

Quantum Lorentz gas in the Boltzmann-Grad limit: random vs periodic

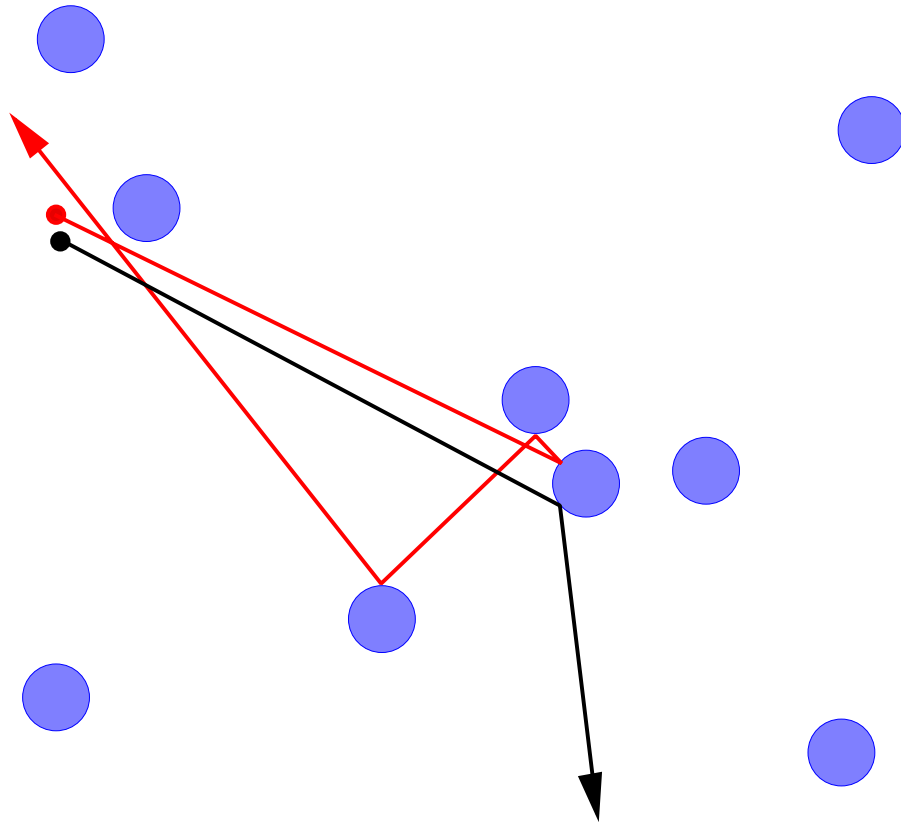
Jens Marklof

School of Mathematics, University of Bristol
<http://www.maths.bristol.ac.uk>

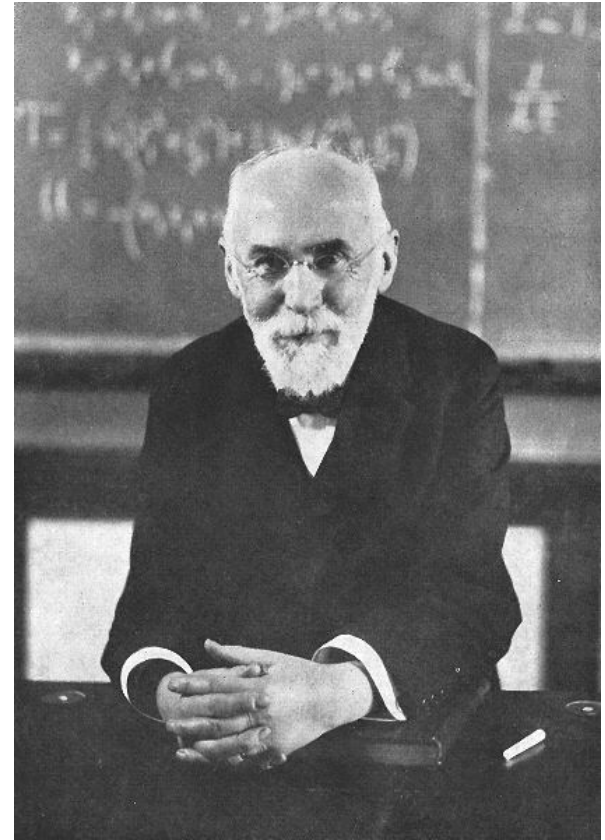
based on joint papers with
Jory Griffin (Oklahoma)

supported by EPSRC grant EP/S024948/1

The Lorentz gas

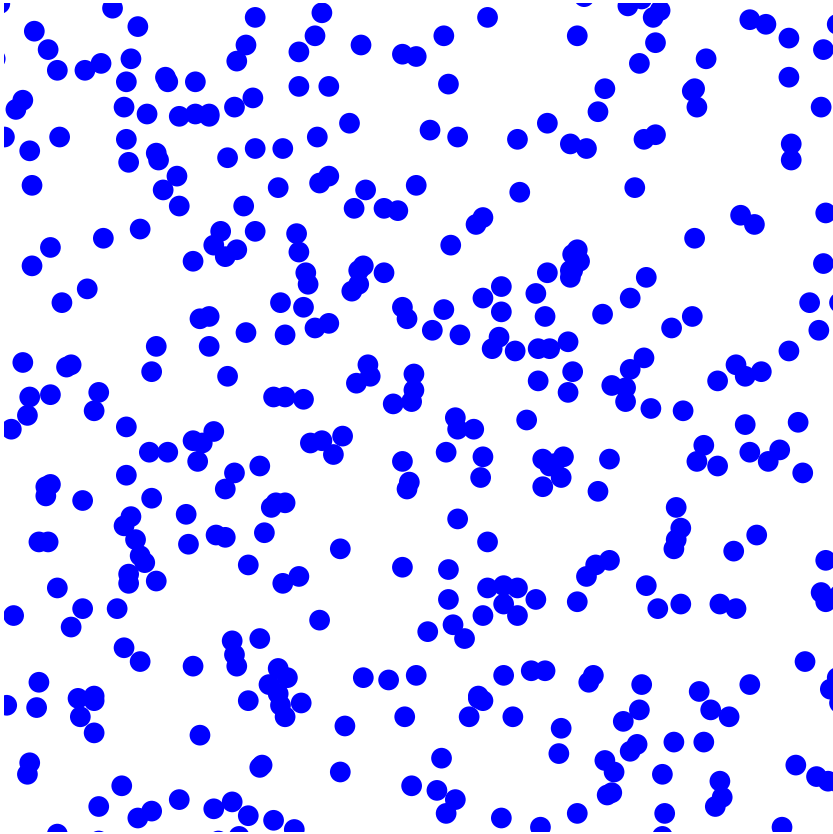


Arch. Neerl. (1905)

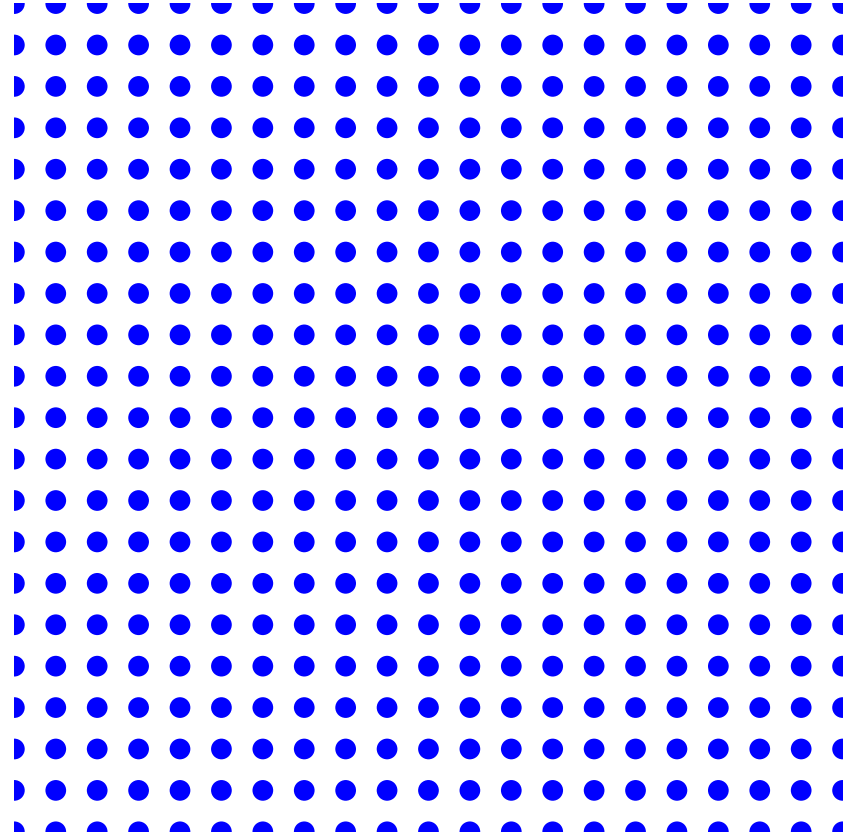


Hendrik Lorentz (1853-1928)

