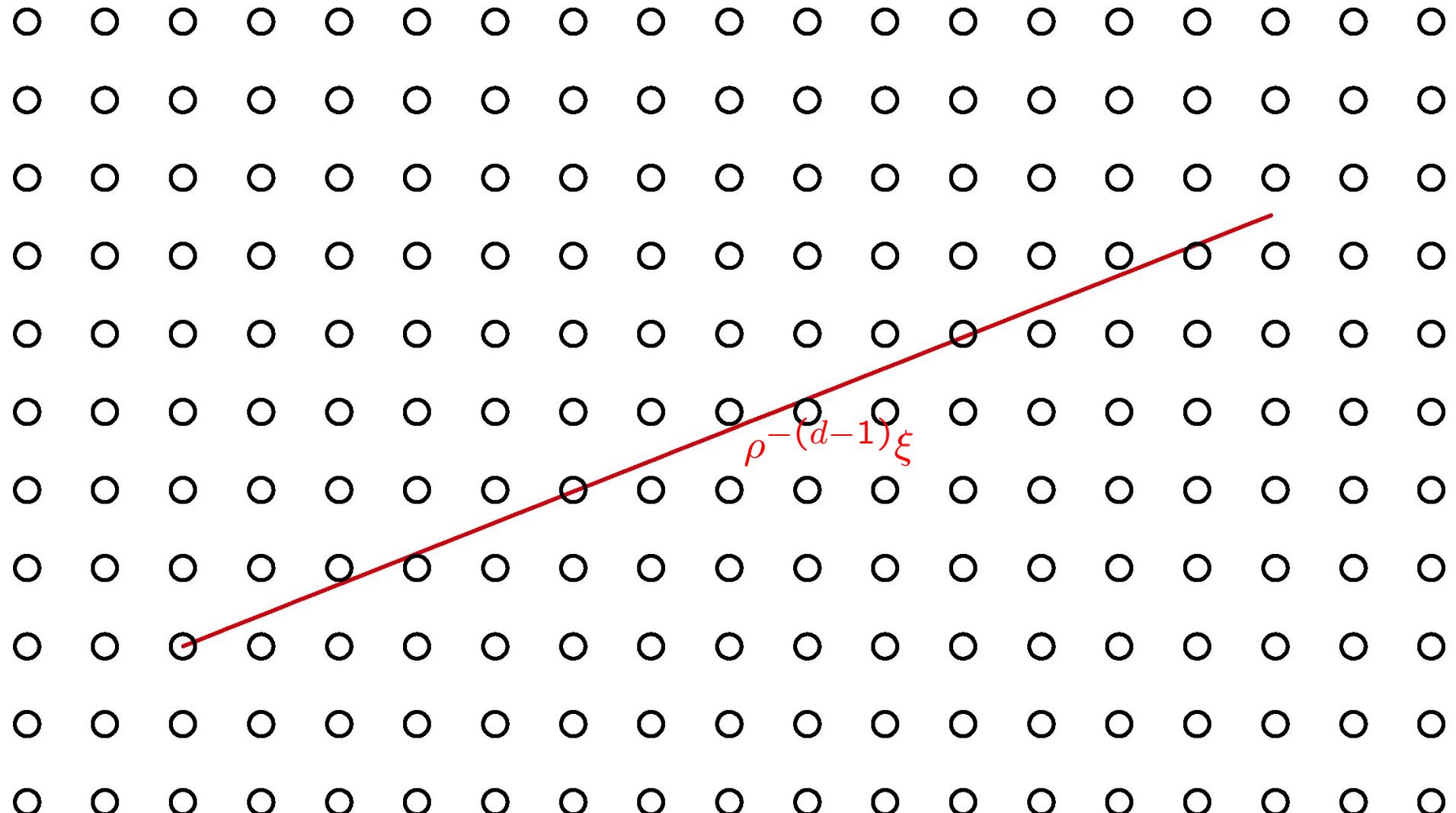
- There are similar formulas for all $q \in \mathbb{Q}\mathcal{L}$.
- Note that in the case $q \notin \mathbb{Q}\mathcal{L}$ the limit $F_{\mathcal{L},q}(\xi) =: F(\xi)$ is independent of q and \mathcal{L} ; in the case $q \in \mathcal{L}$ the limit $F_{\mathcal{L},q}(\xi) =: F_0(\xi)$ is independent of \mathcal{L} .
- Instead of rays emerging from the origin we can also deal with the family of rays starting at the point $\rho\beta(v)$ in direction v . This set-up is important for the joint distribution for the first n path segments in the Lorentz gas.

