

# Coagulation-Fragmentation Models

A (very) brief introduction

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# Coagulation-Fragmentation Models

Lecture 1. Generalities. Existence of solutions via weak  $L^1$  methods

Lecture 2. Aspects of long-time behaviour: phase transitions

Lecture 3. Further aspects of long-time behaviour



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Lecture 2. Aspects of long-time behaviour: phase transitions

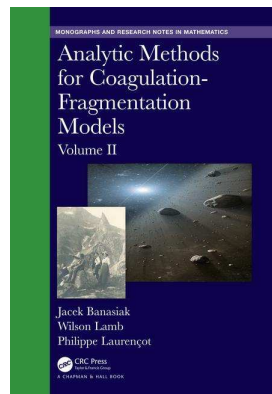
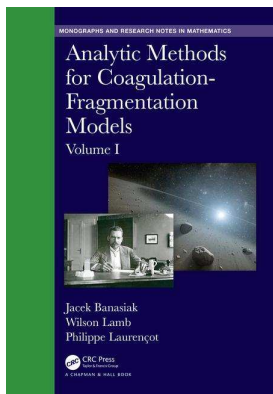
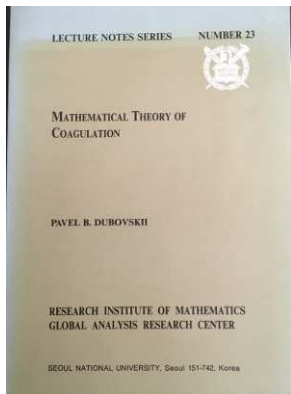
Lecture 3. Further aspects of long-time behaviour



## Some recent mathematical reviews

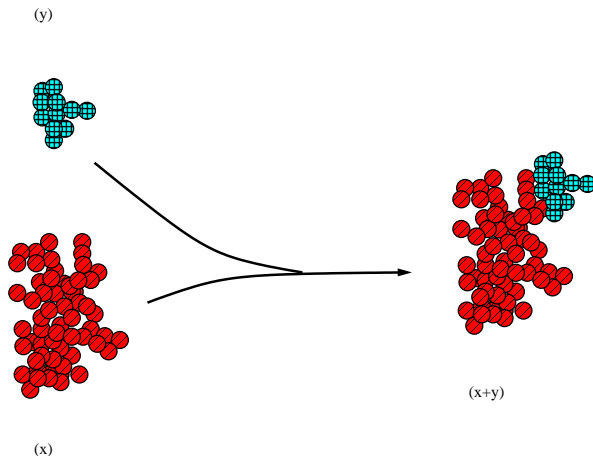
- Ph. Laurençot, S. Mischler, *On Coalescence Equations and Related Models*, in: P. Degond et al (Eds.): *Modelling and Computational Methods for Kinetic Equations*, Birkhäuser, 2004, pp. 321–356.
- R. L. Pego, *Lectures on dynamics in Models of Coarsening and Coagulation*, in: W. Bao, J.-G. Liu (Eds.): *Dynamics in Models of Coarsening, Coagulation, Condensation and Quantization*; Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, vol. 9, World Scientific, 2007, pp. 1–61.
- F.P. da Costa, *Mathematical Aspects of Coagulation-Fragmentation Equations*, in: J.-P. Bourguignon et al (Eds.): *Mathematics of Planet Earth: Energy and Climate Change*, Springer, 2015. pp. 83–162.
- Ph. Laurençot, *Weak Compactness Techniques and Coagulation Equations*, in: J. Banasiak, M. Mokhtar-Kharroubi (Eds.): *Evolutionary Equations with Applications in Natural Sciences*, LNM 2126, Springer, 2015. pp. 199–253.

# Books on mathematical aspects



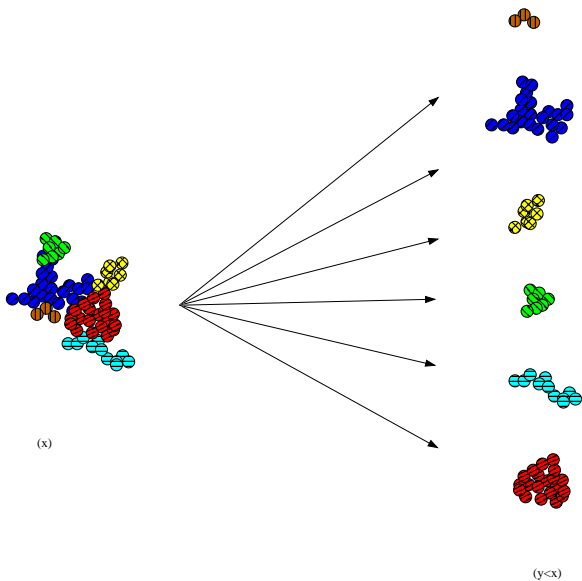
## The “physical” processes

Coagulation-fragmentation systems are models for the kinetics of cluster growth through processes of **coagulation**



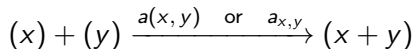
and...

# ... fragmentation



## A mathematical model

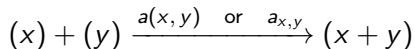
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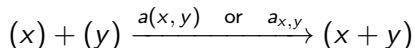


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$c_x(t)$  Concentration of clusters of “size”  $x \in \mathbb{N}^+$  at time  $t$ .

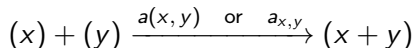
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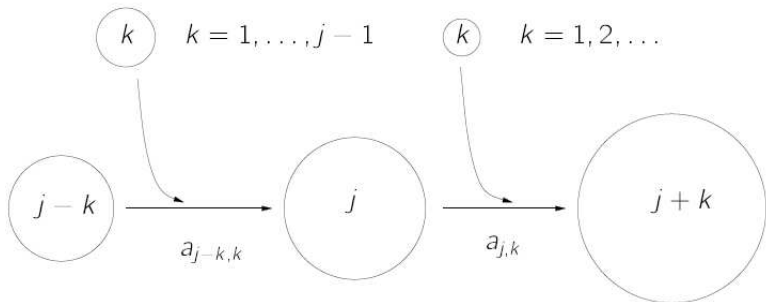
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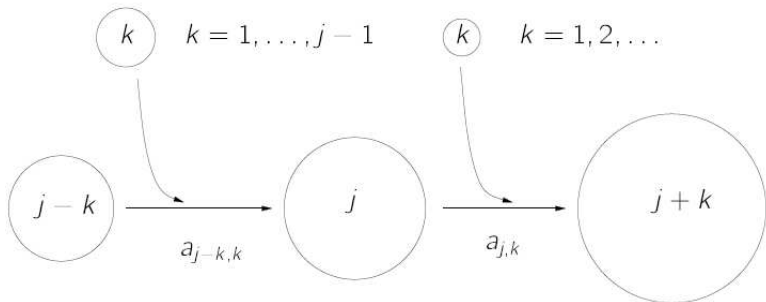
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The “mass action law” of chemical kinetics tells us that for the above reaction scheme the rate of change of  $c_x(t)$  or of  $c(x, t)$  is proportional to the product of the concentrations of the species involved in the reaction, with proportionality coefficient  $a$ .

