The periodic Lorentz gas

in the Boltzmann-Grad limit

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In 1905, H. Lorentz proposed to describe the motion of electrons in metals by the methods of kinetic theory

- Gas of electrons described by its phase-space density $f \equiv f(t, x, v)$ (density of electrons at the position x with velocity v at time t)

- Electron-electron collisions neglected (unlike in the kinetic theory of gases)

- Only the collisions between electrons and metallic atoms are considered

$\Rightarrow$ LINEAR KINETIC EQUATION

unlike Boltzmann's equation in the kinetic theory of gases

The Lorentz kinetic model

•Equation for the phase-space density of electrons $f \equiv f(t, x, v)$:

$$(\partial_t + v \cdot \nabla_x + \frac{1}{m} F(t,x) \cdot \nabla_v) f(t,x,v) = N_{at} r_{at}^2 |v| \mathcal{C}(f(t,x,\cdot))(v)$$

where $\mathcal{C}$ is the Lorentz collision integral

$$\mathcal{C}(\phi)(v) = \int_{\substack{|\omega|=1 \\ \omega \cdot v > 0}} \Big(\phi(\mathcal{R}_\omega v) - \phi(v) \Big) \cos(v, \omega) d\omega$$

and $\mathcal{R}_\omega$ is the specular reflection: $\mathcal{R}_\omega(v) = v - 2(v \cdot \omega)\omega$

Notation: m =mass of the electron; N_{at}, r_{at} density, radius of metallic atoms; $F \equiv F(t,x)$ electric force (given).

Santalò's formula for the mean free path (1942)

•Average length of maximal segments avoiding $\mathcal{N}$ balls in a domain with (large) volume V:

$$\ell = \left(\frac{\mathcal{N}}{V - V_e} \times \Sigma\right)^{-1}$$

where $V_e \ll V$ is the total volume occuped by the balls, and Σ is the equatorial section of each ball.

•**Boltzmann-Grad limit:** $\mathcal{N} \gg 1$, $\Sigma \ll 1$ and $V_e \ll V = O(1)$ so that mean free path ℓ converges to a finite, positive number

Problem

• Can one derive the Lorentz kinetic equation from a microscopic model in the B.-G. limit? — say, without applied electric field: $F \equiv 0$.

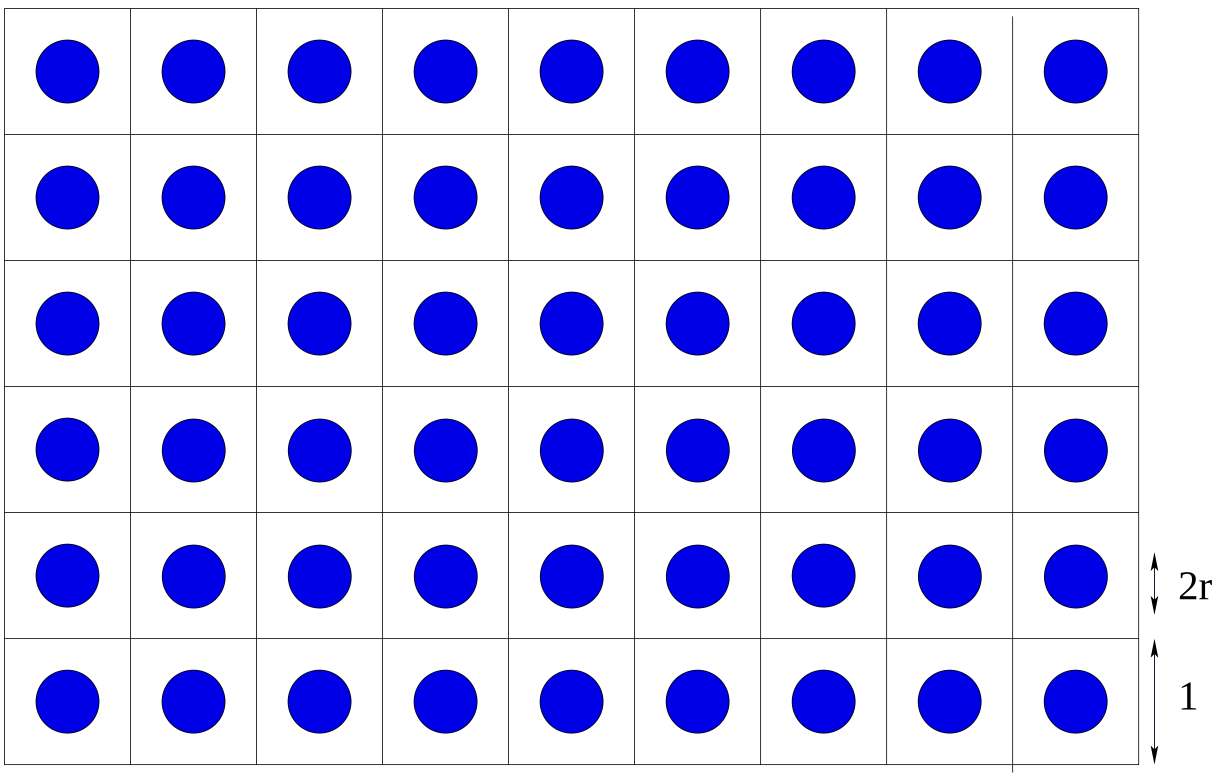
• Microscopic model= billiard system (=gas of point particles moving at a constant speed in a configuration of fixed spherical obstacles, and specularly reflected at the surface of the obstacles).

