Moments estimates for the discrete coagulation-fragmentation equations with diffusion

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Table of Contents

1. Introduction
   - Description of the model
   - About mass conservation and gelation
   - State of the art and new results
2. Moments estimates via duality lemmas
3. Consequences for mass conservation and smoothness

- We denote by $c_i = c_i(t,x) \geq 0$ the concentration of clusters of size $i \in \mathbb{N}^*$, at time $t \geq 0$ and position $x \in \Omega \subset \mathbb{R}^N$.

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- The diffusive coagulation-fragmentation equations are the given by

$$\partial_t c_i - d_i \Delta_x c_i = Q_i(c) + F_i(c), \quad \forall\, i \in \mathbb{N}^*,$$

where the coagulation term $Q_i(c)$ and the fragmentation term $F_i(c)$ take the form

$$Q_i(c) = Q_i^+(c) - Q_i^-(c) = \frac{1}{2}\sum_{j=1}^{i-1} a_{i-j,j} c_{i-j} c_j - \sum_{j=1}^{\infty} a_{i,j} c_i c_j,$$

$$F_i(c) = F_i^+(c) - F_i^-(c) = \sum_{j=1}^{\infty} B_{i+j} \beta_{i+j,i} c_{i+j} - B_i c_i.$$

- This infinite system of reaction-diffusion equations is complemented with Neumann boundary conditions and non negative initial concentrations $c_i^{init} \geq 0$.

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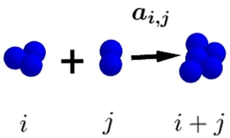

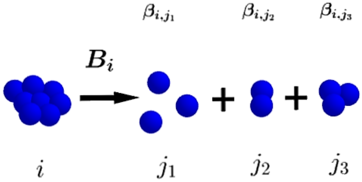

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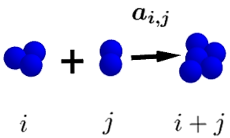

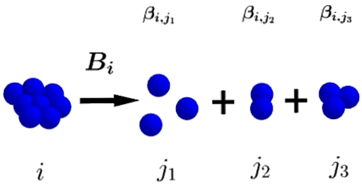

Natural set of assumptions:

$$a_{i,j}, B_i, \beta_{i,j} \geq 0, \quad a_{i,j} = a_{j,i}, \quad B_1 = 0, \quad \text{and} \quad i = \sum_{j=1}^{i-1} j\beta_{i,j}.$$

Weak formulation of the coagulation-fragmentation terms

$$Q_i(c) = Q_i^+(c) - Q_i^-(c) = \frac{1}{2}\sum_{j=1}^{i-1} a_{i-j,j}c_{i-j}c_j - \sum_{j=1}^{\infty} a_{i,j}c_ic_j,$$

$$F_i(c) = F_i^+(c) - F_i^-(c) = \sum_{j=1}^{\infty} B_{i+j}\beta_{i+j,i}c_{i+j} - B_ic_i.$$

For any sequence $(\varphi_i)_{i\in\mathbb{N}^*}$ we have (at least formally)

$$\sum_{i=1}^{\infty}\varphi_i Q_i(c) = \frac{1}{2}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty} a_{i,j}c_ic_j(\varphi_{i+j}-\varphi_i-\varphi_j),$$

$$\sum_{i=1}^{\infty}\varphi_i F_i(c) = -\sum_{i=1}^{\infty} B_ic_i\left(\varphi_i - \sum_{j=1}^{i-1}\beta_{i,j}\varphi_j\right).$$

- Both from a mathematical and from a physical perspective, one of the most interesting questions about coagulation-fragmentation models is the one of mass conservation.
- Starting from the coagulation-fragmentation equations

$$\partial_t c_i - d_i \Delta_x c_i = Q_i(c) + F_i(c), \quad \forall\, i \in \mathbb{N}^*,$$

we get

$$\partial_t \left(\sum_{i=1}^{\infty} i c_i \right) - \Delta_x \left(\sum_{i=1}^{\infty} i d_i c_i \right) = \sum_{i=1}^{\infty} i Q_i(c) + \sum_{i=1}^{\infty} i F_i(c).$$

- Using the previous identity with $\varphi_i = i$, we see that

$$\sum_{i=1}^{\infty} i Q_i(c) = 0 = \sum_{i=1}^{\infty} i F_i(c).$$

- After integrating and using the Neumann boundary conditions, we are left with

$$\int_\Omega \sum_{i=1}^{\infty} ic_i(t,x)dx = \int_\Omega \sum_{i=1}^{\infty} ic_i(0,x)dx, \quad \forall\ t \geq 0,$$

which means that the total mass should stay constant.

