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 $\rho$

• $\left( q(t), v(t) \right) =$ “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

$$\left( Q(t), V(t) \right) = \left( \rho^{d-1} q(\rho^{-(d-1)} t), v(\rho^{-(d-1)} t) \right)$$
The linear Boltzmann equation

- Time evolution of initial data \((Q, V)\):\[ (Q(t), V(t)) = \Phi^t_\rho(Q, V) \]

- Time evolution of a particle cloud with initial density \(f \in L^1\):\[ f_t = L^t_\rho f, \quad [L^t_\rho f](Q, V) := f(\Phi^{-t}_\rho(Q, V)) \]

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

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

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


- 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


- Eng and Erdös (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 $\sqrt{t}$.


- 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).


*“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

• \((q(t), v(t))\) = “microscopic” phase space coordinate at time \(t\)

• Re-define position and time and use the “macroscopic” coordinates

\[
(Q(t), V(t)) = (\rho^{d-1} q(\rho^{-(d-1)} t), v(\rho^{-(d-1)} t))
\]
A limiting random process

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

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

**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 \( A \subset \mathcal{T}^1(\mathbb{R}^d) \) with boundary of Lebesgue measure zero,

\[
\lim_{\rho \rightarrow 0} \int_A [L^t_\rho f](Q, V) \, dQ \, dV = \int_A [L^t f](Q, V) \, dQ \, dV.
\]

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

$$(Q, V) \in T^1(\mathbb{R}^d)$$ — 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:

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

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 \( \xi \) with impact parameter \( b(V, V_+) \)
\[ \rho_s \rho - (d-1) \xi \]
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):

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

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


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

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

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

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

with

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

the latter is a stationary solution of the generalized linear Boltzmann equation.
Why “a generalization” of the linear Boltzmann equation?

\[
\left[ \frac{\partial}{\partial t} + V \cdot \nabla Q - \frac{\partial}{\partial \xi} \right] f_t(Q, V, \xi, V_+) = \int_{S_{d-1}} f_t(Q, V_0, 0, V) p_0(V_0, V, \xi, V_+) dV_0
\]

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

\[ p_0(V_0, V, \xi, V_+) = \sigma(V, V_+) e^{-\text{vol}(B^d_{1-1}) \xi} \]

\[ f_t(Q, V, \xi, V_+) = g_t(Q, V) \sigma(V, V_+) e^{-\text{vol}(B^d_{1-1}) \xi} \]

yields the classical linear Boltzmann equation for \( g_t(Q, V) \).
The key theorem:
Joint distribution of path segments

$S_1$, $S_2$, $S_3$, $S_4$, $S_5$
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 $T^1(\mathbb{R}^d)$. Then, for each $n \in \mathbb{N}$ there exists a probability density $\Psi_{n,\Lambda}$ on $\mathbb{R}^{nd}$ such that, for any set $A \subset \mathbb{R}^{nd}$ with boundary of Lebesgue measure zero,

$$
\lim_{\rho \to 0} \Lambda\left(\left\{(Q_0, V_0) \in T^1(\mathbb{R}^d) : (S_1, \ldots, S_n) \in A\right\}\right) = \int_A \Psi_{n,\Lambda}(S_1', \ldots, S_n') dS_1' \cdots dS_n',
$$

and, for $n \geq 3$,

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

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).
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

- $\mu_1$—right-$\text{SL}(d, \mathbb{R})$ invariant prob measure on $X_1$ (Haar)
Affine lattices

- \textbf{ASL}(d, \mathbb{R}) = \text{SL}(d, \mathbb{R}) \rtimes \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 $X = \text{ASL}(d, \mathbb{Z}) \setminus \text{ASL}(d, \mathbb{R})$

where \text{ASL}(d, \mathbb{Z}) = \text{SL}(d, \mathbb{Z}) \rtimes \mathbb{Z}^d$, i.e.,

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

- $\mu$—right-\text{ASL}(d, \mathbb{R}) invariant prob measure on $X$
Let us denote by $\tau_1 = \tau(q, v)$ the free path length corresponding to the initial condition $(q, v)$. Recall that $\rho^{d-1}\tau_1 = \|S_1\|$.