Considering all coagulation contributions to the the evolution of  $j$ -clusters



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the corresponding differential equations system is

$$\frac{d}{dt}c_j = \frac{1}{2} \sum_{k=1}^{j-1} a_{j-k,k} c_{j-k} c_k - c_j \sum_{k=1}^{\infty} a_{j,k} c_k \quad (1)$$

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$$(x) \xrightarrow{b(x-y, y) \text{ or } b_{x-y, y}} (x-y) + (y).$$

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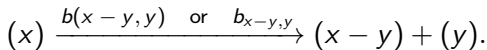
$$(x) \xrightarrow{b(x-y, y) \text{ or } b_{x-y, y}} (x-y) + (y).$$

Again using the mass action law and collecting together all the coagulation *and* the (binary) fragmentation contributions we obtain the **coagulation-fragmentation** system

$$\frac{d}{dt}c_x = \frac{1}{2} \sum_{y=1}^{x-1} (a_{x-y, y} c_{x-y} c_y - b_{x-y, y} c_x) - \sum_{y=1}^{\infty} (a_{x, y} c_x c_y - b_{x, y} c_{x+y})$$



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or

$$\begin{aligned} \frac{\partial}{\partial t}c(x, t) &= \frac{1}{2} \int_0^x (a(x-y, y)c(x-y, t)c(y, t) - b(x-y, y)c(x, t)) dy \\ &\quad - \int_0^{\infty} (a(x, y)c(x, t)c(y, t) - b(x, y)c(x+y, t)) dy. \end{aligned}$$



## Existence of solutions for the continuous Smoluchowski coagulation equation

$$\frac{\partial}{\partial t} c(x, t) = \frac{1}{2} \int_0^x a(x-y, y) c(x-y, t) c(y, t) dy - c(x, t) \int_0^\infty a(x, y) c(y, t) dy.$$

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From this one obtains the “natural” functional space to work in:



- $L_1^1(0, \infty) := \left\{ f \in L^1(0, \infty) : \|f\|_{1,1} := \int_0^\infty (1+x)|f(x)|dx < \infty \right\}$

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With this functional setting it is a natural idea to try to apply a version of the **Picard-Lindelöf** theorem:

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With this functional setting it is a natural idea to try to apply a version of the **Picard-Lindelöf** theorem:

### Theorem

If  $Q : E \rightarrow E$  is a locally Lipschitz function in a Banach space  $E$  and if  $c_0 \in E$ , then there exists a unique maximal solution  $c \in C^1([0, T_*); E)$  to the initial value problem

$$\begin{cases} \frac{dc}{dt} = Q(c) \\ c(0) = c_0 \end{cases}$$

and either  $T_* = \infty$ , or  $T_* < \infty$  and  $\lim_{t \rightarrow T_*} \|c(t)\| = \infty$ .

- The approach based on the **Picard-Lindelöf** theorem is not trivial but it is possible to implement if the coagulation kernel is **bounded**  
 $0 \leq a(x, y) \leq \kappa_0$ .

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- Unbounded kernels are important in applications; e.g.:

$$a(x, y) = \kappa(1 + x)(1 + y),$$

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- 3 prove that  $c(x, t)$  solves the original Cauchy problem for the unbounded kernel.



## (1) Existence of solutions for bounded kernels

$$\frac{\partial c(x, t)}{\partial t} = \underbrace{\frac{1}{2} \int_0^x a(x-y, y) c(x-y, t) c(y, t) dy}_{=: Q_1(c)(x, t)} - \underbrace{c(x, t) \int_0^\infty a(x, y) c(y, t) dy}_{=: Q_2(c)(x, t)}. \quad (2)$$

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### Theorem

Let  $0 \leq a(x, y) = a(y, x) \leq \kappa_0$ ,  $c_0 \in L^1(0, \infty)$ ,  $c_0 \geq 0$  a.e. in  $(0, \infty)$ .

Then,  $\exists^1 c \in C^1([0, \infty); L^1(0, \infty))$  such that  $c$  is a solution of the coagulation equation (2) with initial condition  $c(\cdot, 0) = c_0$ , and  $c(x, t) \geq 0$  a.e.  $x$ , and  $\|c(\cdot, t)\|_1 \leq \|c_0\|_1$ ,  $\forall t \geq 0$ .

Furthermore, if  $c_0 \in L^1_1(0, \infty)$ , then  $c(\cdot, t) \in L^1_1(0, \infty)$  and  $M_1(c) = M_1(c_0)$ , where  $M_1(f) := \int_0^\infty xf(x)dx$ .

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Let us see some of the arguments:

For (a) we need to prove that  $Q_1$  and  $Q_2$  are locally Lipschitz functions from  $L^1(0, \infty)$  to  $L^1(0, \infty)$ .

For  $Q_1$  we have...



## (1) Existence of solutions for bounded kernels

$$\begin{aligned}\|Q_1(c) - Q_1(d)\|_1 &= \\ &= \frac{1}{2} \int_0^\infty \left| \int_0^x a(x-y, y) (c(x-y)c(y) - d(x-y)d(y)) dy \right| dx \\ &\leq \frac{1}{2} \int_0^\infty \int_0^x a(x-y, y) |c(x-y)c(y) - d(x-y)d(y)| dy dx \\ &\leq \frac{1}{2} \kappa_0 \int_0^\infty \int_0^x |c(x-y)c(y) - d(x-y)d(y)| dy dx \\ &\leq \frac{1}{2} \kappa_0 (\|c\|_1 + \|d\|_1) \|c - d\|_1\end{aligned}$$

... and analogously for  $Q_2$ .

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Applying Picard-Lindelöf theorem we conclude the existence of a unique local solution defined on some interval  $[0, T_{\max})$ , and belonging to  $C^1([0, T_{\max}); L^1(0, \infty))$ .

[Note that *no* positivity has been asserted so far!]



## (1) Existence of solutions for bounded kernels

To prove positivity, consider the system

$$\frac{dc}{dt} = Q_1(c)_+ - Q_2(c), \quad (3)$$

where  $r_+ := \max\{r, 0\}$ .

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From

$$\frac{d}{dt}(-c)_+ = -\text{sign}_+(-c) \frac{dc}{dt}$$

we conclude that

$$\begin{aligned} \frac{d}{dt}(-c)_+ &= -\text{sign}_+(-c)(Q_1(c)_+ - Q_2(c)) \leq \text{sign}_+(-c)Q_2(c) \\ &= (-c)_+ \int_0^\infty a(\cdot, y)c(y, t)dy \end{aligned}$$



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Hence  $c_0 \geq 0 \Rightarrow (-c_0)_+ = 0 \Rightarrow (-c)_+ \equiv 0 \Rightarrow c(x, t) \geq 0, \forall x > 0, t \geq 0$ .

Furthermore,  $c \geq 0 \Rightarrow Q_1(c)_+ = Q_1(c)$ , and thus  $c$  is also a solution of

$$\frac{dc}{dt} = Q_1(c) - Q_2(c), \text{ with } c(0) = c_0 \geq 0.$$

By uniqueness (due to Picard-Lindelöf) we conclude that all solutions with nonnegative initial condition are nonnegative.



## (1) Existence of solutions for bounded kernels

By Fubini's theorem we get the following *a priori* estimate

$$\frac{d}{dt} \|c(\cdot, t)\|_1 = -\frac{1}{2} \int_0^\infty \int_0^\infty a(x, y) c(x, t) c(y, t) dy dx \leq 0$$

which ensures the solution is globally defined, i.e., it is defined in  $[0, \infty)$ .

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Again by Fubini's theorem,  $\forall \theta \in L^\infty(0, \infty)$ ,

$$\frac{d}{dt} \int_0^\infty \theta(x) c(x, t) dx = \frac{1}{2} \int_0^\infty \int_0^\infty \tilde{\theta}(x, y) a(x, y) c(x, t) c(y, t) dy dx$$

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## (1) Existence of solutions for bounded kernels

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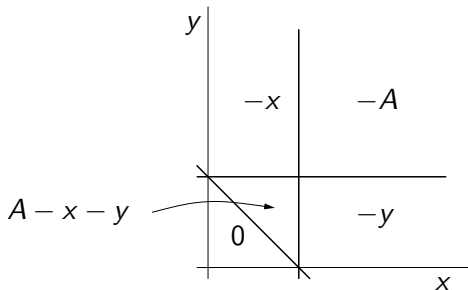
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The technique to handle this problem is typical in coagulation-fragmentation problems:

- truncate the function: use  $\theta_A(x) = \min\{\theta(x), A\}$  instead of  $\theta(x)$ ;
- decompose  $\mathbb{R}^+ \times \mathbb{R}^+$  into subsets adapted to the function  $\tilde{\theta}_A$ ;



- estimate the integrals in each of the subsets separately;
- take the limit  $A \rightarrow \infty$  using an appropriate limit theorem (e.g.: Fatou, dominated convergence, etc.)

## (2) Passing to the limit in a sequence of truncated solutions

### The problem

Let  $(c_n(x, t))$  a sequence of solutions to equations with bounded kernels  
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Now what?



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What can go wrong with a sequence in  $L^1$ ?



What can prevent an  $L^1$  bounded sequence to be weakly convergent ?

