

# Kinetic transport in crystals

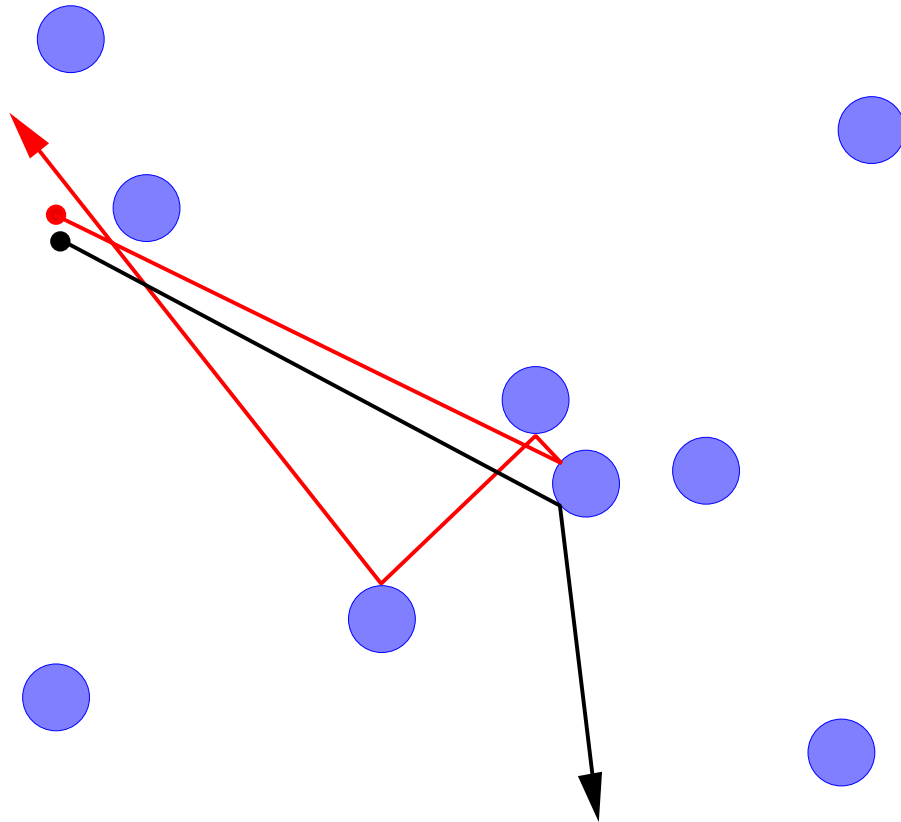
Jens Marklof

University of Bristol

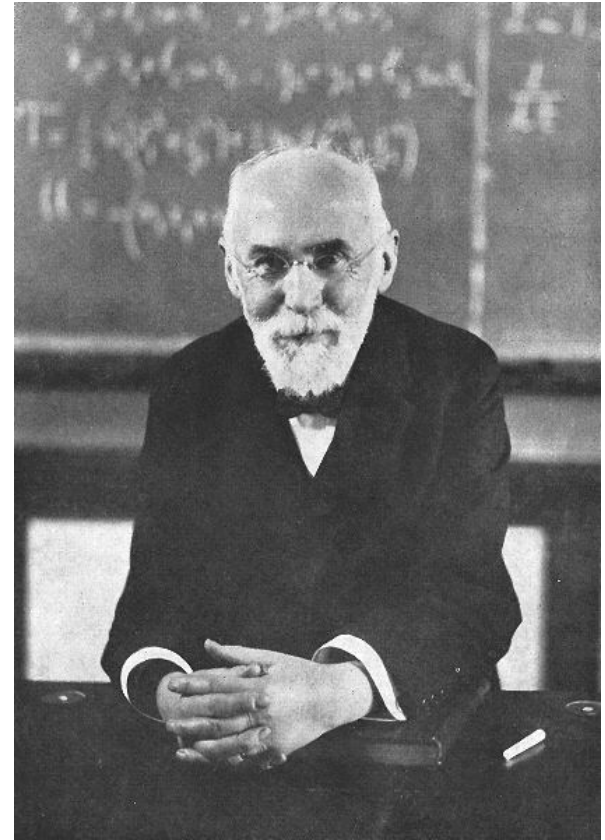
<http://www.maths.bristol.ac.uk>

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  $\rho$
- $(\mathbf{q}(t), \mathbf{v}(t))$  = “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  $f \in L^1$ :

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

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

$$\left[ \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla_Q \right] f_t(Q, \mathbf{V}) = \int_{S_1^{d-1}} [f_t(Q, \mathbf{V}_0) - f_t(Q, \mathbf{V})] \sigma(\mathbf{V}_0, \mathbf{V}) d\mathbf{V}_0$$