Outline of proof of Theorem C

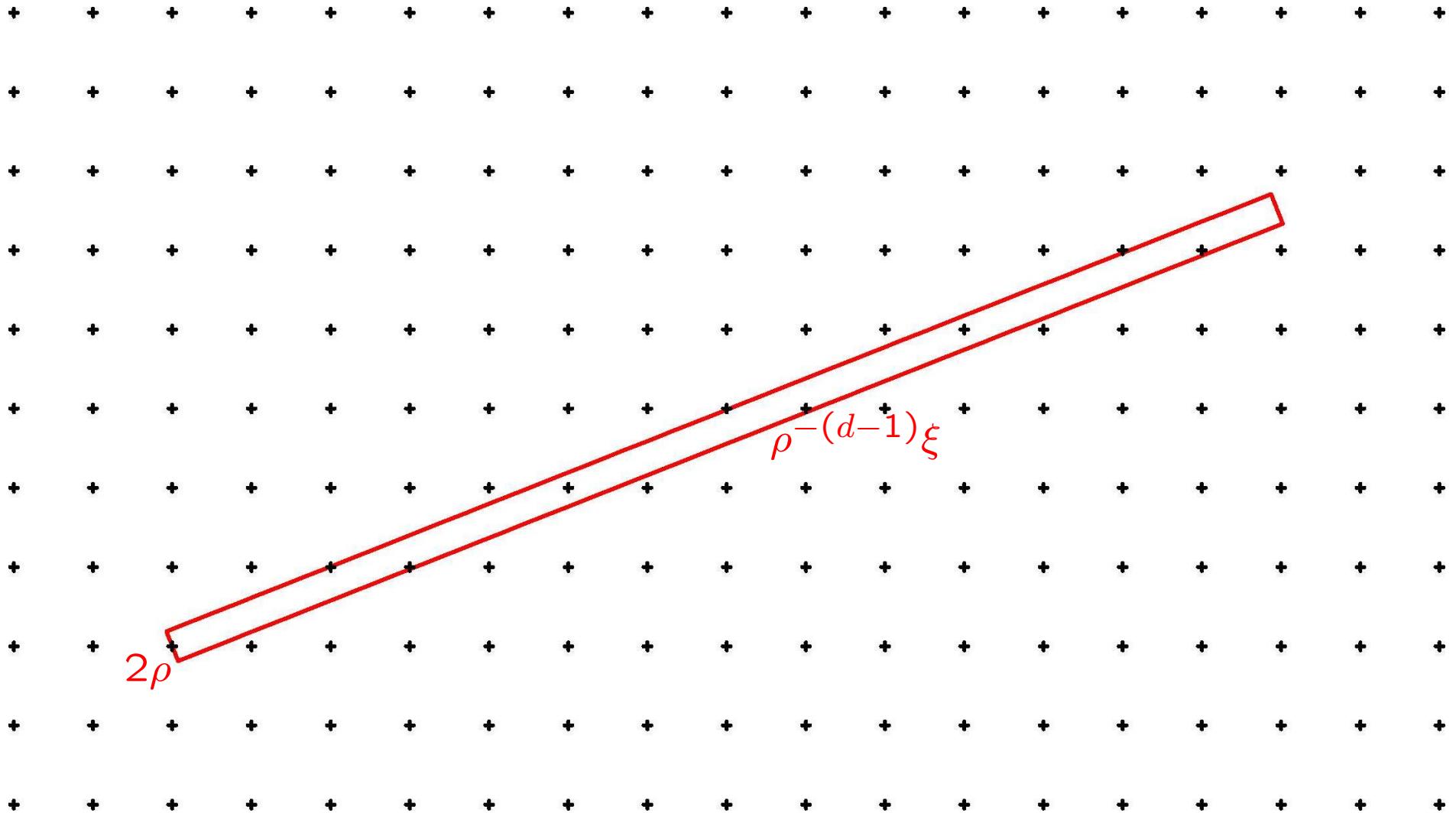
(in the case $q \in \mathcal{L} = \mathbb{Z}^d$)