- **Concentration.** Example:  $f_n(x) = n^p f(nx)$  with  $f \in C^\infty(\mathbb{R}^p)$ ,  $f \geq 0$ ,  $\text{supp} f \subset B_1(0)$ , and  $\|f\|_1 = 1$ .
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## Dunford-Pettis Theorem

Let  $\mathcal{F} \subset L^1(\Omega)$ . Then (i)  $\Leftrightarrow$  (ii), where:

- (i)  $\mathcal{F}$  is relatively weakly sequentially compact in  $L^1(\Omega)$ .
- (ii)  $\mathcal{F}$  is bounded and

$$\eta(\mathcal{F}) := \inf_{\varepsilon > 0} \sup \left\{ \int_A |f| d\mu : f \in \mathcal{F}, A \in \mathcal{B}, \mu(A) \leq \varepsilon \right\} = 0$$

and  $\forall \varepsilon > 0, \exists \Omega_\varepsilon \in \mathcal{B}$  such that  $\mu(\Omega_\varepsilon) < \infty$  and

$$\sup_{f \in \mathcal{F}} \int_{\Omega \setminus \Omega_\varepsilon} |f| d\mu \leq \varepsilon.$$

Back to the sequence  $(c_n(\cdot, t)) \in L^1$ .

The second condition in (ii) of the Dunford-Pettis theorem is easy to get from the *a priori* bound  $M_1(c_n(\cdot, t)) \leq M_1(c_0)$ :

$$\begin{aligned}\int_R^\infty c_n(x, t) dx &= \int_R^\infty \frac{1}{x} x c_n(x, t) dx \\ &\leq \frac{1}{R} \int_R^\infty x c_n(x, t) dx \\ &\leq \frac{1}{R} M_1(c_n(t)) \\ &\leq \frac{1}{R} M_1(c_0) \longrightarrow 0 \quad \text{as } R \rightarrow \infty.\end{aligned}$$

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The uniform integrability condition  $\eta(\mathcal{F}) = 0$  in (ii) is more tricky. It is obtained by a version of the de la Vallée Poussin theorem:



Back to the sequence  $(c_n(\cdot, t)) \in L^1$ .

## de la Vallée Poussin Theorem

Let  $\mathcal{F} \subset L^1(\Omega)$ . Then (a)  $\Leftrightarrow$  (b), where:

(a)  $\mathcal{F}$  is uniformly integrable (i.e.,  $\eta(\mathcal{F}) = 0$ ).

(b)  $\mathcal{F}$  is bounded and there exists  $\Phi \in \mathcal{C}_{VP\infty}$  such that

$$\sup_{f \in \mathcal{F}} \int_{\Omega} \Phi(|f|) d\mu < \infty.$$

where  $\mathcal{C}_{VP\infty}$  is the set of convex functions  $\Phi \in C^\infty([0, \infty))$  such that  $\Phi'$  is concave,  $\Phi(0) = \Phi'(0) = 0$ ,  $\Phi'(x) > 0$  for  $x > 0$ , and

$$\lim_{x \rightarrow \infty} \frac{\Phi(x)}{x} = \lim_{x \rightarrow \infty} \Phi'(x) = \infty.$$

Without these last conditions the set of functions is called  $\mathcal{C}_{VP}$ .



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Now, given  $c_0 \in L^1$ , it's obvious that  $\mathcal{F} = \{c_0\}$  is uniformly integrable, and the de la Vallée Poussin theorem guarantees the existence of  $\Phi \in \mathcal{C}_{VP\infty}$  such that  $\Phi(|c_0|) \in L^1$ .

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Differentiating  $\int_0^R \Phi(c_n(x, t)) dx$  it is not difficult to prove that

$$\int_0^R \Phi(c_n(x, t)) dx \leq \|\Phi(c_0)\|_1 e^{C_1(R)t}.$$

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Hence, the Dunford-Pettis theorem applied to  $\{c_n(\cdot, t)\}$  imply the existence of a subsequence weakly convergent in  $L^1(0, \infty)$ .



Back to the sequence  $(c_n(\cdot, t)) \in L^1$ .

To proceed, we now need to make assumptions on the growth of  $a(x, y)$ .

Let us assume that  $a(x, y) = a(y, x) \leq \kappa(1 + x)(1 + y)$  and

$$\omega_R(y) := \sup_{x \in (0, R)} \frac{a(x, y)}{y} \rightarrow 0 \text{ as } y \rightarrow \infty.$$

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Then,

$$\begin{aligned} \|\partial_t c_n(x, t)\|_1 &= \int_0^\infty |\partial_t c_n(x, t)| dx \\ &\leq \int_0^\infty Q_1(c_n)(x, t) dx + \int_0^\infty Q_2(c_n)(x, t) dx \\ &\leq \frac{3\kappa}{2} \int_0^\infty \int_0^\infty (1+x)(1+y) c_n(x, t) c_n(y, t) dy dx \\ &= \frac{3\kappa}{2} \|c_n(\cdot, t)\|_{1,1}^2 \leq \frac{3\kappa}{2} \|c_0\|_{1,1}^2 =: C_2(\kappa, c_0) \end{aligned}$$



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And hence  $\forall n \geq 1, \|c_n(\cdot, t) - c_n(\cdot, s)\|_1 \leq C_2 |t - s|$ .



## Passing to the limit $n \rightarrow \infty$ in a subsequence

We now have:

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Thus, an appropriate version of the Ascoli-Arzelà theorem implies that:

- there exists a subsequence of  $(c_n(\cdot, t))$  and  $c \in \mathcal{C}([0, T]; w-L^1(0, \infty))$  such that

$$c_n(\cdot, t) \longrightarrow c \quad \text{in } \mathcal{C}([0, T]; w-L^1(0, \infty)), \quad \forall T > 0.$$

Is this limit function  $c$  a (weak) solution to the (limit=untruncated=original) coagulation system?



## The equation solved by the limit function $c(x, t)$

We can now prove that, under appropriate conditions, the limit function  $c(x, t)$  is a *weak solution* of the coagulation equation:

### Theorem

Assume  $a(x, y) = a(y, x) \leq \kappa(1+x)(1+y)$  and

$\omega_R(y) := \sup_{x \in (0, R)} \frac{a(x, y)}{y} \rightarrow 0$  as  $y \rightarrow \infty$ . Let  $c_0 \in L^1_1(0, \infty)$  and  $c_0 \geq 0$

a.e. in  $(0, \infty)$ . Then,  $\forall t > 0, \forall \theta \in L^\infty(0, \infty), \exists c \geq 0$  a.e. such that

$$c \in \mathcal{C}([0, \infty); L^1(0, \infty)) \cap L^\infty(0, \infty; L^1_1(0, \infty)),$$

and

$$\int_0^\infty \theta(x)(c(x, t) - c_0(x)) dx = \frac{1}{2} \int_0^t \int_0^\infty \int_0^\infty \tilde{\theta}(x, y) a(x, y) c(x, s) c(y, s) dy dx ds.$$

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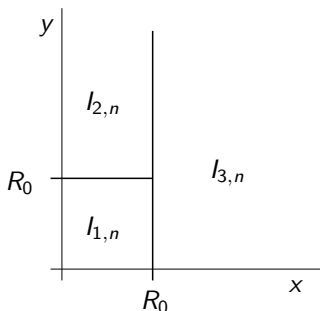
The equation solved by the limit function  $c(x, t)$

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- 1 consider first  $\theta \in L^\infty$  with compact support  $\text{supp}\theta \subset (0, R_0)$ .
- 2 split the triple integral in the rhs as the sum of 3 integrals, corresponding to the decomposition of  $\mathbb{R}^+ \times \mathbb{R}^+$  in the rectangles shown:



## The equation solved by the limit function $c(x, t)$

- 1 The triple integral in the rhs is the sum of

$$I_{1,n}(t) = \int_0^t \int_0^{R_0} \int_0^{R_0} \tilde{\theta}(x, y) a_n(x, y) c_n(x, s) c_n(y, s) dy dx ds.$$

$$I_{2,n}(t) = - \int_0^t \int_0^{R_0} \int_{R_0}^{\infty} \theta(x) a_n(x, y) c_n(x, s) c_n(y, s) dy dx ds.$$

$$I_{3,n}(t) = - \int_0^t \int_{R_0}^{\infty} \int_0^{\infty} \theta(y) a_n(x, y) c_n(x, s) c_n(y, s) dy dx ds.$$

- 2 use the uniform *a priori* bounds on  $M_0(c_n)$  and  $M_1(c_n)$ , the assumptions on  $a(x, y)$ , and Vitali's theorem ("weak- $L^1$  + pointwise convergence = strong  $L^1$  convergence") to pass to the limit  $n \rightarrow \infty$  (in a convenient subsequence. . .) in  $I_{j,n}$  for each  $j$ .
- 3 use a density argument to get the result for arbitrary  $\theta \in L^\infty$ .