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

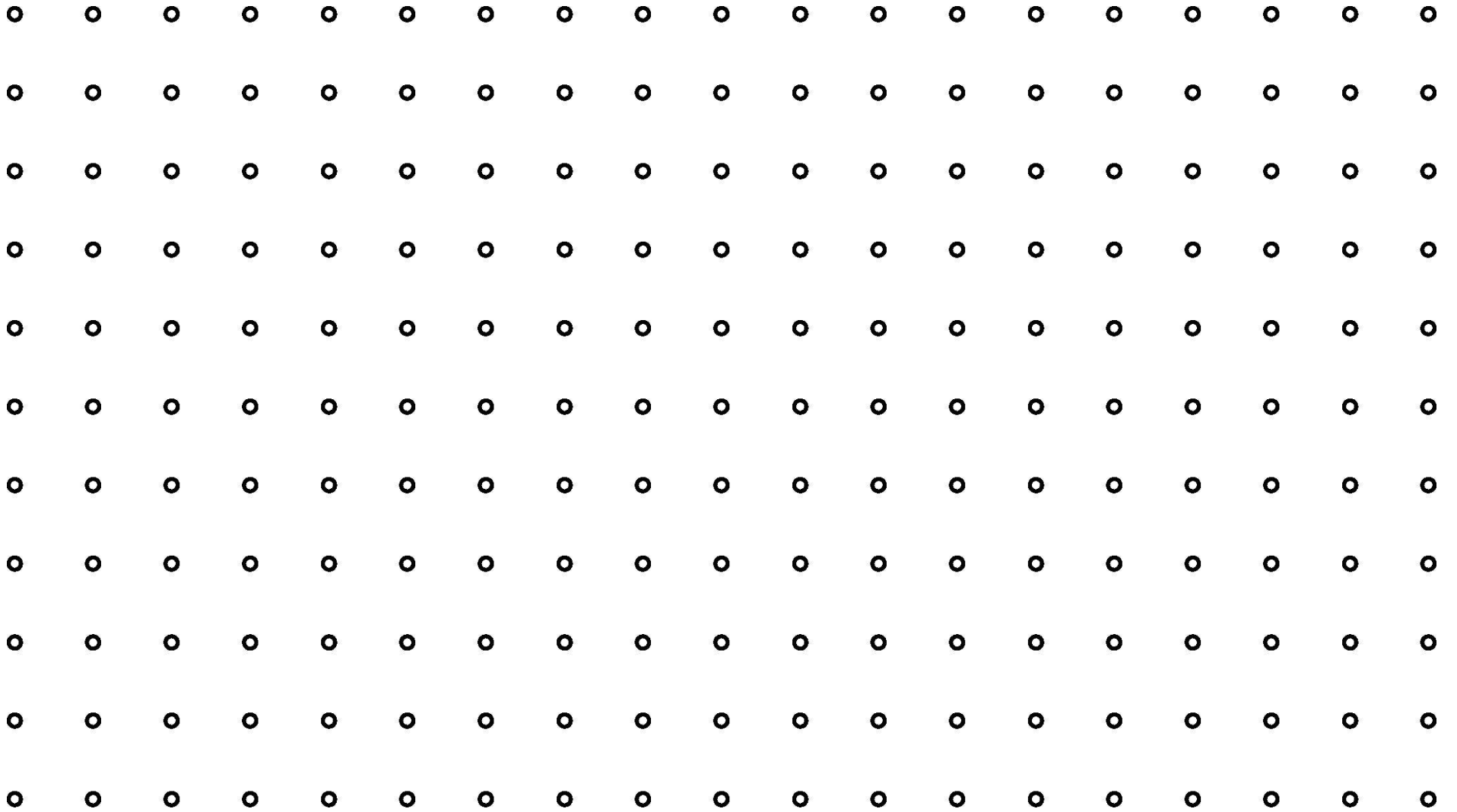
## The linear Boltzmann equation—rigorous proofs

- 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

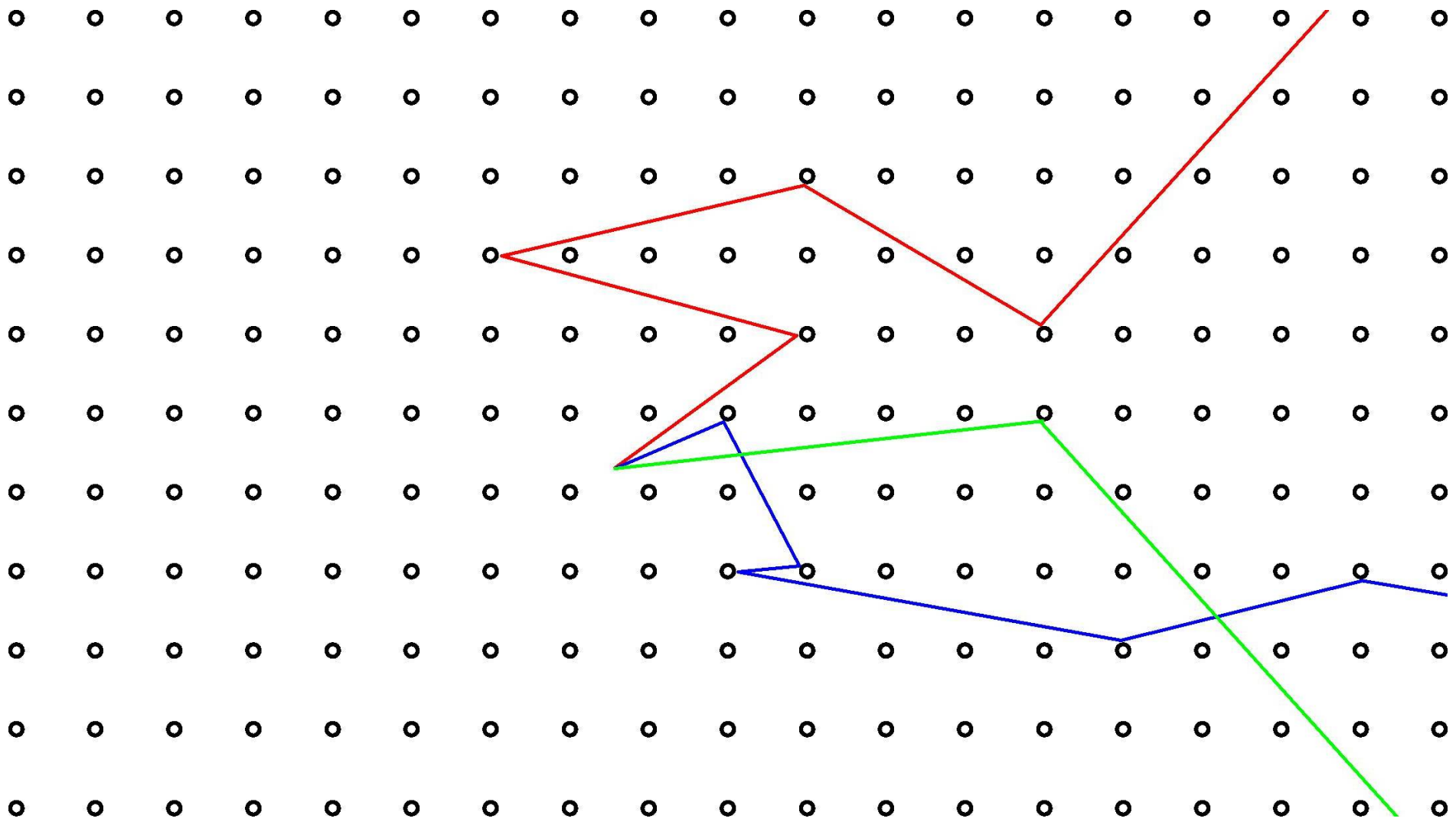
## The quantum linear Boltzmann equation

