Derivation of the Fick's law for the Lorentz model in a low density regime

Alessia Nota

Sapienza, Università di Roma

May 26, 2014

Joint work with G. Basile, F. Pezzotti, M. Pulvirenti



 ρ_2

Nonequilibrium (mass reservoirs at density ρ_1 , ρ_2)

- ρ : macroscopic mass density
- J : macroscopic mass current

$$J = -D\nabla\rho \qquad (Fick's law)$$

D > 0 diffusion coefficient and

$$\varrho(x) = \frac{\rho_1(L-x_1) + \rho_2 x_1}{L}$$
 (Linear profile)

Bunimovich and Sinai, 1981 (Diffusion for the periodic Lorentz gas)

Microscopic description

$$\begin{cases} \dot{x} = v \\ \dot{v} = \mathsf{F}_{obs} \end{cases}$$

Newtonian dynamics (Lorentz gas)

Macroscopic description

$$\partial_t \varrho = D\Delta \varrho, \quad \varrho = \int f \, dv$$

Hydrodynamic equation (diffusion equation)

Mesoscopic description



transport

collisions

Linear kinetic equation

Microscopic description

$$\begin{cases} \dot{x} = v \\ \dot{v} = \mathsf{F}_{obs} \end{cases}$$

Newtonian dynamics (Lorentz gas)

Macroscopic description

$$\partial_t \varrho = D\Delta \varrho, \quad \varrho = \int f \, dv$$

Hydrodynamic equation (diffusion equation)

Mesoscopic description



collisi

Linear kinetic equation

Background

Test particle moving in a random configuration of obstacles in \mathbb{R}^d . μ : intensity of the obstacles; $\varepsilon > 0$ ratio between micro and macro scale.

Low density limit: $t \to \varepsilon t$, $x \to \varepsilon x$, $\mu_{\varepsilon} = \varepsilon^{-(d-1)}\mu$.

(rarefied gas, mean free path O(1))

$(\partial_t + \mathbf{v} \cdot \nabla_x)$	f(x, v, t) = k	f(x, v, t)	(Linear Boltzmann)
transpol	rt	collisions	
	$\mathcal{L}f(\mathbf{v}) = \mu$	$\int_{-1}^{1} d\rho \{f(v'$	$) - f(v) \}$

Gallavotti, 1969 (Poisson distribution of hard sphere scatterers)

- Spohn, 1978 (more general distribution of scatterers)
- Desvillettes, Pulvirenti, 1999 (long range interaction)

Background

Scaling:
$$t \to \varepsilon t, x \to \varepsilon x,$$

 $\mu_{\varepsilon} = \eta_{\varepsilon} \varepsilon^{-(d-1)} \mu, \eta_{\varepsilon}$ slowly diverging.

Asymptotic equation

$$(\partial_t + \mathbf{v} \cdot \nabla_x) f(x, \mathbf{v}, t) \sim \eta_{\varepsilon} \mathcal{L} f(x, \mathbf{v}, t)$$

 $\varepsilon \rightarrow 0?$

- Idea: look at a longer time scale in which the equilibrium starts to evolve $t \rightarrow \eta_{\varepsilon} t$ \implies diffusion for the position variable
 - Erdos, Salmhofer, Yau, 2008 (linear Quantum Boltzmann)
 - Bodineau, Gallagher, and Saint-Raymond, 2013 (linear Boltzmann)
 - Basile, N., Pulvirenti, 2013 (linear Landau)

The model

Poisson distribution of fixed hard disks $\mathbf{c}_N = (c_1, \ldots, c_N)$ in $\Lambda = (0, L) \times \mathbb{R}$. $\mu > 0$ intensity.