• Gallavotti (1969) proved that the expected 1-particle phase-space density converges to a solution of the Lorentz kinetic equation for randomly distributed obstacles (Poisson, possibly overlapping) — improvement by Spohn (1978), a.s. convergence by Boldrighini-Bunimovich-Sinai (1983)

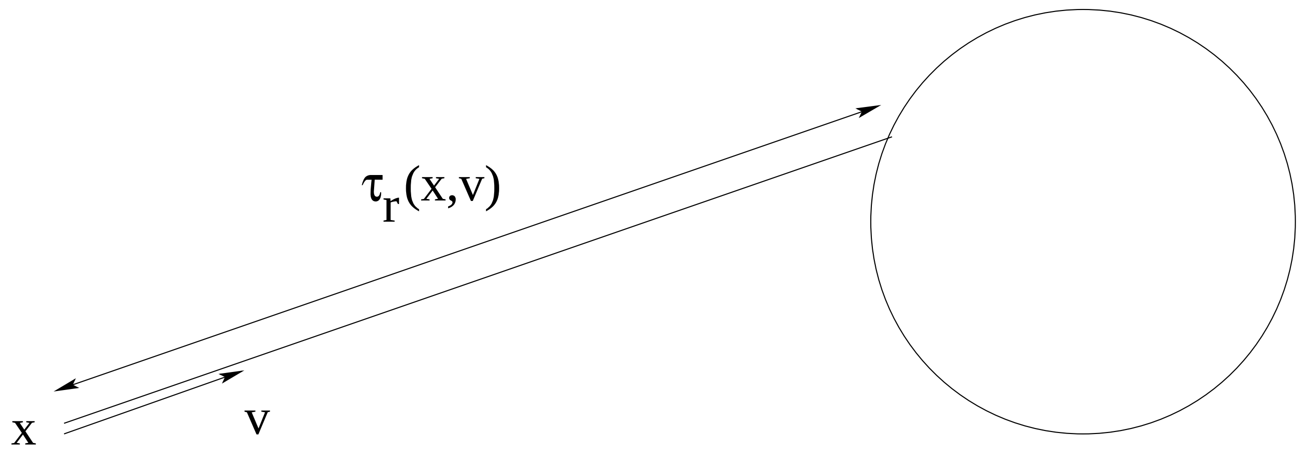
• Periodic configuration of obstacles? homogenization problem for the free transport equation in a perforated domain

Distribution of free path lengths

• For $r \in (0, \frac{1}{2})$, define $Z_r = \{x \in \mathbf{R}^D \,|\, \mathrm{dist}(x, \mathbf{Z}^D) > r\}$;



•Free path length: $\tau_r(x,v) = \min\{t > 0 \,|\, x + tv \in \partial Z_r\}$.