- 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 $\rho$

- 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  $L^t : L^1(T^1(\mathbb{R}^d)) \rightarrow L^1(T^1(\mathbb{R}^d))$ , such that for every  $f \in L^1(T^1(\mathbb{R}^d))$  and any set  $\mathcal{A} \subset T^1(\mathbb{R}^d)$  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  $(Q, V, \xi, V_+)$  where

$$\begin{aligned}(Q, V) &\in T^1(\mathbb{R}^d) \text{ — usual position and momentum} \\ \xi &\in \mathbb{R}_+ \text{ — flight time until the next scatterer} \\ V_+ &\in S_1^{d-1} \text{ — velocity after the next hit}\end{aligned}$$

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

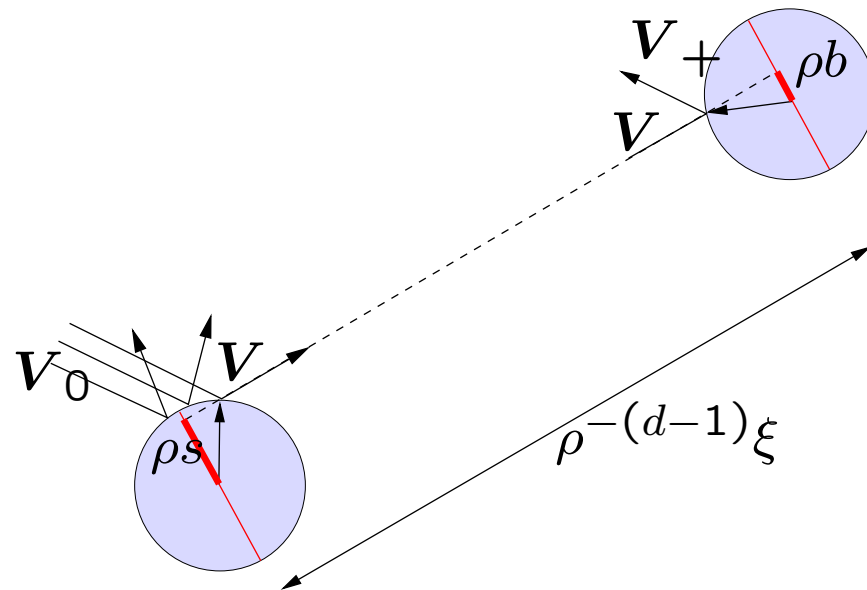
$$\begin{aligned}\left[ \frac{\partial}{\partial t} + V \cdot \nabla_Q - \frac{\partial}{\partial \xi} \right] f_t(Q, V, \xi, V_+) \\ = \int_{S_1^{d-1}} f_t(Q, V_0, 0, V) p_0(V_0, V, \xi, V_+) dV_0\end{aligned}$$

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

## The collision kernel

$$p_0(\mathbf{V}_0, \mathbf{V}, \xi, \mathbf{V}_+) = \sigma(\mathbf{V}, \mathbf{V}_+) \Phi_0(\xi, b(\mathbf{V}, \mathbf{V}_+), -s(\mathbf{V}, \mathbf{V}_0))$$

- $\sigma(\mathbf{V}, \mathbf{V}_+)$  the differential cross section
- $\Phi_0(\xi, b(\mathbf{V}, \mathbf{V}_+), -s(\mathbf{V}, \mathbf{V}_0))$  the transition probability to exit with parameter  $s(\mathbf{V}, \mathbf{V}_0)$  and hit the next scatterer after time  $\xi$  with impact parameter  $b(\mathbf{V}, \mathbf{V}_+)$



## The function $\Phi_0$

... yields the probability to exit a scatterer with parameter  $s$  and hit the next scatterer with impact parameter  $b$  after time  $\xi$ .

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

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

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

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

with

$$p(\mathbf{V}, \xi, \mathbf{V}_+) := \int_\xi^\infty \int_{S_1^{d-1}} \sigma(\mathbf{V}_0, \mathbf{V}) p_0(\mathbf{V}_0, \mathbf{V}, \xi, \mathbf{V}_+) d\mathbf{V}_0 d\xi;$$

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

## Why “a generalization” of the linear Boltzmann equation?

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

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

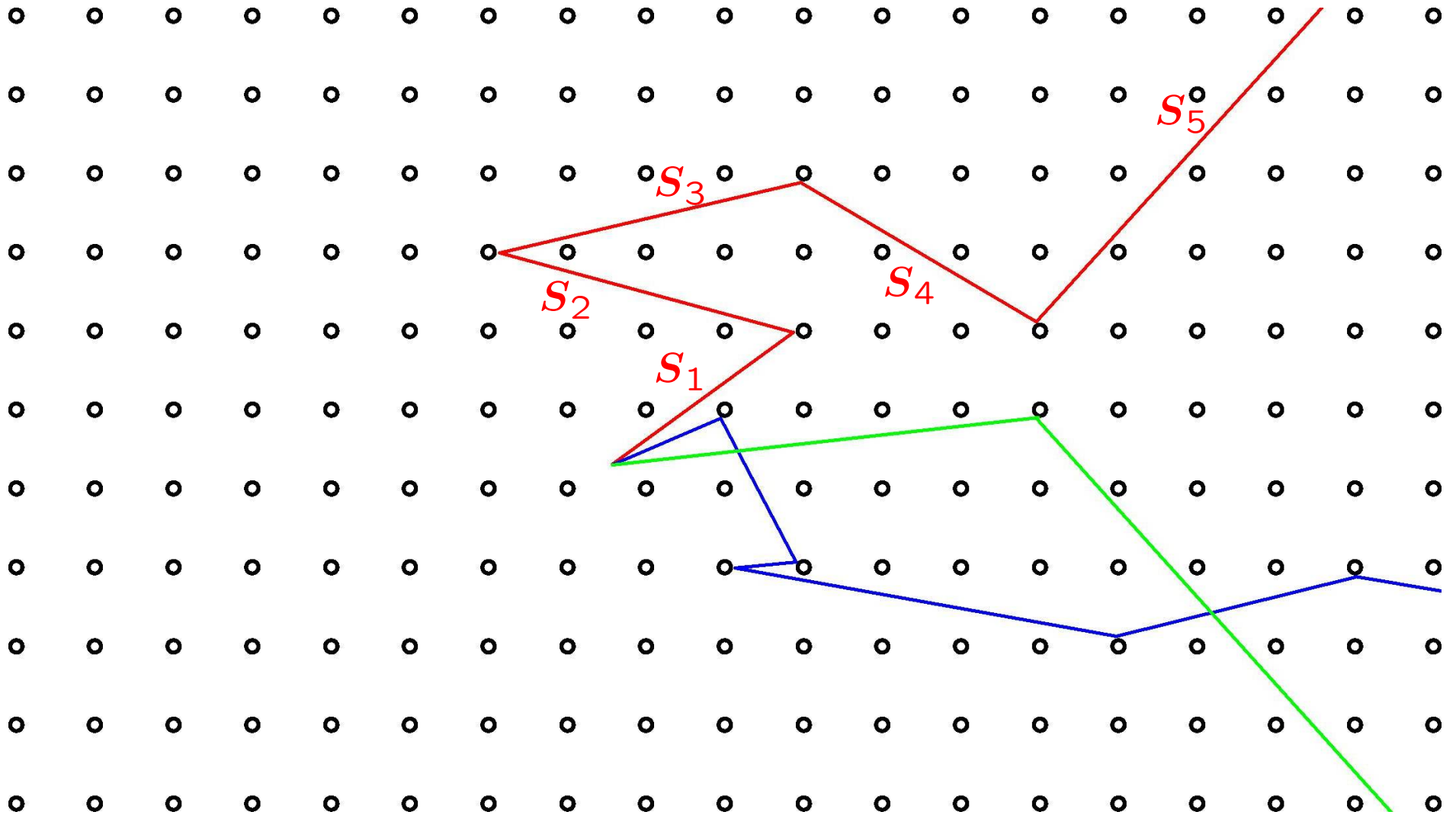
$$p_0(\mathbf{V}_0, \mathbf{V}, \xi, \mathbf{V}_+) = \sigma(\mathbf{V}, \mathbf{V}_+) e^{-\text{vol}(\mathcal{B}_1^{d-1}) \xi}$$

