Kinetic equations describing open systems

J. J. L. Velázquez (Univ. Bonn).

Boltzmann equation (1872)

$$\partial_t f + v \cdot \nabla_x f = Q(f,f) \quad ; \quad f = f(x,v,t) \geq 0$$
$$x \in \mathbb{R}^3, \; v \in \mathbb{R}^3$$

f density of particles in phase space

$$Q(f,f)(x,v,t) = \int_{\mathbb{R}^3} dv_* \int_{S^2} d\omega \, \underbrace{B(v-v_*,\omega)}_{\text{collision kernel}} \Big[\underbrace{f' f_*'}_{\text{Gain term}} - \underbrace{f f_*}_{\text{Loss term}} \Big]$$

$$f = f(x,v,t), \quad f' = f(x,v',t), \quad f_* = f(x,v_*,t), \quad f_*' = f(x,v_*',t)$$

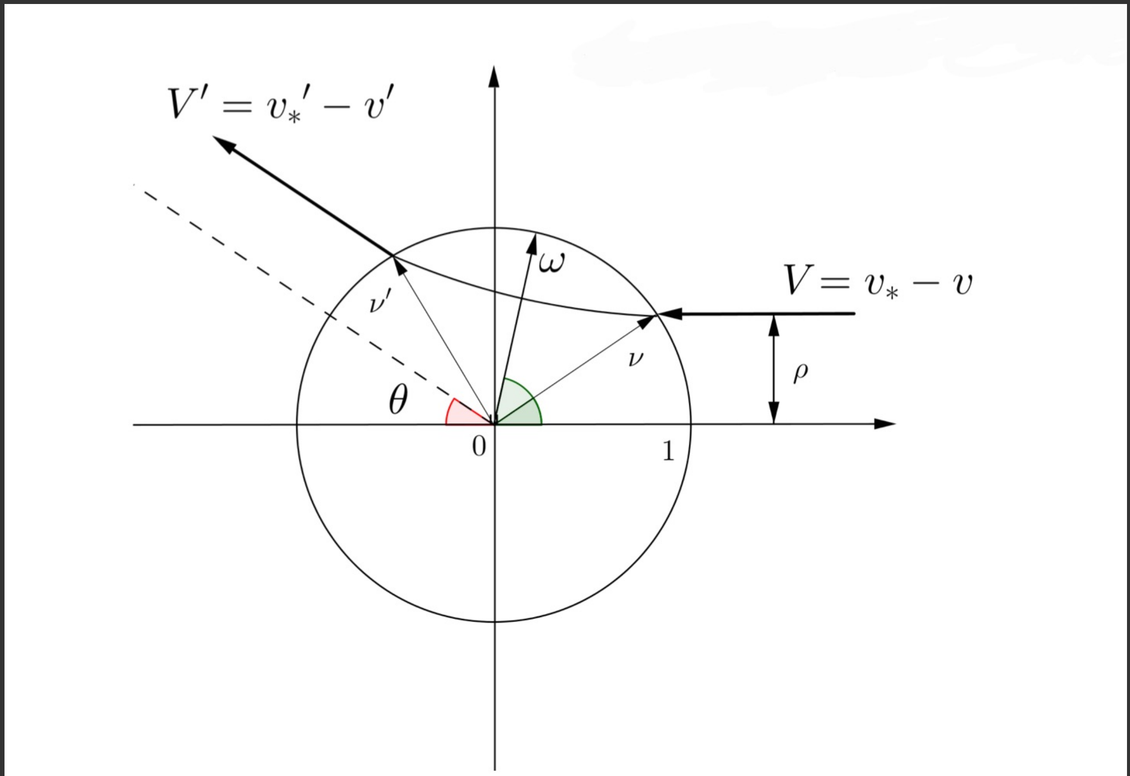
$$v' = v - [(v - v_*) \cdot \omega]\, \omega$$

$$v'_* = v_* + [(v - v_*) \cdot \omega]\, \omega$$

, $\omega \in S^2$

v, v_* Initial velocities

v', v'_* Final velocities



$$v + v_* \rightleftarrows v' + v'_*$$

$B(v - v_*, \omega)$ depends on the interaction potential between the colliding particles

Boltzmann equation (Assumptions)

- Only binary collisions.
- Instantaneous elastic collisions.
- Microreversibility. $(v + v_* \rightleftarrows v' + v'_*)$
- Boltzmann chaos. (Uncorrelated colliding particles)

Lanford (1975), Gallagher, Saint-Raymond, Texier (2013)

Pulvirenti, Simonella (2017), Deng, Hani, Ma (2024), ...

Boltzmann equation ("Fluid mechanics" for rarified gases).

Boltzmann-Grad limit $N a^2 \simeq 1$

N = particle density $\left(N = \frac{\text{particles}}{\text{volume}}\right)$

a = particle radius

$N \to \infty$, $a \to 0$, $N a^3 \to 0$

(the particles fill a very small fraction of the available space).

Boltzmann equation (Conservation laws, Fluid mechanics)

$$\rho(x,t) = \int_{\mathbb{R}^3} f \, dv , \quad V_i(x,t) = \frac{1}{\rho(x,t)} \int_{\mathbb{R}^3} v_i f \, dv$$ (density, mean velocity)

$$e(x,t) = \frac{1}{2\rho(x,t)} \int_{\mathbb{R}^3} (v_i - V_i)^2 f \, dv$$ (internal energy)

$$M_{ij} = \int_{\mathbb{R}^3} (v_i - V_i)(v_j - V_j) f \, dv , \quad q_i = \frac{1}{2} \int_{\mathbb{R}^3} c_i |c|^2 f \, dv$$

(Stress tensor, heat flux).