Lorentz gas in the small scatterer limit



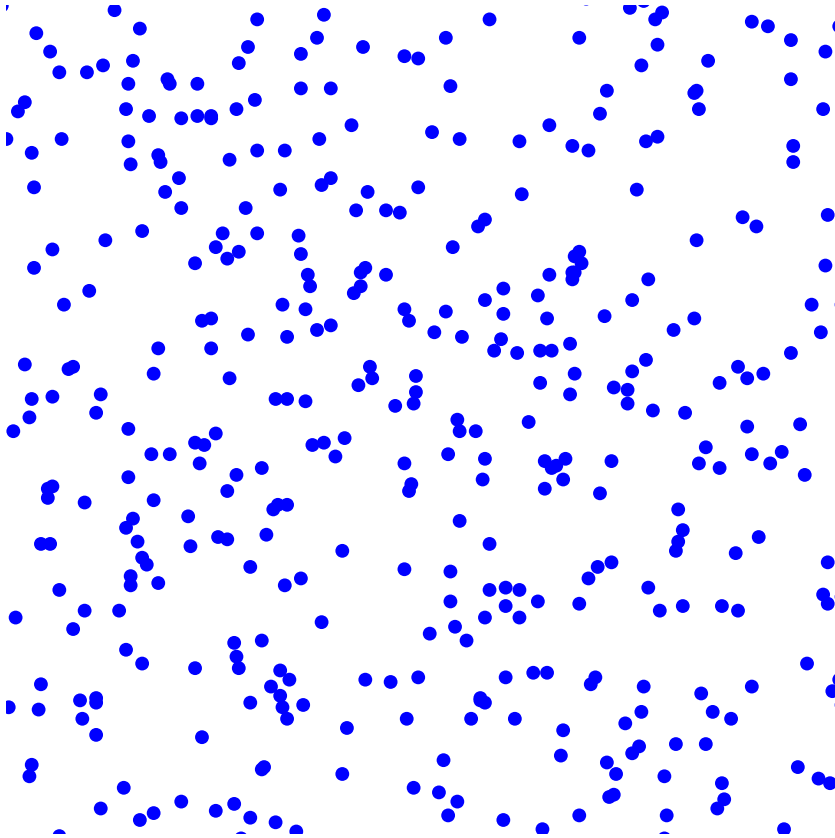
Fixed random scatterer configuration



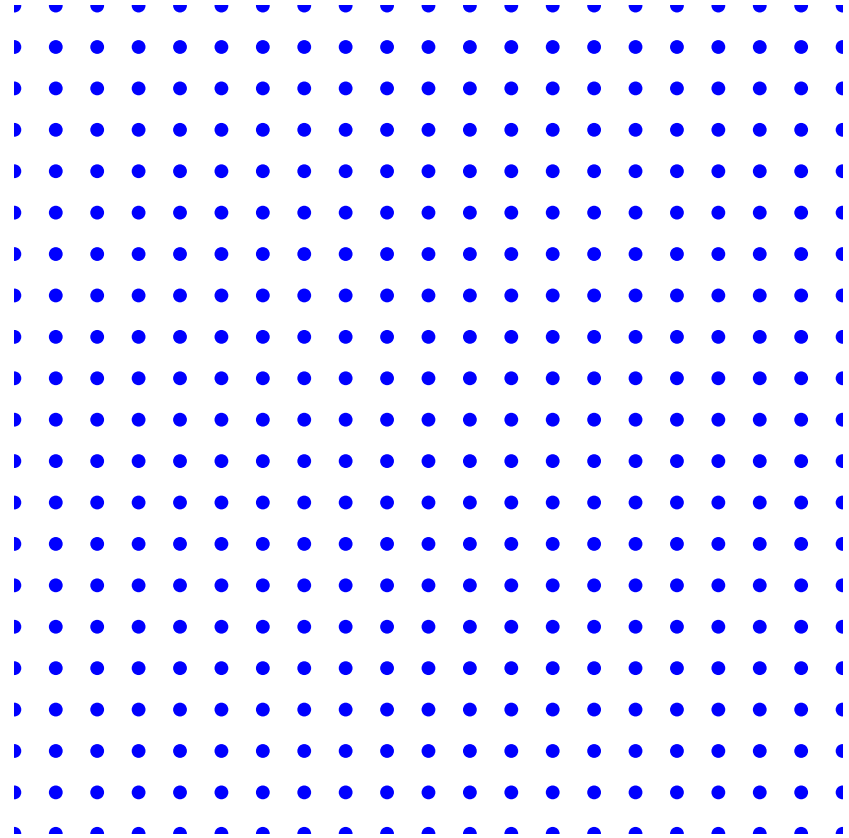
Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/4$, mean free path = $\frac{1}{2r} = 2$

Lorentz gas in the small scatterer limit



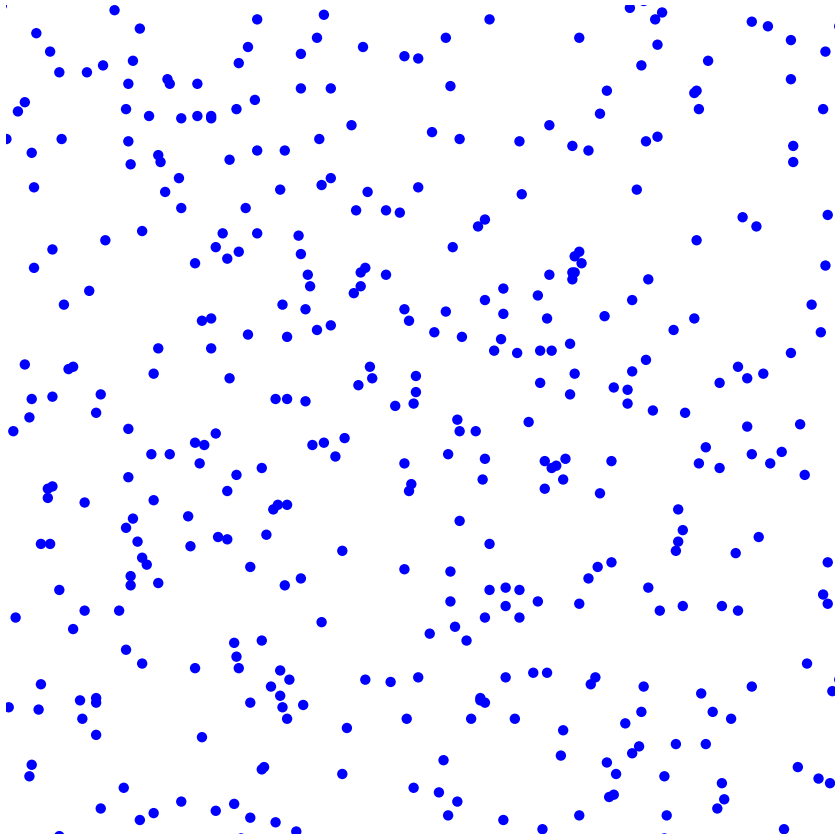
Fixed random scatterer configuration



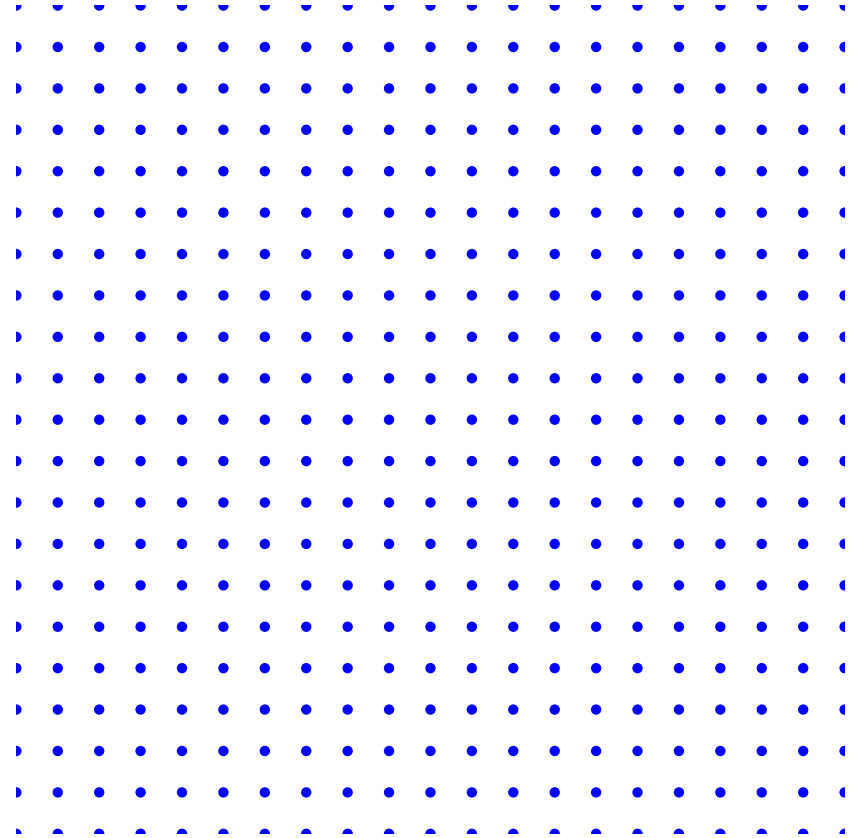
Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/6$, mean free path = $\frac{1}{2r} = 3$

Lorentz gas in the small scatterer limit



Fixed random scatterer configuration



Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/8$, mean free path $= \frac{1}{2r} = 4$

The Boltzmann-Grad (=low-density) limit

- Consider the dynamics in the limit of small scatterer radius r , dimension $d \geq 2$
- $(\mathbf{q}(t), \mathbf{v}(t))$ = “microscopic” phase space coordinate at time t
- A volume argument shows that for $r \rightarrow 0$ the mean free path length (i.e., the average time between consecutive collisions) is asymptotic to

$$\frac{1}{\text{total scattering cross section}} = \frac{1}{r^{d-1} \text{vol } B_1^{d-1}}$$