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

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

$$\begin{aligned} \lim_{\rho \rightarrow 0} \Lambda\left(\left\{(Q_0, V_0) \in \mathbb{T}^1(\mathbb{R}^d) : (S_1, \dots, S_n) \in \mathcal{A}\right\}\right) \\ = \int_{\mathcal{A}} \Psi_{n,\Lambda}(S'_1, \dots, S'_n) dS'_1 \cdots dS'_n, \end{aligned}$$

and, for  $n \geq 3$ ,

$$\Psi_{n,\Lambda}(S_1, \dots, S_n) = \Psi_{2,\Lambda}(S_1, S_2) \prod_{j=3}^n \Psi(S_{j-2}, S_{j-1}, S_j),$$

where  $\Psi$  is a continuous probability density independent of  $\Lambda$  (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  $M \in \mathrm{SL}(d, \mathbb{R})$ , therefore the homogeneous space  $X_1 = \mathrm{SL}(d, \mathbb{Z}) \backslash \mathrm{SL}(d, \mathbb{R})$  parametrizes the space of lattices of covolume one
- $\mu_1$ —right- $\mathrm{SL}(d, \mathbb{R})$  invariant prob measure on  $X_1$  (Haar)

## Affine lattices

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

$$(M, \mathbf{x})(M', \mathbf{x}') = (MM', \mathbf{x}M' + \mathbf{x}').$$

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

$$\mathbf{y} \mapsto \mathbf{y}(M, \mathbf{x}) := \mathbf{y}M + \mathbf{x}.$$

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

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

- $\mu$ —right- $ASL(d, \mathbb{R})$  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  $\rho^{d-1}\tau_1 = \|\mathbf{S}_1\|$ .

**Theorem C.** Fix a lattice  $\mathcal{L}$  and the initial position  $\mathbf{q}$ . Let  $\lambda$  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  $\xi$  and independent of  $\lambda$ . Furthermore