Mass reservoirs: free point particles at equilibrium at densities ρ_1 , ρ_2 .



$$\mathbb{P}(dc_N) = e^{-\mu|A|} \frac{\mu^N}{N!} dc_1 \dots dc_N, \qquad A \subset \Lambda.$$
Scaling: $\mu \to \mu_{\varepsilon} = \varepsilon^{-1} \eta_{\varepsilon} \mu$

$$\begin{bmatrix} Ass : \varepsilon^{\frac{1}{2}} \eta_{\varepsilon}^6 \longrightarrow 0 \\ \varepsilon \to 0 \end{bmatrix}$$
Alessia Nota (Sapienza)
Derivation of the Fick's law.
May 26, 2014

<u>Alessia Nota</u> (Sapienza)

Derivation of the Fick's law

7 / 17

The model

Initial probability distribution $f_0 = f_0(x, v)$. Boundary value

$$f_B(x,v) := \begin{cases} \rho_1 M(v) & \text{if } x \in \{0\} \times \mathbb{R}, \quad v_1 > 0\\ \rho_2 M(v) & \text{if } x \in \{L\} \times \mathbb{R}, \quad v_1 < 0 \end{cases}$$

We look at the one-particle correlation function

 $f_{\varepsilon}(x,v,t) = \mathbb{E}_{\varepsilon}[f_B(T_{c_N}^{-(t-\tau)}(x,v))\chi(\tau>0)] + \mathbb{E}_{\varepsilon}[f_0(T_{c_N}^{-t}(x,v))\chi(\tau=0)]$

$$\begin{split} &\mathbb{E}_{\varepsilon}[\cdot]: \text{ expectation w.r.t. the measure } \mathbb{P}_{\varepsilon}. \\ &\mathcal{T}_{\mathsf{c}_N}^{-t}(x,v): \text{ (backward) Hamiltonian flow.} \\ &t-\tau: \text{ first (backward) hitting time with } \partial \Lambda. \quad (\tau=\tau(x,v,t,\mathsf{c}_N)) \\ &(\tau=0 \text{ if } \mathcal{T}_{\mathsf{c}_N}^{-s}(x,v), \ s\in[0,t], \text{ never hits the boundary}) \end{split}$$

The model

Initial probability distribution $f_0 = f_0(x, v)$. Boundary value

$$f_B(x,v) := \begin{cases} \rho_1 M(v) & \text{if } x \in \{0\} \times \mathbb{R}, \quad v_1 > 0\\ \rho_2 M(v) & \text{if } x \in \{L\} \times \mathbb{R}, \quad v_1 < 0 \end{cases}$$

We look at the one-particle correlation function

$$f_{\varepsilon}(x,v,t) = \mathbb{E}_{\varepsilon}[f_B(T_{\mathbf{c}_N}^{-(t-\tau)}(x,v))\chi(\tau>0)] + \mathbb{E}_{\varepsilon}[f_0(T_{\mathbf{c}_N}^{-t}(x,v))\chi(\tau=0)]$$

$$\begin{split} &\mathbb{E}_{\varepsilon}[\cdot]: \text{ expectation w.r.t. the measure } \mathbb{P}_{\varepsilon}. \\ &\mathcal{T}_{\mathbf{c}_{N}}^{-t}(x,v): \text{ (backward) Hamiltonian flow.} \\ &t-\tau: \text{ first (backward) hitting time with } \partial \Lambda. \quad (\tau = \tau(x,v,t,\mathbf{c}_{N})) \\ &(\tau = 0 \text{ if } \mathcal{T}_{\mathbf{c}_{N}}^{-s}(x,v), s \in [0,t], \text{ never hits the boundary}) \end{split}$$

The Model

 $f_{\varepsilon}^{S}(x, v)$ stationary solution of the microscopic dynamics

Observables

The Model

$f_{\varepsilon}^{S}(x, v)$ stationary solution of the microscopic dynamics

Observables

Stationary mass flux:
$$J^S_{\varepsilon}(x) = \eta_{\varepsilon} \int_{S_1} v f^S_{\varepsilon}(x, v) dv$$

Stationary mass density:

$$\varrho_{\varepsilon}^{S}(x) = \int_{S_{1}} f_{\varepsilon}^{S}(x, v) \, dv$$

 J_{ε}^{S} : total amount of mass through a unit area in a unit time. $\eta_{\varepsilon} \longrightarrow$ (time scaling necessary for diffusion!)

