Hypocoercivity of a model describing the thermalization of a rarefied gas with total energy conservation and chemical reactions

EFI Workshop

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Motivation

- Kinetic model of a gas with chemical reactions, rate depends on the temperature of the background

- Theoretical issues:
  - Existence of solutions
  - Convergence to equilibrium
  - Convergence to macroscopic equations

Kinetic description of gases

mass $m > 0$, position $x \in \mathbb{R}^3$, velocity $v \in \mathbb{R}^3$, time $t \geq 0$
distribution function $f(x, v, t) > 0$
Time evolution:

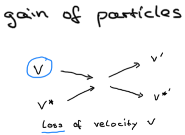
- For fixed $v \in \mathbb{R}^3$, without interactions and external forces, the distributions are just transported with velocity v

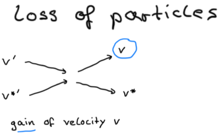
$$\partial_t f(x, v, t) + v \cdot \nabla_x f(x, v, t) = 0,$$

- effect of interactions: change of the velocities + gain and loss of particles

$$\partial_t f(x, v, t) + v \cdot \nabla_x f(x, v, t) = Q(f)(x, v, t)$$

Q collision operator





Examples: Landau-Fokker-Planck, Boltzmann operator, BGK operator

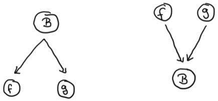
Kinetic model with chemical reactions and background temperature

$$\partial_t f + v \cdot \nabla_x f = \chi_1(v) - \rho_g f, \quad \partial_t f + v \cdot \nabla_x f = \rho_i(T)\chi_1(v,T) - \rho_g f$$

$$\partial_t g + v \cdot \nabla_x g = \chi_2(v) - \rho_f g, \quad \partial_t g + v \cdot \nabla_x g = \rho_i(T)\chi_2(v,T) - \rho_f g$$

$$\rho_f = \int f dv, \rho_g = \int g dv, \quad \rho_i(T) = C \exp(-\frac{E_a}{k_B T}) \quad \text{Arrhenius law}$$

$$\partial_t T - D \triangle T = \text{cons. of total energy}$$



Gas exchanging heat with a background

$$\partial_t f + v \cdot \nabla_x f = \rho M(T) - f$$

$$\partial_t (c_V T) - D \triangle_x T = \int |v|^2 (f - \rho M(T)) dv$$

Gas exchanging heat with a background

$$\partial_t f + v \cdot \nabla_x f = \rho M(T) - f, \quad M(T) = \frac{1}{\sqrt{2\pi T}^d} \exp(-\frac{|v|^2}{2T})$$

$$\partial_t (c_V T) - D \triangle_x T = \int |v|^2 (f - \rho M(T)) dv$$

Hypocoercivity: Let $D > 0$. Then there exist positive constants C and λ such that solutions of the linearized equation satisfy

$$||f - f_\infty||_{L_2} \leq Ce^{-\lambda t}.$$

Existence Under certain assumptions on the boundary and the initial data, there exists a solution (f, T) of the non-linear equation in $d = 1$, where

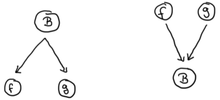
- $(1 + |v|^2 + \log f) f \in L^\infty((0, \tau); L^1(\mathbb{T}^1 \times \mathbb{R}))$, $T \in C^{1/2}(\mathbb{T}^1 \times [0, \tau])$,
- the Cauchy problem for the kinetic equation is interpreted in the distributional sense with interpretation for the term $\rho M(T)$ given by

$$\langle \rho M(T), \phi \rangle = \int_{\mathbb{T}^1 \times \mathbb{R} \times (0,\infty)} \rho(x,t) M(1)(w) \phi(x, w\sqrt{T}, t) dx dw dt$$

- Cauchy problem for the heat equation is interpreted in the mild sense.

Formal macroscopic limit to a cross diffusion system

Kinetic model with generation recombination



$$\partial_t f_1 + v \cdot \nabla_x f_1 = \sigma(\rho_1 \chi_1 - f_1) + \chi_1(v) - \rho_2 f_1 ,$$
$$\partial_t f_2 + v \cdot \nabla_x f_2 = \sigma(\rho_2 \chi_2 - f_2) + \chi_2(v) - \rho_1 f_2 ,$$

Existence Under certain assumptions on χ_1 and the initial data, there exists a unique global solution such that for all $x \in \Omega$, $v \in \mathbb{R}^3$, $t \geq 0$,

$$\rho_m \chi_1(v) \leq f_1(x,v,t) \leq \rho_M \chi_1(v) ,$$
$$\rho_M^{-1} \chi_2(v) \leq f_2(x,v,t) \leq \rho_m^{-1} \chi_2(v) .$$