•For (x,v) independent and uniformly distributed on $Z_r \times \mathbf{S}^{D-1}$

$$\phi_r(t,v) = \text{Prob}\left(\left\{x \,\middle|\, \tau_r(x,v) > \frac{t}{r^{D-1}}\right\}\right) \text{, a.e. in } v \in \mathbf{S}^{D-1}$$

$$\Phi_r(t) = \text{Prob}\left(\left\{(x,v) \,\middle|\, \tau_r(x,v) > \frac{t}{r^{D-1}}\right\}\right) .$$

•Obviously

$$\Phi_r(t) = \frac{1}{|\mathbf{S}^{D-1}|}\int_{\mathbf{S}^{D-1}} \phi_r(t,v)dv$$

Theorem. (Bourgain-G.-Wennberg, 1998-2000) *For each* $D \geq 2$*, there exists* $0 < C_D < C'_D$ *such that*

$$\frac{C_D}{t} \leq \Phi_r(t) \leq \frac{C'_D}{t} \quad \textit{whenever } t > 1 \textit{ and } 0 < r < \tfrac{1}{2}$$

•Upper bound: method based on Fourier series, analogous to Siegel's proof (Acta Math. 1935) of Minkowski's convex body theorem

•Lower bound: based on a precise counting of infinite open strips included in Z_r as in Bleher (JSP 1992); free path length dominates exit time from the strip

Distribution of free path lengths: the case $D = 2$

Theorem. (Caglioti-G. 2003-2006) *For* $t > 0$*, there exists* $\phi(t) \geq 0$ *s.t.*

$$\frac{1}{|\ln \epsilon|} \int_{\epsilon}^{1/4} \phi_r(t, v) \frac{dr}{r} \to \phi(t)\,, \quad \textit{a.e. in } v \in \mathbf{S}^1 \textit{ as } \epsilon \to 0^+\,.$$

Moreover, ϕ *satisfies*

$$\phi(t) = \frac{1}{\pi^2 t} + O\left(\frac{1}{t^2}\right)\,, \quad \textit{as } t \to +\infty\,.$$

•Proof based on 2 ingredients: a) a 3-term partition of the flat 2-torus, and b) the ergodic theory of continued fractions