The Model

$f_{\varepsilon}^{S}(x, v)$ stationary solution of the microscopic dynamics

Observables

Stationary mass flux:
$$J^{\mathcal{S}}_{\varepsilon}(x) = \eta_{\varepsilon} \int_{\mathcal{S}_1} v f^{\mathcal{S}}_{\varepsilon}(x, v) dv$$

Stationary mass density:

$$\varrho_{\varepsilon}^{S}(x) = \int_{S_{1}} f_{\varepsilon}^{S}(x, v) \, dv$$

- J_{ε}^{S} : total amount of mass through a unit area in a unit time.
- $\eta_{arepsilon}$ \rightsquigarrow (time scaling necessary for diffusion!)

Main results

Theorem 1 [Basile, N., Pezzotti, Pulvirenti]

For ε sufficiently small there exists a unique L^∞ stationary solution f_ε^S for the microscopic dynamics. Moreover

$$f_{\varepsilon}^{S}
ightarrow \varrho^{S}$$
 as $\varepsilon
ightarrow 0$

where ρ^{S} is the stationary solution of the heat equation

$$\varrho^{\mathsf{S}}(x) = \frac{\rho_1(L-x_1) + \rho_2 x_1}{L}$$

The convergence is in $L^2((0, L) \times S_1)$.

Boundary conditions depend on the space variable only through x₁
 ⇒ f^S_ε, ρ^S inherits the same feature
 ⇒ convergence in L²((0, L) × S₁) instead of L²(Λ × S₁).

▶ For the convergence of the stationary solutions it is enough $\varepsilon^{\frac{1}{2}}\eta^{5}_{\varepsilon} \rightarrow 0$.

Main results

Theorem 1 [Basile, N., Pezzotti, Pulvirenti]

For ε sufficiently small there exists a unique L^∞ stationary solution f_ε^S for the microscopic dynamics. Moreover

$$f_{\varepsilon}^{S}
ightarrow \varrho^{S}$$
 as $\varepsilon
ightarrow 0$

where ϱ^{S} is the stationary solution of the heat equation

$$\varrho^{\mathsf{S}}(x) = \frac{\rho_1(L-x_1) + \rho_2 x_1}{L}$$

The convergence is in $L^2((0, L) \times S_1)$.

Boundary conditions depend on the space variable only through x₁
 ⇒ f^S_ε, ρ^S inherits the same feature
 ⇒ convergence in L²((0, L) × S₁) instead of L²(Λ × S₁).

▶ For the convergence of the stationary solutions it is enough $\varepsilon^{\frac{1}{2}}\eta^{5}_{\varepsilon} \rightarrow 0$.

Alessia Nota (Sapienza)

Theorem 2 [Fick's law] [Basile, N., Pezzotti, Pulvirenti]

•
$$J_{\varepsilon}^{S} + D\nabla_{x}\varrho_{\varepsilon}^{S} \to 0$$
 as $\varepsilon \to 0$ in $\mathcal{D}'(0, L)$
where $D = \frac{1}{4\pi} \int_{S_{1}} dv \, v \cdot (-\mathcal{L})^{-1} v$ (Green-Kubo).
• $J^{S} = \lim_{\varepsilon \to 0} J_{\varepsilon}^{S}(x)$ in $L^{2}(0, L)$
and $J^{S} = -D \nabla \varrho^{S} = -D \frac{\rho_{2} - \rho_{1}}{L}$ (ϱ^{S} linear profile).

- ▶ J^S does not depend on the space variable.
- Diff. coeff. D determined by the behavior of the system at equilibrium. (Same D of the time dependent problem!)