Boltzmann equation (Conservation laws, Fluid mechanics)

$$\frac{\partial \rho}{\partial t} + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}(\rho V_j) = 0$$ (Continuity equation)

$$\frac{\partial}{\partial t}(\rho V_i) + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}(\rho V_i V_j + M_{i,j}) = 0$$ (Momentum)

$$\frac{\partial}{\partial t}\left(\rho \frac{|V|^2}{2} + \rho e\right) + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\left(\rho V_i \left(\frac{|V|^2}{2} + e\right) + q_j + \sum_{i=1}^{3} V_j M_{i,j}\right) = 0$$

(Energy equation)

$M_{i,j} = M_{i,j}(f)$

$q_j = q_j(f)$

Not a closed system for ρ, V, e.

Boltzmann equation (H-Theorem).

$$\frac{d}{dt}(\mathcal{H}) = -D(f) \quad \Big| \quad \mathcal{H} = \int_{\mathbb{R}^3} f \log(f)\, dv$$ – "entropy"

$$D(f) = \int_{\mathbb{R}^3} dv \int_{\mathbb{R}^3} dv_* \int_{S^2} d\omega\, B(v - v_*, \omega)\left[f' f_*' - f f_*\right] \log\left(\frac{f' f_*'}{f f_*}\right) \geq 0$$

"dissipation"

$$D(f) = 0 \iff f = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|v - V|^2}{2T}\right), \quad \rho \geq 0, \; V \in \mathbb{R}^3, \; T \geq 0$$

(Maxwellian distribution).

The H-Theorem allows to prove rigorously convergence to equilibrium (i.e. Maxwellian distribution) for many collision kernels B.

* Homogeneous Boltzmann $(\partial_t f = Q(f,f))$.
* Non-homogeneous Boltzmann $(\partial_t f + v \nabla_x f = Q(f,f))$
  - $x \in \mathbb{T}^2$, $x \in \partial\Omega$ (elastic boundary conditions).

(local stability of the Maxwellian)

Arkeryd, Cercignani, Ukai, Villani, Mouhot, Guo, Strain, ...

All these results apply to closed systems

What happens in open systems ?

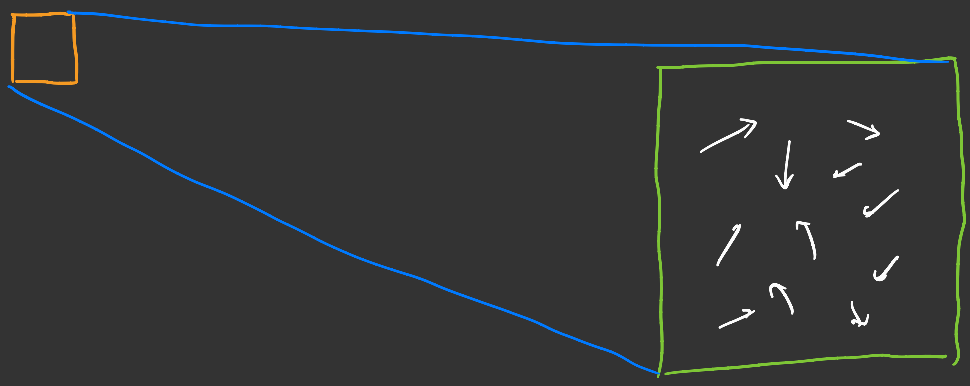
Homoenergetic solutions

$$f(x,v,t) = g(v - \xi(x,t), t)$$

Same distribution of velocities at each point.
(Only the mean value of the velocity changes).

Truesdell, Galkin (1960's).

Homoenergetic solutions



In the Boltzmann description of a gas, each "macroscopic" element contains a very large number of molecules travelling at different speeds.

In the homoenergetic solutions, the distribution of velocities is the same at each point, except for a translation that depends on each point

$$f(x,v,t) = g(v - \xi(x,t), t)$$

Homoenergetic solutions

Very restrictive distribution of velocities.

Are there solutions of Boltzmann with this very particular form? $f(x,v,t) = g(v - \xi(x,t), t)$

$$\xi(x,t) = M(t)\,x \quad , \quad M(t) \in M_{3\times 3}(\mathbb{R})$$

$$\frac{dM}{dt} + M^2 = 0 \quad , \quad \partial_t g(w,t) - M(t)w \cdot \partial_w g = Q(g,g)$$

