Kinetic transport in the Lorentz gas: classical and quantum

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based on joint papers with
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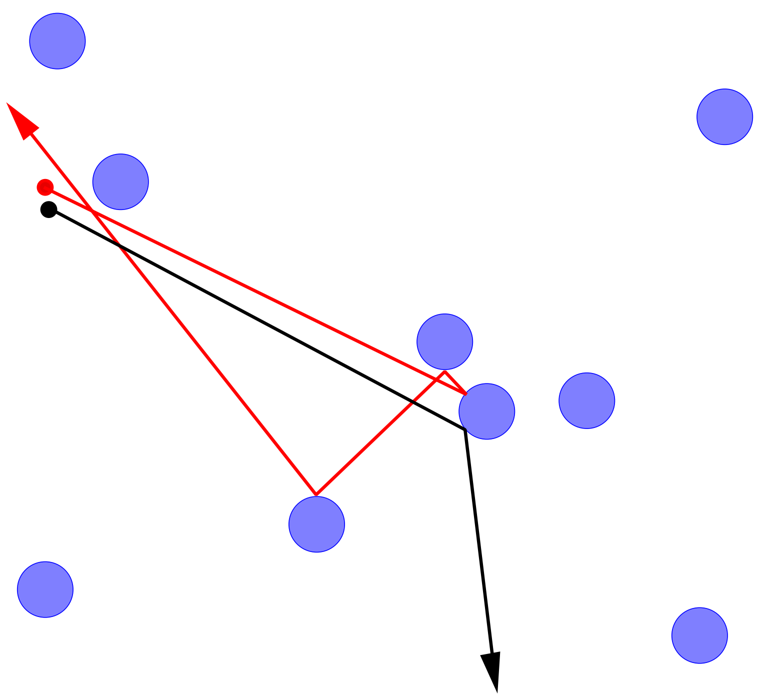
The Lorentz gas



- $\mathcal{P}$ — locally finite subset of $\mathbb{R}^d$ with constant density
- scatterers are fixed open balls of radius r centered at the points in $\mathcal{P}$
- the particles are assumed to be non-interacting
- each test particle moves with constant velocity $\boldsymbol{v}(t)$ between collisions
- the scattering is specular reflection
- we assume w.l.o.g. $\|\boldsymbol{v}(t)\| = 1$

Diffusion in the classical periodic Lorentz gas (dimension two)

In the case of fixed scattering radius r, proofs of CLT for the Lorentz gas are currently restricted to the 2-dim periodic setting.

Finite horizon:

- Bunimovich & Sinai (Comm Math Phys 1980): Standard CLT for finite horizon
- Melbourne & Nicol (Annals Prob 2009): More general invariance principles

Infinite horizon:

- Bleher (J Stat Phys 1992): Heuristics for CLT with $t \log t$ mean square displacement
- Szász & Varjú (J Stat Phys 2007): Proof of CLT for billiard map
- Dolgopyat & Chernov (Russ Math Surveys, 2009): Proof of CLT & invariance principle in continuous time

Diffusion in the classical periodic Lorentz gas (higher dimension)

The problem in higher dimensions is control of complexity of singularities

- Chernov (J Stat Phys 1994)
- Balint & Toth (AHP 2008, Nonlinearity 2012)

and in the case of infinite horizon the subtle geometry of free flight channels

- Dettmann (J Stat Phys 2012)
- Nadori, Szasz & Varju (CMP 2014)

As we will see, the problem becomes tractable if we consider the small scatterer (Boltzmann-Grad) limit $r \to 0$. In particular (taking first $r \to 0$ then $t \to \infty$)

- JM & Balint Toth (CMP 2017): CLT with $t \log t$ mean square displacement in any dimension (with time t measured in units of the mean collision time); builds on JM & Strömbergsson (Annals Math 2010 & 2011, GAFA 2011)

Diffusion in the classical aperiodic/random Lorentz gas

For fixed r, still a major open problem–no CLT established so far.

- Liverani's talk
- Dolgopyat, Szasz & Varju (Duke 2009): finite local perturbations
- Lenci (ETDS 2003/06); Christadoro, degli Esposti, Lenci & Seri (Chaos 2010, J Stat Phys 2011); Lenci & Troubetzkoy (Phys D 2011): recurrence properties

What can be said in the Boltzmann-Grad limit $r \to 0$?