Theorem 2 [Fick's law] [Basile, N., Pezzotti, Pulvirenti]

•
$$J_{\varepsilon}^{S} + D\nabla_{x}\varrho_{\varepsilon}^{S} \to 0$$
 as $\varepsilon \to 0$ in $\mathcal{D}'(0, L)$
where $D = \frac{1}{4\pi} \int_{S_{1}} dv \, v \cdot (-\mathcal{L})^{-1} v$ (Green-Kubo).
• $J^{S} = \lim_{\varepsilon \to 0} J_{\varepsilon}^{S}(x)$ in $L^{2}(0, L)$
and $J^{S} = -D \nabla \varrho^{S} = -D \frac{\rho_{2} - \rho_{1}}{L}$ (ϱ^{S} linear profile).

- J^S does not depend on the space variable.
- Diff. coeff. D determined by the behavior of the system at equilibrium.
 (Same D of the time dependent problem!)

The Boltzmann equation as a bridge

Introduce the stationary linear Boltzmann equation

$$\begin{cases} (\mathbf{v} \cdot \nabla_{\mathbf{x}}) h_{\varepsilon}^{\mathsf{S}}(\mathbf{x}, \mathbf{v}) = \eta_{\varepsilon} \mathcal{L} h_{\varepsilon}^{\mathsf{S}}(\mathbf{x}, \mathbf{v}), \\ h_{\varepsilon}^{\mathsf{S}}(\mathbf{x}, \mathbf{v}) = \rho_{1}, \quad \mathbf{x} \in \{0\} \times \mathbb{R}, \quad \mathbf{v}_{1} > 0, \\ h_{\varepsilon}^{\mathsf{S}}(\mathbf{x}, \mathbf{v}) = \rho_{2}, \quad \mathbf{x} \in \{L\} \times \mathbb{R}, \quad \mathbf{v}_{1} < 0, \end{cases}$$

$$\mathcal{L}f(\mathbf{v}) = \mu \int_{-1}^{1} d\rho [f(\mathbf{v}') - f(\mathbf{v})]$$
$$f \in L^{1}(S_{1})$$
$$\mathbf{v}' = \mathbf{v} - 2(n \cdot \mathbf{v})n, \quad n = n(\rho)$$



 $\{v(t)\}_{t\geq 0}$ Markov jump process $x(t) = \int_0^t v(s) ds$

Strategy

There exists a unique stationary solution h^S_ε ∈ L[∞]((0, L) × S₁) of the linear Boltzmann equation. As ε → 0

$$h^{S}_{arepsilon} o arepsilon^{S}$$
 in $L^{2}((0,L) imes S_{1})$ (Markov part)

② There exists a unique stationary solution f^S_ε ∈ L[∞]((0, L) × S₁) for the microscopic dynamics such that

 $\|h_{\varepsilon}^{S} - f_{\varepsilon}^{S}\|_{\infty} \leq C \varepsilon^{\frac{1}{2}} \eta_{\varepsilon}^{5}$ (Markovian approximation)

(The memory effects preventing the Markovianity are negligible!)

Strategy

There exists a unique stationary solution h^S_ε ∈ L[∞]((0, L) × S₁) of the linear Boltzmann equation. As ε → 0

$$h^{\mathsf{S}}_{arepsilon} o arrho^{\mathsf{S}}$$
 in $L^2((0,L) imes S_1)$ (Markov part)

One and the exists a unique stationary solution $f_{\varepsilon}^{S} \in L^{\infty}((0, L) \times S_{1})$ for the microscopic dynamics such that

 $\|h_{\varepsilon}^{S} - f_{\varepsilon}^{S}\|_{\infty} \leq C \varepsilon^{\frac{1}{2}} \eta_{\varepsilon}^{5}$ (Markovian approximation)

(The memory effects preventing the Markovianity are negligible!)

Stationary solutions as the long time asymptotics of $h_{\varepsilon}(t)$ and $f_{\varepsilon}(t)$? **Pb:** control the convergence rates, as $t \to \infty$, with respect to ε **Trick:** characterize instead h_{ε}^{S} and f_{ε}^{S} in terms of the Neumann series!