$$w = v - \xi(x,t)$$

Homoenergetic solutions

Classification of long time behavior for the solutions of

$$\frac{dM}{dt} + M^2 = 0 \quad , \quad M(t) = (I + tA)^{-1} A$$

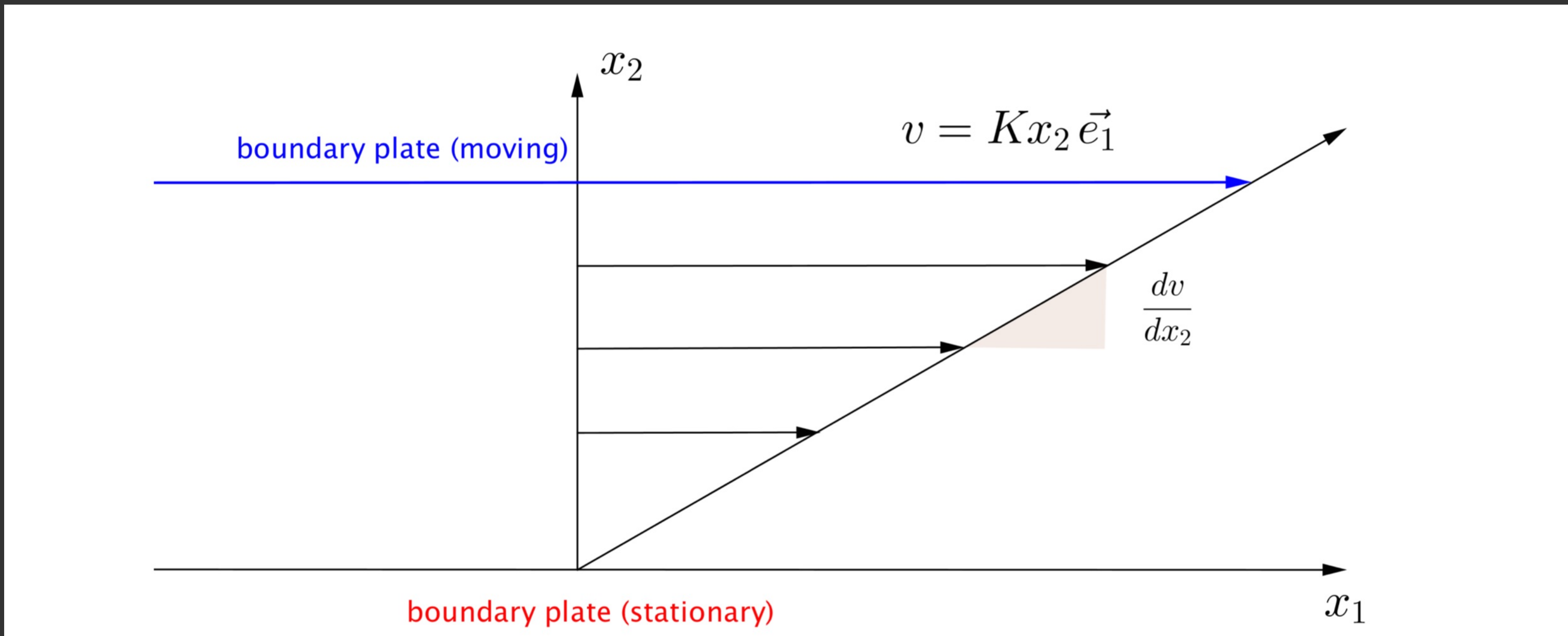
Jordan canonical form (R.L. James, A. Nota, V)

- simple shear
- 3d dilatation (isotropic)
- 1d dilatation
- 2d dilatation
- mixed 1d dilatation and shear
- mixed 2d dilatation and shear
- mixed 3d dilatation and shear
- combined shear in orthogonal directions
- blow-up cases

Homoenergetic solutions (Examples)

Simple shear: $A = a \otimes n$, $a \cdot n = 0$, $a = K e_1$, $n = e_2$

$$\partial_t g - K w_2 \partial_{w_1} g = Q(g,g)$$



Homoenergetic solutions (Examples)

Mixed 1d dilatation and shear: $A = a \otimes n$, $a \cdot n \neq 0$

$$n = e_1 , \quad a = K_1 e_1 + K_2 e_2$$

$$\partial_t g + \frac{K_1}{1 + K_1 t} w_1 \partial_{w_1} g + \frac{K_2}{1 + K_1 t} w_2 \partial_{w_1} g = Q(g,g)$$

Homoenergetic solutions (General features).

$$\partial_t g - \underbrace{M(t)\, w \cdot \partial_w g}_{\text{Hyperbolic term}} = \underbrace{Q(g,g)(w)}_{\text{Collisions}}$$

(competing terms).

$$\rho(t) = \int g(w,t)\, dw$$

(Particle density).

Global well posedness (Adaptation of the tools available for homogeneous Boltzmann) (Cercignani).

Long time asymptotics of the solutions?.

Homoenergetic solutions

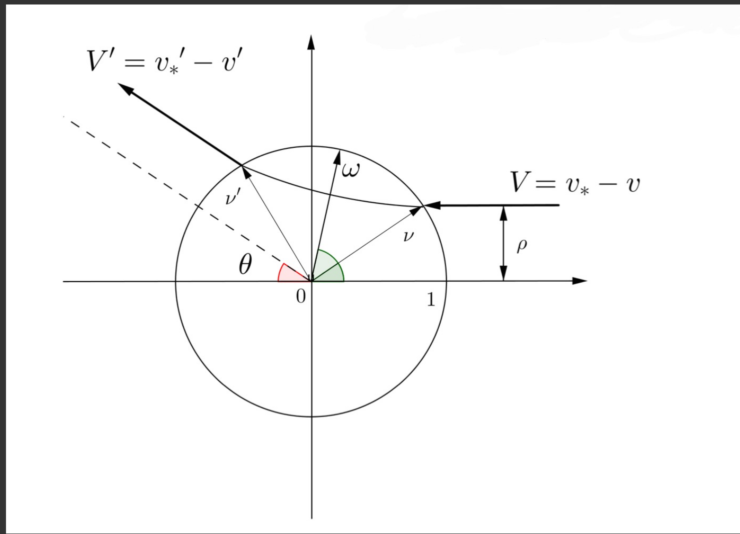
Scaling properties of the collision kernel $B(|v-v_*|,\omega)$

$$Q(f,f)(x,v,t) = \int_{\mathbb{R}^3} dv_* \int_{S^2} d\omega \, \underbrace{B(v-v_*,\omega)}_{\text{collision Kernel}} \left[f' f'_* - f f_* \right]$$

The form of $B(v-v_*,\omega)$ depends on the interaction potential between two particles.