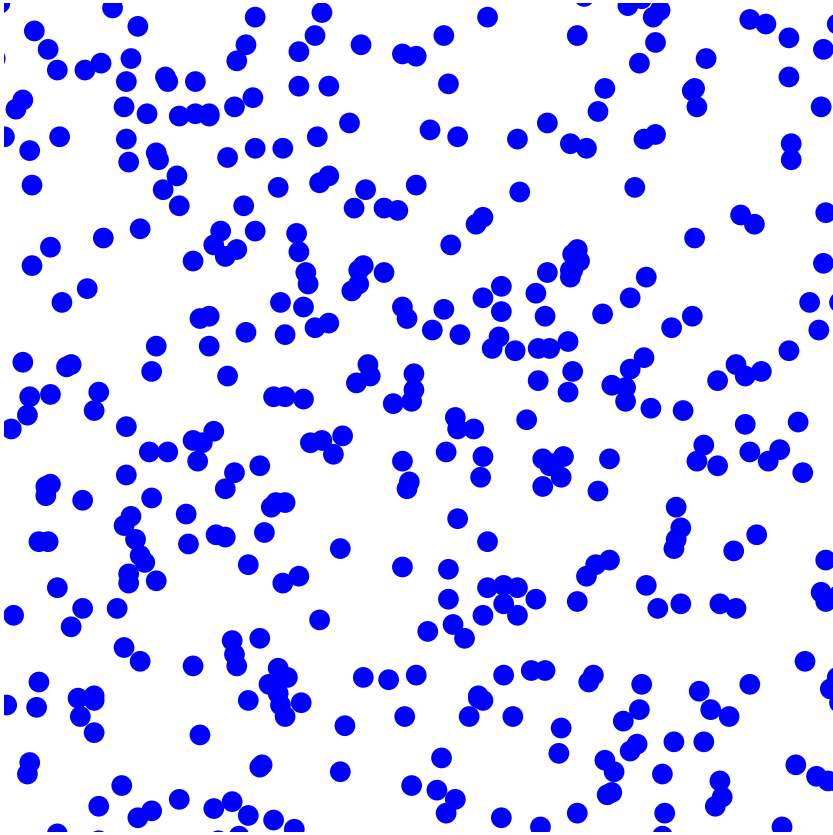
- We thus measure position and time in the “macroscopic” coordinates

$$(\mathbf{x}(t), \mathbf{y}(t)) = (r^{d-1} \mathbf{x}(r^{1-d}t), \mathbf{v}(r^{1-d}t))$$

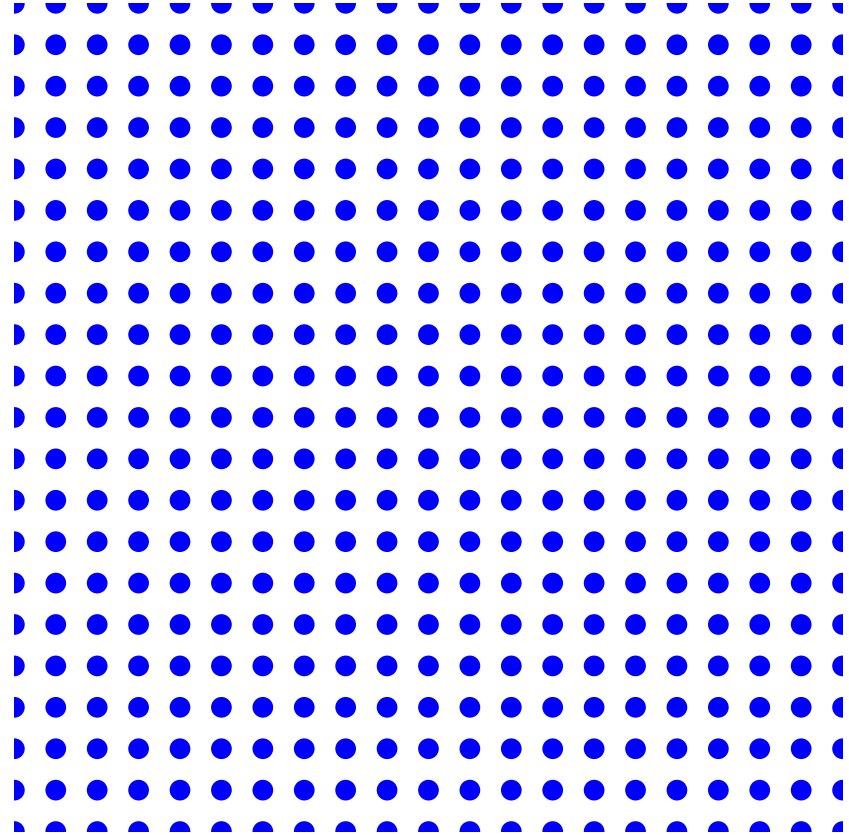
- Time evolution of initial data $(\mathbf{x}_0, \mathbf{y}_0)$:

$$(\mathbf{x}(t), \mathbf{y}(t)) = \Phi_r^t(\mathbf{x}_0, \mathbf{y}_0)$$

The Boltzmann-Grad limit



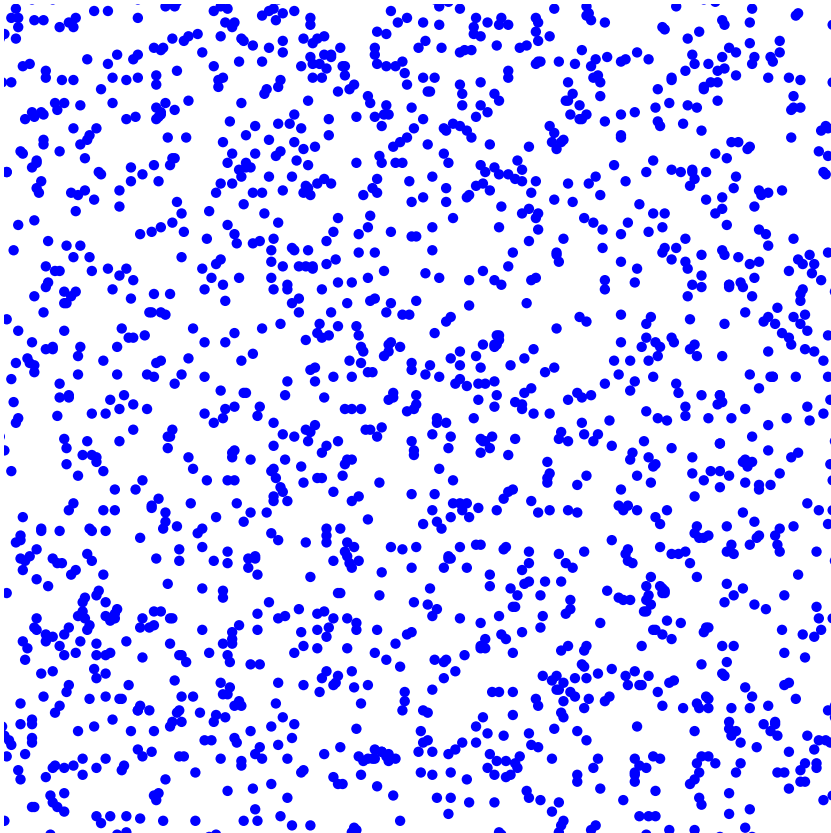
Fixed random scatterer configuration



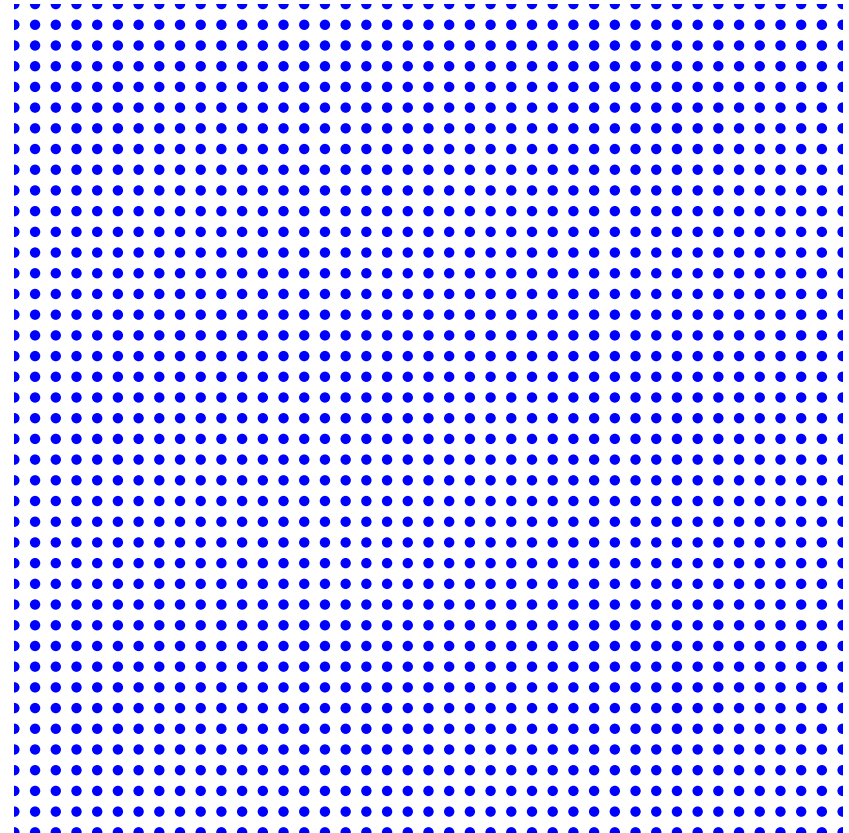
Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/4$, mean free path = $\frac{1}{2r} = 2$