Strategy

There exists a unique stationary solution h^S_ε ∈ L[∞]((0, L) × S₁) of the linear Boltzmann equation. As ε → 0

$$h^{\mathsf{S}}_{arepsilon} o arrho^{\mathsf{S}}$$
 in $L^2((0,L) imes S_1)$ (Markov part)

One and the exists a unique stationary solution $f_{\varepsilon}^{S} \in L^{\infty}((0, L) \times S_{1})$ for the microscopic dynamics such that

 $\|h_{\varepsilon}^{S} - f_{\varepsilon}^{S}\|_{\infty} \leq C \varepsilon^{\frac{1}{2}} \eta_{\varepsilon}^{5}$ (Markovian approximation)

(The memory effects preventing the Markovianity are negligible!)

Stationary solutions as the long time asymptotics of $h_{\varepsilon}(t)$ and $f_{\varepsilon}(t)$? **Pb:** control the convergence rates, as $t \to \infty$, with respect to ε **Trick:** characterize instead h_{ε}^{S} and f_{ε}^{S} in terms of the Neumann series!

Markov part

 \Rightarrow

 h_{ε} solution of the linear Boltzmann equation with boundary conditions ρ_1 , ρ_2 and initial data f_0 .

$$h_{\varepsilon}(x,v,t) = h_{\varepsilon}^{out}(x,v,t) + h_{\varepsilon}^{in}(x,v,t) = h_{\varepsilon}^{out}(x,v,t) + S_{\varepsilon}^{0}(t)f_{0}$$

$$\underset{Markov sgr.}{\overset{Markov sgr.}{\longrightarrow}}$$

 h_{ε}^{out} : backward trajectories hitting the boundary.

 h_{ε}^{in} : trajectories which never leave Λ .

$$h_{\varepsilon}^{S} = h_{\varepsilon}^{out}(t_{0}) + S_{\varepsilon}^{0}(t_{0})h_{\varepsilon}^{S}, \qquad t_{0} > 0$$

$$h_{\varepsilon}^{S} = \sum_{n \ge 0} (S_{\varepsilon}^{0}(t_{0}))^{n} h_{\varepsilon}^{out}(t_{0}) \quad (Neumann \ series)$$

Convergence of the Neumann series \Rightarrow existence and uniqueness of h_{ε}^{S} $h_{\varepsilon}^{S} \rightarrow \varrho^{S}$ Hilbert expansion technique

Pathological configuration in the Markovian approximation



Backward Interference

Backward Recollision

Proof of Theorem 2

By standard computations (Hilbert expansion technique)

$$h_arepsilon^{\mathcal{S}} = arrho^{\mathcal{S}} + rac{1}{\eta_arepsilon} h^{(1)} + rac{1}{\eta_arepsilon} extbf{R}_{\eta_arepsilon}$$

But

$$h^{(1)}(v) = \mathcal{L}^{-1}(v \cdot \nabla_{x} \varrho^{S}) = \frac{\rho_{2} - \rho_{1}}{L} \mathcal{L}^{-1}(v_{1})$$

$$R_{\eta_{\varepsilon}} = O(\frac{1}{\sqrt{\eta_{\varepsilon}}}), \qquad \int_{S_{1}} v \varrho^{S} dv = 0$$

$$\downarrow$$

$$\eta_{\varepsilon} \int_{S_{1}} v h_{\varepsilon}^{S}(x, v) dv = -D \nabla_{x} \varrho^{S} + O(\frac{1}{\sqrt{\eta_{\varepsilon}}})$$

$$\sim J_{\varepsilon}^{S}(x) \text{ in } L^{\infty} \qquad \sim D \nabla_{x} \varrho_{\varepsilon}^{S} \text{ in } \mathcal{D}'$$
(Theorem 1)

Thanks for your attention!