Theorem. (Boca-Zaharescu, 2005) *For each* $t > 0$

$$\lim_{r \to 0^+} \Phi_r(t) = \frac{6}{\pi^2} \int_t^{\infty} (s - t) g(s) ds$$

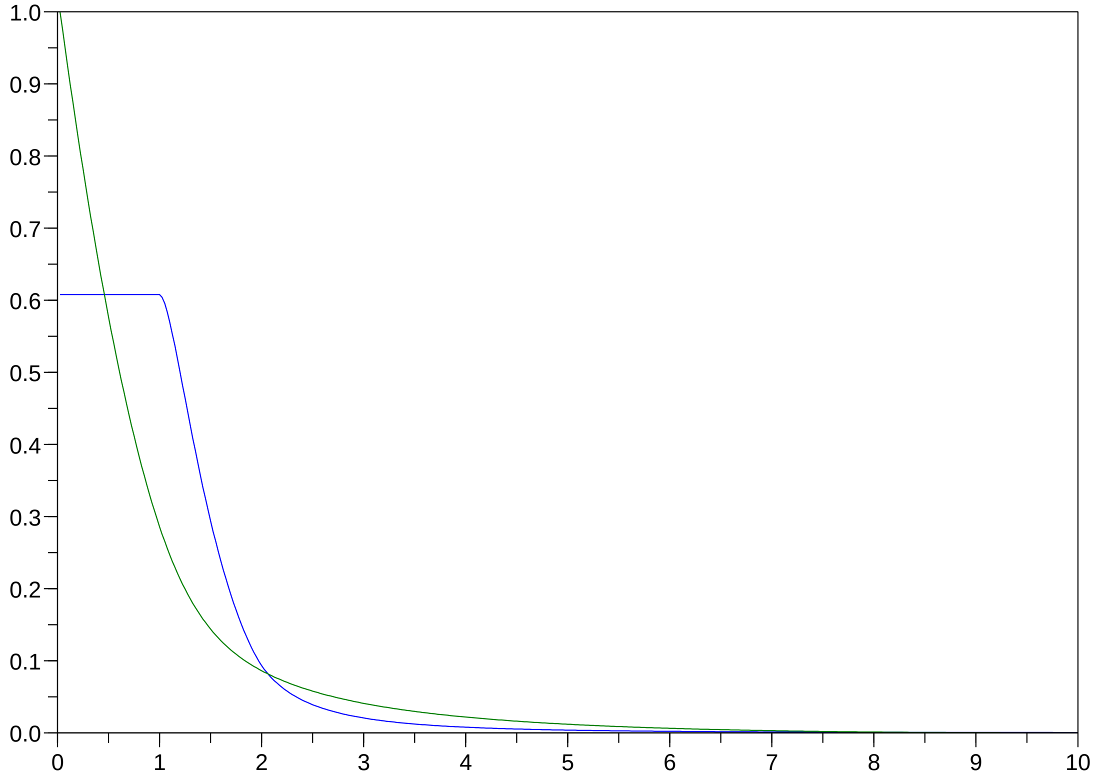
where

$$g(s) = \begin{cases} 1 & s \in [0, 1] \\ \frac{1}{s} + 2\left(1 - \frac{1}{s}\right)^2 \ln(1 - \frac{1}{s}) - \frac{1}{2}\left|1 - \frac{2}{s}\right|^2 \ln|1 - \frac{2}{s}| & s \in (1, \infty) \end{cases}$$

•**Remark:** By the Caglioti-G. thm, one has

$$\lim_{r \to 0^+} \Phi_r(t) = \frac{1}{|\ln \epsilon|} \int_{\epsilon}^{1/4} \phi_r(t, v) \frac{dr}{r} = \phi(t)$$

Proof uses: a) same partition of the flat 2-torus as above, and b) asymptotic estimates for sums on coprime lattice points (Kloosterman sums)



Graph of $\phi(t)$ (green curve) and $g(t) = \phi''(t)$ (blue curve)

The homogenization problem

•Write the free transport equation for the density of point particles in Z_r:

$$\partial_t F_r + v \cdot \nabla_x F_r = 0\,, \qquad (x,v) \in Z_r \times \mathbf{S}^{D-1}$$
$$F_r(t,x,\mathcal{R}_x v) = F_r(t,x,v)\,, \qquad (x,v) \in \partial Z_r \times \mathbf{S}^{D-1}$$

(where $\mathcal{R}_x$ is the specular reflection on ∂Z_r at the point x). Assume that

$$F_r\Big|_{t=0} = f^{in}(r^{D-1}x, v)\,, \qquad (x,v) \in Z_r \times \mathbf{S}^{D-1}$$

•If f^{in} is bounded on $\mathbf{R}^D \times \mathbf{S}^{D-1}$, then

$$|F_r(t,x,v)| \le \|f^{in}\|_{L^\infty} \text{ for each } (t,x,v) \in \mathbf{R}_+ \times \mathbf{R}^D \times \mathbf{S}^{D-1}$$

•**Pbm:** to find the weak-* limit points in $L^\infty(\mathbf{R}_+ \times \mathbf{R}^D \times \mathbf{S}^{D-1})$ of

$$f_r(t,x,v) := F_r\left(\frac{t}{r^{D-1}}, \frac{x}{r^{D-1}}, v\right) \text{ as } r \to 0^+$$

A negative result

Theorem. *Assume* $f^{in} \equiv f^{in}(x)$ *periodic and* $r = \frac{1}{n}$ *with* $n \geq 2$. *Then, no weak-* limit point of* f_r *in* $L^\infty(\mathbf{R}_+ \times \mathbf{R}^D \times \mathbf{S}^{D-1})$ *as* $r \to 0^+$ *satisfies the Lorentz kinetic equation — nor can it satisfy any equation of the form*

$$(\partial_t + v \cdot \nabla_x) f(t,x,v) = \sigma \int_{\mathbf{S}^{D-1}} p(v,v')(f(t,x,v') - f(t,x,v))dv'$$

$$f\Big|_{t=0} = f^{in}$$

where $\sigma > 0$ *and* p *is the kernel of a compact operator on* $L^2(\mathbf{S}^{D-1})$ *s.t.*

$$p(v,v') = p(v',v) \geq 0\,, \quad \int_{\mathbf{S}^{D-1}} p(v,v')dv' = 1$$

• Proof: $f(t,\cdot,\cdot)$ converges exponentially fast to a constant as $t \to \infty$; but BGW lower bound implies $\|f(t,\cdot,\cdot)\|_{L^2_{x,v}} \geq \frac{C_D}{t}\|f^{in}\|_{L^2_x}$: contradiction.