Homoenergetic solutions

$B(v-v_*, \omega)$ is computed studying the collision between two particles. (Newton equation)



Power law potentials (Maxwell)

$$\phi(r) = \frac{1}{r^{s-1}}, \quad s > 2 \quad ; \quad B(v-v_*; \omega) = b(\cos(\theta))\, |v-v_*|^{\gamma}$$

$$\gamma = \frac{s-5}{s-1}$$

Homogeneous potentials (Homogeneity $= \gamma$)

Homoenergetic solutions (Scaling properties, $\phi(r) = \frac{1}{r^{s-1}}$)

$$\partial_t g - M(t) w \cdot \partial_w g = Q(g,g)(w)$$

$$\rho(t) = \int g \, dw \quad \text{(density)} \quad , \quad \| M(t) \| \simeq 2(t)$$

Scaling

Hyperbolic term

$$M(t) w \cdot \partial_w g \simeq 2(t) [g]$$

Collision term

$$Q(g,g) \simeq \rho(t) [w]^{\gamma} [g]$$

Which one is the dominant term (if any)?

Homoenergetic solutions (Scaling properties, simple shear).

Which term is the dominant one as $t \to \infty$ depends on the homogeneity of the collision Kernel B.

$\gamma > 0$ Collision dominated case

$\gamma < 0$ Hyperbolic dominated

$\gamma = 0$ Critical behaviour

$B(v - v_*, \omega) = b(\cos(\theta))$, $\gamma = 0$ (Maxwellian molecules)

$\phi(r) = \frac{1}{r^4}$, $s = 5$, $\gamma = \frac{s-5}{s-1}$

Long time asymptotics of homoenergetic solutions

Simple shear.

Maxwellian molecules $(\gamma = 0)$.

$$(E) \qquad \partial_t g - K w_2 \partial_{w_1} g = Q(g,g)$$

$$g(w,0) = g_0(w) \quad , \quad \int g_0(w)\, w \, dw = 0$$

(w.l.o.g)

$$g_0 \in \mathcal{M}_+(\mathbb{R}^3)$$

Theorem : • Assume $\gamma = 0$, $|K| \le \varepsilon_0$ (small).

There exists a self-similar solution of (E) with the form $\bar{g}_s(w,t) = e^{-3\beta t} G\left(\frac{w}{e^{\beta t}}\right)$, for some $\beta = \beta(K) > 0$

(unique up to time translations $t \to t + t_0$)

• Suppose that $g(w,0) = g_0(w)$.

with $\int g_0(w) |w|^p \, dw$, $p > 2$. Then, the corresponding

solution of (E) satisfies

$$e^{3\beta t} g(e^{\beta t} \xi, t + t_0) \longrightarrow G(\xi) \quad \text{as } t \to \infty$$

(for some $t_0 \in \mathbb{R}$)

Homoenergetic solutions. Simple shear. Maxwellian molecules

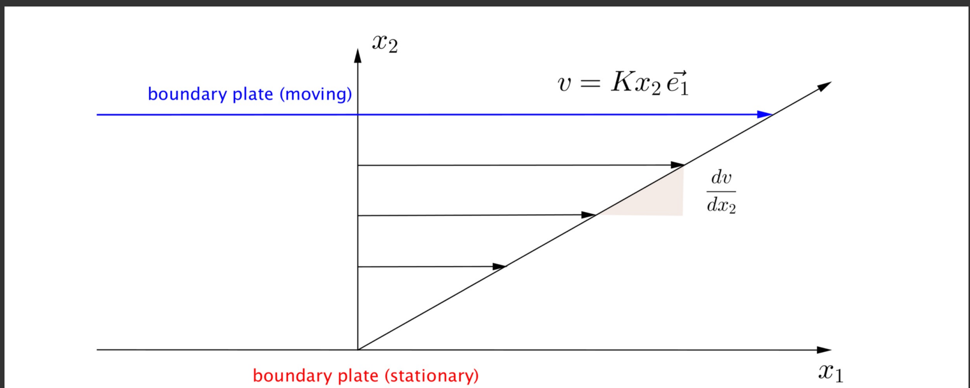
$(\gamma = 0)$

$$\bar{g}_s(w,t) = e^{-3\beta t}\, G\left(\frac{w}{e^{\beta t}}\right), \quad \beta = \beta(K) > 0$$

$$\rho(t) = \int \bar{g}_s(w,t)\, dw = \rho_0 \quad \text{(constant).}$$

$$T = \frac{1}{\rho_0} \int |w|^2 \bar{g}_s(w,t)\, dw = e^{2\beta t}$$

(exponential growth of the temperature).



* Friction between the different layers (heating).
* Energy injected from "infinity". (Non-equilibrium).