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

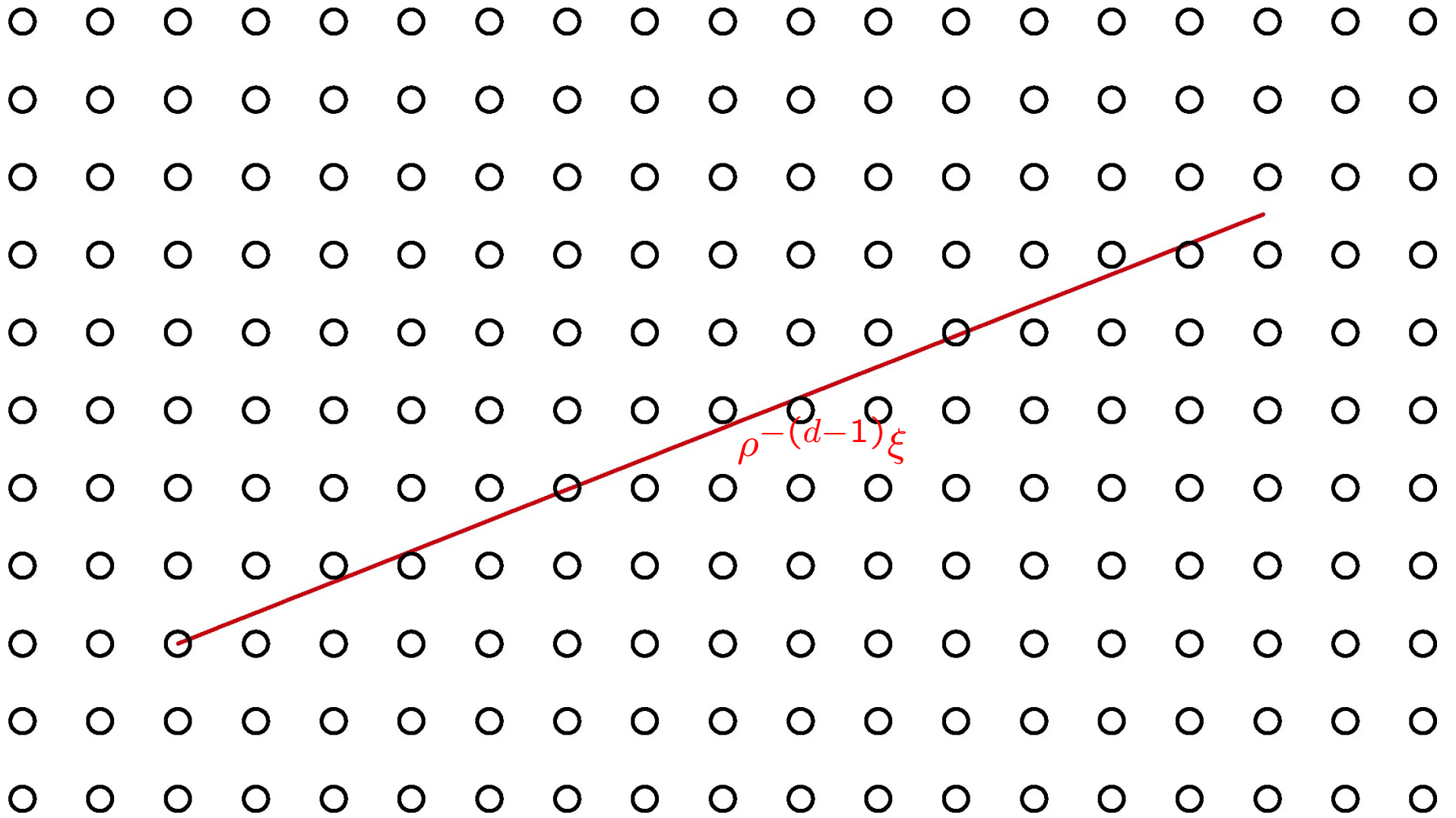
with the cylinder

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

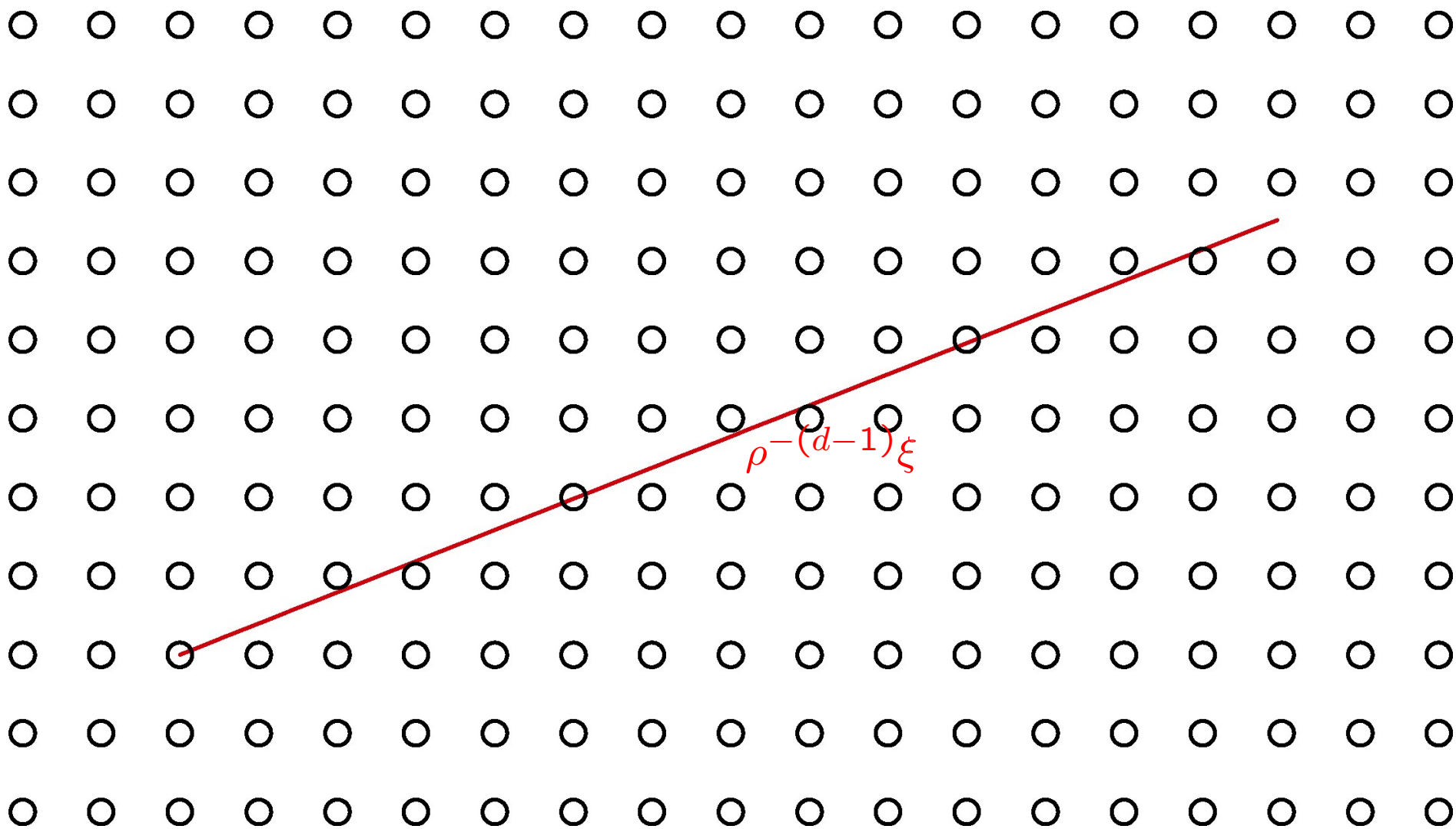
## Remarks

- 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.