Case of absorbing obstacles, $D = 2$

- In that case, the density of point particles in Z_r satisfies

$$\begin{aligned}
&\partial_t F_r + v \cdot \nabla_x F_r = 0\,, && (x,v) \in Z_r \times \mathbf{S}^1\\
&F_r(t, k + r\omega, v) = 0\,, && k \in \mathbf{Z}^2\,,\ v,\omega \in \mathbf{S}^1\,,\ v\cdot\omega > 0\\
&F_r\Big|_{t=0} = f^{in}(rx, v)\,, && (x,v) \in Z_r \times \mathbf{S}^1
\end{aligned}$$

Theorem. *For each* $f^{in} \in L^\infty(\mathbf{R}^2 \times \mathbf{S}^1)$

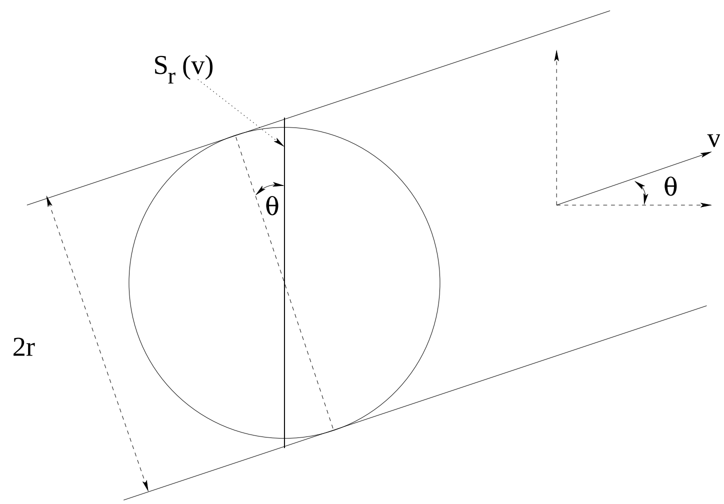
$$\frac{1}{|\ln \epsilon|}\int_\epsilon^{1/4} F_r\left(\frac{t}{r}, \frac{x}{r}, v\right)\frac{dr}{r} \to f \equiv f(t,x,v)$$

in $L^\infty(\mathbf{R}_+ \times \mathbf{R}^2 \times \mathbf{S}^1)$ *weak-* as* $r \to 0^+$*, where* f *is the solution of*

$$\begin{aligned}
&\partial_t f + v \cdot \nabla_x f = \frac{\phi'(t)}{\phi(t)} f\,, \quad (x,v) \in \mathbf{R}^2 \times \mathbf{S}^1\\
&f\Big|_{t=0} = f^{in}
\end{aligned}$$