Homoenergetic solutions. Simple shear. Maxwellian molecules ($\gamma = 0$)

The self-similar profile $G(\xi)$ is not a Maxwellian

Detailed balance fails. (At equilibrium each reaction and its reverse one are balanced).

$$Q(f,f)(x,v,t) = \int_{\mathbb{R}^3} dv_* \int_{S^2} d\omega \; B(v-v_*,\omega)\left[f' f'_* - f f_* \right]$$

$$v' = v - [(v-v_*)\cdot\omega]\,\omega \quad , \omega \in S^2$$

$$v'_* = v_* + [(v-v_*)\cdot\omega]\,\omega$$

Homoenergetic solutions. Simple shear. Maxwellian molecules

$(\gamma = 0)$

Detailed balance (Boltzman collisions)

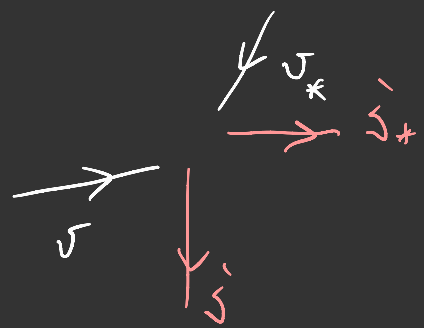
$$f_e = \frac{\rho_0}{(2\pi T)^{3/2}} \exp\left(-\frac{|v-V|^2}{2T}\right)$$

$$f_e' f_{e,*}' = f_e f_{e,*}$$ (Balance of individual collisions).

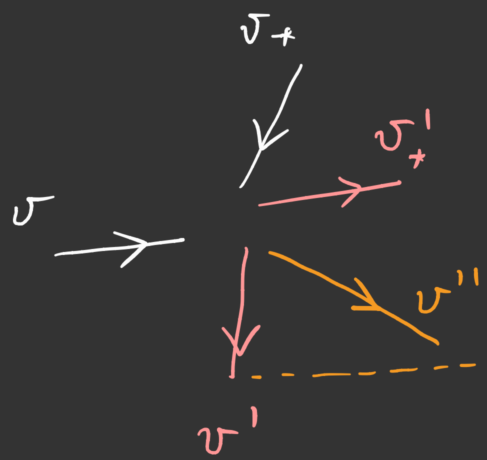
For the self-similar solutions above, detailed balance fails $G' G_*' \neq G G_*$

Lack of detailed balance is a common feature of open systems.

Stationarity is due to an involved balance of collisions and transport



Detailed balance



+ Additional collisions

Absence of detailed balance

Equation for the self-similar profile

$$-\beta\, \partial_w (w G) - \partial_{w_1}(w_2 G) = Q(G,G)(w)$$

None of the terms vanishes individually.

Homoenergetic solutions. General case. Maxwellian molecules ($\gamma=0$)

Similar results. (Existence and uniqueness of self-similar solutions, that are global attractors).

Example: Combined 1d dilatation and shear

$$\partial_t g + \frac{K_1}{1+K_1 t} w_1 \partial_{w_1} g + \frac{K_2}{1+K_1 t} w_2 \partial_{w_1} g = Q(g,g)$$

Competition between dilatation (cooling) and shear (heating)

Homoenergetic solutions. Maxwellian molecules

$(\gamma = 0)$

1d dilatation : (Rate K_1)

Shear : (Rate K_2)

$$\bar{g}_s(w,t) = t^{-3\alpha} G\left(\frac{w}{t^{\alpha}}\right),$$

$\alpha = \alpha(K_1, K_2)$

$\alpha > 0$ if $K_2^2 > K_1$

$\alpha < 0$ if $K_2^2 < K_1$

Homoenergetic solutions. Collision dominated and hyperbolic dominated cases. (Simple shear)

$$\partial_t g + K w_2 \partial_{w_1} g = Q(g,g)(w)$$

$$[g] \qquad \rho_0 [w]^{\gamma} [g]$$

* If $\gamma > 0$ and the temperature (i.e. $\langle |w|^2 \rangle$) increases the collision term becomes more important as $t \to \infty$.

$$|K w_2 \partial_{w_1} g| \ll |Q(g,g)| \quad \text{as } t \to \infty$$

* If $\gamma < 0$ and the temperature increases, the shear term becomes dominant as $t \to \infty$

$$|K w_2 \partial_{w_1} g| \gg |Q(g,g)|, \quad t \to \infty$$

Homoenergetic solutions. Simple shear. Collision dominated ($\gamma > 0$)

Tools to describe solutions of Boltzmann equations when the collisions are dominant are available (Hilbert expansions).

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f,f)$$

$$f = f_e + \varepsilon f_1 + \varepsilon^2 f_2 + \dots$$

$$f_e = \frac{\rho_0}{(2\pi T)^{3/2}} \exp\left(-\frac{|v-V|^2}{2T}\right) \; ; \quad \begin{aligned} T &= T(x,t) \\ \rho_0 &= \rho_0(x,t) \\ V &= V(x,t) \end{aligned}$$

$\rightarrow$ Hydrodynamic equations.

Homoenergetic solutions. Simple shear. Collision dominated

$(\gamma > 0)$

The method of Hilbert expansions can be adapted to study the long time asymptotics of the homoenergetic solutions in this case

$$\partial_t T = a T^{1-\frac{\gamma}{2}}, \quad a > 0 \implies T \sim C_0 t^{2/\gamma}, \quad t \to \infty$$

$$g(w,t) \simeq \frac{\rho_0}{(2\pi T)^{3/2}} \exp\left(-\frac{|v|^2}{2T}\right), \quad t \to \infty$$

(Similar results for general homoenergetic solutions).

