UNIVERSITÀ DEGLI STUDI DELL'AQUILA

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Università degli Studi dell'Aquila

On the Smoluchowski equation for aggregation phenomena: stationary non-equilibrium solutions

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Joint works with M.A. Ferreira, J. Lukkarinen, J.J.L. Velázquez

Scaling limits and generalized hydrodynamics, GSSI, L'Aquila

Outline

Introduction

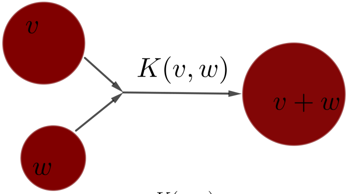
One-component Smoluchowski equation with source terms:
existence and non-existence of stationary non-equilibrium solutions

Multi-component equation: stationary non-equilibrium solutions
and localization properties

Perspectives

Smoluchowski coagulation equation (1916)

- Model: irreversible aggregation of spherical clusters through collisions
- $f(v,t)$: number density of particles (clusters) of size $v \geq 0$ at time t
- $K(v,w) \geq 0$ rate kernel, symmetric and $K(\alpha v, \alpha w) = \alpha^\gamma K(v,w)$



$$[v] + [w] \xrightarrow{K(v,w)} [v+w]$$

Goal: description of the **particle size distribution** as a function of time (mesoscopic/kinetic model)

Rate equation:

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

No detailed balance!

Smoluchowski coagulation equation (1916)

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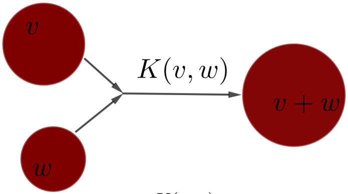

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Well-posedness:

[Ball, Carr '92; Norris '01; Laurencot, Mischler '02, Fournier, Laurencot '06, ...]

Dynamical scaling Hp.: Is there a dynamic equilibrium, i.e. a solution that becomes stationary after a similarity transformation?

Smoluchowski coagulation equation (1916)

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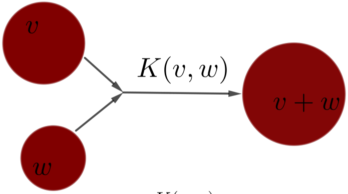

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Well-posedness:

[Ball, Carr '92; Norris '01; Laurencot, Mischler '02, Fournier, Laurencot '06, ...]

Dynamical scaling Hp.: [Menon and Pego '04] (explicit solvable kernels)

[Bonacini, Escobedo, Laurencot, Mischler, Niethammer, Pego, N., Velázquez, ...]

Mass conservation and current

- **Moment identity**:

$$\frac{d}{dt}\int_0^\infty \psi(v)f(v,t)dv$$
$$= \frac{1}{2}\int_0^\infty\int_0^\infty K(v,w)f(v,t)f(w,t)\left[\psi(v+w)-\psi(v)-\psi(w)\right]dvdw$$

- **Total mass (volume) = 1st moment**:

$$M_1(t) := \int_0^\infty v\, f(v,t)dv \quad \Longrightarrow \quad \frac{d}{dt}M_1(t) = 0$$

This is only formal! Indeed, for kernels with

- $\gamma \leq 1$ *mass conservation* for all times
- $\gamma > 1$ *gelation* (loss of mass at finite time, phase-transition)
  [Ex: $K(v,w) = vw$]

Mass conservation and current

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- **Continuity equation**:

$$\partial_t(v\, f(v,t)) + \partial_v J(v; f(\cdot,t)) = 0\,,$$

- **Mass current** :

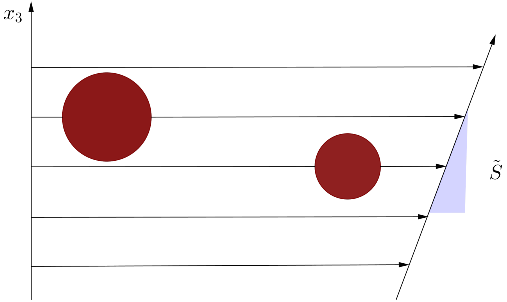
$$J(v;f) = \int_0^v dw \int_{v-w}^\infty du\, K(w,u)\, w\, f(w)\, f(u)$$

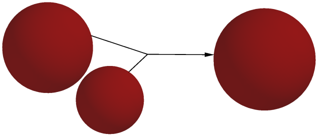
Some examples of physically relevant coagulation kernels

Coagulation mechanism in shear flows

Spherical particles in $\mathbb{R}^3$ with speed $u(x) = \left(\tilde{S}x_3, 0, 0\right)$

$\tilde{S} = \frac{\partial u_1}{\partial x_3}$ shear coeff.



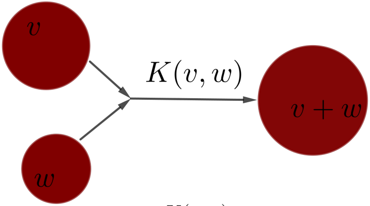


Coagulation kernel: $K(v, w) = \dfrac{4}{3} S (v^{\frac{1}{3}} + w^{\frac{1}{3}})^3$

[Smoluchowski 1917, Friedlander 2000]

Coagulation mechanism for aerosols (particle sizes $\sim$ 1nm)

Model: spheres dispersed in $\mathbb{R}^3$ moving independently until they collide and coalesce, forming growing spheres (irreversible aggregation)



$$[v] + [w] \xrightarrow{K(v,w)} [v + w]$$

+ gas of background particles (air) which do not coalesce

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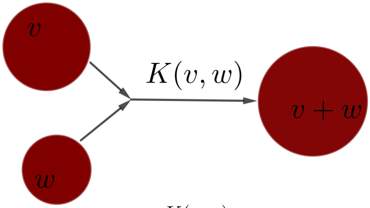


$$[v] + [w] \xrightarrow{K(v,w)} [v+w]$$

+ gas of background particles (air) which do not coalesce

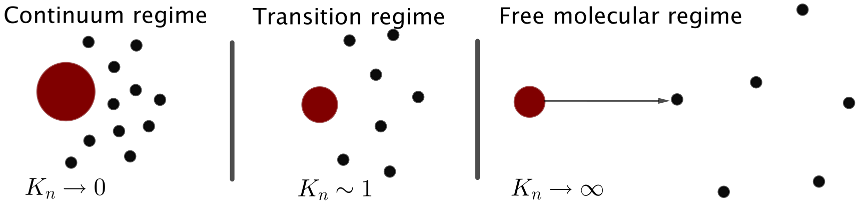
Assumptions [Friedlander, 2000]:

- many more collisions with "background" particles (gas molecules at thermal equilibrium) than between coalescing particles
- all collisions between coalescing particles yield merging particles
- different regimes depending on the ratio between the particles **size** (d) and the **mean-free path** in air ℓ

Coagulation mechanism for aerosols (particle sizes $\sim$ 1nm)

Different regimes depending on the ratio between the particles **size** (d) and the **mean-free path** in air ℓ:

$$K_n = \frac{\ell}{d}$$



Physical kernels

- Free molecular regime (or Ballistic) kernel ($d \ll \ell$)

$$K(v,w) = \left(\frac{3}{4\pi}\right)^{\frac{1}{6}} \sqrt{6k_B T} \left(\frac{1}{v} + \frac{1}{w}\right)^{\frac{1}{2}} \left(v^{\frac{1}{3}} + w^{\frac{1}{3}}\right)^2$$

k_B : Boltzmann constant, T : absolute temperature

[Friedlander 2000]

- Diffusion limited aggregation (or Brownian) kernel ($d \gg \ell$)

$$K(v,w) = 4\pi D \left(v^{\frac{1}{3}} + w^{\frac{1}{3}}\right) \qquad D : \text{diffusion constant}$$

$$D = \frac{k_B T}{6\mu\pi} \left(\frac{1}{v^{\frac{1}{3}}} + \frac{1}{w^{\frac{1}{3}}}\right) \qquad \text{(Einstein-Stokes law)}$$

$\mu > 0$: viscosity of the fluid in which the clusters move

[Smoluchowski 1916, Friedlander 2000]

Derivation of the Smoluchowski equation from particle systems: some ideas in a linear regime

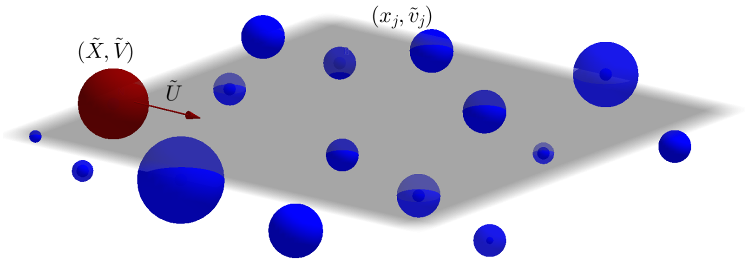
- Brownian coagulation:

  Lang and Nguyen 1980, Grosskinsky, Klingenberg, Oelschläger 2004, Norris 1999-2004, Hammond and Rezakhanlou 2007, Yaghouti, Rezakhanlou, and Hammond 2009, ...

- Convergence of the Markov-Lushnikov process:

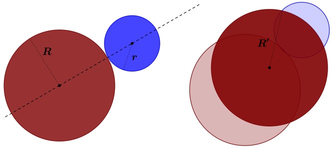
  Lushnikov 1978-1979, ..., Deaconu and Fournier 2002, Fournier and Giet 2004 ....

A coalescing particle in a random background



$\phi > 0$ volume fraction; μ_ϕ s. t. $\{\tilde{x}_j\}_j \sim \mathcal{P}(1)$, $\{\tilde{v}_j\}_j \sim \frac{1}{\phi} G(\frac{v}{\phi})$,

$G(v) \sim v^{-\sigma}$, $\sigma > \frac{5}{3}$



$$\mathcal{A}(Y, V; \omega) = \underbrace{\left(\frac{VY + \sum_{k \in J} x_k v_k}{V + \sum_{k \in J} v_k}, V + \sum_{k \in J} v_k; \omega \setminus J \right)}_{\text{merging operator}}$$

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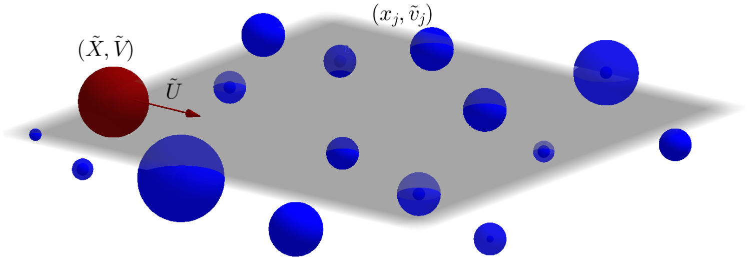

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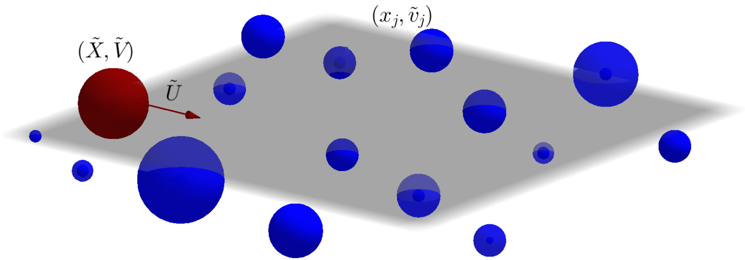
Main difficulties: (change of size of the tagged particle)

- coalescing particles could trigger sequences of coagulation events

  $\rightsquigarrow$ formation of an infinite cluster (dynamic percolation theory)

A coalescing particle in a random background



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  $\rightsquigarrow$ formation of an infinite cluster (dynamic percolation theory)

- the free flights between coagulation events become shorter

  $\rightsquigarrow$ runaway growth of the tagged particle in finite time

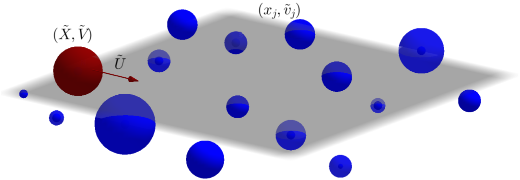
A coalescing particle in a random background

- Scaling limit:

  $$\tilde{V} = \phi V,\ \tilde{v} = \phi v,$$

  $$\tilde{Y} = \phi^{\frac{1}{3}} Y,\ \tilde{U} = \phi^{-\frac{2}{3}} U$$

  (one collision for unit of time)