The Boltzmann-Grad limit

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

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

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

- We thus measure position and time the "macroscopic" coordinates

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

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

$$\big(\boldsymbol{Q}(t), \boldsymbol{V}(t)\big) = \Phi_r^t(\boldsymbol{Q}, \boldsymbol{V})$$

The linear Boltzmann equation

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

$$f_t^{(r)}(\boldsymbol{Q},\boldsymbol{V}) := f\Big(\Phi_r^{-t}(\boldsymbol{Q},\boldsymbol{V})\Big)$$

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

$$\left[\frac{\partial}{\partial t} + \boldsymbol{V}\cdot\nabla_{\boldsymbol{Q}}\right] f_t(\boldsymbol{Q},\boldsymbol{V}) = \int_{\mathsf{S}_1^{d-1}} \Big[f_t(\boldsymbol{Q},\boldsymbol{V}') - f_t(\boldsymbol{Q},\boldsymbol{V})\Big]\sigma(\boldsymbol{V},\boldsymbol{V}')\,d\boldsymbol{V}'$$

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

Applications: Neutron transport, radiative transfer, . . .

The linear Boltzmann equation—rigorous proofs

Classical:

- Galavotti (Phys Rev 1969 & report 1972): Poisson distributed hard-sphere scatterer configuration $\mathcal{P}$
- Spohn (Comm Math Phys 1978): extension to more general random scatterer configurations $\mathcal{P}$ and potentials
- Boldrighini, Bunimovich and Sinai (J Stat Phys 1983): prove convergence for almost every scatterer configuration $\mathcal{P}$ (w.r.t. the Poisson random measure)
- Implies CLT for limit process (standard CLT for Markovian random flight process)

The linear Boltzmann equation—rigorous proofs

Quantum:

- Spohn (J Stat Phys 1977): Gaussian random potentials, weak coupling limit & small times
- Erdös and Yau (Contemp Math 1998, Comm Pure Appl Math 2000): General random potentials, weak coupling limit
- Eng and Erdös (Rev Math Phys 2005): smooth potentials, Boltzmann-Grad limit

Part I: Boltzmann-Grad limit of classical Lorentz gas for general scatterer configurations

(joint with A. Strömbergsson)

Part II: Boltzmann-Grad limit of quantum Lorentz gas for periodic scatterer configurations

(joint with J. Griffin)

Part I: Boltzmann-Grad limit of classical Lorentz gas for general scatterer configurations

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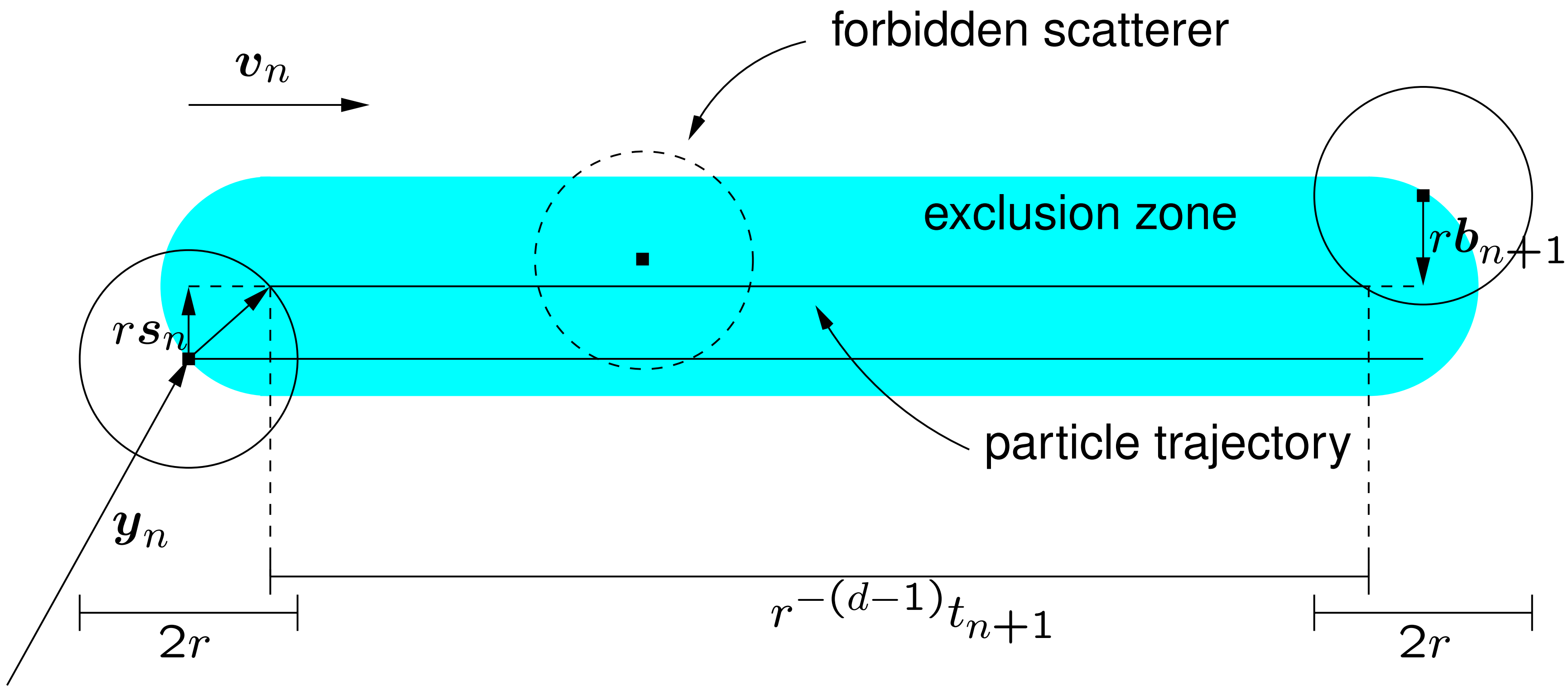
Intercollision flights