The Boltzmann-Grad limit



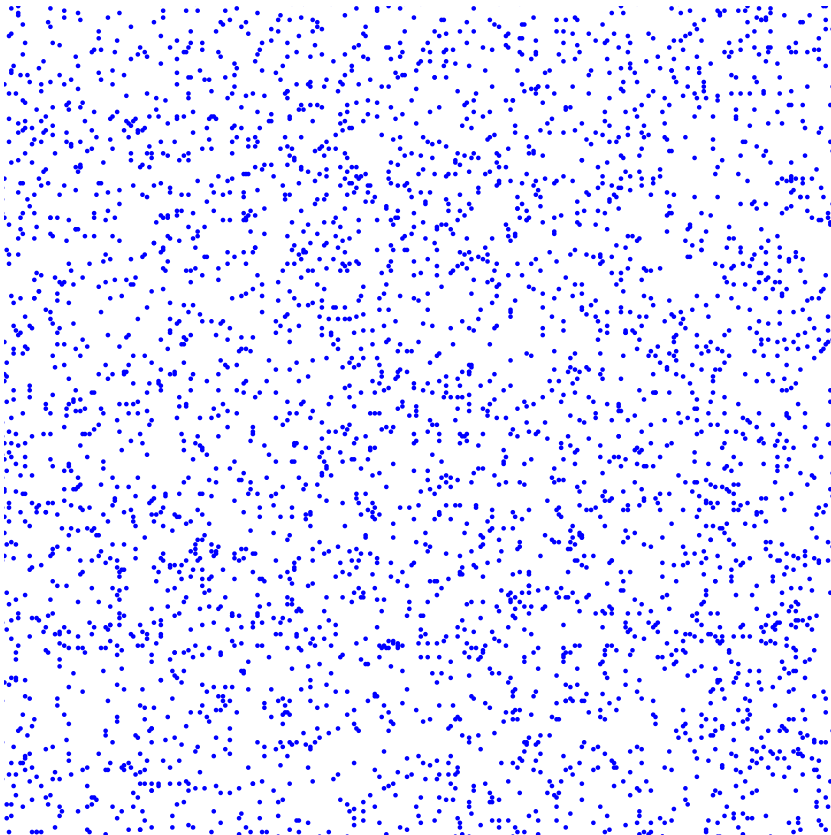
Fixed random scatterer configuration



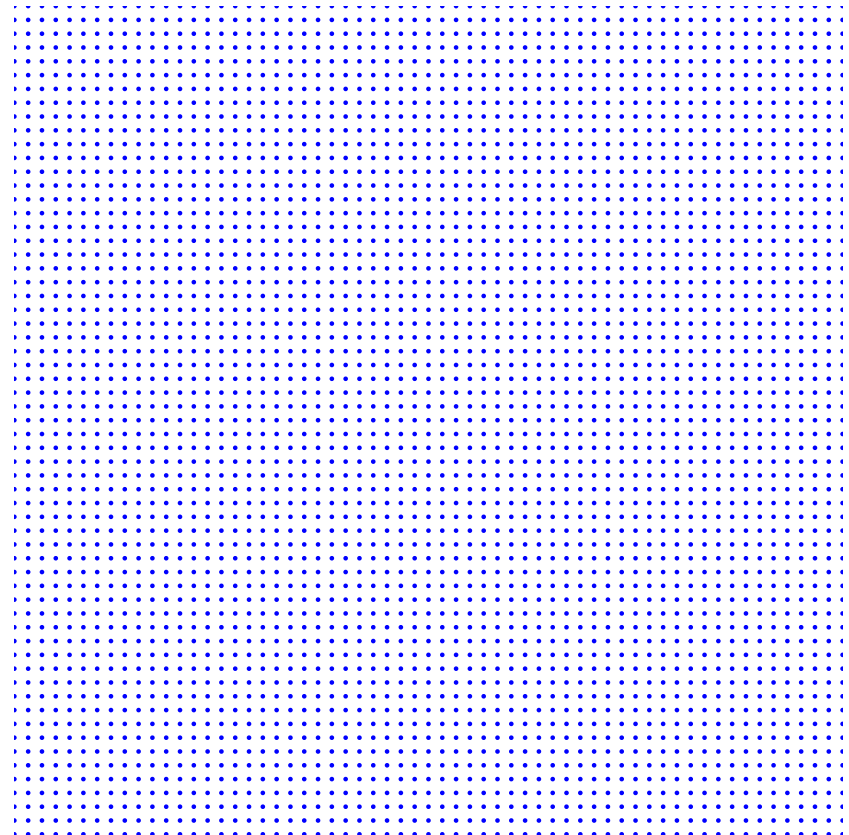
Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/4$; 1/2-zoom: macroscopic mean free path=1

The Boltzmann-Grad limit



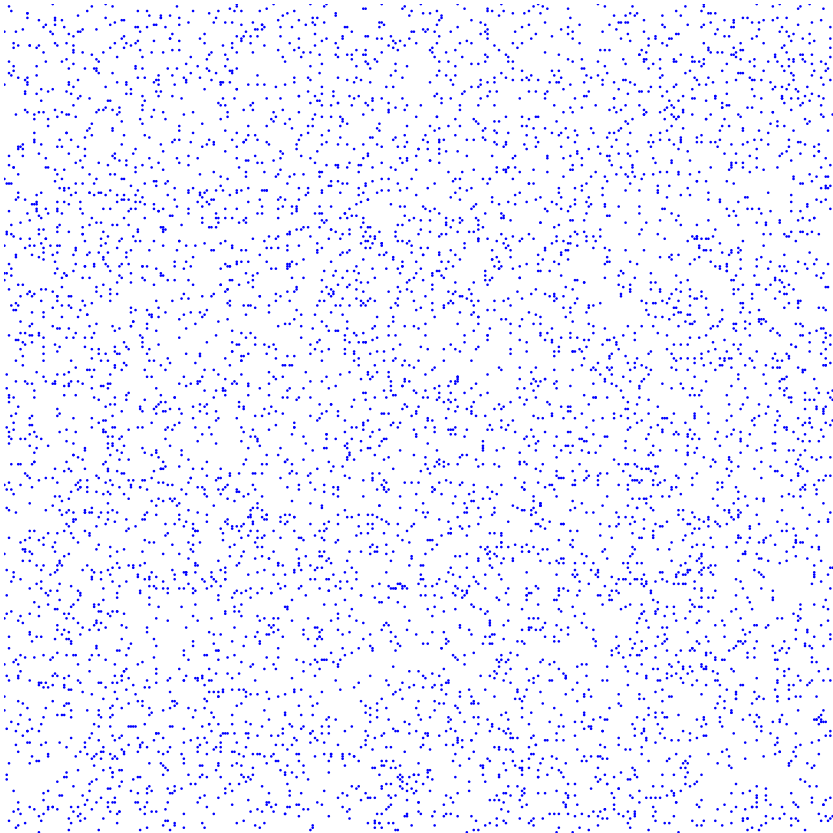
Fixed random scatterer configuration



Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/6$; 1/3-zoom: macroscopic mean free path=1

The Boltzmann-Grad limit



Fixed random scatterer configuration



Periodic scatterer configuration \mathbb{Z}^2

Scattering radius $r = 1/8$; 1/4-zoom: macroscopic mean free path=1

The linear Boltzmann equation

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

$$f_t^{(r)}(\mathbf{x}, \mathbf{y}) := f(\Phi_r^{-t}(\mathbf{x}, \mathbf{y}))$$

In his 1905 paper Lorentz suggested that $f_t^{(r)}$ is governed, as $r \rightarrow 0$, by the linear Boltzmann equation:

$$(\partial_t + \mathbf{y} \cdot \nabla_{\mathbf{x}}) f(t, \mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^d} [\Sigma(\mathbf{y}, \mathbf{y}') f(t, \mathbf{x}, \mathbf{y}') - \Sigma(\mathbf{y}', \mathbf{y}) f(t, \mathbf{x}, \mathbf{y})] d\mathbf{y}'$$

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

Applications: Neutron transport, radiative transfer, ...

The linear Boltzmann equation—rigorous proofs

Random

- Galavotti (Phys Rev 1969 & report 1972): Poisson distributed hard-sphere scatterer configuration
- 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 (w.r.t. the Poisson process)

Periodic

- Golse (Ann Fac Toulouse 2008): failure of linear Boltzmann equation; Caglioti and Golse (Comptes Rendus 2008, J Stat Phys 2010): identified limit process in two dimensions
- JM and Strömbergsson (Nonlinearity 2008, Annals Math 2010, Annals Math 2011, GAFA 2011): proof of convergence of Lorentz gas to limit process (in arbitrary dimension); extension to quasicrystals and other aperiodic scatterer configurations (Memoirs AMS, to appear)

The quantum Lorentz gas

Random

- Spohn (J Stat Phys 1977): Gaussian random potentials, weak coupling limit & 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): random scatterer configuration with smooth potential, Boltzmann-Grad limit

Periodic “easy”... ? >>>**this talk**<<<

- Griffin and JM (Pure Applied Math 2019, J Stat Phys 2021): periodic scatterer configuration, new limit process in Boltzmann-Grad limit

The setting

- Schrödinger equation

$$i\frac{h}{2\pi} \partial_t f(t, \mathbf{x}) = H_{h,\lambda} f(t, \mathbf{x}), \quad f(0, \mathbf{x}) = f_0(\mathbf{x})$$