Homoenergetic solutions. Simple shear. Hyperbolic dominated

($\gamma < 0$)

$$\partial_t g + K w_2 \partial_{w_1} g = Q(g,g)(w)$$

$$[g] \qquad\qquad \rho_0 [w]^\gamma [g]$$

Increasing temperature yields $|Q(g,g)| << |K w_2 \partial_{w_1} g|$

$\gamma < -1 \longrightarrow$ Frozen collisions

$-1 \leq \gamma < 0 \longrightarrow$? (Simplified models).

References

R. D. James, A. Nota, V. ARMA (2019), $\gamma = 0$

R. D. James, A. Nota, V. JNLS (2019), $\gamma > 0$

R. D. James, A. Nota, V. Nonlinearity (2020), $\gamma < 0$

A. Bobylev, A. Nota, V. CMP (2020), $\gamma = 0$ (Uniq. Stab)

B. Kepka, JSP (2023)

B. Kepka, PAA (2024)

R. Duan, S. Liu (2024).

Becker-Döring model. A class of kinetic models arising in polymerization, nucleation, bubble aggregation, ...

(ℓ) = Clusters of size ℓ.

(1) = Monomers

n_ℓ = concentration of clusters of size ℓ.

$$(\ell) + (1) \underset{b_\ell}{\overset{a_\ell}{\rightleftarrows}} (\ell+1)$$

a_ℓ, b_ℓ = reaction rates

(Aggregation-fragmentation model).

Becker-Döring model

System of infinitely many ODEs

$$\partial_t n_1 = -J_1 - \sum_{k=1}^{\infty} J_k$$

$$\partial_t n_k = J_{k-1} - J_k \quad , \quad k \geq 2$$

$$J_k = a_k n_k n_1 - b_k n_{k+1} \quad , \quad k \geq 1$$

$$a_k = k^{\alpha} \quad , \quad b_k = a_k \left(1 + \frac{q}{k^{\gamma}}\right) \quad , \quad \alpha \in (0,1) \quad , \quad \gamma \in [0,1)$$

Ball, Carr, Penrose (CMP, 1986)

("Simplest" model of phase transitions).

This model describes a "closed" system. There is a decreasing "free energy"

Detailed balance holds.

$$F = -\sum_{k=1}^{\infty} n_k \log\left(\frac{n_k}{Q_k}\right) \quad ; \quad a_k Q_k = b_k Q_{k+1}$$

$$\frac{dF}{dt} \leq 0$$

(Dissipation formula)

Convergence to equilibrium, with a possible escape of mass to infinity in "supercritical" cases. (Phase transitions).

Becker-Döring models describing open systems.

(a) Becker-Döring with atomization

$$(K) + (1) \rightleftharpoons (K+1)$$

$$(M) \xrightarrow[\text{open}]{} M(1) \longrightarrow \text{Atomization}$$ (Detailed balance fails)

$$\partial_t n_\ell = J_{\ell-1} - J_\ell \,, \quad 2 \leq \ell \leq N \,,$$

$$\partial_t n_M = J_{M-1} - K n_M \,, \quad M = N+1$$

$$\partial_t n_1 = -J_1 - \sum_{\ell=1}^{N} J_\ell + M K n_M$$

$$J_\ell = n_1 n_\ell - n_{\ell+1}$$

This model exhibits periodic solutions

B. Pego, V (2020)

(Hopf bifurcation).

Becker-Döring model with atomization

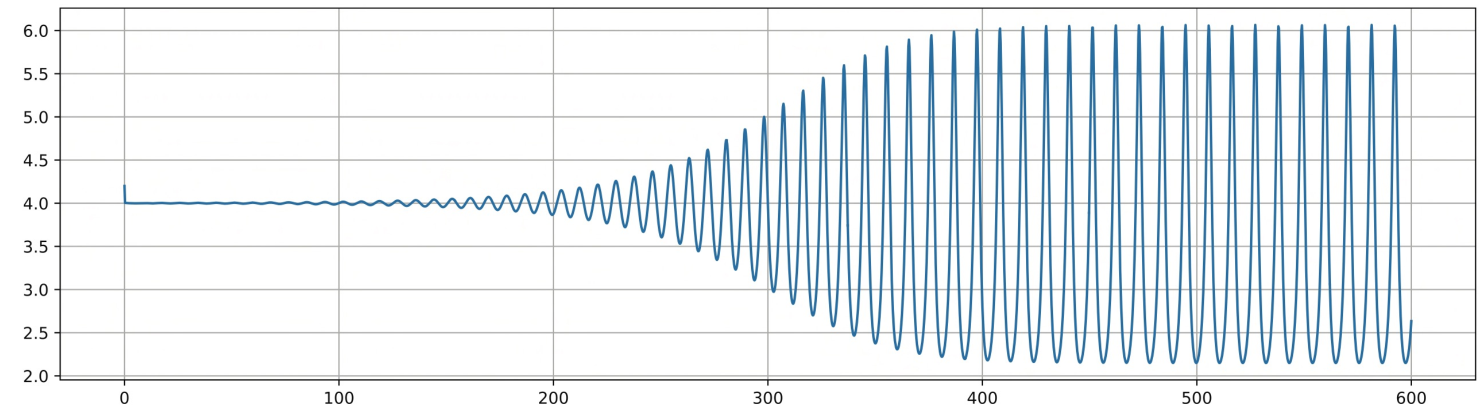


Figure 1. Monomer density n_1 versus t for a numerical solution of (2)–(4).