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  - ▶ further regularity whenever possible.
- This general approach is, of course, also used in many studies of PDEs!

to be continued. . .

# Coagulation-Fragmentation Models

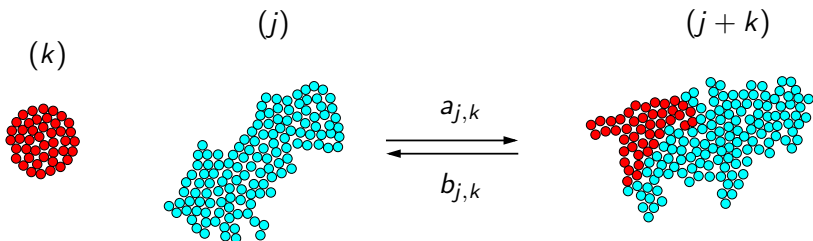
Lecture 1. Generalities. Existence of solutions via weak  $L^1$  methods

Lecture 2. Aspects of long-time behaviour: phase transitions

Lecture 3. Further aspects of long-time behaviour



We will consider the *discrete* coagulation-fragmentation process:



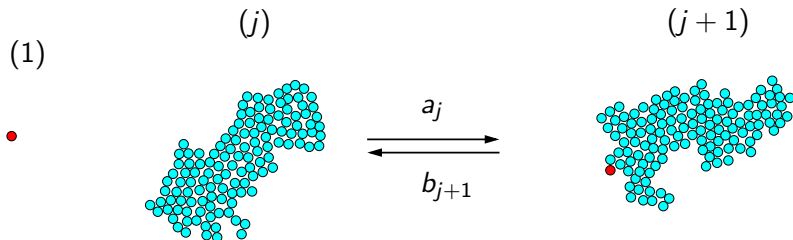
modelled by the system:

$$\frac{dc_j}{dt} = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k}(c) - \sum_{k=1}^{\infty} W_{j,k}(c) \quad (4)$$

where

$$W_{j,k}(c) := a_{j,k}c_jc_k - b_{j,k}c_{j+k}.$$

We will also consider the special case of the Becker-Döring model:



modelled by the system:

$$\begin{cases} \frac{dc_j}{dt} = \widetilde{W}_{j-1}(c) - \widetilde{W}_j(c), & j \geq 2 \\ \frac{dc_1}{dt} = -\widetilde{W}_1 - \sum_{j=1}^{\infty} \widetilde{W}_j(c) \end{cases} \quad (5)$$

where

$$\widetilde{W}_j(c) := a_j c_j c_1 - b_{j+1} c_{j+1}.$$

- We shall consider the following subspaces of  $\ell^1$ :

$$X_p := \left\{ c = (c_j) \in \mathbb{R}^{\mathbb{N}^+} : \|c\|_p = \sum_{j=1}^{\infty} j^p |c_j| < \infty \right\}, \quad \text{with } p \geq 0.$$

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- Basic assumptions on the rate coefficients:

- ▶ *growth type* assumptions, e.g.:

$$0 \leq a_j \leq j^\alpha, \quad \alpha \in [0, 1];$$

- ▶ *structural type* assumptions, e.g.: the *detailed balace assumption*:

$$\exists(Q_j) : Q_1 = 1, \quad a_j Q_j Q_1 = b_{j+1} Q_{j+1}.$$



## Definition of a (mild) solution of the Becker-Döring system

### Definition

A (mild) solution of the Becker-Döring system on  $[0, T)$  is a function  $c = (c_j) : [0, T) \rightarrow X_1$  such that:

- 1  $c_j \geq 0, \quad \forall j;$
- 2  $c_j : [0, T) \rightarrow \mathbb{R}^+$  is continuous and  $\sup_{t \in [0, T)} \|c(t)\|_1 < \infty;$
- 3  $\int_0^t \sum_{j=1}^{\infty} a_j c_j < \infty, \quad \int_0^t \sum_{j=1}^{\infty} b_{j+1} c_j < \infty, \quad \forall t \in [0, T);$

4

$$c_j(t) = c_j(0) + \int_0^t \left( \widetilde{W}_{j-1}(c(s)) - \widetilde{W}_j(c(s)) \right) ds,$$

$$c_1(t) = c_1(0) - \int_0^t \left( \widetilde{W}_1(c(s)) + \sum_{j=1}^{\infty} \widetilde{W}_j(c(s)) \right) ds$$

## On solutions to the Becker-Döring system

Under physically reasonable conditions, such as

$$0 \leq a_j \leq Kj, \quad 0 \leq b_j \leq Bj, \quad c(0) \in X_{1+\varepsilon}^+ := X_{1+\varepsilon} \cap \{c \geq 0\}$$

or

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one can prove existence and uniqueness of global (i.e., defined in  $[0, \infty)$ ) solution, and also density conservation (i.e.,  $\|c(t)\|_1 = \|c(0)\|_1, \forall t > 0$ .)

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one can prove existence and uniqueness of global (i.e., defined in  $[0, \infty)$ ) solution, and also density conservation (i.e.,  $\|c(t)\|_1 = \|c(0)\|_1, \forall t > 0$ .)

Assume the *detailed balance* condition:

$$\exists(Q_j) : \quad Q_1 = 1, \quad a_j Q_j Q_1 = b_{j+1} Q_{j+1}.$$

Then,

$$c^{\text{eq}} = (c_j^{\text{eq}}), \quad \text{with} \quad c_j^{\text{eq}} = Q_j z^j$$

is a formal equilibrium solution (i.e.,  $\widetilde{W}_j(c^{\text{eq}}) = 0, \forall j$ ) of (5).



## Equilibria of the Becker-Döring system

For a formal equilibrium to be really an equilibrium of (5) we must have

$$c^{\text{eq}} \in X_1 \quad \iff \quad \sum_{j=1}^{\infty} j Q_j z^j < \infty$$

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Assume  $z_s \neq 0$ . Define the *critical density*  $\rho_s := \sup_{[0, z_s)} F(z)$ .

$$\begin{cases} z_s = \infty \Rightarrow \rho_s = \infty \\ z_s < \infty \Rightarrow \rho_s \in (0, \infty], \text{ and if } \rho_s \neq \infty \text{ then } \rho_s = F(z_s) \end{cases}$$



## Equilibria of the Becker-Döring system

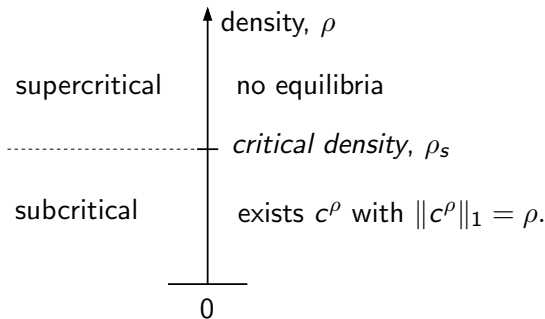
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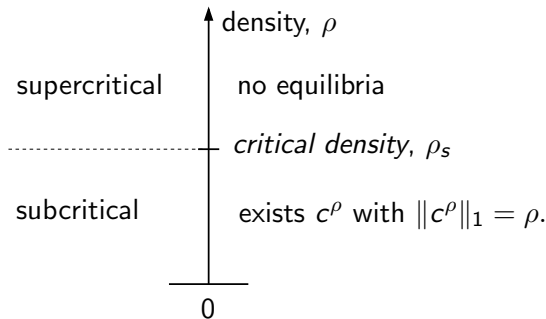


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This looks like a phase transition of *condensation type*:

“Subcritical”  $\Leftrightarrow$  “subsaturated vapor”

“Supercritical”  $\Leftrightarrow$  “supersaturated vapor”



## Dynamic phase transition

The dynamics of the Becker-Döring system is very interesting.

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Under appropriate assumptions (such as those stated previously) we have

### Dynamic phase transition behaviour

Let  $z_s = \infty$  (hence also  $\rho_s = \infty$ ).

Then  $c(t) \rightarrow c^{\rho_0}$  strongly in  $X_1$ , where  $c^{\rho_0}$  is the unique equilibrium solution of (5) with  $\|c^{\rho_0}\|_1 = \rho_0$ , and  $\rho_0 := \|c(0)\|_1$ .