- quantum Hamiltonian

$$H_{h,\lambda} = -\frac{h^2}{8\pi^2} \Delta + \lambda V(\mathbf{x})$$

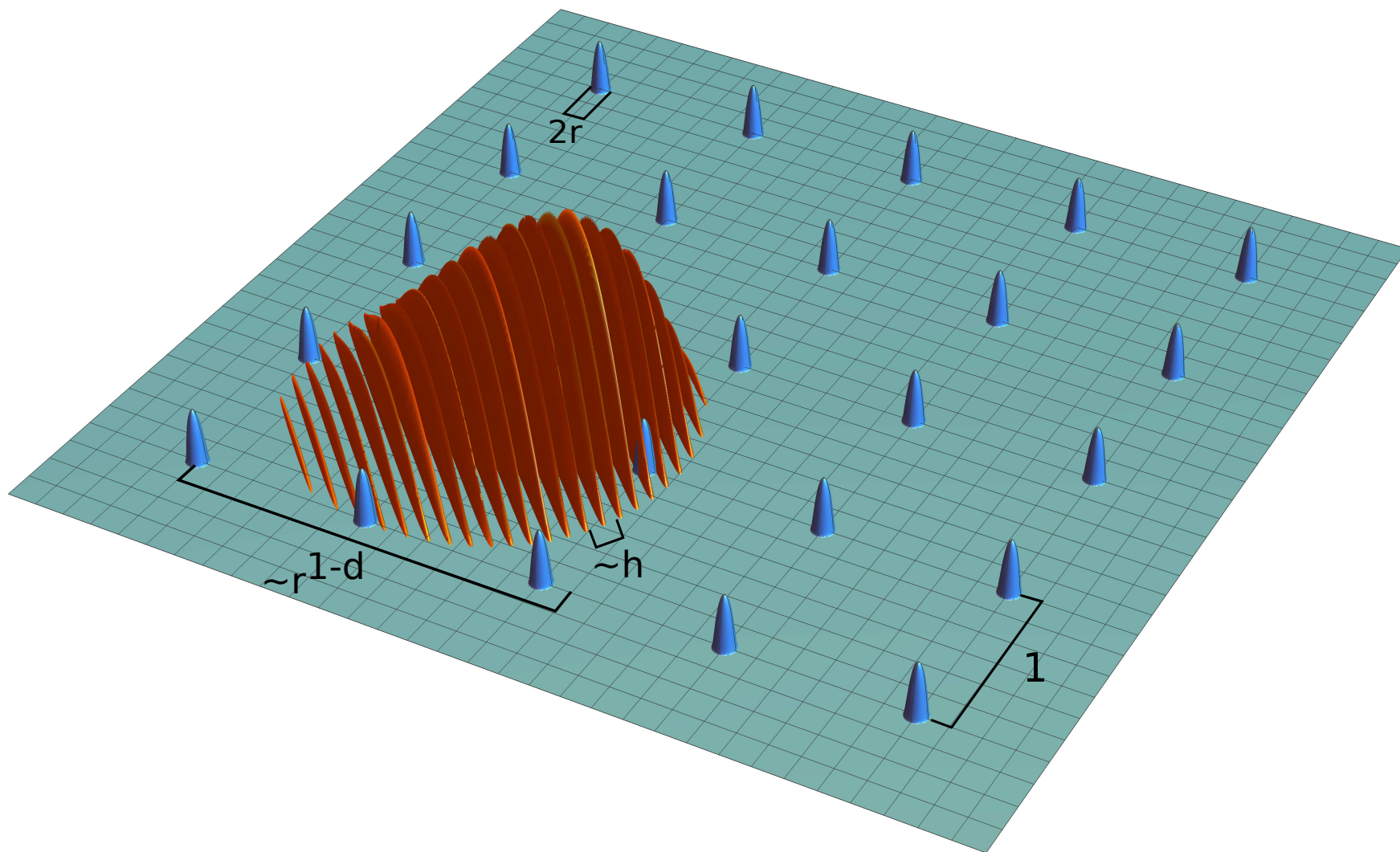
- potential

$$V(\mathbf{x}) = V_r(\mathbf{x}) = \sum_{m \in \mathcal{P}} W(r^{-1}(\mathbf{x} + m)), \quad W \in \mathcal{S}(\mathbb{R}^d)$$

with \mathcal{P} point set describing location of scatterers (e.g. $\mathcal{P} = \mathbb{Z}^d$)

- solution

$$f(t, \mathbf{x}) = U_{h,\lambda}(t) f_0(\mathbf{x}), \quad U_{h,\lambda}(t) = e^{-2\pi i H_{h,\lambda} t / h}$$



Observables

- time evolution of linear operators $A(t)$ (“quantum observables”) given by Heisenberg evolution $A(t) = U_{h,\lambda}(t) A U_{h,\lambda}(t)^{-1}$.
- L^2 inner product on classical phase space

$$\langle a, b \rangle = \int_{\mathbb{R}^d \times \mathbb{R}^d} a(\mathbf{x}, \mathbf{y}) \overline{b(\mathbf{x}, \mathbf{y})} d\mathbf{x} d\mathbf{y},$$

- Hilbert-Schmidt inner product $\langle A, B \rangle_{\text{HS}} = \text{Tr} AB^\dagger$.
- semiclassical Boltzmann-Grad scaling

$$D_{r,h} a(\mathbf{x}, \mathbf{y}) = r^{d(d-1)/2} h^{d/2} a(r^{d-1} \mathbf{x}, h \mathbf{y}),$$

- standard Weyl quantisation of $a \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$,

$$\text{Op}(a) f(\mathbf{x}) = \int_{\mathbb{R}^d \times \mathbb{R}^d} a\left(\frac{1}{2}(\mathbf{x} + \mathbf{x}'), \mathbf{y}\right) e(i(\mathbf{x} - \mathbf{x}') \cdot \mathbf{y}) f(\mathbf{x}') d\mathbf{x}' d\mathbf{y}$$

- Set $\text{Op}_{r,h} = \text{Op} \circ D_{r,h}$ and $\text{Op}_h = \text{Op}_{1,h}$.

A limiting transport process?

Pick your favourite scatterer configuration \mathcal{P} (random or deterministic).

Questions.

(i) Does there exist a family of operators $L(t) : L^1(\mathbb{R}^d \times \mathbb{R}^d) \rightarrow L^1(\mathbb{R}^d \times \mathbb{R}^d)$ such that for all $a, b \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, $A = \text{Op}_{r,h}(a)$, $B = \text{Op}_{r,h}(b)$,

$$\lim_{r \rightarrow 0} \langle A(tr^{-(d-1)}), B \rangle_{\text{HS}} = \langle L(t)a, b \rangle \quad ?$$

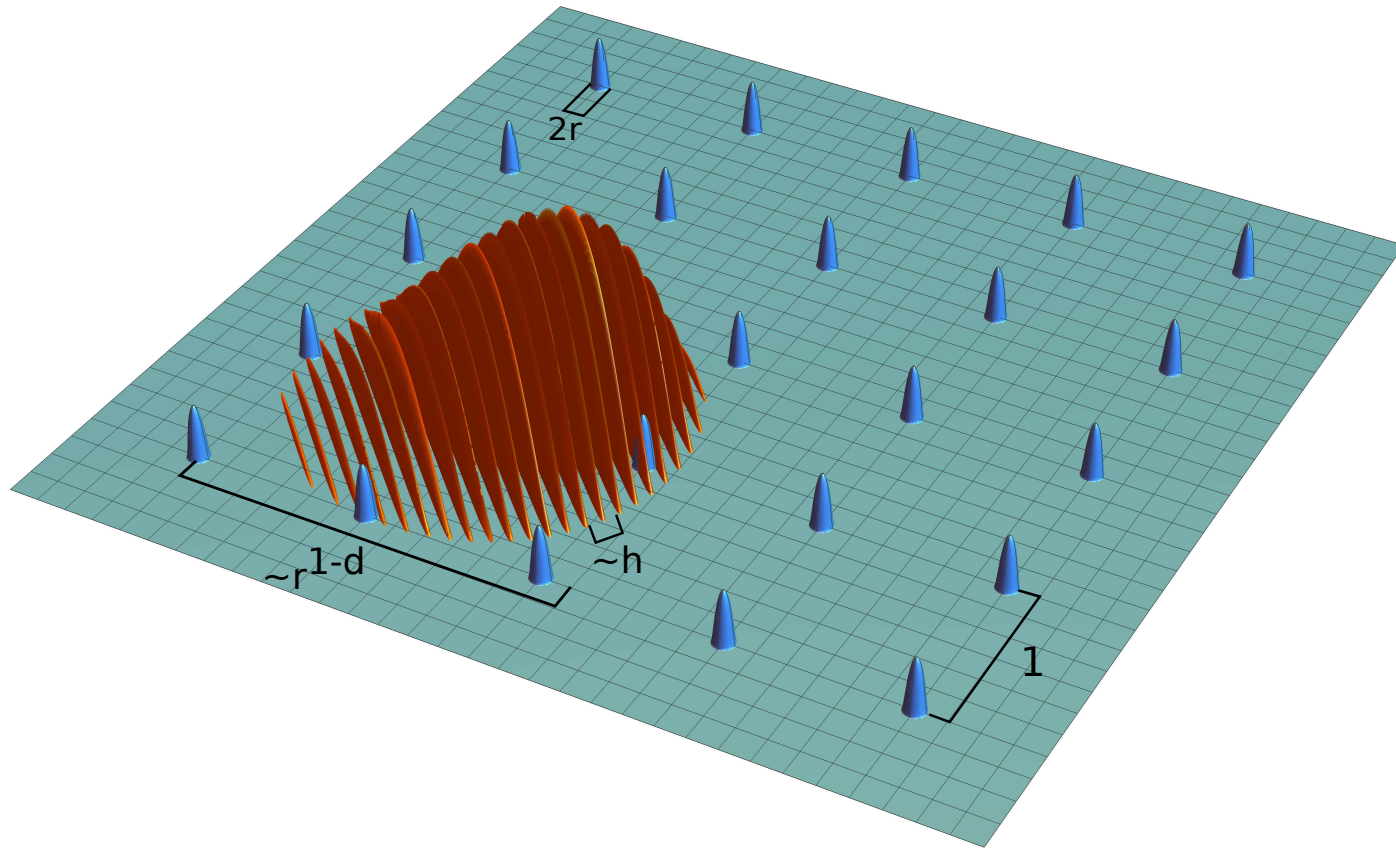
(ii) Is $f(t, \mathbf{x}, \mathbf{y}) = L(t)a(\mathbf{x}, \mathbf{y})$ a solution of the linear Boltzmann equation?