- The distribution function f for the particle position and volume in the scaling limit $\phi \to 0$ satisfies

$$\partial_t f(Y,V,t) = U \int_0^{\frac{\pi}{2}} d\theta \int_0^{2\pi} d\varphi \Big[\int_0^V dv\, K(V-v,v,\theta) f(Y'(v,\theta,\varphi), V-v, t)$$

$$- \int_0^\infty dv\, K(V,v,\theta) f(Y,V,t) \Big], \qquad Y = X - Ut\vec{e}_1$$

$$K(V,v,\theta) = \left(\frac{3}{4\pi}\right)^{\frac{2}{3}} \sin\theta\cos\theta\, G(v)(V^{\frac{1}{3}} + v^{\frac{1}{3}})^2 \qquad \text{(coagulation kernel)}$$

- Global well-posedness of the particle system with probability one for any $\phi < \phi_*$ with $\phi_* = \phi_*(v) > 0$.
- Rigorous Derivation of the lin. Smoluchowski equation as $\phi \to 0$:

Solution of the microscopic coalescence process:

$f_0 \in \mathcal{P}$. For any Borel set A of $\mathbb{R}^3 \times \mathbb{R}^+$ we define $f_\phi \in L^\infty([0,T);\mathcal{M}_+)$ as

$$\int_A f_\phi(Y,V,t)dY\,dV = \int_{\mathbb{R}^3\times\mathbb{R}^+} \mu_\phi(\{\omega\ :\ T^t_\phi(Y_0,V_0;\omega) \in A\}) f_0(Y_0,V_0)dY_0\,dV_0$$

Solutions of the equation in the sense of measures:

$f \in C([0,T];\mathcal{M}_+)$ is a weak sol. if $f_0 \in \mathcal{P}$ and $\forall\,\Psi \in C^1_c([0,T)\times\mathbb{R}^3\times[0,\infty))$

$$-\int_0^T \int_{\mathbb{R}^3\times\mathbb{R}^+} f(Y,V,t)\{\partial_t\psi(Y,V,t) + \mathcal{C}[\psi](Y,V,t)\}dYdVdt$$
$$= \int_{\mathbb{R}^3\times\mathbb{R}^+} f_0(Y,V)\psi_0(Y,V)dYdV$$

- Global well-posedness of the particle system with probability one for any $\phi < \phi_*$ with $\phi_* = \phi_*(v) > 0$.

- Rigorous Derivation of the lin. Smoluchowski equation as $\phi \to 0$:

$G \in \mathcal{M}_+(\mathbb{R}^+))$ s.t. $\displaystyle\int_0^\infty v^\gamma G(v)dv < \infty$, for $\gamma > 2$.

Let be $f_0 \in \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^+)$, $f_\phi \in L^\infty([0,T); \mathcal{M}_+(\mathbb{R}^3 \times \mathbb{R}^+))$ and $T > 0$.

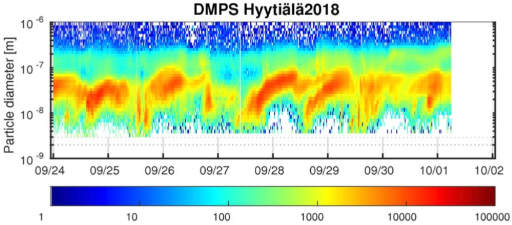
Then

$$\forall\ A \in \mathbb{R}^3 \times \mathbb{R}^+ \quad \int_A f_\phi(t) \underset{\phi \to 0}{\longrightarrow} \int_A f(t) \quad \text{uniformly in } [0,T]$$

where f is the unique weak solution of the lin. Smoluchowski eq.

[N., Velázquez CMP '17]

The Smoluchowski equation with source terms: existence and non-existence of NESS



https://wiki.helsinki.fi/display/SMEAR/Aerosol+Measurements

Smoluchowski coagulation equation with source

Motivation: aerosol dynamics in the atmosphere (sizes from $1nm$ to $100\mu m$)

- intermittent **source** of small molecules (vegetation)
- **coagulation** of molecules to produce larger particles

Rate equation (discrete):

$n_\alpha(t)$ density of clusters with size $\alpha \in \mathbb{N}_*$ at time $t \geq 0$ satisfies

$$\partial_t n_\alpha(t) = \frac{1}{2} \sum_{\beta<\alpha} K_{\alpha-\beta,\beta} n_{\alpha-\beta}(t) n_\beta(t) - n_\alpha(t) \sum_{\beta>0} K_{\alpha,\beta} n_\beta(t) + s_\alpha .$$

(Smoluchowski eq.)

Assumption: the **source term** is localized at small cluster sizes

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Rate equation (continuous):

$f(v, t)$ density of clusters of size $v \in \mathbb{R}_*$ at time $t \geq 0$ satisfies

$$\begin{aligned} \partial_t f(v,t) = \frac{1}{2} \int_0^v K(v-w,w) f(v-w,t) f(w,t) dw \\ - \int_0^\infty K(v,w) f(v,t) f(w,t) dw + \eta(v). \end{aligned}$$

(Smoluchowski eq.)

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(Smoluchowski eq.)

Allowing f and η to be positive measures we can study the continuous and discrete equations simultaneously using

$$f(v) = \sum_{\alpha=1}^\infty n_\alpha \delta(v-\alpha) \quad , \qquad \eta(v) = \sum_{\alpha=1}^\infty s_\alpha \delta(v-\alpha)$$

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(Smoluchowski eq.)

Source terms lead to nontrivial stationary solutions towards which the time-dependent solutions could be expected to evolve as $t \to \infty$.

Stationary solutions are non-equilibrium steady states

Smoluchowski coagulation equation with source

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(Smoluchowski eq.)

- Existence and properties of stationary sol. $K = 1$: [Dubovskii, Gajewski '83]
- Existence and non-existence results of stationary sol. [Laurencot 2020]

Stationary solutions (Informal)

The stationary solutions satisfy

$$0 = \frac{1}{2}\int_0^v K(v-w,w)\, f(v-w)\, f(w)\, dw - \int_0^\infty K(v,w)\, f(v)\, f(w)\, dv + \eta(v) \qquad (\star)$$

For sufficiently regular functions f $(\star)$ can be written as

$$\partial_v J(v;f) = v\eta(v) \qquad \text{where} \qquad \underbrace{J(v;f)}_{\textit{flux}} = \int_0^v dy \int_{v-w}^\infty du\, K(w,u) w f(w)\, f(u)$$

- $J(v;f)$ is constant for v sufficiently large (η compactly supported)

Constant flux solutions: solutions to $(\star)$ with $\eta \equiv 0$ satisfying

$$J(v;f) = J_0\,, \quad \text{for } v > 0 \quad (\diamond)$$

- power law solutions to $(\diamond)$: $f(v) = c_s(v)^{-\frac{(3+\gamma)}{2}}$ with $c_s > 0$
- not all the solutions to $(\diamond)$ are power laws! Indeed ....