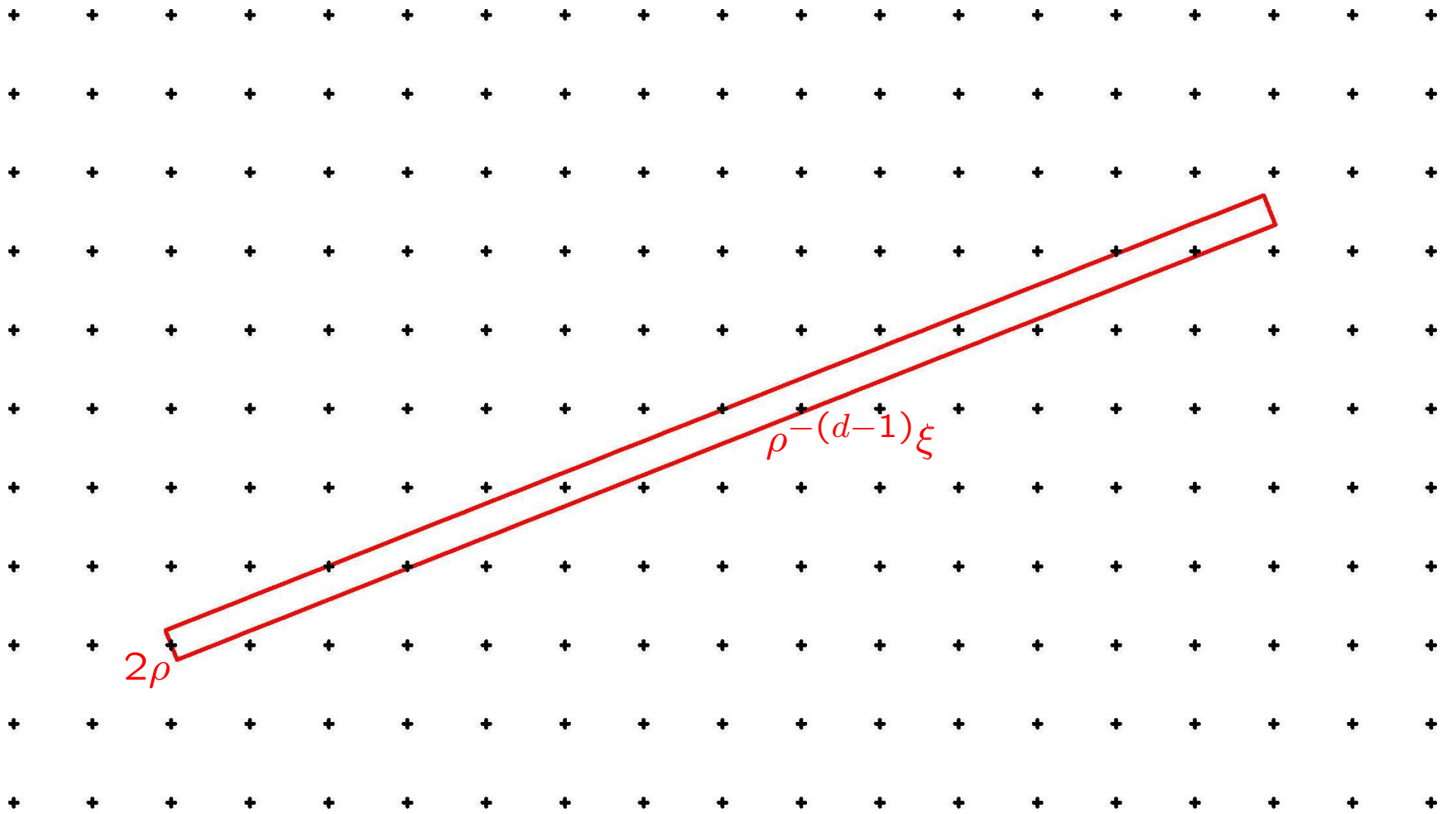
**Outline of proof of Theorem C**  
(in the case  $q \in \mathcal{L} = \mathbb{Z}^d$ )



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

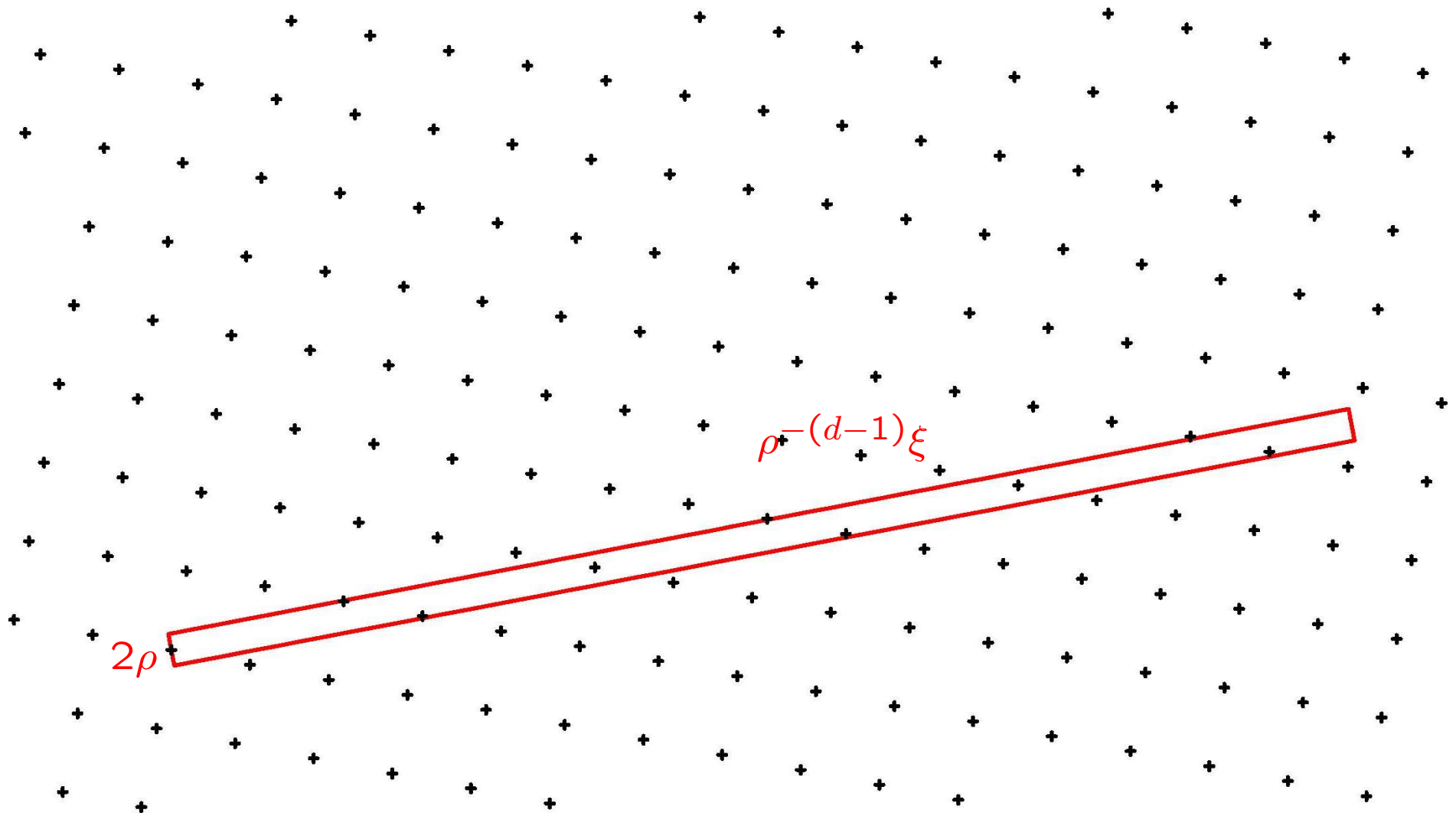


$$= \lambda\left(\left\{v \in S_1^{d-1} : \text{at least one scatterer intersects } \text{ray}(v, \rho^{-(d-1)}\xi)\right\}\right)$$