Let  $\rho_s \in (0, \infty)$ .

Let  $\rho_0$  be the density of the initial condition, let  $c^{\rho_0}$  be as above, and  $c^{\rho_s}$  be the unique equilibrium solution with critical density  $\rho_s$ . Then:

- 1 if  $\rho_0 \in [0, \rho_s]$ , then  $c(t) \rightarrow c^{\rho_0}$  strongly in  $X_1$ ;
- 2 if  $\rho_0 > \rho_s$ , then  $c(t) \xrightarrow{*} c^{\rho_s}$ , but *not* strongly, in  $X_1$ .

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This is essentially the great result in the 1986 Becker-Döring paper by John Ball, Jack Carr, and Oliver Penrose.



## Dynamic phase transition

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For (4) there is a crucial distinction between “strong” and “weak” fragmentation coefficients (given the coagulation ones, which typically are at most bilinear, like  $a_{j,k} \leq C \cdot (j + k)$ ,  $a_{j,k} \leq C \cdot (jk)$ , or  $a_{j,k} \leq C \cdot (j^\alpha k^\beta + j^\beta k^\alpha)$  with  $\alpha + \beta \leq 1$ , etc.).

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Let us see the main distinction between these two classes.

A *strong enough fragmentation* (when compared with the coagulation coefficients) regularizes the solution, relative to the space where  $c(0)$  is given. Since  $X_\mu \stackrel{c}{\subset} X_\nu$  when  $\mu > \nu$ , the regularization provides a priori bounds and pre-compactness of orbits.



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Let us state the result.



### Long time behaviour under a strong fragmentation condition

Assume:

- $a_{j,k} = a_{k,j} \geq 0$ ,  $b_{j,k} = b_{k,j} \geq 0, \forall j, k$ , and  $a_{1,j}, b_{1,j} > 0, \forall j$ ;
- $a_{j,k} \leq C \cdot (j^\alpha + k^\alpha)$  [or  $a_{j,k} \leq C \cdot (jk)^\alpha$ ],  $\alpha \leq 1$ ;
- $\sum_{j=1}^{\lfloor r-1/2 \rfloor} j^\mu b_{j,r-j} > C_f(\mu) r^{\gamma+\mu}$ , for  $\gamma > \alpha$ ;
- $\liminf Q_j^{1/j^q} > 0$  for some  $q \geq 1$ .

Then:

For every  $\rho \geq 0$  there exists  $c^\rho$ , an equilibrium solution with  $\|c^\rho\|_1 = \rho$ , such that, for every  $c_0 \in X_1^+$  with  $\|c_0\|_1 = \rho$ , the unique solution of (4) with constant density satisfies  $\|c(t) - c^\rho\|_m \rightarrow 0$  as  $t \rightarrow \infty, \forall m \geq 1$ .

## Main ideas and sketch of proof

- Consider the  $N$ -truncated coagulation-fragmentation system

$$\frac{dc_j^N}{dt} = \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k}(c^N) - \sum_{k=1}^{N-j} W_{j,k}(c^N), \quad 1 \leq j \leq N.$$

and prove that,  $\forall \mu > 1$  and with  $\delta = 1 + \frac{\gamma}{\mu-1}$ , its solutions satisfy

$$\frac{d}{dt} \|c^N\|_{\mu} \leq C_0 \|c^N\|_{\mu} - C_1 \|c^N\|_{\mu}^{\delta} \quad \left[ \frac{d}{dt} \|c^N\|_{\mu} \leq D_0 + D_1 \|c^N\|_{\mu}^{\theta} - D_2 \|c^N\|_{\mu}^{\delta} \right]$$

(where  $\theta = 1 + \frac{2\alpha-1}{\mu-1}$ .)

We can solve this differential inequality and pass to the limit  $N \rightarrow \infty$  to obtain

$$\|c(t)\|_{\mu} \leq A \cdot \left(1 - e^{-Bt}\right)^{-\frac{\mu-1}{\gamma}} \quad \left[ \|c(t)\|_{\mu} \leq ((\nu-1)At)^{-\frac{1}{\nu-1}} \right] \quad (6)$$

(for any  $\nu \in (1, \delta)$  and an adequately chosen constant  $A$ .)



## Dynamic phase transition

- The strong fragmentation condition implies that the  $(1 + \gamma - \varepsilon)$ -moments of every density conserving solution not only *exist* (as we already know by (6)) but are actually *integrable* in  $[0, t)$  for all  $t < \infty$ , which implies the uniqueness of the density conserving solutions.

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- Hence, there exists a semigroup of operators  $T(\cdot)$  such that  $T(\cdot)c_0$  is the solution of the coagulation-fragmentation system (4), and (6) implies that the orbit  $\cup_{t \geq \tau} T(t)c_0$  is bounded in  $X_\mu$ , hence precompact in  $X_1^+$ . This implies the omega-limit set  $\omega(c_0) \subset X_\mu$  is nonempty.



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- For the characterization of  $\omega(c_0)$  we now use the detailed balance condition and the Lyapunov function

$$V(c) := \sum_{j=1}^{\infty} c_j \cdot \left( \log \frac{c_j}{Q_j} - 1 \right)$$



in the following way:

- - ▶ Using the assumption on  $Q_j$  we can prove that  $V$  is bounded in  $X_m \cap X_{1,\rho}^+$ , and continuous if  $m \geq q$ .
  - ▶ Using  $c^N \rightarrow c$  strongly in  $X_m^+$ ,  $\forall m \geq 1$ , (due to the strong fragmentation condition), and the continuity of  $V$ , we conclude that

$$V(c(t)) + \int_{\tau}^t D_{CF}(c(s)) ds \leq V(c(\tau)), \quad (7)$$

where

$$D_{CF}(c) := \frac{1}{2} \sum_{j,k \geq 1} H_{j,k}(c)$$

and

$$H_{j,k}(c) := (a_{j,k} c_j c_k - b_{j,k} c_{j+k}) (\log a_{j,k} c_j c_k - \log b_{j,k} c_{j+k}) \geq 0.$$

- The detailed balance condition and inequality (7) are used to prove the *uniqueness of an equilibrium*  $c^\rho$  with density  $\rho$ , which must be of the form  $c_j^\rho = Q_j z^j$ , for  $z$  the unique solution of  $F(z) = \rho$ .

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- Thus we conclude that, for every  $c_0 \in X_1^+$  with  $\|c_0\|_1 = \rho$ , we have  $\omega(c_0) = \{c^\rho\}$ .

## Dynamic phase transition

### “Weak fragmentation” conditions

The crucial difference to the “strong fragmentation” case is that now *orbits are not precompact* in the strong (norm) topology of  $X_1$ .

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The precise assumption can be stated as follows:

- $a_{j,k} = a_{k,j} \geq 0$ ,  $b_{j,k} = b_{k,j} \geq 0$ ,  $\forall j, k$ , and there exists  $\lambda \in [0, 1)$  such that  $a_{1,j} > C_1 j^\lambda$ ,  $\forall j$ ;

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- $(Q_j z_s^j)_j$  is a monotone decreasing sequence;
- $c_0 \in X_\mu^+$ ,  $\mu := \max\{2 - \lambda, 1 + \lambda, 1 + \gamma\}$ .

### The result

- With these *weak fragmentation* conditions, the dynamic phase transition theorem that was proved for the Becker-Döring system (5) is also true for the coagulation-fragmentation system (4).

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### General strategy of the proof

- The general strategy of the proof consists in showing that if a solution converges weak-\* to an equilibrium with subcritical density, then the convergence is strong (i.e., in the norm topology of)  $X_1$ , and hence the density of the limit is equal to the initial density.