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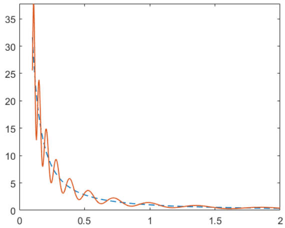
- not all the solutions to $(\diamond)$ are power laws! Indeed ....

Existence of non-power law constant flux solutions

[Ferreira, Lukkarinen, N., Velázquez, Preprint '22]

$$f(x) \simeq \frac{C_0}{x^{\frac{\gamma+3}{2}}}\left[1 + \varepsilon \cos(\alpha \log(x))\right]$$



Main questions

1. Do such stationary solutions yielding a constant flux of monomers towards clusters with large sizes exist?
2. When such stationary non-equilibrium solutions exist, can we compute the rate of formation of macroscopic (infinitely large) particles?
3. Which collisions contribute more to the transport of monomers to large clusters?
4. Atmospheric aerosols are typically constituted by different chemicals leading to multicomponent systems. Existence/non-existence of stationary solutions for multicomponent systems? Properties?

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One-component Coagulation equation with source

$$\partial_t f(v,t) = \frac{1}{2}\int_0^v K(v-w,w)\, f(v-w,t)\, f(w,t)\, dw - \int_0^\infty K(v,w)\, f(v,t)\, f(w,t)\, dw + \eta(v)$$

Assumption on the source rate:

$$\eta \in \mathcal{M}_+(\mathbb{R}_*), \quad \mathrm{supp}\ (\eta) \subset [1,L] \text{ for some } L \geq 1.$$

Assumptions on the coagulation kernel:

$$K : \mathbb{R}_* \times \mathbb{R}_* \to \mathbb{R}_+ \text{ continuous}, \quad K(v,w) = K(w,v)$$

$$K(v,w) \geq c_1 \left(v^{\gamma+\lambda} w^{-\lambda} + w^{\gamma+\lambda} v^{-\lambda} \right), \qquad \lambda, \gamma \in \mathbb{R}$$

$$K(v,w) \leq c_2 \left(v^{\gamma+\lambda} w^{-\lambda} + w^{\gamma+\lambda} v^{-\lambda} \right), \qquad 0 < c_1 \leq c_2 < \infty.$$

γ : yields the behaviour of K under the scaling of the particle size

λ : measures the relevance of coagulation events between particles of different sizes

Stationary solutions

Definition

Assume that K satisfies

$$K\left(v,w\right)\leq c_2\left(v^{\gamma+\lambda}w^{-\lambda}+w^{\gamma+\lambda}v^{-\lambda}\right)$$

We say that $f\in\mathcal{M}_+\left(\mathbb{R}_*\right)$, satisfying $f\left(0,1\right)=0$ and:

$$M_{\gamma+\lambda}+M_{-\lambda}=\int_{\mathbb{R}_*}v^{\gamma+\lambda}f\left(dv\right)+\int_{\mathbb{R}_*}v^{-\lambda}f\left(dv\right)<\infty$$

is a **stationary injection solution** if the following identity holds for any test function $\varphi\in C_c(\mathbb{R}_*)$:

$$\frac{1}{2}\int_{\mathbb{R}_*}\int_{\mathbb{R}_*}K\left(v,w\right)\left[\varphi\left(v+w\right)-\varphi\left(v\right)-\varphi\left(w\right)\right]f\left(dv\right)f\left(dw\right)$$
$$+\int_{\mathbb{R}_*}\varphi\left(v\right)\eta\left(dv\right)=0.$$

Existence and non-existence of stationary solutions

The parameters $\gamma,\ \lambda$ determine whether there exists a stationary solution

Theorem [Ferreira, Lukkarinen, N., Velázquez, ARMA '21]

- If $|\gamma + 2\lambda| < 1$ then **there exists** a stationary injection solution $f \in \mathcal{M}_+(\mathbb{R}_*)$, $f \neq 0$, in the sense of Definition.
- If $|\gamma + 2\lambda| \geq 1$ then **there is not** any stationary injection solution in the sense of Definition.

- Brownian kernel $(\gamma = 0,\ \lambda = \frac{1}{3})$ $\Rightarrow\ \gamma + 2\lambda < 1$ (existence)
- Free molecular kernel $(\gamma = \frac{1}{6},\ \lambda = \frac{1}{2})$ $\Rightarrow\ \gamma + 2\lambda > 1$ (non-existence)

Some ideas on the proof of existence

Step 1 Well posedness of the corresponding truncated time-dependent problem

$$\partial_t f(v,t) = \frac{\zeta_{R_*}(v)}{2} \int_0^v K_{R_*,\varepsilon}(v-w,w)\, f(v-w,t)\, f(w,t)\, dw - \int_0^\infty K_{R_*,\varepsilon}(v,w)\, f(v,t)\, f(w,t)\, dw + \eta(v)$$

$K_{R_*,\varepsilon}$: continuous, compactly supported, bounded kernel

Step 2 Existence of a stationary solution f_{ε,R_*} (Schauder fixed-point):

Step 3 Extension to general unbounded kernels supported in $\mathbb{R}^2$.
Uniform estimates in the cut-off parameters R_*, ε allow to remove the truncation and to obtain the existence result for the original problem.

Step 4 $|\gamma + 2\lambda| < 1$ implies the moments estimates $M_{\gamma+\lambda} + M_{-\lambda} < \infty$ and $\eta \neq 0$ implies $f \neq 0$.