Oscillatory behaviour of $n_1(t)$

(b) Becker-Döring with monomer sources and sedimentation

$$\partial_t n_1 = -J_1 - \sum_{k=1}^{\infty} J_k + S$$

Source

Sedimentation

$$\partial_t n_k = J_{k-1} - J_k - r k^b n_k \quad , \quad k \geq 2 \, , \; r > 0 \, , \; b \geq 0$$

$$J_k = a_k n_k n_1 - b_{k+1} n_{k+1} \quad , \quad k \geq 1$$

$$a_k = k^\alpha \quad , \quad \alpha \in (0,1) \quad ; \quad b_k = a_k \left(1 + \frac{q_s}{k^\gamma} \right) \quad , \quad \gamma \in (0,1)$$

This model exhibits also oscillatory behaviour

B. Pego, A. Schlichting, B. Niethammer, " (2022)

(b) Becker-Döring with monomer sources and sedimentation

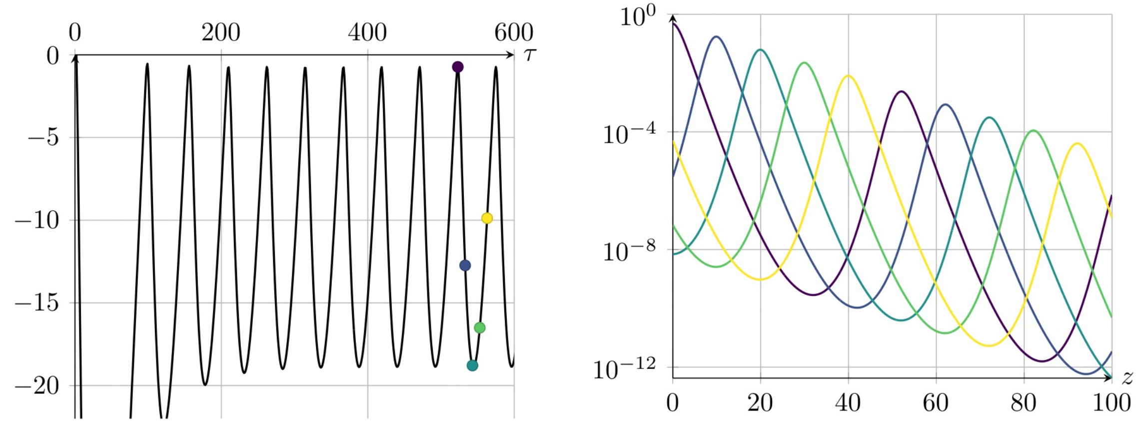


Fig. 1: Time evolution of u (left) and the profile h (right, semi-log plot) at times $t = 523$ (—), $t = 533$ (—), 543 (—), $t = 553$ (—), 563 (—).
Parameters: $\theta = 0.1$, $\nu = 2$, $\beta = 1$ ($\alpha = \frac{1}{3}$, $\gamma = \frac{1}{3}$, $b = \frac{3}{2}$).

$u \to$ Rescaled n_1

$h \to$ Rescaled $\{n_k\}_{k=1}^{\infty}$

Smoluchowski coagulation equations (1916)

$$\partial_t f(v,t) = \underbrace{\frac{1}{2}\int_0^v K(v-\xi,\xi)\, f(v-\xi,t)\, f(\xi,t)\, d\xi - \int_0^\infty K(v,\xi)\, f(v,t)\, f(\xi,t)\, d\xi}_{\mathbb{K}[f](v,t)} + s(v)$$

Source

$$f(v,0) = f_0(v)$$

$$(v_1) + (v_2) \longrightarrow (v_1+v_2)$$

$K(v,\xi) = K(\xi,v)$ (collision rate)

$f(v,t)$ = density of particles in the space of volumes v

$$c_0\left[(v)^{\gamma+\lambda}(\xi)^{-\lambda} + (\xi)^{\gamma+\lambda}(v)^{-\lambda}\right] \leq K(v,\xi) \leq c_1\left[(v)^{\gamma+\lambda}(\xi)^{-\lambda} + (\xi)^{\gamma+\lambda}(v)^{-\lambda}\right]$$

Examples:

$$K(v,\xi) = \left[(v)^{-1/3} + (\xi)^{-1/3}\right]\left[(v)^{1/3} + (\xi)^{1/3}\right]$$ (Brownian Kernel) $\gamma = 0$, $\lambda = 1/3$

$$K(v,\xi) = \left[(v)^{1/3} + (\xi)^{1/3}\right]^2 \left[(v)^{-1} + (\xi)^{-1}\right]^{1/2}$$ (Free molecular coagulation). $\gamma = 1/6$, $\lambda = 1/2$

Smoluchowski coagulation equations

In the absence of sources, the behavior of the solutions is usually self-similar

$$\partial_t f(v,t) = \frac{1}{2}\int_0^v K(v-\xi,\xi)\, f(v-\xi,t)\, f(\xi,t)\, d\xi - \int_0^\infty K(v,\xi)\, f(v,t)\, f(\xi,t)\, d\xi$$

$$f(v,t) = \frac{1}{t^{2/1-\gamma}} F\left(\frac{v}{t^{1/1-\gamma}}\right) \quad ; \quad \gamma < 1$$

$$K(v,\xi) \simeq (v)^{\gamma+\lambda}(\xi)^{-\lambda} + (\xi)^{\gamma+\lambda}(v)^{-\lambda}$$

Smoluchowski coagulation equations

$$\partial_t f(v,t) = \frac{1}{2}\int_0^v K(v-\xi,\xi) f(v-\xi,t) f(\xi,t)\, d\xi - \int_0^\infty K(v,\xi) f(v,t) f(\xi,t)\, d\xi + \underbrace{s(v)}_{\text{Source.}}$$

(Natural problem in many applications).