Intercollision flight in the Lorentz gas between the nth and $(n+1)$st collision. The exclusion zone is a long and thin cylinder of radius r with spherical caps. Scatterers are centered at $\mathcal{P}$.

Rescaling

- Define $R(\boldsymbol{v}) : \mathsf{S}_1^{d-1} \to \mathsf{SO}(d)$ such that $\boldsymbol{v}R(\boldsymbol{v}) = \boldsymbol{e}_1 = (1, 0, \ldots, 0)$ and

$$D_r = \begin{pmatrix} r^{d-1} & \mathbf{0} \\ {}^{t}\mathbf{0} & r^{-1} 1_{d-1} \end{pmatrix} \in \mathsf{SL}(d, \mathbb{R})$$

- Applying $R(\boldsymbol{v})D_r$ to the above this cylinder orients it along the e_1-axis and makes it well proportioned.

- If at nth scattering event scatterer is located at $\boldsymbol{y}_n \in \mathcal{P}$, and particle velocity is $\boldsymbol{v}_n$, consider

$$\Xi_r^{(n)} = (\mathcal{P} - \boldsymbol{y}_n) R(\boldsymbol{v}_n) D_r$$

- Since $\boldsymbol{v}_n$ and $\boldsymbol{y}_n$ are random (they are functions of the initial random position and velocity of the particle) we may think of $\Xi_r^{(n)}$ as a random point set (random point process)

Assumptions on the scatterer configuration $\mathcal{P}$ (I)

- Assume point set $\mathcal{P}$ has constant density, i.e., there is $c_{\mathcal{P}} > 0$ such that

$$\lim_{R\to\infty} \frac{\#(\mathcal{P} \cap R\mathcal{D})}{R^d} = c_{\mathcal{P}} \operatorname{vol} \mathcal{D}$$

  for all bounded sets $\mathcal{D} \subset \mathbb{R}^d$ with $\operatorname{vol} \partial\mathcal{D} = 0$

- For $\boldsymbol{y}$ fixed and $\boldsymbol{v}$ random, limit distribution of $(\mathcal{P} - \boldsymbol{y})R(\boldsymbol{v})D_r$ can in general depend on $\boldsymbol{y} \in \mathcal{P}$; in order to keep track of this, need to assign a **mark** to each $\boldsymbol{y}$; we want the space of marks to be nice

Assumptions on the scatterer configuration $\mathcal{P}$ (II)

- Let Σ compact metric space with Borel probability measure $\mathfrak{m}$, and map $\varsigma : \mathcal{P} \to \Sigma$ (the marking)