Estimates

- When stationary solutions do exist ($\gamma + 2\lambda < 1$) we have

$$\boxed{\frac{C_1}{z^{(\gamma+3)/2}} \leq \frac{1}{z}\int_{[z/2,z]} f(dv) \leq \frac{C_2}{z^{(\gamma+3)/2}} \quad \text{for all } z \geq L_\eta}$$

Stationary solutions cannot decay too fast for large sizes

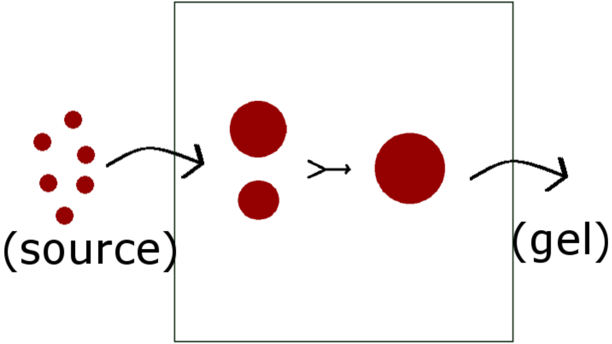
Moments estimates

- $\displaystyle\int_{\mathbb{R}_+} v^{\mu} f(dv) < \infty, \quad \text{for} \quad \mu < \frac{\gamma+1}{2},$
- $\displaystyle\int_{\mathbb{R}_+} v^{\frac{\gamma+1}{2}} f(dv) = \infty.$

$$\left(\text{the condition } \gamma + 2\lambda < 1 \text{ implies that } \max\{\gamma+\lambda, -\lambda\} < \tfrac{\gamma+1}{2}\right)$$

Physical meaning

- When stationary solutions do exist ($|\gamma + 2\lambda| < 1$) monomers are transported towards large clusters at the same rate at which monomers are added into the system.



Physical meaning

- When stationary solutions do exist ($|\gamma + 2\lambda| < 1$) monomers are transported towards large clusters at the same rate at which monomers are added into the system.

Can we compute the flux of mass at the stationary state ?

$$\underbrace{\int_{(0,R]} \int_{(R-v,\infty)} K(v,w) v f(dv) f(dw)}_{J(R)} = \int_{(0,R]} v\eta(dv) \quad R > 0$$

(the flux is constant in regions involving large clusters sizes!)

Main transport mechanism ?

The fluxes of monomers towards infinity are mostly due to collisions between clusters of comparable sizes

Physical meaning

- When stationary solutions do exist ($|\gamma + 2\lambda| < 1$) monomers are transported towards large clusters at the same rate at which monomers are added into the system.

- When stationary solutions do not exist ($|\gamma + 2\lambda| \geq 1$) the aggregation of monomers with large clusters is too fast. It cannot be compensated by the constant addition of monomers due to the injection term.

Multi-component equation:
stationary non-equilibrium solutions
and localization properties

Multicomponent coagulation equation with source

A particle/cluster may be characterized not only by its size but also by its composition (different monomer types).

Example: clusters composed of sulfuric acid and ammonia monomers

- **Discrete equation**:

  $n_\alpha(t)$ density of clusters with composition $\alpha \in \mathbb{N}^d_* := \mathbb{N}^d \setminus \{0\}$
  at time $t \geq 0$

$$\partial_t n_\alpha(t) = \frac{1}{2} \sum_{\beta < \alpha} K_{\alpha-\beta,\beta} n_{\alpha-\beta}(t) n_\beta(t) - n_\alpha(t) \sum_{\beta > 0} K_{\alpha,\beta} n_\beta(t) + s_\alpha$$

$\alpha = (\alpha_1, \alpha_2, ..., \alpha_d)$ $\quad \alpha < \beta \iff \alpha_i \leq \beta_i$ and $\alpha \neq \beta, \quad |\alpha| = \sum_{i=1}^d \alpha_i$

$s_\alpha \geq 0$ supported on a finite set of values α.

(Explicit) stationary sol. in the discrete case for $K_{\alpha,\beta} = 1, \quad K_{\alpha,\beta} = \alpha + \beta$

[Lushnikov 1976; Krapivksy and Ben-Naim, 1996]

Multicomponent coagulation equation with source

A particle/cluster may be characterized not only by its size but also by its composition (different monomer types).

Example: clusters composed of sulfuric acid and ammonia monomers

- **Multicomponent coagulation equation**:

  $f(v,t)$ density of clusters of composition $v \in \mathbb{R}^d_* := \mathbb{R}^d_+ \setminus \{\mathbf{0}\}$ at time $t \geq 0$

$$\partial_t f(v,t) = \frac{1}{2}\int_{\{0<w<v\}} K(v-w,w)f(v-w,t)f(w,t)dw - \int_{w>0} K(v,w)f(v,t)f(w,t)dw \quad + \quad \eta(v)$$

Source rate: $\eta \in \mathcal{M}_+\left(\mathbb{R}^d_*\right)$ with support in $\left\{v \in \mathbb{R}^d_* \,:\, 1 \leq |v| \leq L\right\}$, $L > 1$.

Multicomponent Coagulation equation with source

$$\partial_t f(v,t) = \frac{1}{2}\int_{\{0<w<v\}} K(v-w,w) f(v-w,t) f(w,t) dw$$
$$- \int_{w>0} K(v,w) f(v,t) f(w,t) dw \quad + \quad \eta(v)$$

Assumptions on the coagulation kernel: K continuous, $K(v,w) = K(w,v)$

$$c_1 \left(|v| + |y|\right)^{\gamma} \Phi\left(\frac{|v|}{|v|+|w|}\right) \le K(v,w) \le c_2 \left(|v|+|w|\right)^{\gamma} \Phi\left(\frac{|v|}{|v|+|w|}\right) \quad (*)$$

for $v, w \in \mathbb{R}_*^d$ with $0 < c_1 \le c_2 < \infty$ and

$$\Phi(s) = \Phi(1-s) \text{ for } 0 < s < 1 \quad , \quad \Phi(s) = \frac{1}{s^p (1-s)^p}, \quad p \in \mathbb{R}$$

(This class of kernels is strictly larger than the class of kernels considered in the case $d = 1$. Choose $p = \max\{\lambda, -(\gamma+\lambda)\}$ when $d = 1$)

Stationary injection solutions in the multicomponent case

Definition

Let $\eta \in \mathcal{M}_+\left(\mathbb{R}_*^d\right)$ with $supp(\eta) \subset \left\{v \in \mathbb{R}_*^d \,:\, 1 \leq |v| \leq L\right\}$, $L > 1$.