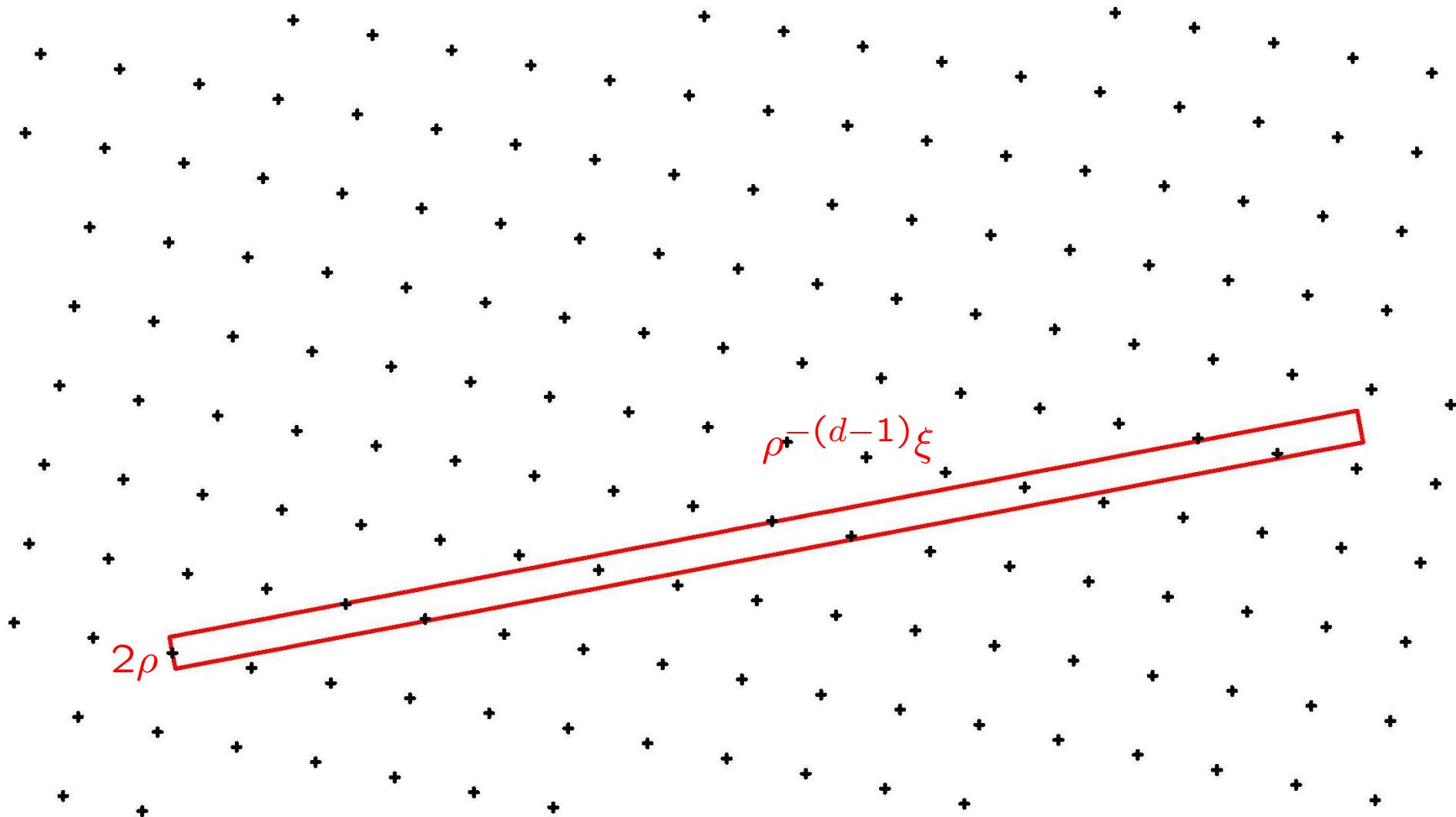
$$\lambda\left(\left\{v \in S_1^{d-1} : \rho^{d-1}\tau_1 \leq \xi\right\}\right) = \dots$$