Exponential convergence Let (f_1, f_2) be solution under the same assumptions as for the existence, then there exist λ and c positive constants such that for all $t \geq 0$ it holds

$$\| f_k(t) - f_{k,\infty} \|^2 \leq c, e^{-\lambda t} .$$

Rigorous macroscopic limit to reaction-diffusion equations

Hypocoercivity

$$\partial_t f(x,v,t) + v\partial_x f(x,v,t) = m(x,t)\chi(v) - f(x,v,t) =: L(f)(x,v,t),$$

$$\int \chi(v)dv = 1 \qquad m(x,t) = \int f(x,v,t)dv\ \chi(v), \quad \int f_0 dv = 0$$

Denote $f(x,v,t) = m(x,t)\chi(v) + h(x,v,t)$
Entropy $\mathcal{H}(f) = ||f||^2 + \delta < Af, f >$ with $A := [1 + (T\Pi)^*(T\Pi)]^{-1}(T\Pi)^*$
If we can prove

$$\frac{d}{dt}\mathcal{H}(f) \leq -c\mathcal{H}(f) \quad \text{and} \quad c||f||^2 \leq \mathcal{H}(f) \leq C||f||^2,$$

we can deduce $||f||^2 \leq C\mathcal{H}(f(t)) \leq C\exp(-2Ct)\mathcal{H}(f_0)$
Strategy:

$$\frac{d}{dt}||f||^2 =< Lf, f >=< -h, m\chi + h >= -||h||^2$$

deviation of f from local equicibrium

one ingredient: Poincaré inequality

$$\frac{d}{dt}\mathcal{H}(f) \leq -||h||^2 - \delta c||m||^2$$

deviation of local equilibrium from global equilibrium

Main issues in our case:

- no conservation of mass due to chemical reactions
- entropy $\int\int f \ln f dv dx$ (non-linear equation)

J. Dolbeault, C. Mouhot, C. Schmeiser, Hypocoercivity for linear kinetic equations conserving mass, 2015

Hypocoercivity for generation recombination model

$$\partial_t f_1 + v \cdot \nabla_x f_1 = \sigma(\rho_1 \chi_1 - f_1) + \chi_1(v) - \rho_2 f_1,$$
$$\partial_t f_2 + v \cdot \nabla_x f_2 = \sigma(\rho_2 \chi_2 - f_2) + \chi_2(v) - \rho_1 f_2,$$

Entropy $H(f_1, f_2) = \sum_{k=1,2} \int \int f_k (\ln \frac{f_k}{f_{k,\infty}} - 1) + f_{k,\infty}) dvdx$,

Entropy dissipation $\frac{d}{dt} H(f_1, f_2) = -\sigma \sum_{k=1,2} D_k - D_3$

term from relaxation

term from generation recombination

Global equilibrium $f_{1,\infty} = \rho_\infty \chi_1$, $f_{2,\infty} = \frac{1}{\rho_\infty} \chi_2$, 3 steps of relaxation:

- f_1, f_2 to local equilibria $\rho_1 \chi_1, \rho_2 \chi_2$
- ρ_1, ρ_2 to average densities $\rho_{1,\Omega} = \frac{1}{\Omega} \int_\Omega \rho_1 dx$, $\frac{1}{\Omega} \int_\Omega \rho_2 dx$
- $\rho_{1,\Omega}, \rho_{2,\Omega}$ to ρ_∞, $\frac{1}{\rho_\infty}$

$(f_k - \rho_k \chi_k)$ — deviation from local equilibrium

$(\rho_k \chi_k - \rho_{k,\Omega} \chi_k)$ — deviation from constant density → same mass, Poincaré inequality

$(\rho_{k,\Omega} \chi_k - f_{k,\infty})$ — deviation from global equilibrium

Terms in $\frac{d}{dt}(H(f_1, f_2) + \delta < A(f_1, f_2), (f_1, f_2) >)$

deviation from local equilibrium

D_3

deviation from global equilibrium

deviation from constant densities

Summary

G. Favre, M. Pirner, C. Schmeiser, Hypocoercivity and reaction diffusion limit for a nonlinear pairwise generation-recombination model, manuscript, 2021

- Existence of mild solutions
- Exponential convergence to equilibrium through hypocoercivity
- Macroscopic limit: reaction diffusion equations

G. Favre, M. Pirner, C. Schmeiser, Thermalization of a rarefied gas with total energy conservation: existence, hypocoercivity, macroscopic limit submitted, 2021

- Hypocoerivity for the linearized problem
- Formal macroscopic limit: cross diffusion
- Global existence for the non-linear problem in one dimension

Thank you for your attention!