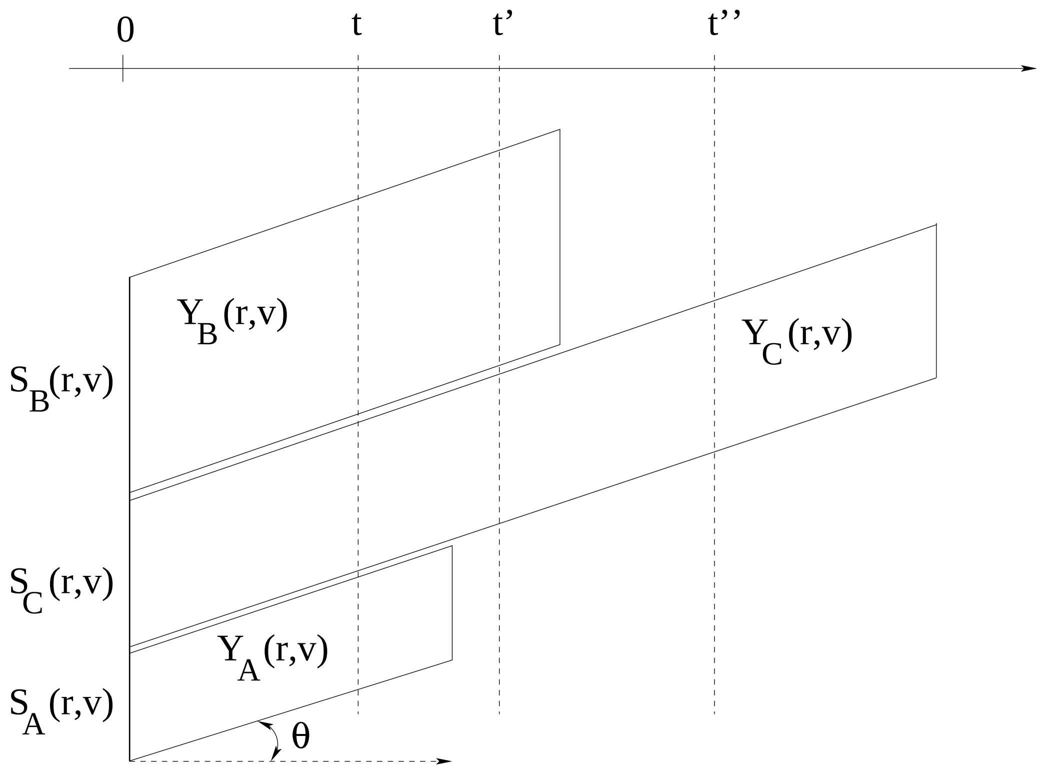
Proof of the Caglioti-G. result

Idea no.1 Given a linear flow with irrational slope on a 2-torus with a disk removed, what is the longest orbit of this flow? (R. Thom in 1989)

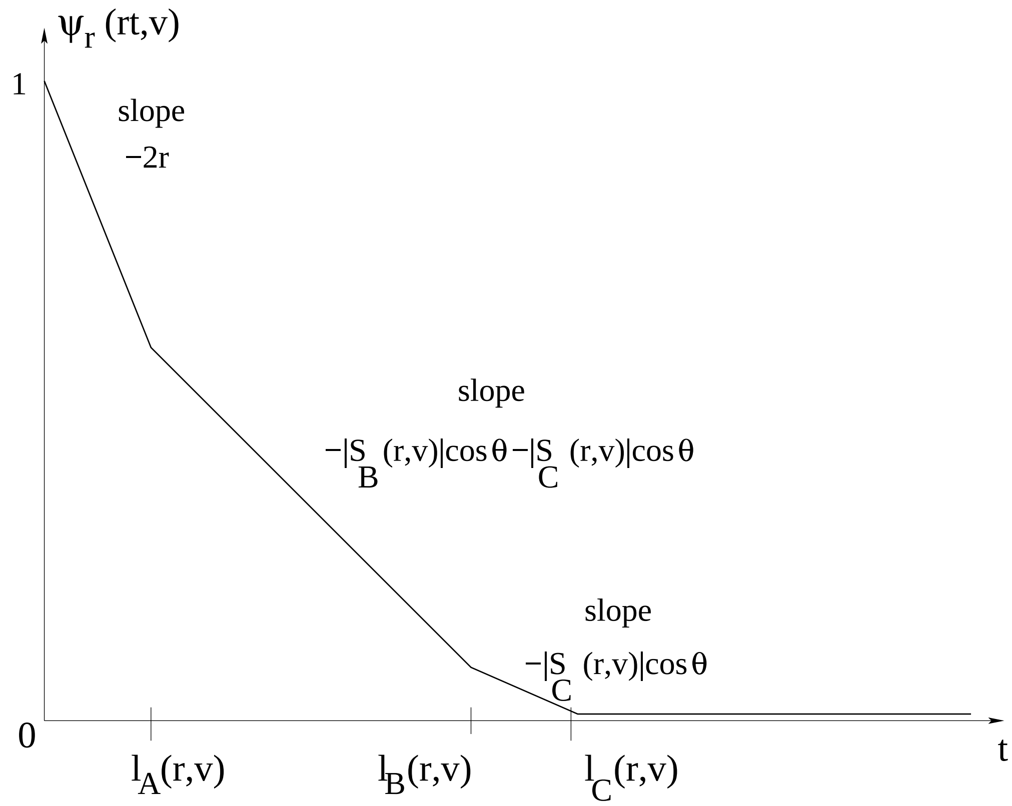


Blank-Krikorian, IJM'93: Instead of a disk, remove a slit parallel to one of the coordinate axis; generically 3 classes of orbits with same length