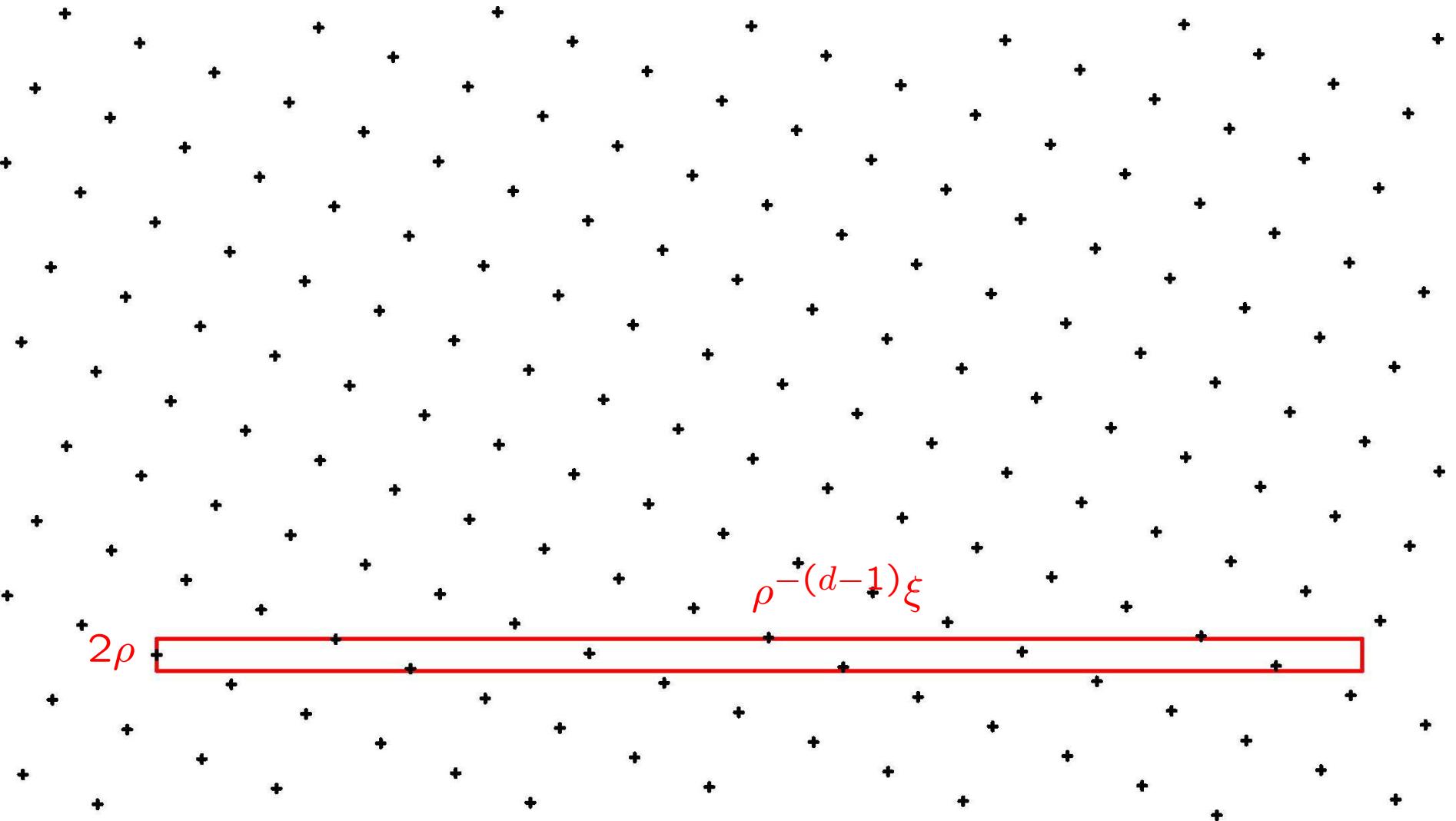
$$= \lambda \left(\{ \mathbf{v} \in \mathbb{S}_1^{d-1} : \text{at least one scatterer intersects } \text{ray}(\mathbf{v}, \rho^{-(d-1)}\xi) \} \right)$$