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

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

exists, is continuous in $\xi$ and independent of $\lambda$. Furthermore

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

with the cylinder

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

- There are similar formulas for all \( q \in \mathbb{Q}L \).

- Note that in the case \( q \notin \mathbb{Q}L \) the limit \( F_{L,q}(\xi) =: F(\xi) \) is independent of \( q \) and \( L \); in the case \( q \in L \) the limit \( F_{L,q}(\xi) =: F_0(\xi) \) is independent of \( L \).

- Instead of rays emerging from the origin we can also deal with the family of rays starting at the point \( \rho_B(v) \) 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 $q \in \mathcal{L} = \mathbb{Z}^d$)
\[ \lambda\left(\{ \mathbf{v} \in S^{d-1}_1 : \rho^{d-1} \tau_1 \leq \xi \} \right) = \ldots \]
\[
\begin{align*}
\rho - (d-1) \xi = \lambda \left( \left\{ v \in S^{d-1}_1 : \text{at least one scatterer intersects } \text{ray}(v, \rho^{-(d-1)} \xi) \right\} \right)
\end{align*}
\]
\[ \approx \lambda \left( \left\{ \mathbf{v} \in S^{d-1}_1 : \mathbb{Z}^d \cap \mathbb{Z}(\mathbf{v}, \rho^{-(d-1)} \xi, \rho) \neq \emptyset \right\} \right) \]
\[ \rho^{-(d-1)} \xi \]

(Rotate by \( K(v) \in SO(d) \) such that \( v \mapsto e_1 \))
\[ \lambda \left( \left\{ \mathbf{v} \in S_{d-1}^1 : \mathbb{Z}^d K(\mathbf{v}) \cap \mathbb{Z}(\mathbf{e}_1, \rho^{-(d-1)} \xi, \rho) \neq \emptyset \right\} \right) \]
(Apply $D_{\rho} = \text{diag}(\rho^{d-1}, \rho^{-1}, \ldots, \rho^{-1}) \in \text{SL}(d, \mathbb{R})$)
\[ \lambda \left( \{ v \in S^{d-1}_1 : \mathbb{Z}^d K(v) D_\rho \cap \mathbb{Z}(e_1, \xi, 1) \neq \emptyset \} \right) \]
The following Theorem shows that in the limit $\rho \to 0$ the lattice

$$\mathbb{Z}^d K(v) \begin{pmatrix} \rho^{d-1} & 0 \\ t_0 & \rho^{-1} \end{pmatrix}$$

behaves like a random lattice with respect to Haar measure $\mu_1$.

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

$$\Phi^t = \begin{pmatrix} e^{-(d-1)t} & 0 \\ t_0 & e^t \end{pmatrix}, \quad t = \log 1/\rho.$$

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

$$\lim_{t \to \infty} \int_{S_1^{d-1}} f(M_0 K(v) \Phi^t) d\lambda(v) = \int_{X_1} f(M) d\mu_1(M).$$
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 $q \notin \mathcal{Q}_L$

Recall:

\[
F(\xi) := \lim_{\rho \to 0} \lambda(\{v \in S^{d-1}_1 : \rho^{d-1} \tau_1 \leq \xi\})
= \mu(\{(M, x) \in X : (\mathbb{Z}^d M + x) \cap \mathbb{Z}(\xi) \neq \emptyset\}).
\]

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

\[
F(\xi) = \text{vol}(B_1^{d-1}) \xi + O(\xi^2) \quad \text{as } \xi \to 0
\]

with $\text{vol}(B_1^{d-1}) = \frac{\pi^{(d-1)/2}}{\Gamma((d+1)/2)}$.

Note: for a random scatterer configuration $F(\xi) = 1 - e^{-\text{vol}(B_1^{d-1})\xi}$.
Asymptotics of the limiting distribution for $q \in \mathcal{L}$

Recall:

$$F_0(\xi) := \lim_{\rho \to 0} \lambda(\{v \in S_{1}^{d-1} : \rho^{d-1} \tau_1 \leq \xi\})$$

$$= \mu_1(\{M \in X_1 : \mathbb{Z}^d M \cap \mathbb{Z}(\xi) \neq \emptyset\}).$$

$$F_0(\xi) = 1 \quad \text{for } \xi \text{ sufficiently large}$$

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

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

$1/\zeta(d)$ 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