- In some cases (depending on the coagulation and the fragmentation coefficients $a_{i,j}$, B_i and $\beta_{i,j}$), these formal computations can be justified, to prove that the total mass is indeed conserved. To do so, we need an a priori estimate on a higher order moment, of the form

$$\int_0^T \int_\Omega \sum_{i=1}^{\infty} i\eta_i c_i(t,x)dxdt \leq C_T, \quad \text{where } \eta_i > 0,\ \eta_i \to \infty.$$

- However, in some other situations the total mass is NOT conserved, and instead decreases strictly in finite time, a phenomenon called *gelation*.

- Gelation occurs when some of the mass escapes as $i \to \infty$, which can be interpreted as the formation of clusters of infinite size.
- Gelation is not a mathematical artifact, it can be observed and explained physically. It corresponds to a phase transition of the system, the lost mass being transferred to the newly created phase.
- One example is the formation of colloidal gels in chemistry, which leads to this loss of mass being referred to as *gelation*.

For given coagulation and fragmentation coefficients $a_{i,j}$, B_i and $\beta_{i,j}$, can we predict whether gelation is going to occur or not?

An explicit example

- We introduce the moments ρ_k, $k \in \mathbb{N}$: $\rho_k = \sum_{i=1}^{\infty} i^k c_i$.

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- We consider the specific case where $d_i = 0$, $B_i = 0$ and $a_{i,j} = ij$. The weak formulation becomes

$$\frac{d}{dt} \sum_{i=1}^{\infty} \varphi_i c_i = \frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} i c_i j c_j (\varphi_{i+j} - \varphi_i - \varphi_j).$$

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- With $\varphi_i = i^2$, we get

$$\frac{d}{dt}\rho_2 = \frac{d}{dt}\left(\sum_{i=1}^{\infty} i^2 c_i\right) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} i^2 c_i j^2 c_j = (\rho_2)^2 .$$

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- We have a blow-up at time $T^* = \frac{1}{\rho_2(0)}$, for the second order moment, therefore mass conservation is only guaranteed for $t < T^*$.

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- With $\varphi_i = 1$, we obtain

$$\frac{d}{dt} \rho_0 = \frac{d}{dt} \left(\sum_{i=1}^{\infty} c_i \right) = -\frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} i c_i j c_j = -\frac{1}{2} (\rho_1)^2 .$$

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- We then get $\frac{1}{2} \int_0^T (\rho_1(t))^2 \, dt \leq \rho_0(0), \ \forall \ T \geq 0$, which implies that gelation does indeed occur.

Known results: the spatially homogeneous case

- For *sublinear* or *linear* coagulation rates:

$$a_{i,j} \leq C(i+j),$$

the total mass is conserved [White 1980; Ball, Carr 1990]. This includes any coagulation coefficients of the form

$$a_{i,j} = i^\alpha j^\beta + i^\beta j^\alpha, \quad \alpha, \beta \geq 0,\ \alpha + \beta \leq 1.$$

- For *superlinear* coagulation rates, of the form

$$a_{i,j} = i^\alpha j^\beta + i^\beta j^\alpha, \quad \alpha, \beta \geq 0,\ \alpha + \beta > 1,$$

gelation occurs if there is no fragmentation [Jeon 1998; Escobedo, Mischler, Perthame 2002], but the total mass is still conserved if the fragmentation rates are *large enough* [Carr 1992; Da Costa 1995; Escobedo, Laurençot, Mischler, Perthame 2003].