## Main ideas and sketch of proof

- Using the continuity of

$$V_{z_s}(c) := V(c) - (\log z_s) \sum_{j=1}^{\infty} j c_j = \sum_{j=1}^{\infty} c_j \cdot \left( \log \frac{c_j}{Q_j} - 1 \right) - (\log z_s) \sum_{j=1}^{\infty} j c_j$$

in the metric space  $B_{\rho_0}^+ := \{c \in X_1^+ : \|c\|_1 \leq \rho_0\}$  with distance  $\text{dist}(c, e) := \|c - e\|_0$ , and using the fact that  $V_{z_s}$  satisfies

$$V_{z_s}(c(t)) + \int_0^t D_{CF}(c(s)) ds = V_{z_s}(c_0) \quad (8)$$

we can use the precompactness of the orbits in  $B_{\rho_0}^+$  to conclude that  $\omega(c)$  is made of solutions along which  $V_{z_s}$  has a constant value

$$V_{z_s}^{\infty} := \lim_{t \rightarrow \infty} V_{z_s}(c(t))$$



## Dynamic phase transition

### Main ideas and sketch of proof

- Take any  $\bar{c}(\cdot) \in \omega(c)$ , then  $V_{z_s}(\bar{c}(t)) = V_{z_s}(\bar{c}_0)$  and (8) implies that  $D(\bar{c}(s)) \equiv 0$ , which implies that  $\bar{c}_j = Q_j(\bar{c}_1(t))^j$ .

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- From conservation of density:

$$\sum_{j=1}^{\infty} j \bar{c}_j(t) = \sum_{j=1}^{\infty} j Q_j(\bar{c}_1(t))^j = \sum_{j=1}^{\infty} j Q_j(\bar{c}_1(0))^j$$

which implies that  $\bar{c}_1(t) = \text{constant}$ .

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- Since  $V_{z_s}(c^\rho)$  is a monotone strictly decreasing function of  $\rho$ , we must have  $\omega(c) = \{c^\rho\}$ , for a unique value of  $\rho \in [0, \min\{\rho_0, \rho_s\}]$  and  $\text{dist}(c(t), c^\rho) \rightarrow 0$  as  $t \rightarrow \infty$ , i.e.

$$c(t) \xrightarrow{*} c^\rho.$$



### Main ideas and sketch of proof

- To prove that the convergence is strong if  $\rho < \rho_s$  we use the inequality

$$\|c\|_1 - \sum_{j=1}^{\infty} j Q_j c_1^j \leq C \sqrt{D_{\text{BD}}} \|c\|_{2-\lambda}^{1/2}, \quad (9)$$

where  $D_{\text{BD}}$  is the free-energy dissipation rate for the Becker-Döring system

$$D_{\text{BD}}(c) := \sum_{j=1}^{\infty} a_j Q_j \left( \frac{c_1 c_j}{Q_j} - \frac{c_{j+1}}{Q_{j+1}} \right) \left( \log \frac{c_1 c_j}{Q_j} - \log \frac{c_{j+1}}{Q_{j+1}} \right),$$

i.e., is the function such that

$$V(c_{\text{BD}}(t)) = V(c_{\text{BD}}(\tau)) - \int_{\tau}^t D_{\text{BD}}(c_{\text{BD}}(s)) ds,$$

for solutions  $c_{\text{BD}}$  of the Becker-Döring system (5).



### Main ideas and sketch of proof

- Working with the  $N$ -truncated system and passing to the limit  $N \rightarrow \infty$  we can prove that

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- Using (9) and (10), and being  $\rho_1(t) := \|Q_j(c_1(t))^j\|_1$ , we conclude

$$\rho - \rho_1(t) \leq C \sqrt{D_{\text{BD}}} \sqrt{1+t} \iff D_{\text{BD}} \geq \frac{1}{C^2} \frac{(\rho - \rho_1(t))^2}{1+t}.$$



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- Computing  $V$  along solutions we obtain...



## Dynamic phase transition

### Main ideas and sketch of proof

$$\begin{aligned} V(t) &= V(t_1) - \int_{t_1}^t D_{CF} \\ &\leq V(t_1) - \int_{t_1}^t D_{BD} \\ &\leq V(t_1) - \frac{1}{C^2} \int_{t_1}^t \frac{(\rho - \rho_1(s))^2}{1+s} ds \end{aligned}$$

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- Since  $c(t) \xrightarrow{*} c^{\text{eq}}$  and  $\|c(t)\|_1 = \rho = \rho_z = \|c^{\text{eq}}\|_1$   
we finally conclude that

$$c(t) \rightarrow c^{\text{eq}} \quad \text{strongly in } X_1$$

## What else?

The phase transition problem just visited is but one of the many interesting issues in the dynamic behaviour of solutions of the coagulation-fragmentation equations.

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There are, of course, a large number of other problems that we have no time to speak about!



to be continued. . .

# Coagulation-Fragmentation Models

Lecture 1. Generalities. Existence of solutions via weak  $L^1$  methods

Lecture 2. Aspects of long-time behaviour: phase transitions

Lecture 3. Further aspects of long-time behaviour



## Aspects of long time behaviour: convergence rates

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### Rate of convergence to equilibria, Fournier & Mischler (2004)

Assume

- $a_{j,k} \leq K_c(jk)^\alpha$ , with  $\alpha \in [0, 1]$ ;
- $L(j+k)^\gamma \leq b_{j,k} \leq K_f(j+k)^s$ , with  $s, \gamma \in (-1, \infty)$ ,  $\gamma > -2(1 - \alpha)$ ;
- $\rho = \|c_0\|_1$  is sufficiently small.

Then the solution  $T(t)c_0$  of the coagulation-fragmentation equation satisfies

$$\|T(t)c_0 - \hat{c}\|_2 \leq Ke^{-\kappa t}, \quad \text{for all } t \geq 1,$$

where  $K$  and  $\kappa$  are constants and  $\hat{c}$  is the only equilibrium solution with density  $\rho$ .

## Convergence rates with strong fragmentation

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## Convergence rates with strong fragmentation

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The proof uses in a crucial way the fact that the strong fragmentation assumption provided by the lower bound on the coefficients  $b_{j,k}$  imply higher order moments are bounded.

The main ingredient is the establishment of the inequality

$$\frac{d}{dt} \|c(t) - d(t)\|_2 \leq \left( 2K \|c(t) + d(t)\|_3 - \frac{L}{16} \right) \|c(t) - d(t)\|_2$$

and uniformly bounding  $2K \|c + d\|_3$  by a constant smaller than  $L/16$  provided the initial density is sufficiently small.



## Convergence rates in Becker-Döring

Remember the two distinct cases:

- 1 subcritical solutions:  $\|c(t)\|_1 = \|c_0\|_1 < \rho_s$ ;
- 2 supercritical solutions:  $\|c(t)\|_1 = \|c_0\|_1 > \rho_s$ .

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With appropriate assumptions the following is true:

$$\begin{aligned} \sum_{j=1}^{\infty} e^{\nu j} c_j(0) < \infty &\implies \\ \implies \exists \bar{\nu} \in (0, \nu), \lambda_* > 0 : \forall \eta \in (0, \bar{\nu}), \exists C > 0 : \forall t \geq 0, \\ \sum_{j=1}^{\infty} e^{\eta j} |c_j(t) - Q_j z^j| &\leq C e^{-\lambda_* t}. \end{aligned}$$



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The proof is highly nontrivial from a technical point of view.



Although the proof is technically quite hard, the **main idea** used is classical:

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- 2 prove a linear spectral gap in appropriate spaces;
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The techniques are related to / inspired by those developed for the study of exponential convergence in the Navier-Stokes and in the Boltzmann equations.

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$$\text{Mass conservation} \implies \sum_{j=1}^{\infty} j Q_j z^j h_j = 0.$$

In the new variable  $h = (h_j)_j$  the Becker-Döring system becomes

$$\frac{dh}{dt} = F(h_1(t))h, \tag{11}$$

where  $F(g) = L + g\Gamma$ , with the linear operators  $L, \Gamma$  given by...



## Convergence rates in Becker-Döring

$$\sum_{i=1}^{\infty} Q_i z^i (Lh)_i \varphi_i := \sum_{i=1}^{\infty} a_i Q_i Q_1 z^{i+1} (h_1 + h_i - h_{i+1}) (\varphi_{i+1} - \varphi_i - \varphi_1),$$

$$\sum_{i=1}^{\infty} Q_i z^i (\Gamma h)_i \varphi_i := \sum_{i=1}^{\infty} a_i Q_i Q_1 z^{i+1} h_i (\varphi_{i+1} - \varphi_i - \varphi_1).$$

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In an appropriately defined Hilbert space of sequences with exponential weight,  $\mathcal{H} = \ell^2((1 + \sigma_i) Q_i z^i)$ , it can be proved that there exists a positive constant  $\lambda_0$  such that

$$\langle Lh, h \rangle_{\mathcal{H}} \leq -\lambda_0 \|h\|_{\mathcal{H}}^2.$$



## Convergence rates in Becker-Döring

To control the nonlinear terms, a careful enlargement of the space to the weighted  $\ell^1$  space (where  $\eta \in (0, 1)$  is sufficiently small) defined by

$$X_\eta := \left\{ h = (h_i) : \|h\| := \sum_{i=1}^{\infty} Q_i e^{\eta i} |h_i| < \infty, \sum_{i=1}^{\infty} Q_i i h_i = 0 \right\}$$

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That result, which essentially says that if the tail of the initial condition decays exponentially fast then the solution to the Becker-Döring system converges exponentially fast to the equilibrium as  $t \rightarrow \infty$ , was proved by Cañizo & Lods (2013), extending a slightly less general result by Niethammer (2008).