•The 2-torus minus the slit is then metrically equivalent to 3 strips $Y_A(r,v)$, $Y_B(r,v)$ and $Y_C(r,v)$ of lengths $l_A(r,v)$, $l_B(r,v)$ and $l_C(r,v)$



•For $v = (\cos\theta, \sin\theta)$, denoting $\psi_r(t, v)$ the analogue of $\phi_r(t, v)$ with the disk of radius r replaced with the slit of length $\frac{2r}{\cos\theta}$;



•Set $\alpha = \tan\theta \in (0,1) \setminus \mathbf{Q}$ with continued fraction expansion

$$\alpha = [a_1, a_2, a_3, \ldots] := \frac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \ldots}}} \;; \qquad \frac{p_n}{q_n} := [a_1, \ldots, a_{n-1}]$$

and

$$d_n(\alpha) = (-1)^{n-1}(q_n \alpha - p_n) > 0 \,,$$
$$N(\alpha, r) = \min \left\{ n \in \mathbf{N} \,\middle|\, d_n(\alpha) \leq 2r\sqrt{1+\alpha^2} \right\} \,.$$

Then

$$\psi_r(t,v) = E\left(t, -\left[\frac{2r\sqrt{1+\alpha^2} - d_{N-1}}{d_N}\right], \frac{d_N}{d_{N-1}}, \frac{d_{N-1}}{d_{N-2}}, d_{N-1}q_N, d_{N-2}q_{N-1}\right)$$

where E is uniformly Lipschitz continuous in its last 2 variables.

Idea no. 2 The Gauss map $T: (0,1) \setminus \mathbf{Q} \to (0,1) \setminus \mathbf{Q}$ defined by

$$T(\alpha) = \frac{1}{\alpha} - \left[\frac{1}{\alpha}\right] \text{ is ergodic with invariant measure } \frac{1}{\ln 2}\frac{d\alpha}{1+\alpha}$$

- Birkhoff's theorem: for each $\phi \in L^1(0,1; \frac{d\alpha}{1+\alpha})$

$$\frac{1}{n}\sum_{k=0}^{n-1} \phi(T^k\alpha) \to \frac{1}{\ln 2}\int_0^1 \phi(\beta)\frac{d\beta}{1+\beta} \text{ a.e. in } \alpha \text{ as } n \to \infty$$

- Two facts about continued fractions:

$$d_n(\alpha) = \prod_{k=1}^{n-1} T^k\alpha$$

$$\left| d_{n-1}q_n - \sum_{j=n-m}^{n-1} (-1)^{n-1-j}\, \frac{d_n d_{n-1}}{d_j d_{j-1}} \right| \leq 2^{-m}$$

Use this for fixed $m \ll n \to \infty$.

- This helps approximating q_n in terms of finitely many $T^k\alpha$ as $n \to \infty$

- Next we apply Birkhoff's ergodic theorem to the expression

$$\psi_r(t,v) = E\left(t, -\left[\frac{2r\sqrt{1+\alpha^2} - d_{N-1}}{d_N}\right], \frac{d_N}{d_{N-1}}, \frac{d_{N-1}}{d_{N-2}}, d_{N-1}q_N, d_{N-2}q_{N-1}\right)$$

after replacing $d_{N-1}q_N$ and $d_{N-2}q_{N-1}$ with the finite sum involving only the d_ns as above

- Error in $O(2^{-m})$ since E is uniformly Lipschitz in its last two arguments

•Hence

$$\frac{1}{|\ln\epsilon|}\int_\epsilon^{1/4}\psi_r(t,v)\frac{dr}{r}$$ satisfies Cauchy's convergence criterion

as $\epsilon \longrightarrow 0^+$ and, as a consequence of Birkhoff's theorem

its limit $\phi(t)$ is independent of the direction v

•Same with ϕ_r replacing ψ_r since $\phi_r(t) = \psi_r(t + O(r^2)) + O(r^2)$

•For the $t \longrightarrow \infty$ limit, replace the exact expression E with its approximation

$$\psi_r(t,v) \simeq \left(1 - \frac{2r\sqrt{1+\alpha^2}}{d_{N-1}} - 2t\frac{d_N}{2r\sqrt{1+\alpha^2}}\right)_+$$