For random scatterer configurations Eng and Erdős (Rev Math Phys 2005) have proved convergence (in the annealed case) to a limit $L(t)$, which in fact is a solution to the linear Boltzmann equation with the standard quantum mechanical collision kernel

$$\Sigma(\mathbf{y}, \mathbf{y}') = 8\pi^2 \delta(\|\mathbf{y}\|^2 - \|\mathbf{y}'\|^2) |T(\mathbf{y}, \mathbf{y}')|^2.$$

Here $T(\mathbf{y}, \mathbf{y}')$ is the (single scatterer) T -matrix.

>>> **Semiclassical propagation with quantum scattering** <<<



>>> Semiclassical propagation with quantum scattering <<<

A limiting transport process!

Consider the periodic scatterer configuration $\mathcal{P} = \mathbb{Z}^d$ (or any other lattice in \mathbb{R}^d of full rank).

Theorem (Griffin & JM, J Stat Phys 2021).

Conditional on a generalised Berry-Tabor conjecture:

(i) There exists a family of operators $L(t) : L^1(\mathbb{R}^d \times \mathbb{R}^d) \rightarrow L^1(\mathbb{R}^d \times \mathbb{R}^d)$ such that for all $a, b \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, $A = \text{Op}_{r,h}(a)$, $B = \text{Op}_{r,h}(b)$, $t > 0$ and $0 < \lambda \leq \lambda_0$ (λ_0 sufficiently small)

$$\lim_{r \rightarrow 0} \langle A(tr^{-(d-1)}), B \rangle_{\text{HS}} = \langle L(t)a, b \rangle$$

(ii) $f(t, x, y) = L(t)a(x, y)$ is **NOT** a solution of the linear Boltzmann equation.

The statement can be proved unconditionally up to second order in perturbation theory (in λ): Griffin and JM, Pure & Applied Analysis 2019.

Collision series for linear Boltzmann

Total scattering cross section $\Sigma_{\text{tot}}(\mathbf{y}) = \int_{\mathbb{R}^d} \Sigma(\mathbf{y}', \mathbf{y}) \mathbf{y}'$

Collision series for solution of the linear Boltzmann equation

$$f_{\text{LB}}(t, \mathbf{x}, \mathbf{y}) = \sum_{k=1}^{\infty} f_{\text{LB}}^{(k)}(t, \mathbf{x}, \mathbf{y})$$

with the zero-collision term

$$f_{\text{LB}}^{(1)}(t, \mathbf{x}, \mathbf{y}) = a(\mathbf{x} - t\mathbf{y}, \mathbf{y}) e^{-t\Sigma_{\text{tot}}(\mathbf{y})},$$

and the $(k - 1)$ -collision term ...

Collision series for linear Boltzmann

... and the $(k - 1)$ -collision term

$$f_{\text{LB}}^{(k)}(t, \mathbf{x}, \mathbf{y}) = \int_{(\mathbb{R}^d)^k} \int_{\mathbb{R}_{\geq 0}^k} \delta(\mathbf{y} - \mathbf{y}_1) a\left(\mathbf{x} - \sum_{j=1}^k u_j \mathbf{y}_j, \mathbf{y}_k\right) \\ \times \rho_{\text{LB}}^{(k)}(\mathbf{u}, \mathbf{y}_1, \dots, \mathbf{y}_k) \delta\left(t - \sum_{j=1}^k u_j\right) d\mathbf{u} d\mathbf{y}_1 \cdots d\mathbf{y}_k$$

with

$$\rho_{\text{LB}}^{(k)}(\mathbf{u}, \mathbf{y}_1, \dots, \mathbf{y}_k) = \prod_{i=1}^k e^{-u_i \Sigma_{\text{tot}}(\mathbf{y}_i)} \prod_{j=1}^{k-1} \Sigma(\mathbf{y}_j, \mathbf{y}_{j+1}).$$

The product form of the density $\rho_{\text{LB}}^{(k)}$ shows that the corresponding random flight process is Markovian, and describes a particle moving along a random piecewise linear curve with momenta \mathbf{y}_i and exponentially distributed flight times u_i .

Collision series for our limit process

Collision series

$$f(t, \mathbf{x}, \mathbf{y}) = \sum_{k=1}^{\infty} f^{(k)}(t, \mathbf{x}, \mathbf{y})$$

with the zero-collision term (as for LB)

$$f^{(1)}(t, \mathbf{x}, \mathbf{y}) = f_{\text{LB}}^{(1)}(t, \mathbf{x}, \mathbf{y}) = a(\mathbf{x} - t\mathbf{y}, \mathbf{y}) e^{-t\Sigma_{\text{tot}}(\mathbf{y})},$$

and the $(k - 1)$ -collision term ...

$$f^{(k)}(t, \mathbf{x}, \mathbf{y}) = \frac{1}{k!} \sum_{\ell, m=1}^k \int_{(\mathbb{R}^d)^k} \int_{\mathbb{R}_{\geq 0}^k} \delta(\mathbf{y} - \mathbf{y}_\ell) a\left(\mathbf{x} - \sum_{j=1}^k u_j \mathbf{y}_j, \mathbf{y}_m\right) \\ \times \rho_{\ell m}^{(k)}(\mathbf{u}, \mathbf{y}_1, \dots, \mathbf{y}_k) \delta\left(t - \sum_{j=1}^k u_j\right) d\mathbf{u} d\mathbf{y}_1 \cdots d\mathbf{y}_k,$$

with the collision densities ...

Collision series for our limit process

... with the **positive** collision densities

$$\rho_{\ell m}^{(k)}(\mathbf{u}, \mathbf{y}_1, \dots, \mathbf{y}_k) = \left| g_{\ell m}^{(k)}(\mathbf{u}, \mathbf{y}_1, \dots, \mathbf{y}_k) \right|^2 \omega_k(\mathbf{y}_1, \dots, \mathbf{y}_k) \prod_{i=1}^k e^{-u_i \Sigma_{\text{tot}}(\mathbf{y}_i)}.$$

Here

$$\omega_k(\mathbf{y}_1, \dots, \mathbf{y}_k) = \prod_{j=1}^{k-1} \delta\left(\frac{1}{2}\|\mathbf{y}_j\|^2 - \frac{1}{2}\|\mathbf{y}_{j+1}\|^2\right)$$

and $g_{\ell m}^{(k)}$ are the coefficients of the matrix valued function

$$\mathbb{G}^{(k)}(\mathbf{u}, \mathbf{y}_1, \dots, \mathbf{y}_k) = \frac{1}{(2\pi i)^k} \oint \cdots \oint (\mathbb{D}(\mathbf{z}) - \mathbb{W})^{-1} \exp(\mathbf{u} \cdot \mathbf{z}) dz_1 \cdots dz_k,$$

where $\mathbb{D}(\mathbf{z}) = \text{diag}(z_1, \dots, z_k)$ and $\mathbb{W} = \mathbb{W}(\mathbf{y}_1, \dots, \mathbf{y}_k)$ with entries

$$w_{ij} = \begin{cases} 0 & (i = j) \\ -2\pi i T(\mathbf{y}_i, \mathbf{y}_j) & (i \neq j). \end{cases}$$

>>> **Strong correlation with past momenta** <<<

Collision series for our limit process

Explicitly, for the one collision terms

$$\rho_{11}^{(2)}(\mathbf{u}, \mathbf{y}_1, \mathbf{y}_2) = \rho_{\text{LB}}^{(2)}(\mathbf{u}, \mathbf{y}_1, \mathbf{y}_2) \left| \frac{u_1 T(\mathbf{y}_2, \mathbf{y}_1)}{u_2 T(\mathbf{y}_1, \mathbf{y}_2)} \right| \times \left| J_1 \left(4\pi [u_1 u_2 T(\mathbf{y}_1, \mathbf{y}_2) T(\mathbf{y}_2, \mathbf{y}_1)]^{1/2} \right) \right|^2.$$

and

$$\rho_{12}^{(2)}(\mathbf{u}, \mathbf{y}_1, \mathbf{y}_2) = \rho_{\text{LB}}^{(2)}(\mathbf{u}, \mathbf{y}_1, \mathbf{y}_2) \left| J_0 \left(4\pi [u_1 u_2 T(\mathbf{y}_1, \mathbf{y}_2) T(\mathbf{y}_2, \mathbf{y}_1)]^{1/2} \right) \right|^2$$

with J_k the standard Bessel functions.

The remaining matrix elements can be computed via the identities

$$\rho_{22}^{(2)}(u_1, u_2, \mathbf{y}_1, \mathbf{y}_2) = \rho_{11}^{(2)}(u_2, u_1, \mathbf{y}_2, \mathbf{y}_1),$$

$$\rho_{21}^{(2)}(u_1, u_2, \mathbf{y}_1, \mathbf{y}_2) = \rho_{12}^{(2)}(u_2, u_1, \mathbf{y}_2, \mathbf{y}_1).$$

- Above formulas strikingly similar to those for two-point spectral statistics in diffractive systems (Bogomolny and Giraud, Nonlinearity 2002)

Key steps in proof

- Use Floquet-Bloch decomposition to reduce problem to L^2 subspaces of functions

$$\psi(\mathbf{x} + \mathbf{k}) = e(\mathbf{k} \cdot \boldsymbol{\alpha})\psi(\mathbf{x}), \quad \forall \mathbf{k} \in \mathbb{Z}^d$$

with $\boldsymbol{\alpha} \in [0, 1)^d$

- Consider each $\boldsymbol{\alpha}$ -subspace separately (random or fixed)
- Use iterated application of Duhamel formula for quantum propagator,

$$U_{\lambda,h}(t) = U_{0,h}(t) - 2\pi i \lambda \int_0^t U_{\lambda,h}(t-s) \text{Op}(V)U_{0,h}(s)ds,$$

to produce perturbation expansion

- The eigenphases of $U_{0,h}(t)$ restricted to $\boldsymbol{\alpha}$ -subspace are of the form

$$\pi t \|\mathbf{m} + \boldsymbol{\alpha}\|^2, \quad \mathbf{m} \in \mathbb{Z}^d$$

Key steps in proof

- Set $\mathcal{P}_\alpha = \mathbb{Z}^d + \alpha$
- The $(n - 1)$ collision term can be expressed in the form

$$r^d \sum_{\substack{\mathbf{p}_1, \dots, \mathbf{p}_n = \mathbf{p}_0 \in \mathcal{P}_\alpha \\ \text{non-consec}}} H_{t,\ell,n} \left(r^{2-d} \left(\frac{1}{2} \|\mathbf{p}_0\|^2, \dots, \frac{1}{2} \|\mathbf{p}_n\|^2 \right), r\mathbf{p}_0, \dots, r\mathbf{p}_n \right)$$

form some (not so well behaved) function $H_{t,\ell,n}$, which has translation invariance in the first coordinates so that it only depends on the differences between the $\|\mathbf{p}_j\|^2$

- The above expression is thus the n -point correlation density of \mathcal{P} tested against $H_{t,\ell,n}$ — measured on the scale of their mean separation
- **Our key assumption in this work is that we can replace \mathcal{P}_α , for typical (or random) α by a Poisson point process in \mathbb{R}^d of intensity one**

How random is $\mathcal{P}_\alpha = \mathbb{Z}^d + \alpha$?