Known results: the spatially inhomogeneous case

- Existence of global weak solutions [Wrzosek 1997; Laurençot, Mischler 2002].
- For *sublinear* coagulation rates:

$$a_{i,j} = i^\alpha j^\beta + i^\beta j^\alpha, \quad \alpha, \beta \geq 0, \ \alpha + \beta < 1.$$

  the total mass is conserved [Hammond, Rezakhanlou 2007; Cañizo, Desvillettes, Fellner 2010]. Notice that the linear case $a_{i,j} = i + j$ is still open.
- For *superlinear* coagulation rates, of the form

$$a_{i,j} = i^\alpha j^\beta + i^\beta j^\alpha, \quad \alpha, \beta \geq 0, \ \alpha + \beta > 1,$$

  gelation occurs if there is no fragmentation.

New results in the inhomogeneous case

- Smoothness of the solutions, in essentially every case where mass conservation is known to hold [B., Desvillettes, Fellner 2016].
- For *superlinear* coagulation rates, of the form

$$a_{i,j} = i^\alpha j^\beta + i^\beta j^\alpha, \quad \alpha, \beta \geq 0, \ \alpha + \beta > 1,$$

the total mass is still conserved if the fragmentation rate satisfies

$$B_i \geq i^\gamma,$$

with $\gamma > \alpha + \beta$ [B. 2017].

▶ These results rely on a crucial assumption on the diffusion coefficients:

$$d_i > 0, \ \forall\ i \in \mathbb{N}^* \qquad \text{and} \qquad d_i \underset{i\to\infty}{\longrightarrow} d_\infty > 0.$$

1 Introduction

2 Moments estimates via duality lemmas

- Using duality lemmas ...
- ... to get moments estimates

3 Consequences for mass conservation and smoothness

How to get moments estimates for discrete coagulation-fragmentation equations with diffusion?

$$\partial_t c_i - d_i \Delta_x c_i = Q_i(c) + F_i(c), \quad \forall\ i \in \mathbb{N}^*$$

How to get moments estimates for discrete coagulation-fragmentation equations with diffusion?

$$\partial_t c_i - d_i \Delta_x c_i = Q_i(c) + F_i(c), \quad \forall\ i \in \mathbb{N}^*$$

- In a specific case, without diffusion and fragmentation, using the weak form of the reaction term we obtained

$$\frac{d}{dt}\rho_2 = (\rho_1)^2, \quad \text{where } \rho_k = \sum_{i=1}^{\infty} i^k c_i.$$

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$$\frac{d}{dt}\rho_2 = (\rho_1)^2, \quad \text{where } \rho_k = \sum_{i=1}^{\infty} i^k c_i.$$

- When diffusion and fragmentation are taken into account (i.e. $d_i \neq 0$ and $B_i \neq 0$), a similar computation yields

$$\partial_t \rho_2 - \Delta_x \sum_{i=1}^{\infty} i^2 d_i c_i \leq (\rho_1)^2 .$$

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- We rewrite this equation as

$$\partial_t \rho_2 - \Delta_x \left(\frac{\sum_{i=1}^{\infty} i^2 d_i c_i}{\sum_{i=1}^{\infty} i^2 c_i} \sum_{i=1}^{\infty} i^2 c_i \right) \leq (\rho_1)^2 .$$

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- Therefore we get an equation on ρ_2, of the form

$$\partial_t \rho_2 - \Delta_x (M_2 \rho_2) \leq (\rho_1)^2 ,$$

where

$$\inf_{i \in \mathbb{N}^*} d_i \leq M_2 \leq \sup_{i \in \mathbb{N}^*} d_i.$$

Some a priori estimates for parabolic equations

What a priori estimates can we get for a function u satisfying

$$\partial_t u - \Delta_x (Mu) = 0, \quad \text{with } 0 < a \leq M \leq b < \infty \ ?$$

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  testing the equation against $\boldsymbol{\Delta_x u}$ we would get an estimate in $\boldsymbol{H^2}$.

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- If we had
$$\partial_t u - \operatorname{div}(M\nabla_x u) = 0,$$
testing the equation against $\boldsymbol{u}$ we would get an estimate in $\boldsymbol{H^1}$.