Perspectives, open problems

• Find analogues of the results above for 2-dimensional lattices other than $\mathbf{Z}^2$: in particular find the intrinsic meaning of the constant $\frac{1}{\pi^2}$ in the Caglioti-G. theorem

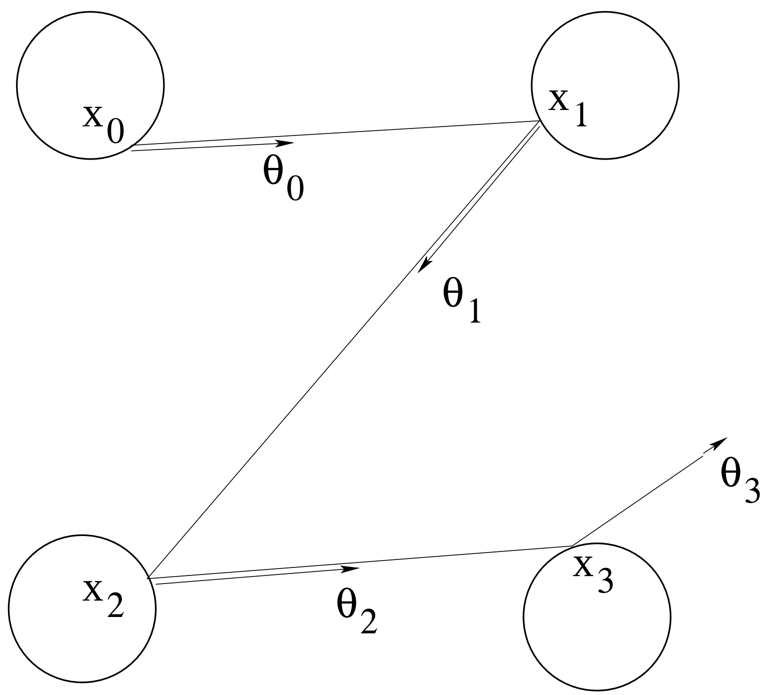
• Does the introduction of an external force field accelerating the particles between collisions modify the results above, and if yes, in which way?

• What replaces the Lorentz kinetic equation in the simplest case of the $\mathbf{Z}^2$ lattice considered in this talk?

• Does $\phi_r(t, v)$ — or even its angle average $\Phi_r(t)$ — converge as $r \to 0^+$ in the case of space dimension $D > 2$? (might require accurate estimates on simultaneous rational approximation)

A (plausible?) conjecture

•Start from a particle located at the surface of an obstacle with initial position x_0^r and direction θ_0^r; denote by x_n^r and θ_n^r the position and directions of that particle as it leaves the n-th encountered obstacle.



•Assume that the sequence of impact parameters and free path lengths

$$h_n^r := \cos\left(\frac{\theta_{n-1}^r - \theta_n^r}{2}\right)\ , \quad \tau_n^r := |x_n^r - x_{n-1}^r|$$

can be simulated in the small r (obstacle radius) limit by a Markov chain $(h_n, \tau_n) \in [-1,1] \times [1,\infty)$.

•Call $f(t,x,\theta,h,\tau)$ be the limiting density of particles which, at time t, are located at x with velocity $v = (\cos\theta, \sin\theta)$, and whose next collision with an obstacle will occur at time $t+\tau$ with impact parameter h

•Then

$$(\partial_t + v\cdot\nabla_x)f(t,x,\theta,h,\tau)$$
$$= \partial_\tau f(t,x,\theta,h,\tau) + \int_{-1}^{1} k(h,\tau|h')f(t,x,\theta',h',0)dh'\,,$$
$$\text{with } \theta' = \theta - \pi + 2\arcsin(h)\,,\quad \tau > 0$$

while the transition kernel k satisfies

$$k(h,\tau|h') \geq 0\,,\quad \iint_{[-1,1]\times\mathbf{R}_+} k(h,\tau|h')dhd\tau = 1$$

•Should the conjecture above be true, the Lorentz equation should be replaced with this **kinetic model on an extended phase space**