Illustrative example for $d = 2$:

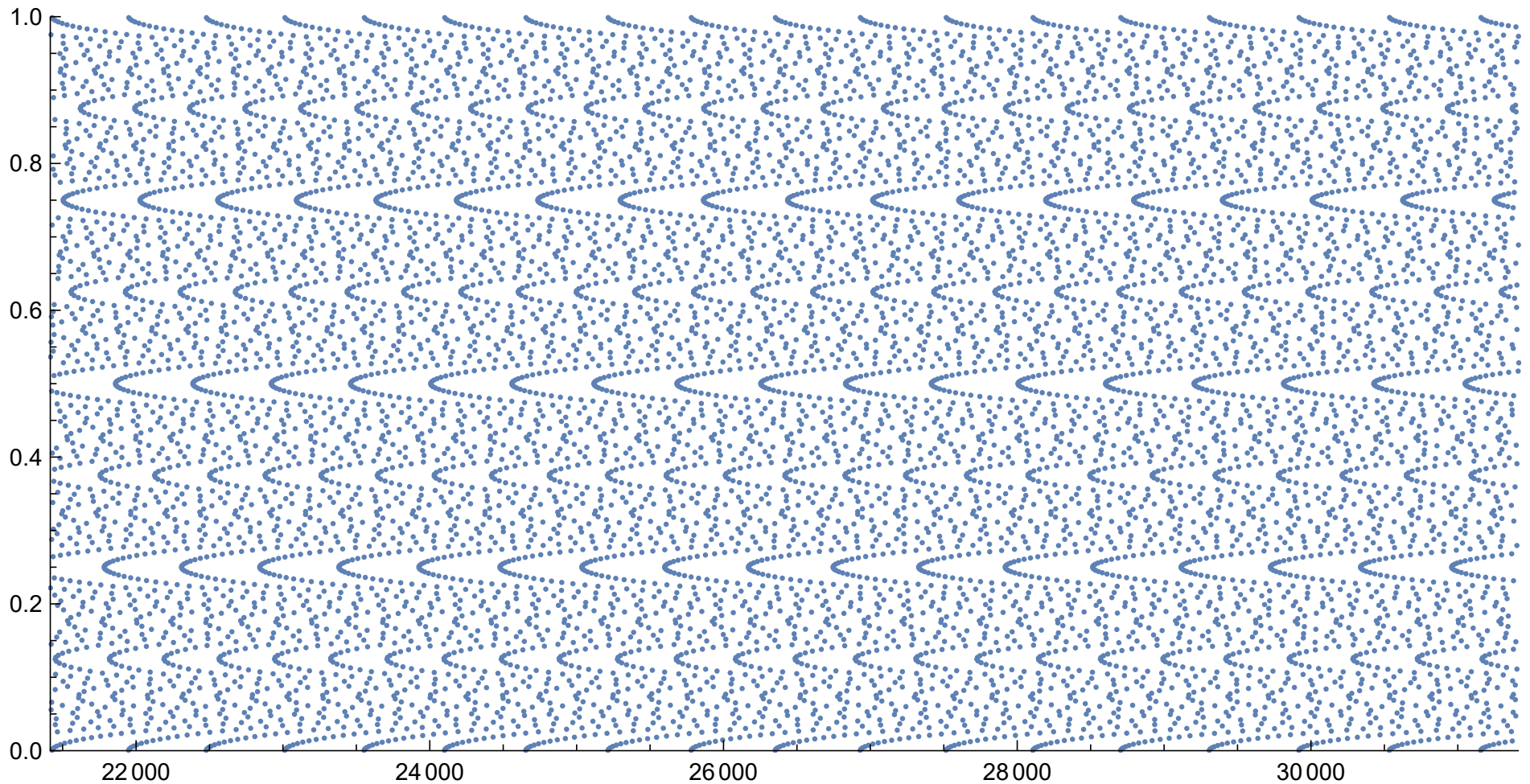
- Fix $\alpha = (\sqrt{2}, \sqrt{3})$ ← not even generic/random

- Consider the sequence $(\lambda_i, \theta_i)_{i \in \mathbb{N}}$ of elements of the set

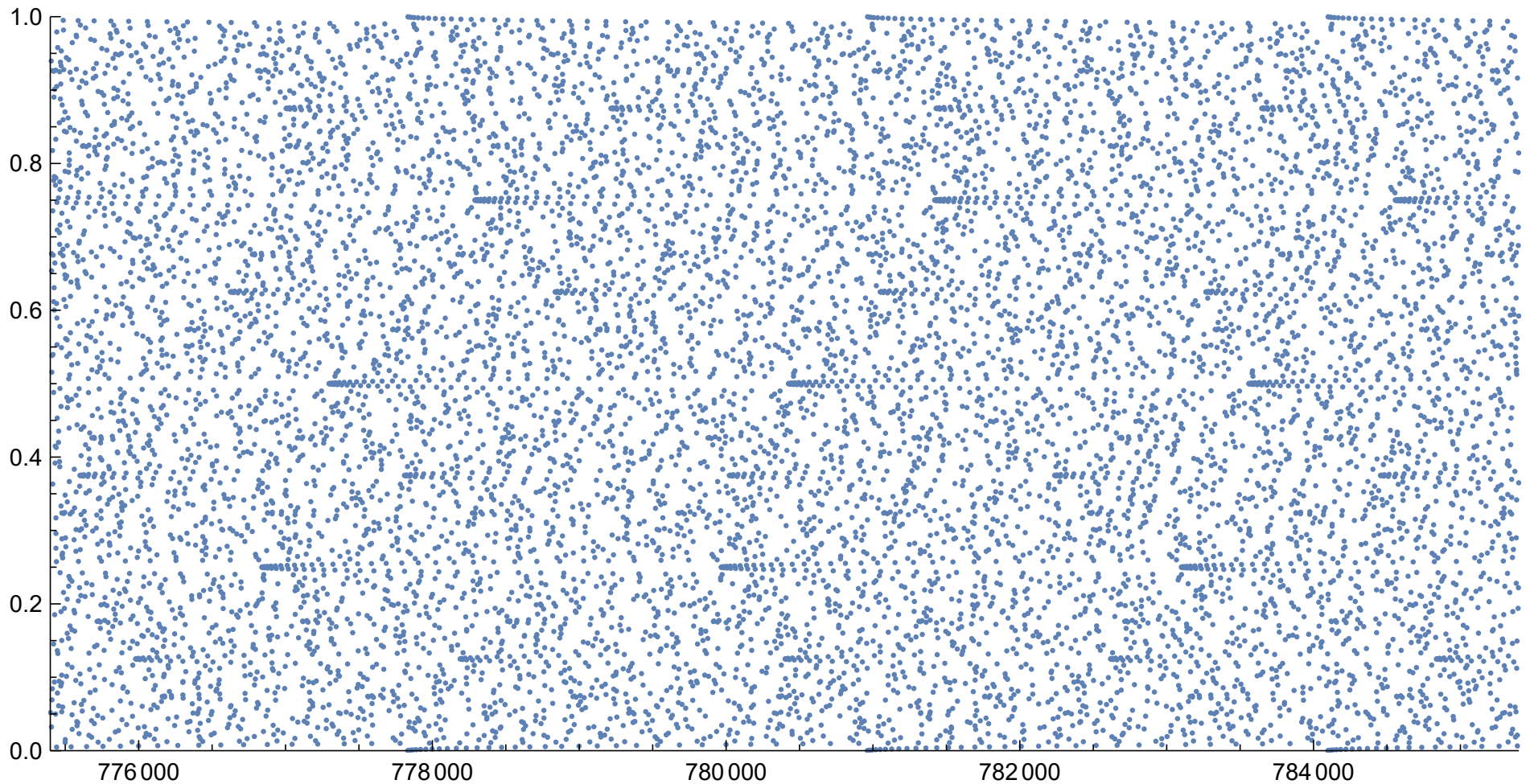
$$\left\{ \left(\pi \|n + \alpha\|^2, \frac{1}{2\pi} \arg(n + \alpha) \right) \in \mathbb{R}_{\geq 0} \times [0, 1) \mid n \in \mathbb{Z}^2 \right\}$$