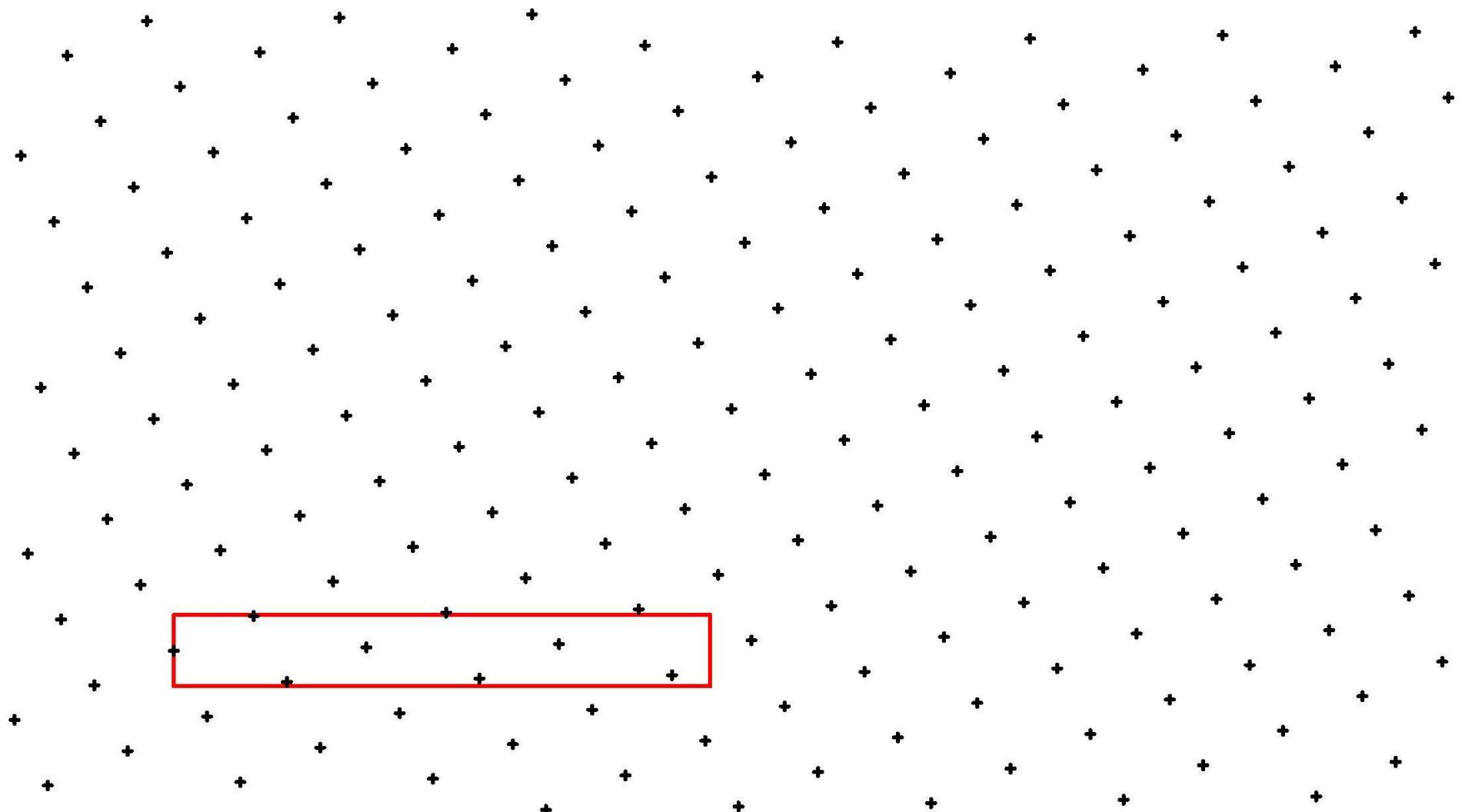
$$\approx \lambda \left(\left\{ \mathbf{v} \in \mathbb{S}_1^{d-1} : \mathbb{Z}^d \cap \mathcal{Z}(\mathbf{v}, \rho^{-(d-1)}\xi, \rho) \neq \emptyset \right\} \right)$$