$f \in \mathcal{M}_+(\mathbb{R}_*^d)$ is a stat. inj. sol. if $supp(f) \subset \left\{v \in \mathbb{R}_*^d :\ |v| \geq 1\right\}$ and

$$\int_{\mathbb{R}_*^d} |v|^{\gamma+p} f(dv) < \infty$$

and

$$\begin{aligned} 0 =& \frac{1}{2}\int_{\mathbb{R}_*^d}\int_{\mathbb{R}_*^d} K(v,w)\left[\varphi(v+w)-\varphi(v)-\varphi(w)\right] f(dv)\, f(dw) \\ &+ \int_{\mathbb{R}_*^d} \varphi(v)\,\eta(dv) \qquad\quad \forall\ \varphi \in C_c^1\left(\mathbb{R}_*^d\right) \end{aligned}$$

Change of variable: $v = (r,\theta)$, $r = |v| > 0$, $\theta = \frac{v}{|v|} \in \Delta_{d-1}$, $v = r\theta$;

$$dv = \frac{r^{d-1}}{\sqrt{d}} dr \underbrace{d\tau(\theta)} = \frac{r^{d-1}}{\sqrt{d}} dr \underbrace{\sqrt{d}\, d\theta_1 d\theta_2, ... d\theta_{d-1}}; \quad f(x) = F(r,\theta)$$

Stationary injection solutions in the multicomponent case

Definition

Let $\eta \in \mathcal{M}_+\left(\mathbb{R}^d_*\right)$ with $supp(\eta) \subset \left\{v \in \mathbb{R}^d_* \,:\, 1 \leq |v| \leq L\right\}$, $L > 1$.

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$$\int_{\mathbb{R}^d_*} |v|^{\gamma+p} f(dv) < \infty$$

and

$$0 = \frac{1}{2}\int_{\mathbb{R}^d_*}\int_{\mathbb{R}^d_*} K(v,w)\left[\varphi(v+w) - \varphi(v) - \varphi(w)\right] f(dv)\, f(dw) + \int_{\mathbb{R}^d_*} \varphi(v)\,\eta(dv) \qquad \forall\, \varphi \in C^1_c\left(\mathbb{R}^d_*\right)$$

- $\gamma + 2p < 1$: **there exists** a stationary injection sol. $f \in \mathcal{M}_+\left(\mathbb{R}^d_*\right)$
- $\gamma + 2p \geq 1$: **there is not** any stationary injection solution

[Ferreira, Lukkarinen, N., Velázquez, Preprint '22]

Stationary injection solutions in the multicomponent case

Definition

Let $\eta \in \mathcal{M}_+\left(\mathbb{R}_*^d\right)$ with $supp(\eta) \subset \left\{v \in \mathbb{R}_*^d\ :\ 1 \leq |v| \leq L\right\}$, $L > 1$.

$f \in \mathcal{M}_+(\mathbb{R}_*^d)$ is a stat. inj. sol. if $supp(f) \subset \left\{v \in \mathbb{R}_*^d :\ |v| \geq 1\right\}$ and

$$\int_{\mathbb{R}_*^d} |v|^{\gamma+p} f(dv) < \infty$$

and

$$0 = \frac{1}{2}\int_{\mathbb{R}_*^d}\int_{\mathbb{R}_*^d} K(v,w)\left[\varphi(v+w) - \varphi(v) - \varphi(w)\right] f(dv)\, f(dw) + \int_{\mathbb{R}_*^d} \varphi(v)\, \eta(dv) \qquad \forall\ \varphi \in C_c^1\left(\mathbb{R}_*^d\right)$$

- Main feature:

  when stationary solutions exist, their mass concentrates for large values of the clusters size $|v|$ along a specific direction of the cone $\mathbb{R}_+^d$

  (Asymptotic localization)

Localization along a line ($K = 1$)

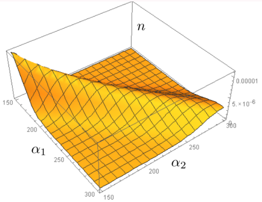
$$\partial_t n_\alpha(t) \quad = \quad \frac{1}{2}\sum_{\beta<\alpha} n_{\alpha-\beta}(t) n_\beta(t) - n_\alpha(t)\sum_{\beta>0} n_\beta(t) + \sum_{|\beta|=1} \delta_{\alpha,\beta} s_\beta,$$

A **stationary solution** is approximated for large sizes by :

$$\bar{n}_\alpha \sim \sqrt{s}(\alpha_1+\alpha_2)^{-2}\exp\left(-\frac{(\alpha_1-\alpha_2)^2}{2(\alpha_1+\alpha_2)}\right),$$

with source $s_\alpha = s \geq 0$,

$|\alpha| = 1,\ \alpha = (\alpha_1, \alpha_2)$



Tool : moments generating function

[Krapivksy and Ben-Naim, 1996]

If there is no source we also observe localization in the time-dependent solution: the localization along a diagonal is an intrinsic phenomenon of this system!

Localization for steady states and general kernels

Theorem [Ferreira, Lukkarinen, N., Velázquez, CMP '21]

Let $\gamma + 2p < 1$. Let $f \in \mathcal{M}_+\left(\mathbb{R}^d_*\right)$, $\mathbb{R}^d_* := \mathbb{R}^d_+ \setminus \{0\}$, be a stationary injection solution. Then, there exists $b \in (0,1)$ and $\delta : \mathbb{R}_* \to \mathbb{R}_+$ with $\delta(R) \underset{R\to\infty}{\longrightarrow} 0$ s.t.

$$\lim_{R\to\infty}\left(\frac{\int_{[R,R/b]} dr \int_{\Delta^{d-1}\cap\{|\theta-\theta_0|\leq\delta(R)\}} d\tau(\theta)\, F(r,\theta)}{\int_{[R,R/b]} dr \int_{\Delta^{d-1}} d\tau(\theta)\, F(r,\theta)}\right) = 1$$

where $$\theta_0 = \frac{\int_{\mathbb{R}^d_*} v\eta(v)\, dv}{\int_{\mathbb{R}^d_*} |v|\,\eta(v)\, dv} \in \Delta^{d-1}.$$

$\Big($Using $v \to (r, \theta_1, \theta_2, \ldots, \theta_{d-1})$, $r = |v|$, $\theta = \frac{v}{|v|} \in \Delta^{d-1} = \left\{\theta \in \mathbb{R}^d_* : |\theta| = 1\right\}\Big)$

- the direction θ_0 is uniquely determined from the source term η (the fluxes of monomers only depend on the injection rates!)