arranged in increasing order according to the first component

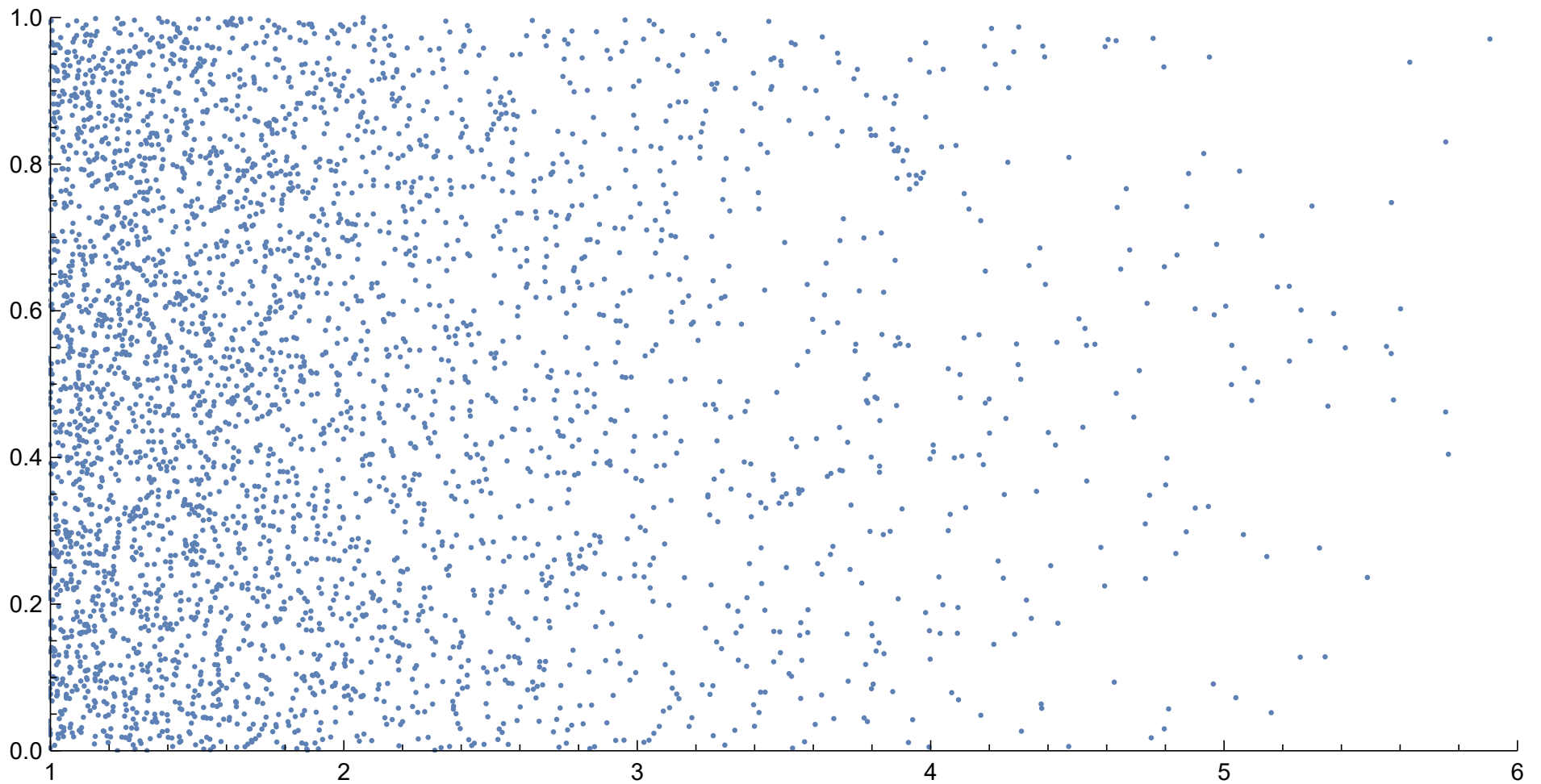
- Our assumption is concerned with the distribution of points (λ_i, θ_i) restricted to a strip $[R - \Delta R, R) \times [0, 1)$ for $\Delta R > 0$ fixed and $R \rightarrow \infty$



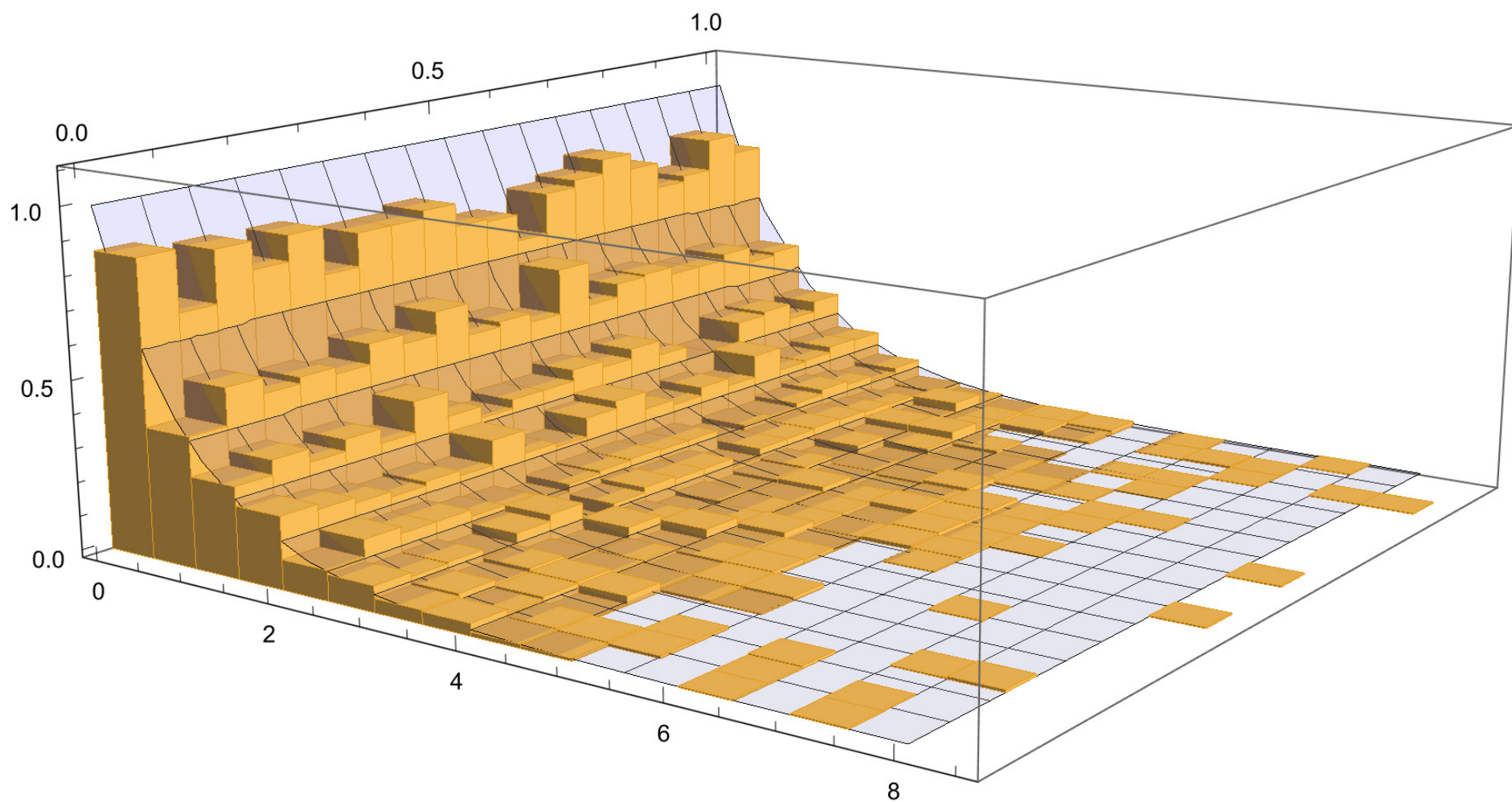
Scatter plots of (λ_i, θ_i) in the strip $[R - \Delta R, R) \times [0, 1)$ for $R = \pi \times 100^2$, with $\Delta R = 10^4$. For large R we expect the point set to be modelled by a Poisson point process.



Scatter plots of (λ_i, θ_i) in the strip $[R - \Delta R, R) \times [0, 1)$ for $R = \pi \times 500^2$, with $\Delta R = 10^4$. For large R we expect the point set to be modelled by a Poisson point process.



Scatter plot for the sequence $(\lambda_{i+1} - \lambda_i, \theta_i)$ for $R = \pi \times 500^2$ and $\Delta R = 10^4$



Histogram for the sequence $(\lambda_{i+1} - \lambda_i, \theta_i)$ for $R = \pi \times 500^2$ and $\Delta R = 10^4$

Theoretical evidence

- Our key assumption can be established for two-point correlations, in the case of random, generic and Diophantine $\alpha \in \mathbb{R}^d$ (JM, Annals Math 2003, Duke Math J 2002)
- Can be used to prove macroscopic limit up to order λ^2 (Griffin & JM, Pure & Applied Analysis 2019)

Outlook

- Can our hypothesis on the Poisson nature of

$$\|m + \alpha\|^2, \quad m \in \mathbb{Z}^d$$

can be made rigorous?

- Is the long-time limit of the macroscopic process (super-) diffusive?

(Cf. superdiffusive CLT for kinetic limit of classical periodic Lorentz gas, JM & Toth 2016)

- Other scaling limits: $h \ll r$ or $r \ll h$

- Extension to quasicrystals or other scatterer configurations with long-range correlations

Further reading

- J. Griffin and J. Marklof, Quantum transport in a low-density periodic potential: homogenisation via homogeneous flows, *Pure and Applied Analysis* 1 (2019) 571-614
- J. Griffin and J. Marklof, Quantum transport in a crystal with short-range interactions: The Boltzmann-Grad limit, *Journal of Statistical Physics* 184 (2021) no. 16; 46pp