- Set $\mathcal{X} = \mathbb{R}^d \times \Sigma$, $\mu_{\mathcal{X}} = \mathrm{vol} \times \mathfrak{m}$
- $\tilde{\mathcal{P}} = \{(\boldsymbol{y}, \varsigma(\boldsymbol{y})) : \boldsymbol{y} \in \mathcal{P})\} \subset \mathcal{X}$ (the marked point set)
- for $M \in \mathrm{SL}(d, \mathbb{R})$ set $(\boldsymbol{y}, \varsigma(\boldsymbol{y}))M = (\boldsymbol{y}M, \varsigma(\boldsymbol{y}))$

- **Assumption 1** (density)

$$\lim_{R\to\infty} \frac{\#(\tilde{\mathcal{P}} \cap R\mathcal{D})}{R^d} = c_{\mathcal{P}} \mu_{\mathcal{X}}(\mathcal{D})$$

  for all bounded sets $\mathcal{D} \subset \mathcal{X}$ with $\mu_{\mathcal{X}}(\partial\mathcal{D}) = 0$
- **Assumption 2** (spherical equidistribution) For $\boldsymbol{v}$ random according to λ a.c. w.r.t. vol measure on S_1^{d-1}

$$\tilde{\Xi}_{r,\boldsymbol{y}} = (\tilde{\mathcal{P}} - \boldsymbol{y})R(\boldsymbol{v})D_r \xrightarrow{\mathrm{d}} \tilde{\Xi}_{\varsigma(\boldsymbol{y})} \qquad (r \to 0)$$

  uniformly for all $\boldsymbol{y} \in \mathcal{P}$ in balls of radius $\asymp r^{-(d-1)}$, where $\tilde{\Xi}_\varsigma$ **depends only on** $\varsigma \in \Sigma$

Examples for admissible $\mathcal{P}$

Example 1: $\mathcal{P} =$ a realization of the Poisson process in $\mathbb{R}^d$ with intensity 1, and $\Sigma = \{1\}$; proof non-trivial, follows ideas of Boldrighini, Bunimovich and Sinai (J Stat Phys 1983)

Example 2: $\mathcal{P} = \mathbb{Z}^d$ and $\Sigma = \{1\}$ (periodic Lorentz gas); proof uses spherical equidistribution on space of lattices (JM & Strömbergsson, Annals of Math 2010/11)

Example 3: $\mathcal{P} = \mathbb{Z}^d$ and $\Sigma = \{1\}$ (periodic Lorentz gas with random defects); proof uses spherical equidistribution on space of marked lattices (JM & Vinogradov, Geom. Dedicata 2017)

Example 4: $\mathcal{P} =$ Euclidean cut-and-project set (e.g. the vertex set of a Penrose tiling) and $\Sigma = \mathbb{R}^k$ (the internal space in the c&p construction); proof uses uses equidistribution of lower dimensional spheres in space of lattices and Ratner's theorem (JM & Strömbergsson, CMP 2014)

A limiting random process

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

$$[L_r^t f](\boldsymbol{Q},\boldsymbol{V}) = f\Big(\Phi_r^{-t}(\boldsymbol{Q},\boldsymbol{V})\Big).$$

Theorem A [JM & Strömbergsson 2018; for $\mathcal{P}=\mathbb{Z}^d$ Annals of Math 2011]. Assume $\mathcal{P}$ is as above (+ more). Then 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 Liouville measure zero,

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

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

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

A generalized linear Boltzmann equation

Consider extended phase space coordinates $(\boldsymbol{Q}, \boldsymbol{V}, \varsigma, \xi, \boldsymbol{V}_+)$:

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

$\varsigma \in \Sigma$ — the mark of current scatterer location

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

$\boldsymbol{V}_+ \in \mathrm{S}_1^{d-1}$ — velocity after the next hit

$$\left[\frac{\partial}{\partial t} + \boldsymbol{V} \cdot \nabla_{\boldsymbol{Q}} - \frac{\partial}{\partial \xi}\right] f_t(\boldsymbol{Q}, \boldsymbol{V}, \varsigma, \xi, \boldsymbol{V}_+)$$
$$= \int_\Sigma \int_{\mathrm{S}_1^{d-1}} f_t(\boldsymbol{Q}, \boldsymbol{V}', \varsigma', 0, \boldsymbol{V})\, p_0(\boldsymbol{V}', \varsigma', \boldsymbol{V}, \varsigma, \xi, \boldsymbol{V}_+) d\boldsymbol{V}' d\mathbb{m}(\varsigma').$$

with a collision kernel $p_0(\boldsymbol{V}', \varsigma', \boldsymbol{V}, \varsigma, \xi, \boldsymbol{V}_+)$, which can be expressed as a product of the scattering cross section of an individual scatterer and a certain transition probability for hitting a given point on the next scatterer with mark ς after time ξ, given the present scatterer has mark ς'.