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This was further complemented by Murray & Pego (2016) who, under appropriate conditions, proved the following:



*For initial conditions with a polynomially decaying tail, the solutions to the Becker-Döring system converge to equilibria at an algebraic rate, namely, for  $h$  as before,*

$$\|h(t)\|_{X_{1+k}} \leq C \cdot (1+t)^{-(k-m-1)} \|h(0)\|_{X_{1+k}},$$

where  $k > m + 2 > 2$  and, for  $k \geq 1$ ,

$$X_k := \left\{ h = (h_i) : \|h\| := \sum_{i=1}^{\infty} Q_i z^i i^k |h_i| < \infty, \sum_{i=1}^{\infty} Q_i z^i i h_i = 0 \right\}.$$

## Convergence rates in Becker-Döring

An alternative approach, used by Jabin & Niethammer (2003) and Cañizo, Einav & Lods (2017) is based on so called “energy / energy dissipation inequalities”

$$\underbrace{D_{\text{BD}}(c)}_{\substack{\text{energy} \\ \text{dissipation}}} \geq K \cdot \underbrace{V(c | Q_i z^i)}_{\text{energy}}^A \quad (12)$$

where  $V(c | Q_i z^i)$  is the relative energy of the solution  $c$  (relative to the equilibrium  $Q_i z^i$ ), defined by

$$\begin{aligned} V(c | Q_i z^i) &:= V_z(c) + \sum_{i=1}^{\infty} Q_i z^i \\ &= \left( \sum_{i=1}^{\infty} c_i \left( \log \frac{c_i}{Q_i} - 1 \right) - (\log z) \sum_{i=1}^{\infty} i c_i \right) + \sum_{i=1}^{\infty} Q_i z^i. \end{aligned}$$

## Convergence rates in Becker-Döring

and  $D_{BD}$  is (remember lecture 2) the free-energy dissipation rate for the Becker-Döring system

$$D_{BD}(c) := \sum_{j=1}^{\infty} a_j Q_j \left( \frac{c_1 c_j}{Q_j} - \frac{c_{j+1}}{Q_{j+1}} \right) \left( \log \frac{c_1 c_j}{Q_j} - \log \frac{c_{j+1}}{Q_{j+1}} \right),$$

i.e., is the function such that  $\frac{d}{dt} V(c | Q_i z^i) = -D_{BD}(c)$ .

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i.e., is the function such that  $\frac{d}{dt} V(c | Q_i z^i) = -D_{\text{BD}}(c)$ .

The energy / energy dissipation inequality (12) allows one to deduce the decay rate of  $V(c | Q_i z^i)$  and then, using the Csiszár-Kullback (or Pinsker) inequality

$$\|c - (Q_i z^i)\|_{\ell^1} \leq \sqrt{2\rho V(c | Q_i z^i)},$$

to get the convergence rate result.

## Convergence rates in Coagulation-Fragmentation

For the general discrete coagulation-fragmentation (with weak fragmentation type coefficients) Cañizo (2007) proved that solutions with subcritical mass converge to the equilibrium (with the same mass) with the following rate

$$\|c(t) - (Q_i z^i)\|_1 := \sum_{i=1}^{\infty} i |c_i(t) - Q_i z^i| \leq \frac{(\text{constant})}{\sqrt{1 + \log(1 + t)}}. \quad (13)$$

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This was done by obtaining the estimate

$$0 < \sum_{i=1}^{\infty} i c_i - \sum_{i=1}^{\infty} i Q_i z^i \leq \max\left\{2V(c | Q_i z^i), K_z \sqrt{V(c | Q_i z^i)}\right\}$$

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The decay estimate (13) is believed not to be optimal.



## Excess mass and the Lifschitz-Slyozov-Wagner PDE

Consider again the Becker-Döring equations.

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We saw in lecture 2 that if the initial density  $\rho$  is larger than the critical density  $\rho_s$  then  $c(t) \xrightarrow{*} c^{\rho_s}$  in  $X_1$ , as  $t \rightarrow \infty$ , where  $c^{\rho_s}$  is the unique equilibrium with density  $\rho_s$ .

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Since  $\|c(t)\|_1 = \rho$ ,  $\forall t$ , and  $\|c^{\rho_s}\|_1 = \rho_s < \rho$ , a natural question is:

*What happens with the distribution of clusters corresponding to the excess mass  $\rho - \rho_s$  when  $t \rightarrow \infty$ ?*

This problem was investigated by several mathematicians (Carr, Laurençot, Niethammer, Penrose, etc.) and the answer provides a very interesting connection with an hyperbolic equation developed in the 1960s in the classical theory of coarsening: the **Lifschitz-Slyozov-Wagner** equation.



## Excess mass and the Lifschitz-Slyozov-Wagner PDE

Assume the following coagulation and fragmentation coefficients:

$$a_i = i^\alpha, \quad \text{for some } \alpha \in [0, 1),$$

$$b_i = a_i \left( z_s + \frac{q}{i^\gamma} \right), \quad \text{with } z_s > 0, q > 0, \gamma \in (0, 1), \text{ and where}$$

$z_s$  is the unique  $z$  such that  $\|(Q_i z^i)\|_1 = \rho_s$ .



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$z_s$  is the unique  $z$  such that  $\|(Q_i z^i)\|_1 = \rho_s$ .

Consider large times  $t$  and let  $\tau$  be defined by  $\tau = \varepsilon^{1+\gamma-\alpha} t$  with  $0 < \varepsilon \ll 1$ .



## Excess mass and the Lifschitz-Slyozov-Wagner PDE

Assume the following coagulation and fragmentation coefficients:

$$a_i = i^\alpha, \quad \text{for some } \alpha \in [0, 1),$$
$$b_i = a_i \left( z_s + \frac{q}{i^\gamma} \right), \quad \text{with } z_s > 0, q > 0, \gamma \in (0, 1), \text{ and where}$$
$$z_s \text{ is the unique } z \text{ such that } \|(Q_i z^i)\|_1 = \rho_s.$$

Consider large times  $t$  and let  $\tau$  be defined by  $\tau = \varepsilon^{1+\gamma-\alpha} t$  with  $0 < \varepsilon \ll 1$ .

Adequately choosing a separation  $i_*$  between small and large clusters, where  $i_* = i_*(\varepsilon) \rightarrow \infty$  as  $\varepsilon \rightarrow 0$ , and considering the rescalings  $x = \varepsilon i$  and

$$c_i(t) = \varepsilon^2 \nu(\tau, x), \quad \widetilde{W}_i(c(t)) = \varepsilon^{2+\alpha-\gamma} \nu(\tau, x), \quad c_1(t) = z_s + \varepsilon^\gamma u(\tau),$$

it can be proved that, to first order in  $\varepsilon$  as  $\varepsilon \rightarrow 0$ , the rescaled variables satisfy...



... the Lifschitz-Slyozov-Wagner equations

$$\frac{\partial \nu}{\partial \tau} + \frac{\partial}{\partial x} \left( x^\alpha (u(\tau, x) - qx^{-\gamma}) \nu \right) = 0$$
$$\int_0^\infty x \nu(\tau, x) dx = \rho - \rho_s.$$

A similar problem can be considered in the case of the Smoluchowski coagulation equation studied in lecture 1:

$$\frac{\partial}{\partial t} c(x, t) = \frac{1}{2} \underbrace{\int_0^x a(x-y, y) c(x-y, t) c(y, t) dy - c(x, t) \int_0^\infty a(x, y) c(y, t) dy}_{=: Q(c)(x, t)} \quad (14)$$

## Excess mass and self-similarity in Smoluchowski coagulation system

A similar problem can be considered in the case of the Smoluchowski coagulation equation studied in lecture 1:

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If  $a(x, y) > 0$  we have that  $c(x, t) \rightarrow 0$  as  $t \rightarrow \infty$ , for (a.e.) all  $x$ .