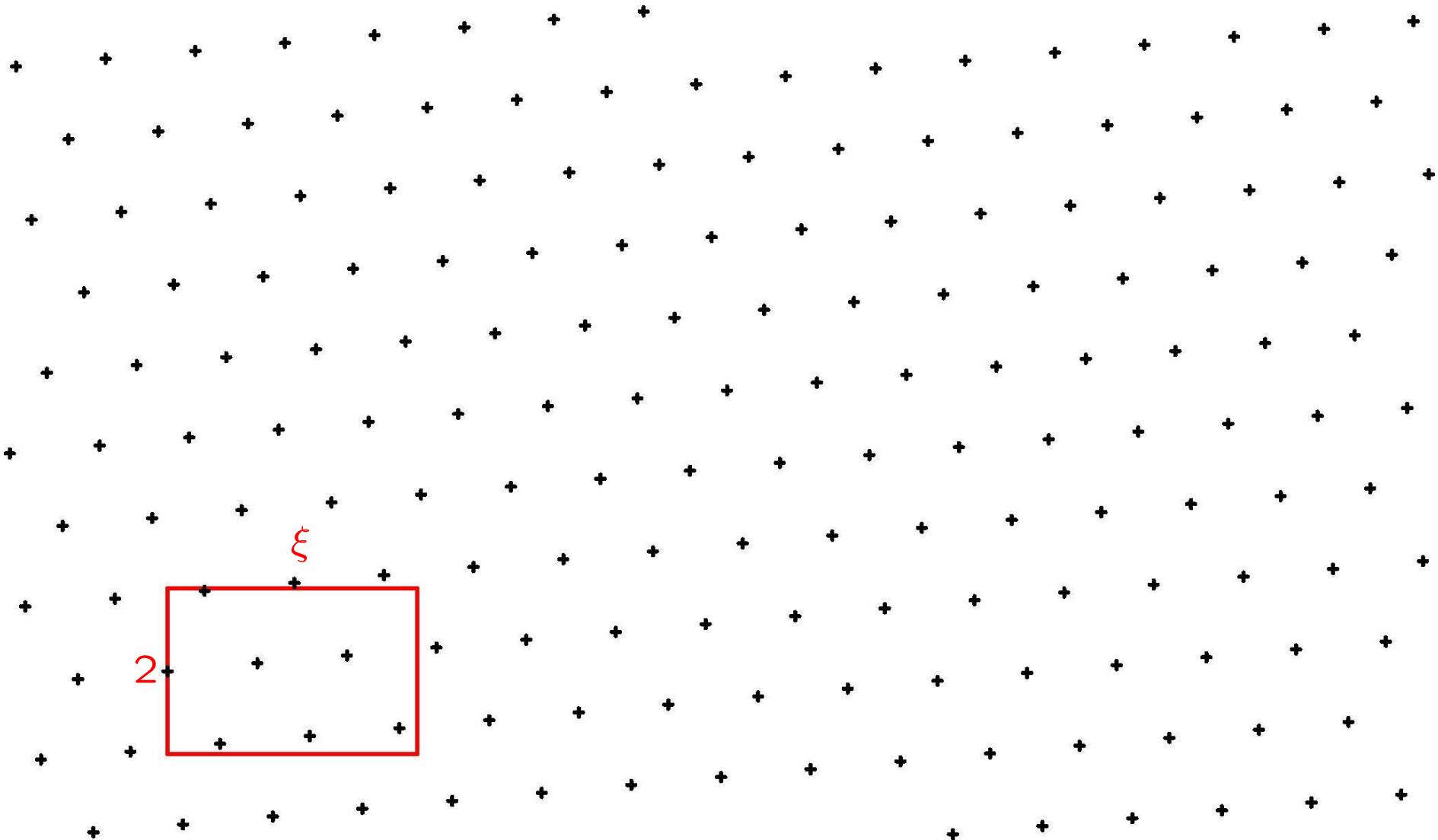
$\left(\text{Rotate by } K(v) \in \text{SO}(d) \text{ such that } v \mapsto e_1 \right)$



$$\lambda\left(\left\{v \in S_1^{d-1} : \mathbb{Z}^d K(v) \cap \mathcal{Z}(e_1, \rho^{-(d-1)}\xi, \rho) \neq \emptyset\right\}\right)$$