Part II: Boltzmann-Grad limit of quantum Lorentz gas for periodic scatterer configurations

(joint with J. Griffin)

The setting

- Schrödinger equation

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

- quantum Hamiltonian

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

- potential

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

- solution

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

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

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

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

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

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

$$\mathrm{Op}(a)f(\boldsymbol{x}) = \int_{\mathbb{R}^d\times\mathbb{R}^d} a(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{x}'),\boldsymbol{y})\,\mathrm{e}((\boldsymbol{x}-\boldsymbol{x}')\cdot\boldsymbol{y})\,f(\boldsymbol{x}')\,d\boldsymbol{x}'d\boldsymbol{y}$$

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

A limiting transport process?

Conjecture. There exists a family of operators $L(t) : \mathsf{L}^1(\mathbb{R}^d \times \mathbb{R}^d) \to \mathsf{L}^1(\mathbb{R}^d \times \mathbb{R}^d)$ such that (i) for all $a, b \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, $A = \mathrm{Op}_{r,h}(a)$, $B = \mathrm{Op}_{r,h}(b)$, $\lambda > 0$ and $t > 0$,

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

and (ii) $L(t)a(\boldsymbol{x}, \boldsymbol{y})$ is in general **not** a solution to the linear Boltzmann equation.

For random scatterer configurations Eng and Erdös (Rev Math Phys 2005) have proved convergence to a limit $L(t)a(\boldsymbol{x}, \boldsymbol{y})$, which in fact is a solution to the linear Boltzmann equation with the standard quantum mechanical collision kernel

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

Here $T(\boldsymbol{y}, \boldsymbol{y}')$ is the kernel of the T-matrix in momentum representation.

Evidence for conjecture up to order λ^2

- Consider the formal expansion $L(t) \sim \sum_{n=0}^{\infty} L_n(t)\lambda^n$,
- $L_0(t)a(\boldsymbol{x},\boldsymbol{y}) = a(\boldsymbol{x} - t\boldsymbol{y}, \boldsymbol{y})$, $\qquad L_1(t)a(\boldsymbol{x},\boldsymbol{y}) = 0$,
- $L_2(t)a(\boldsymbol{x},\boldsymbol{y})$

$$= \int_0^t \int_{\mathbb{R}^d} \Sigma_2(\boldsymbol{y},\boldsymbol{y}')[a(\boldsymbol{x} - s\boldsymbol{y} - (t-s)\boldsymbol{y}', \boldsymbol{y}') - a(\boldsymbol{x} - t\boldsymbol{y}, \boldsymbol{y})]d\boldsymbol{y}'ds.$$

- These are consistent with $L(t)$ generating solutions of the linear Boltzmann equation.

Evidence for conjecture up to order λ^2

Theorem B [JM & Griffin 2018] Let $t > 0$ and $a, b \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$, $A = \mathrm{Op}_{r,h}(a)$, $B = \mathrm{Op}_{r,h}(b)$. Then there exist linear operators $A_0^{(r)}(t)$, $A_1^{(r)}(t)$, $A_2^{(r)}(t)$, such that

$$\langle A(tr^{-(d-1)}), B\rangle_{\mathrm{HS}} = \sum_{n=0}^{2} \langle A_n^{(r)}(tr^{-(d-1)}), B\rangle_{\mathrm{HS}}\, \lambda^n + \sum_{n=3}^{6} O(r^{-nd/2}\lambda^n).$$

and

$$\lim_{r\to 0} \langle A_n^{(r)}(tr^{-(d-1)}), B\rangle_{\mathrm{HS}} = \langle L_n(t)a, b\rangle \qquad (n = 0, 1, 2).$$

- We expect terms of order 4 and higher to not match the expansion for the linear Boltzmann equation (hence the conjecture)

Key steps in proof

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

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

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

- Prove first Theorem for almost every $\boldsymbol{\alpha}$ (in fact under explicit Diophantine conditions) and use dominated convergence
- Use Duhamel expansion for quantum propagator up to order 3

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

- Exploit a phase-space extension of the convergence of the pair correlation statistics of

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

to that of a Poisson process (JM, Duke Math J 2002, Annals of Math 2003)

Thank you!