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  testing the equation against $\boldsymbol{u}$ we would get an estimate in $\boldsymbol{H^1}$.
- For

$$\partial_t u - \Delta_x (Mu) = 0,$$

  we thus expect to get an estimate in $\boldsymbol{L^2}$.

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- Testing the equation against the solution v of

$$\begin{cases} \partial_t v + M\Delta_x v = -u \\ v(T,\cdot) = 0, \end{cases}$$

  we get

$$\int_0^T \int_\Omega u^2 = \int_\Omega u(0,\cdot)v(0,\cdot) \leq C \int_\Omega u(0,\cdot)^2.$$

- This kind of result is often attributed to [Pierre, Schmitt 1997], who first used such estimates for finite reaction-diffusion systems.

Generalized duality lemmas

- We can also get estimates in L^p, $p < \infty$, for a function u satisfying

$$\partial_t u - \Delta_x (Mu) = 0, \quad \text{with } 0 < a \leq M \leq b < \infty,$$

provided that a and b satisfy a *closeness condition* of the form

$$\frac{b-a}{b+a} C_{\frac{a+b}{2},p'} < 1.$$

This generalization was introduced by [Cañizo, Desvillettes, Fellner 2014], to study reaction-diffusion systems coming out of chemistry.

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- We can also get L^p estimates, $p < \infty$, still assuming this closeness condition, if $u \geq 0$ satisfies

$$\partial_t u - \Delta_x (Mu) \leq \mu_1 u + \mu_2, \quad \text{with } \mu_1 \in L^\infty, \ \mu_2 \in L^p,$$

or

$$\partial_t u - \Delta_x (Mu) \leq \mu_1 u^{1-\varepsilon} + \mu_2, \quad \text{with } \mu_1 \in L^{\frac{p}{\varepsilon}}, \ \mu_2 \in L^p.$$

Estimates for the first moment

- Remember that we have

$$\partial_t \left(\sum_{i=1}^{\infty} i c_i \right) - \Delta_x \left(\sum_{i=1}^{\infty} i d_i c_i \right) = 0,$$

which we can rewrite as

$$\partial_t \rho_1 - \Delta_x \left(M_1 \rho_1 \right) = 0, \quad \text{where } M_1 = \frac{\sum_{i=1}^{\infty} i d_i c_i}{\sum_{i=1}^{\infty} i c_i}.$$

- Therefore, we can use a generalized duality lemma to get an L^p estimate:

Proposition

If $\rho_1^{init} \in L^p(\Omega)$, $p < \infty$, and $d_i > 0$, $d_i \underset{i \to \infty}{\longrightarrow} d_\infty > 0$, then (under some technical assumptions), $\rho_1 \in L^p([0, T] \times \Omega)$.

Estimates for higher order moments

$$\partial_t \rho_2 - \Delta_x \left(M_2 \rho_2 \right) \leq \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_{i,j} i c_i j c_j$$

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- For higher order moment, the assumptions on the coagulation rates are really crucial.
- Assuming $a_{i,j} \leq C(i+j)$, we get

$$\partial_t \rho_2 - \Delta_x \left(M_2 \rho_2 \right) \leq 2C \rho_1 \rho_2.$$

  To apply a duality lemma here we would need an L^∞ bound for ρ_1. However, we only have L^p estimates with $p < \infty$.

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  To apply a duality lemma here we would need an L^∞ bound for ρ_1. However, we only have L^p estimates with $p < \infty$.
- Assuming $a_{i,j} \leq C(i^{1-\varepsilon} + j^{1-\varepsilon})$, with $\varepsilon > 0$, we get

$$\partial_t \rho_2 - \Delta_x \left(M_2 \rho_2 \right) \leq 2C\rho_1\rho_{2-\varepsilon}.$$

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- Assuming $a_{i,j} \leq C(i^{1-\varepsilon} + j^{1-\varepsilon})$, with $\varepsilon > 0$, we get

$$\partial_t \rho_2 - \Delta_x (M_2 \rho_2) \leq 2C \rho_1 \rho_{2-\varepsilon}.$$