However, in the presence of sources $s(v)$, there might be a rich structure of behaviors.

Smoluchowski coagulation equations (with source)

* Self-similar solutions due to coagulation of comparable particles
* Self-similar solutions due to the coagulation of comparable particles and also the coagulation of particles with very different sizes
* "Propagating Dirac mass behaviour"
* Critical cases with logarithmic singularities

Smoluchowski coagulation equations with source $(\gamma < 1)$

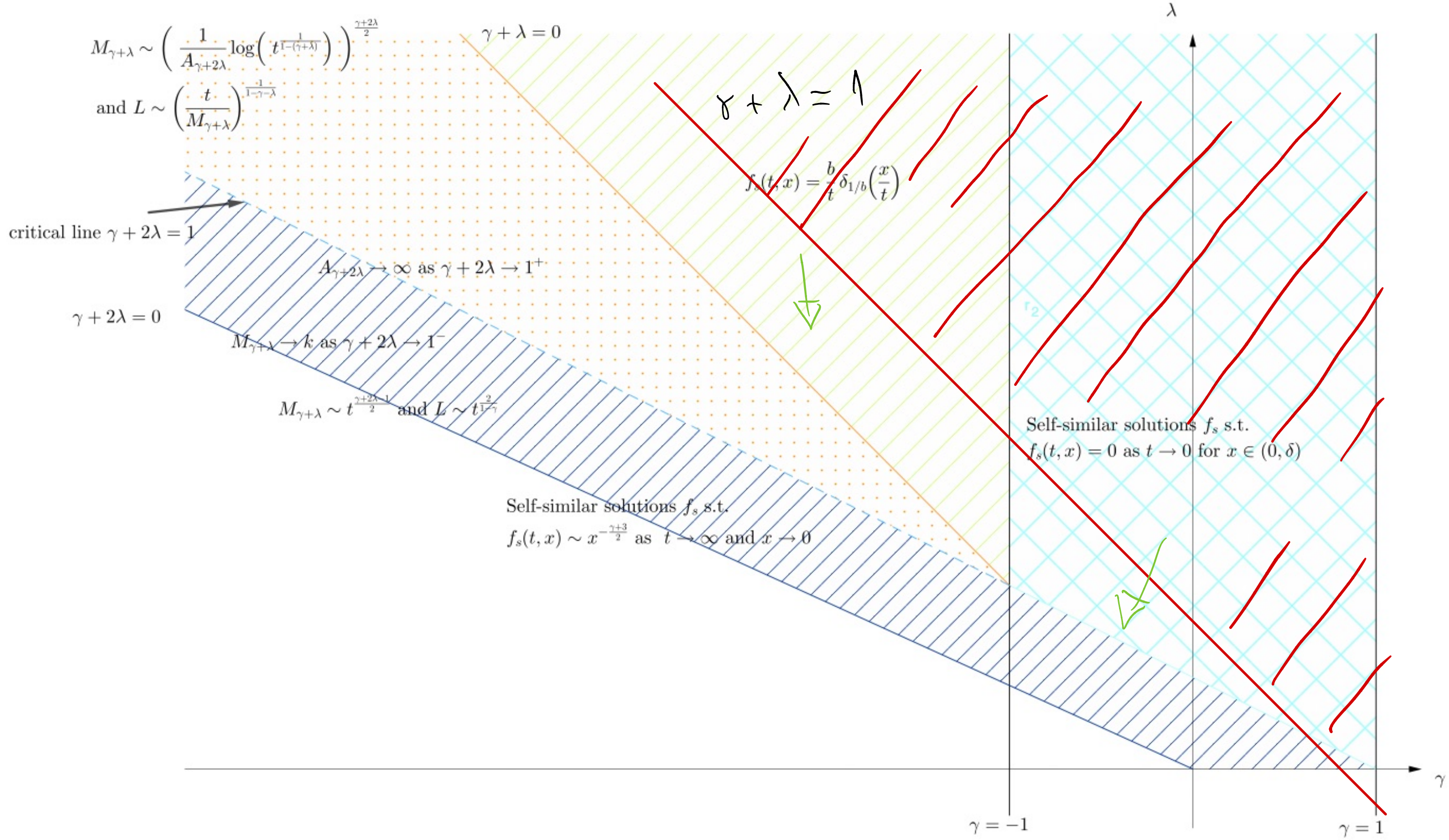


Figure 6 In this picture we show the different behaviours near the critical line $\gamma + 2\lambda = 1$ in the different regimes $\gamma < -1$, $\gamma = -1$ and $-1 < \gamma < 1$.

Cristian, Ferreira, Franco, Lukkarinen, Nota, V

ARMA. CMP. JSP, AIHP. ARMA. SIMA. PAA. J Phys A

General remarks about the study of the behavior of solutions of Kinetic equations describing open systems.

* The dissipation formulas do not allow to prove convergence to equilibrium
* Richer set of possible behaviors as $t \to \infty$ (periodic solutions, multistability, ...)
* Ad hoc methods. (Bifurcation theory, Asymptotic methods, general functional analysis results).

Thanks for your attention