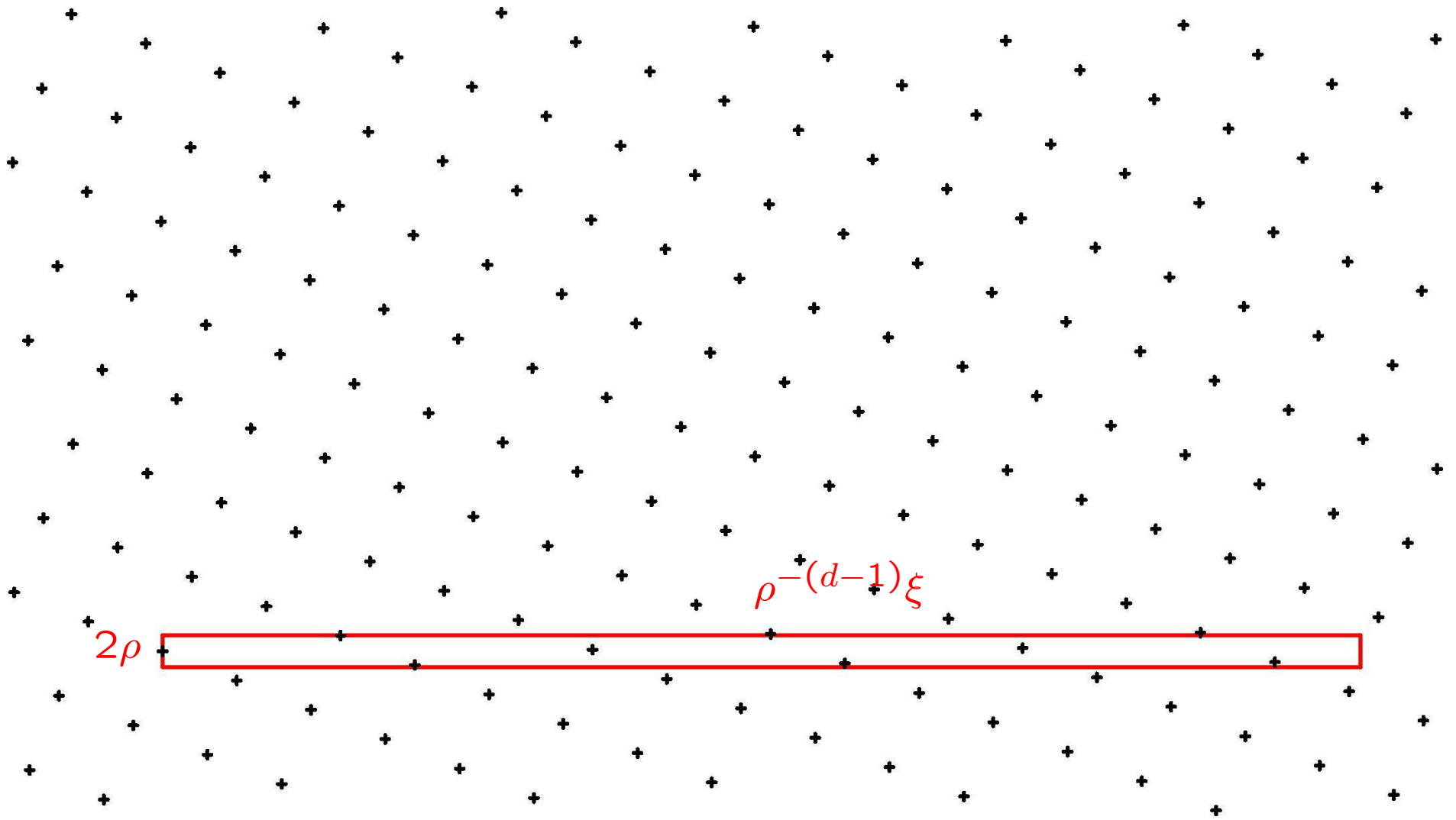


$$\approx \lambda(\{v \in S_1^{d-1} : \mathbb{Z}^d \cap \mathcal{Z}(v, \rho^{-(d-1)}\xi, \rho) \neq \emptyset\})$$