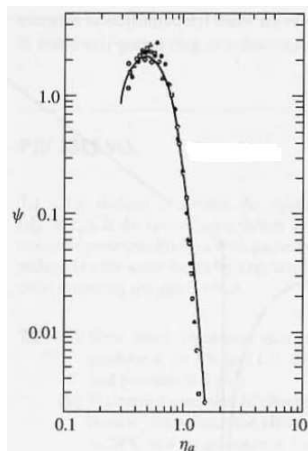
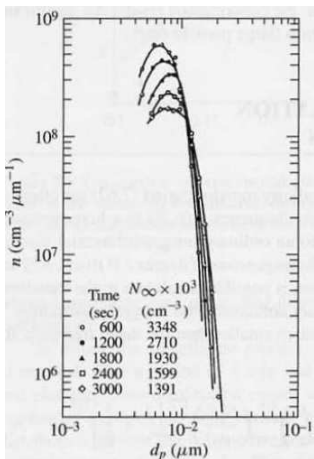
Note that the null function is the only equilibrium solution of (14) and its density is (obviously) equal to 0.

When the rate coefficient  $a(x, y)$  is such that the solution conserve the initial density  $\rho = \|c(\cdot, 0)\|_1$ , how is the excess density  $\rho$  distributed among the various  $x$ -clusters ?



## Excess mass and self-similarity in Smoluchowski coagulating system

It is an experimental observation that in many coagulation systems, after a transient time has elapsed and a specific transformation of variables is performed to the data, a “typical” cluster distribution emerges:



(in: S.K. Friedlander: *Smoke, Dust, and Haze: Fundamentals of Aerosol Dynamics*, 2nd ed., OUP, 2000.)

## Excess mass and self-similarity in Smoluchowski coagulation system

So it seems that, at least in some cases, when  $t \rightarrow \infty$  the cluster size distribution  $c(x, t)$  that is a solution of the Smoluchowski coagulation equation (14) approaches, after an appropriate rescaling, a *universal self-similar form*

$$c(x, t) \sim \frac{1}{r(t)} \psi(\eta), \quad \text{where } \eta = x/s(t)$$

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A natural necessary condition for this to take place is that the cluster system must be “scale-free” (or maybe “asymptotically scale-free”).

Mathematically this means that the coagulation rate function must satisfy the homogeneity condition

$$a(ux, uy) = u^\lambda a(x, y), \quad \forall x, y, u \in \mathbb{R}^+ \quad (15)$$

for some real number  $\lambda$ .



## Excess mass and self-similarity in Smoluchowski coagulation system

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At present nothing has rigorously been proved about the case  $\lambda \geq 1$  except for the so called “solvable cases”  $a(x, y) = x + y$  and  $a(x, y) = xy$  (for which one can use Laplace transforms to work out the solution explicitly: see the work of Menon & Pego (2004, 2005, 2008)) and for some special cases, like the diagonal kernel  $a(x, y) = x^\lambda \delta(x - y)$ .

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For the case of homogeneity degree  $\lambda < 1$  the situation is much different: until recently only the solvable case  $a(x, y) = (\text{constant})$  was well understood (Kreer & Penrose (1994), dC (1996), Menon & Pego (2004, 2005, 2008), Laurençot & Mischler (2005), Cañizo et al (2010)), but recently a large number of papers have been appearing that have considered advanced our knowledge about existence, uniqueness, properties of the scaling profile, and convergence issues (see works by Fournier & Laurençot (2005), Niethammer & Velázquez (2013, 2014), Laurençot (2018, 2019), Throm (2019), etc., etc.).

## Excess mass and self-similarity in Smoluchowski coagulation system

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Consider an homogeneous coagulation rate kernel with homogeneity degree  $\lambda < 1$ .

It is easy to observe that if  $c(x, t)$  is a solution of (14), then, for all constants  $a, b > 0$ , the function  $\tilde{c}(x, t) := a^{1+\lambda}b^{-1}c(ax, bt)$  is also a solution of (14).



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This scale invariance leads to the expectation of existence of solutions with the form

$$c(x, t) = t^{-\alpha}\Phi(\xi), \quad \text{with } \xi := x/t^\beta, \quad (16)$$

with  $\alpha = 1 + (1 + \lambda)\beta$ .



## Excess mass and self-similarity in Smoluchowski coagulation system

If we require such a solution to conserve density we have

$$\begin{aligned}\rho_0 &:= \|c(\cdot, 0)\|_1 = \|c(\cdot, t)\|_1 \\ &= \int_0^\infty xc(x, t)dx = \int_0^\infty xt^{-\alpha}\Phi\left(\frac{x}{t^\beta}\right)dx \\ &= t^{2\beta-\alpha} \int_0^\infty \xi\Phi(\xi)d\xi\end{aligned}$$

and thus  $\alpha = 2\beta$  which, together with the previous relation  $\alpha = 1 + (1 + \lambda)\beta$  gives  $\alpha = \frac{2}{1-\lambda}$  and  $\beta = \frac{1}{1-\lambda}$

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Plugging the *ansatz* with this values of the parameters into the coagulation equation (14) and making use of the homogeneity condition (15) we get that  $\Phi$  should solve the equation

$$\xi \frac{d\Phi}{d\xi} + 2\Phi = (1 - \lambda)Q(\Phi)(\xi), \quad \text{with } \|\Phi\|_1 = \rho_0. \quad (17)$$



## Excess mass and self-similarity in Smoluchowski coagulation system

The integro-differential (note that  $Q$  is the coagulation integral operator) equation (17) is extremely difficult to study for at least two reasons:

- 1 it is not an initial value problem: at any given  $\tilde{\xi} \in \mathbb{R}^+$  the right-hand side  $Q(\Phi)(\tilde{\xi})$  depends on the “past values”  $(0, \tilde{\xi})$  of  $\xi$ , as well as on the “future”  $(\tilde{\xi}, \infty)$ ,
- 2 it is degenerate: the derivative term disappears when  $\xi = 0$ .

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Some authors prefer to further modify (17) transforming it into an integral equation as follows: under the assumption  $\xi^2 \Phi(\xi) \rightarrow 0$  as  $\xi \rightarrow \infty$  we can multiply the equation (17) by  $\xi$  and integrate from  $\xi$  to  $\infty$  to obtain

$$\xi^2 \Phi(\xi) = (1 - \lambda) \int_0^\xi \int_{\xi-\eta}^\infty \eta a(\eta, \zeta) \Phi(\eta) \Phi(\zeta) d\zeta d\eta \quad (18)$$

still with the normalizing condition  $\|\Phi\|_1 = \rho_0$ .



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The study of (18) does not seem to be easier than (17).

Both equations have been used in various recent studies (see, for example, Laurençot (2019), Niethammer (2014), Throm (2019), etc.)

## Excess mass and self-similarity in Smoluchowski coagulation system

Although equations (17) and (18) are extremely hard to study in general, there are an extremely small number of rate coefficients  $a(\cdot, \cdot)$  for which they can be explicitly solved.

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At present only three explicitly “solvable cases” are known and the study heavily depends on the hability to use the Laplace transform. The solvable case for homogeneity degree  $\lambda < 1$  is just  $a(x, y) = (\text{constant})$ . (The others solvable cases are  $a(x, y) = x + y$  with degree  $\lambda = 1$ , and  $a(x, y) = xy$  with  $\lambda > 1$ ).



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Although a full study of the self-similar dynamics in the solvable cases is far from trivial (see Menon & Pego (2004, 2005, 2008)) at least an explicit self-similar solution can be obtain in those cases.



We finish with the following easy. . .

### Exercise

Let  $a(x, y) = 2$  for all  $x, y > 0$ . Use (17) or (18) to check that (14) has a self-similar solution of the form  $\Phi(\xi) = Ae^{-B\xi}$  and determine the precise values of the constants  $A$  and  $B$ .

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Thank you for staying till **THE END** !

## Works referred to in these lectures

Besides the four review papers pointed out at the beginning of lecture 1, the following papers were referred to and some of them were used in the preparation of these talks:

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