Localization for steady states and general kernels

Theorem [Ferreira, Lukkarinen, N., Velázquez, CMP '21]

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where
$$\theta_0 = \frac{\int_{\mathbb{R}^d_*} v\eta(v)\,dv}{\int_{\mathbb{R}^d_*} |v|\,\eta(v)\,dv} \in \Delta^{d-1} .$$

- the ratio between monomers of a given type to the total number of monomers in the cluster becomes close to a predetermined ratio as $|v| \to \infty$

Localization for steady states and general kernels

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where
$$\theta_0 = \frac{\int_{\mathbb{R}^d_*} v\eta(v)\, dv}{\int_{\mathbb{R}^d_*} |v|\, \eta(v)\, dv} \in \Delta^{d-1} .$$

- localization is a non-equilibrium property. It cannot be derived from a variational principle. It is a consequence of the coagulation mechanism
- localization is a **universal property**, specific of multicomponent systems . . .

Localization for steady states and general kernels

Theorem [Ferreira, Lukkarinen, N., Velázquez, CMP '21]

Let $\gamma + 2p < 1$. Let $f \in \mathcal{M}_+\left(\mathbb{R}^d_*\right)$, $\mathbb{R}^d_* := \mathbb{R}^d_+ \setminus \{0\}$, be a stationary injection solution. Then, there exists $b \in (0,1)$ and $\delta : \mathbb{R}_* \to \mathbb{R}_+$ with $\delta(R) \underset{R\to\infty}{\longrightarrow} 0$ s.t.

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where
$$\theta_0 = \frac{\int_{\mathbb{R}^d_*} v\eta(v)\, dv}{\int_{\mathbb{R}^d_*} |v|\,\eta(v)\, dv} \in \Delta^{d-1}\,.$$

- localization is a **universal property**, specific of multicomponent systems ...

  it can be proved that localization holds also for mass-conserving solutions !

[Ferreira, Lukkarinen, N., Velázquez, Preprint '22]

Localization for steady states and general kernels

Theorem [Ferreira, Lukkarinen, N., Velázquez, CMP '21]

Let $\gamma + 2p < 1$. Let $f \in \mathcal{M}_+\left(\mathbb{R}^d_*\right)$, $\mathbb{R}^d_* := \mathbb{R}^d_+ \setminus \{0\}$, be a stationary injection solution. Then, there exists $b \in (0,1)$ and $\delta : \mathbb{R}_* \to \mathbb{R}_+$ with $\delta(R) \underset{R\to\infty}{\longrightarrow} 0$ s.t.

$$\lim_{R\to\infty}\left(\frac{\int_{[R,R/b]} dr \int_{\Delta^{d-1}\cap\{|\theta-\theta_0|\leq\delta(R)\}} d\tau(\theta)\, F(r,\theta)}{\int_{[R,R/b]} dr \int_{\Delta^{d-1}} d\tau(\theta)\, F(r,\theta)}\right) = 1$$

where $$\theta_0 = \frac{\int_{\mathbb{R}^d_*} v\eta(v)\, dv}{\int_{\mathbb{R}^d_*} |v|\,\eta(v)\, dv} \in \Delta^{d-1}\ .$$

Strategy: growth bounds to derive estimates for a family of prob. measures

$$\lambda(\theta; R) = \frac{\int_{[R,\infty)} F(r,\theta)\, r^{\gamma+d-1} dr}{\int_{[R,\infty)\times\Delta^{d-1}} F(r,\sigma)\, r^{\gamma+d-1} dr d\tau(\sigma)}$$

A measure concentration estimate $\quad\Rightarrow\quad \lambda(\theta; R) \rightharpoonup \delta(\theta-\theta_0) \quad$ as $\quad R\to\infty$

Perspectives

- Uniqueness of stationary non-equilibrium states?
- Long-time behaviour of time-dependent solutions to coagulation systems with injection in the existence and non-existence regime: self-similarity?
- Include **fragmentation**: Coagulation–fragmentation models with source terms.
- Include other particles growth mechanism as **condensation**, i.e. growth of particles by exchange of matter with the surrounding medium.
(Example: liquid droplets in gaseous phase as in raindrops)
- Rigorous **derivation** of the coagulation equation with physically relevant kernels from particle systems in suitable scaling limits

M.A. Ferreira, J. Lukkarinen, A. Nota, J.J.L. Velàzquez, Stationary non-equilibrium solutions for coagulation systems. *Arch. Rational Mech. Anal.* **240**, 809–875 (2021)

M.A. Ferreira, J. Lukkarinen, A. Nota, J.J.L. Velàzquez, Localization in stationary non-equilibrium solutions for multicomponent coagulation systems. *Commun. Math. Phys.* **388**(1), 479–506 (2021)

M.A. Ferreira, J. Lukkarinen, A. Nota, J.J.L. Velàzquez, Multicomponent coagulation systems: existence and non-existence of stationary non-equilibrium solutions. arXiv:2103.12763 (2022)

M.A. Ferreira, J. Lukkarinen, A. Nota, J.J.L. Velàzquez, Asymptotic localization in multicomponent mass conserving coagulation equations. arXiv:2203.08076 (2022)

M.A. Ferreira, J. Lukkarinen, A. Nota, J.J.L. Velàzquez, Non-power law constant flux solutions for the Smoluchowski coagulation equation. arXiv:2207.09518 (2022)

Thank you for your attention !

Backup slides

Strategy of the proof: existence

Step 1 Well posedness of the corresponding truncated time-dependent problem

$$\partial_t f(v,t) = \frac{\zeta_{R_*}(v)}{2}\int_0^v K_{R_*,\varepsilon}(v-w,w)\, f(v-w,t)\, f(w,t)\, dw \\ - \int_0^\infty K_{R_*,\varepsilon}(v,w)\, f(v,t)\, f(w,t)\, dw + \eta(v)$$

$K_{R_*,\varepsilon}$: continuous, compactly supported, bounded kernel

$$K_{R_*,\varepsilon}(v,w) \in [a_1(\varepsilon), a_2(\varepsilon)] \quad \text{for } (v,w) \in [1, 2R_*]^2$$

$$\text{with} \quad \operatorname{supp} K_{R_*,\varepsilon} \subset [0, 4R_*], \qquad R_* > L$$

ζ_{R_*} : cut-off function

$$\zeta_{R_*}(v) = 1 \text{ for } v \in [0, R_*], \qquad \operatorname{supp} \zeta_{R_*} \subset [0, 2R_*]$$