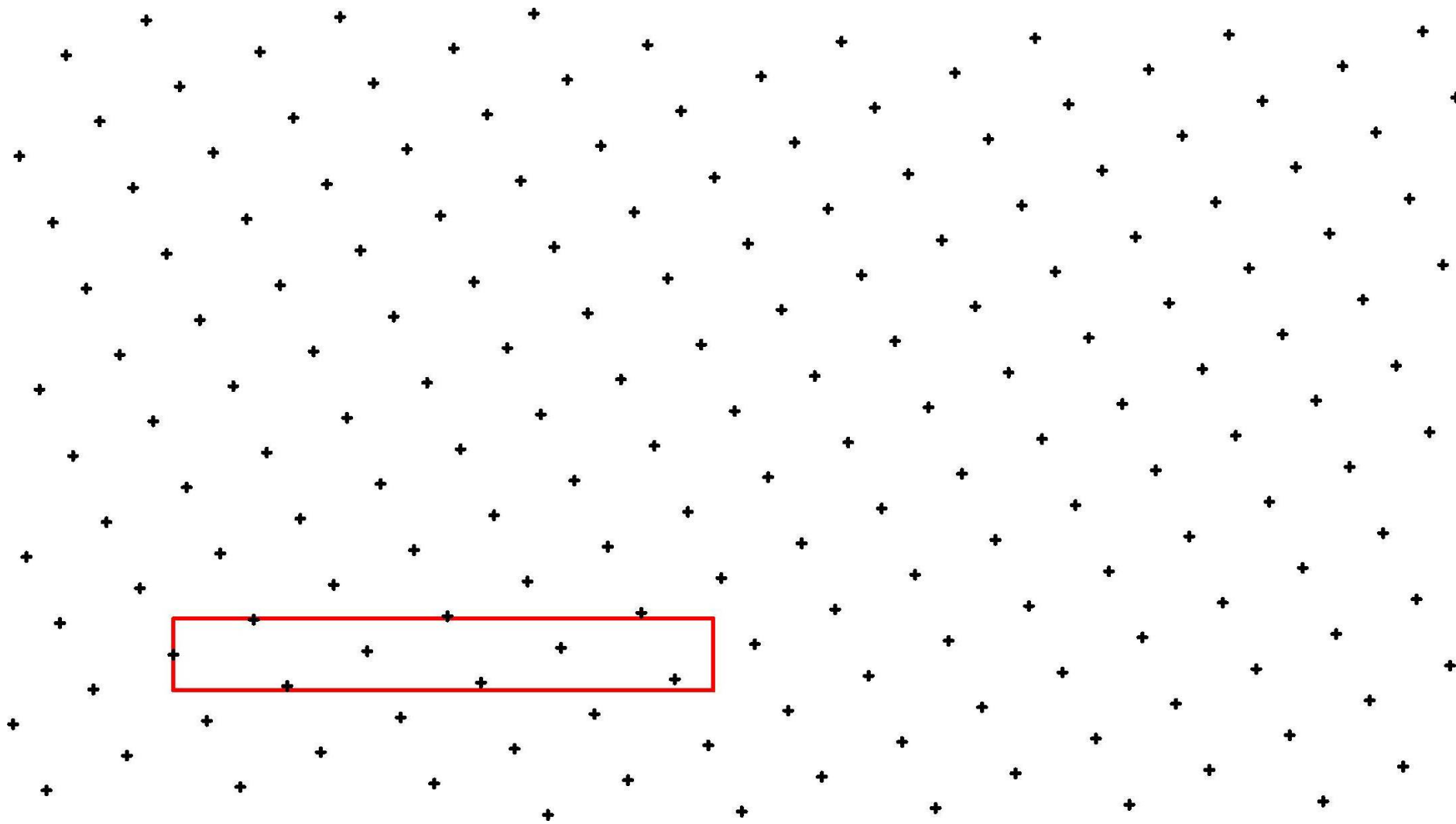




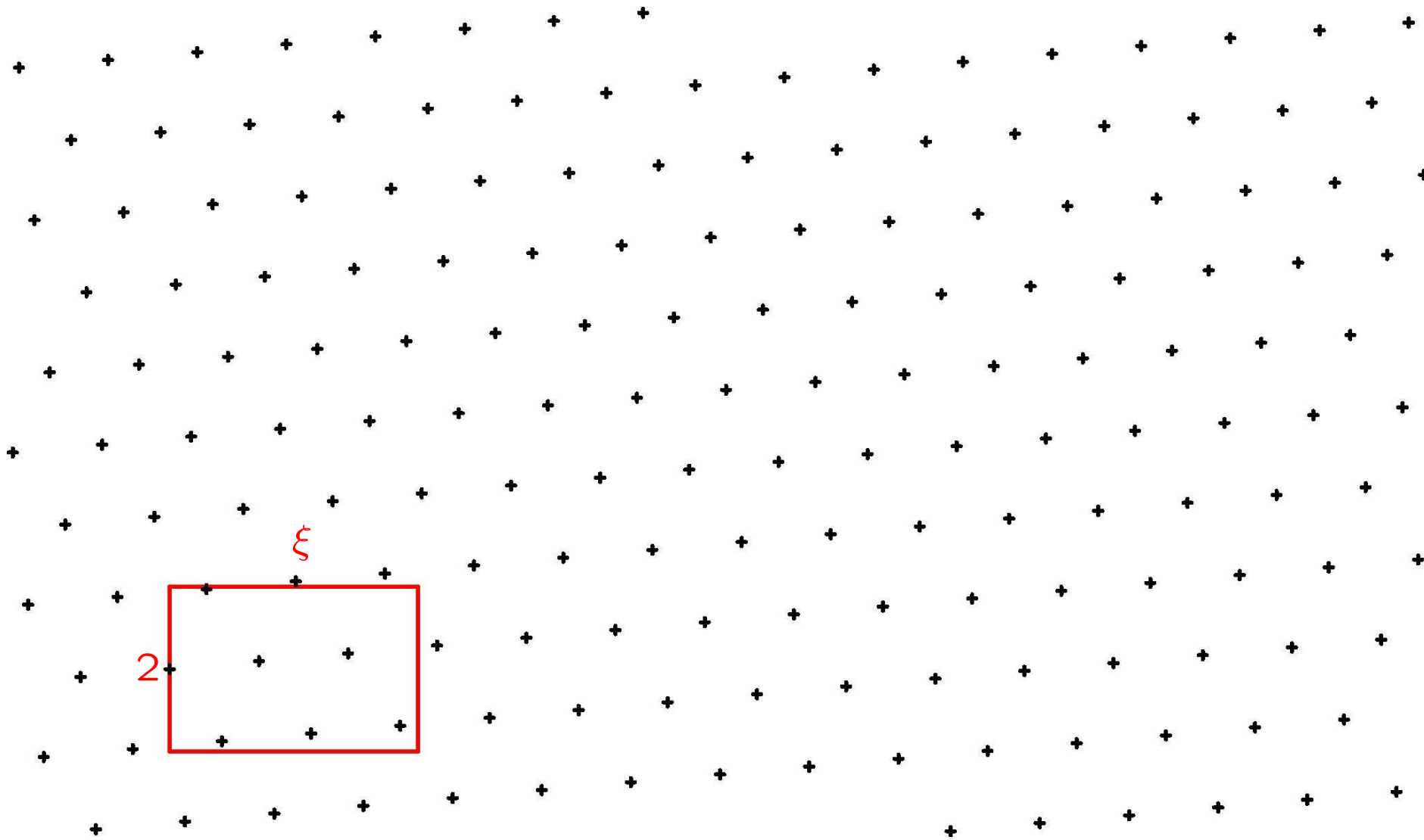
(Rotate by  $K(v) \in \text{SO}(d)$  such that  $v \mapsto e_1$ )



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



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



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

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  $\mu_1$ .

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  $\lambda$  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  $\Phi^t$ .

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 $q \notin \mathbb{QL}$

Recall:

$$\begin{aligned} F(\xi) &:= \lim_{\rho \rightarrow 0} \lambda(\{\mathbf{v} \in \mathbb{S}_1^{d-1} : \rho^{d-1} \tau_1 \leq \xi\}) \\ &= \mu(\{(M, \mathbf{x}) \in X : (\mathbb{Z}^d M + \mathbf{x}) \cap \mathcal{Z}(\xi) \neq \emptyset\}). \end{aligned}$$

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

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

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  $\xi$  sufficiently large

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

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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