$\left(\text{Apply } D_\rho = \text{diag}(\rho^{d-1}, \rho^{-1}, \dots, \rho^{-1}) \in \text{SL}(d, \mathbb{R})\right)$



$$\lambda\left(\left\{v \in S_1^{d-1} : \mathbb{Z}^d K(v) D_\rho \cap \mathcal{Z}(e_1, \xi, 1) \neq \emptyset\right\}\right)$$

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

$$\mathbb{Z}^d K(\mathbf{v}) \begin{pmatrix} \rho^{d-1} & \mathbf{0} \\ \mathbf{t}_0 & \rho^{-1} \mathbf{1} \end{pmatrix}$$

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

$$\Phi^t = \begin{pmatrix} e^{-(d-1)t} & \mathbf{0} \\ \mathbf{t}_0 & e^{t} \mathbf{1} \end{pmatrix}, \quad t = \log 1/\rho.$$

Theorem D. 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 $f : X_1 \rightarrow \mathbb{R}$,

$$\lim_{t \rightarrow \infty} \int_{S_1^{d-1}} f(M_0 K(\mathbf{v}) \Phi^t) d\lambda(\mathbf{v}) = \int_{X_1} f(M) d\mu_1(M).$$

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

This concludes the proof of Theorem C when $q \in \mathcal{L} = \mathbb{Z}^d M_0$.

The generalization of Theorem D 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.

Asymptotics

Asymptotics of the limiting distribution for $q \notin \mathbb{Q}\mathcal{L}$

Recall:

$$\begin{aligned} F(\xi) &:= \lim_{\rho \rightarrow 0} \lambda(\{v \in S_1^{d-1} : \rho^{d-1} \tau_1 \leq \xi\}) \\ &= \mu(\{(M, x) \in X : (\mathbb{Z}^d M + x) \cap \mathcal{Z}(\xi) \neq \emptyset\}). \end{aligned}$$

$$F(\xi) = 1 - \frac{\pi^{\frac{d-1}{2}}}{2^d d \Gamma(\frac{d+3}{2}) \zeta(d)} \xi^{-1} + O\left(\xi^{-1-\frac{2}{d}}\right) \quad \text{as } \xi \rightarrow \infty$$

$$F(\xi) = \text{vol}(\mathcal{B}_1^{d-1}) \xi + O\left(\xi^2\right) \quad \text{as } \xi \rightarrow 0$$

$$\text{with } \text{vol}(\mathcal{B}_1^{d-1}) = \frac{\pi^{(d-1)/2}}{\Gamma((d+1)/2)}.$$

Note: for a random scatterer configuration $F(\xi) = 1 - e^{-\text{vol}(\mathcal{B}_1^{d-1})\xi}$.

Asymptotics of the limiting distribution for $q \in \mathcal{L}$

Recall:

$$\begin{aligned} F_0(\xi) &:= \lim_{\rho \rightarrow 0} \lambda(\{v \in S_1^{d-1} : \rho^{d-1} \tau_1 \leq \xi\}) \\ &= \mu_1(\{M \in X_1 : \mathbb{Z}^d M \cap \mathcal{Z}(\xi) \neq \emptyset\}). \end{aligned}$$

$$F_0(\xi) = 1$$

for ξ sufficiently large

$$F_0(\xi) = \frac{\text{vol}(\mathcal{B}_1^{d-1})}{\zeta(d)} \xi + O(\xi^2) \quad \text{as } \xi \rightarrow 0.$$

Note: for a random scatterer configuration $F_0(\xi) = F(\xi) = 1 - e^{-\text{vol}(\mathcal{B}_1^{d-1})\xi}$.

$1/\zeta(d)$ is the relative density of primitive lattice points (i.e., the lattice points visible from the origin).

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?

References

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