Step 2 Existence of a stationary solution f_{ε,R_*} (Schauder fixed-point):

- continuity of the evolution semigroup $S(t)$, s.t. $f(\cdot,t) = S(t)f_0$, in the $*-$weak topology
- existence of an invariant convex set of functions for $S(t)$

$$\mathcal{U}_{M_\varepsilon} = \left\{ f \in \mathcal{M}_+(\mathbb{R}_*) : \int_{[1,2R_*]} f(dv) \le M_\varepsilon \right\}$$

Step 3 Extension to general unbounded kernels supported in $\mathbb{R}^2$ satisfying the conditions of the theorem:

- estimate independent of R_*:

$$\int_{[1,2R_*/3]} f_{\varepsilon,R_*}(dx) \leq \bar{C}_\varepsilon,$$

$$\Rightarrow \quad \exists\; f_\varepsilon \in \mathcal{M}_+(\mathbb{R}_+), \quad R_*^n \to \infty \;(n \to \infty), \quad \text{s.t.}$$

$$f_{\varepsilon,R_*^n} \rightharpoonup f_\varepsilon \text{ in the } * \text{-weak topology}$$

- estimate independent of ε:

$$\int_{[1,\infty)} f_\varepsilon(dx) \leq \bar{C},$$

$$\Rightarrow \quad \exists\; f \in \mathcal{M}_+(\mathbb{R}_+), \quad \varepsilon_n \to 0 \;(n \to \infty), \quad \text{s.t.}$$

$$f_{\varepsilon_n} \rightharpoonup f \quad \text{in the } * \text{-weak topology}$$

Step 4 $|\gamma + 2\lambda| < 1$ implies the moments estimates $M_{\gamma+\lambda} + M_{-\lambda} < \infty$ and $\eta \neq 0$ implies $f \neq 0$.

Strategy of the proof: non-existence (by contradiction)

Step 1 Suppose that $f \in \mathcal{M}_+(\mathbb{R}_+)$ is a stationary solution in the sense of Definition satisfying $M_{\gamma+\lambda} < \infty$.

Step 2 Function J: $$J(R) = J_1(R) + J_2(R)$$

$$J_k(R) = \iint_{\Sigma_R \cap D_\delta^{(k)}} [K(x,y)x] f(dx) f(dy), \quad k = 1,2$$

$$\Sigma_R = \{x \geq 1,\ y \geq 1 : x + y > R,\ x \leq R\}$$

$$D_\delta^{(1)} = \{x \geq 1,\ y \geq 1 : y \leq \delta x\}$$

$$D_\delta^{(2)} = \{x \geq 1,\ y \geq 1 : y > \delta x\}$$

Step 3 Contribution of J_2 vanishes as $R \to \infty$:

$$\lim_{R\to\infty} J_2(R) = 0 \quad \Rightarrow \quad \lim_{R\to\infty} J_1(R) = \lim_{R\to\infty} J(R) = J(L)$$

Step 4 Using bounds for K:

$$\liminf_{R\to\infty}\left(R^{\gamma+\lambda+1}\iint_{\Sigma_R\cap D_\delta^{(1)}} y^{-\lambda} f\left(dx\right) f\left(dy\right)\right) \geq \frac{J\left(L_\eta\right)}{c_2\left(1+\delta^{|\gamma+2\lambda|}\right)} =: C_1$$

Step 5 Define

$$F(R) := \int_{(R,\infty)} f(dx)\,, \quad \gamma+\lambda \geq 0$$
$$F(R) := \int_{[1,R]} f(dx)\,, \quad \gamma+\lambda < 0$$

Then there is R_0 such that

$$-\int_{[1,\delta R]}\left[F\left(R-y\right)-F\left(R\right)\right] y^{-\lambda} f\left(dy\right) \leq -\frac{C_1}{2}\frac{1}{R^{\gamma+\lambda+1}} \text{ for } R \geq R_0.$$

Step 6 Contradiction since then

$$M_{\gamma+\lambda} \geq \int_{[R_0,\infty)} x^{\gamma+\lambda} f(dx) = \infty.$$

Decay estimates for “inverse fractional Laplacian”

Lemma

Let a and b be constants satisfying $a > 0$ and $a - b \geq 1$. Let $F : \mathbb{R}_* \to \mathbb{R}$ be a right-continuous non-increasing function with $F \geq 0$. Assume that $f \in \mathcal{M}_+(\mathbb{R}_*)$ satisfies $f \neq 0$ and

$$\int_{[1,\infty)} x^a f(dv) < \infty$$

Suppose that there is δ such that $0 < \delta < 1$ and the following inequality holds for some $R_0 > 1/\delta$ and $C > 0$:

$$-\int_{[1,\delta R]} [F(R-y) - F(R)]\, y^b f(dy) \leq -\frac{C}{R^{a+1}} \quad \text{for } R \geq R_0$$

Then there is a constant $B > 0$ such that

$$F(R) \geq \frac{B}{R^a} \quad \text{for} \quad R \geq R_0$$

A measure concentration estimate

Lemma

There is a constant $C_d > 0$ which depends only on the dimension $d \geq 1$ and for which the following alternative holds.
Suppose a Borel probability measure $\lambda \in \mathcal{M}_{+,b}\left(\Delta^{d-1}\right)$ and parameters $\varepsilon, \delta \in (0,1)$ are given.
Then at least one of the following alternatives is true:

(i) *There exists a measurable set $A \subset \Delta^{d-1}$ with $\operatorname{diam}(A) \leq \varepsilon$ such that $\int_A \lambda(d\theta) > 1 - \delta$.*

(ii) $\int_{\Delta^{d-1}} \lambda(d\theta) \int_{\Delta^{d-1}} \lambda(d\sigma) \left\|\theta - \sigma\right\|^2 \geq C_d \delta \varepsilon^{d+1}$.

Define $\lambda(\theta; R) d\tau(\theta) \in \mathcal{M}_{+,b}\left(\Delta^{d-1}\right)$ via the formula

$$\lambda(\theta; R) = \frac{\int_{[R,\infty)} F(r,\theta) r^{\gamma+d-1} dr}{\int_{[R,\infty)\times\Delta^{d-1}} F(r,\sigma) r^{\gamma+d-1} dr d\tau(\sigma)}$$