- We can interpolate $\rho_{2-\varepsilon} \leq \rho_1^{\varepsilon} \rho_2^{1-\varepsilon}$, to get

$$\partial_t \rho_2 - \Delta_x (M_2 \rho_2) \leq 2C \rho_1^{1+\varepsilon} \rho_2^{1-\varepsilon}.$$

Theorem

Assume $a_{i,j} \leq C(i^{1-\varepsilon} + j^{1-\varepsilon})$, with $\varepsilon > 0$. If

- $\rho_2^{init} \in L^p(\Omega)$, $p < \infty$,
- $\rho_1^{init} \in L^q(\Omega)$, $q = \frac{1+\varepsilon}{\varepsilon} p$,
- $d_i > 0$, $d_i \underset{i \to \infty}{\longrightarrow} d_\infty > 0$,

then (under some technical assumptions), $\rho_2 \in L^p([0, T] \times \Omega)$.

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Theorem

Assume $a_{i,j} \leq C(i^{1-\varepsilon} + j^{1-\varepsilon})$, with $\varepsilon > 0$. If

- $\rho_k^{init} \in L^p(\Omega)$, for all $p < \infty$, for all $k \in \mathbb{N}^*$,
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then (under some technical assumptions), $\rho_k \in L^p([0, T] \times \Omega)$, for all $p < \infty$, for all $k \in \mathbb{N}^*$.

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- For coagulation rates of the form $a_{i,j} \leq C(i^\alpha j^\beta + i^\beta j^\alpha)$, we have

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whereas we in fact have

$$\sum_{i=1}^{\infty} i^2 F_i(c) \leq -\sum_{i=1}^{\infty} B_i i c_i.$$

- Assuming $a_{i,j} \leq C(i^\alpha j^\beta + i^\beta j^\alpha)$, $B_i \geq C i^\gamma$ and putting all the estimates together, we get

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- Therefore, even if $\alpha + \beta \geq 1$ we can hope to close the estimate if γ is large enough.
- Indeed, if $\gamma > \alpha + \beta$, we can interpolate

$$\rho_{1+\alpha+\beta} \leq (\rho_1)^{\frac{\gamma-(\alpha+\beta)}{\gamma}} (\rho_{1+\gamma})^{\frac{\alpha+\beta}{\gamma}}$$

to obtain

$$\partial_t \rho_2 - \Delta_x (M_2 \rho_2) \lesssim (\rho_1)^{1+\frac{\gamma-(\alpha+\beta)}{\gamma}} (\rho_{1+\gamma})^{\frac{\alpha+\beta}{\gamma}} - \rho_{1+\gamma}.$$

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and then an integration over $[0, T]$ yields

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- Finally, using Hölder's inequality we get
$$\int_\Omega \rho_2(T) + \int_0^T \int_\Omega \rho_{1+\gamma} \lesssim$$
$$\int_\Omega \rho_2(0) + \left(\int_0^T \int_\Omega \left(\rho_1 \right)^{1+\frac{\gamma}{\gamma-(\alpha+\beta)}} \right)^{\frac{\gamma-(\alpha+\beta)}{\gamma}} \left(\int_0^T \int_\Omega \rho_{1+\gamma} \right)^{\frac{\alpha+\beta}{\gamma}}.$$

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- Since we can get estimates in any L^p, $p < \infty$, for the first moment, we have that
$$\left(\int_0^T \int_\Omega (\rho_1)^{1+\frac{\gamma}{\gamma-(\alpha+\beta)}}\right)^{\frac{\gamma-(\alpha+\beta)}{\gamma}} < \infty.$$
Since $\frac{\alpha+\beta}{\gamma} < 1$, we then get an estimate in $L^1([0,T]\times\Omega)$ for $\rho_{1+\gamma}$.

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Since $\frac{\alpha+\beta}{\gamma} < 1$, we then get an estimate in $L^1([0,T]\times\Omega)$ for $\rho_{1+\gamma}$.
- Notice that, if $\gamma > 1$ we get an estimate for of moment $\rho_{1+\gamma}$ of order strictly larger than 2, just by assuming that the initial moment of order 2 $\rho_2(0)$ is in $L^1(\Omega)$. Therefore, if $\gamma > 1$, we can bootstrap the estimate to get bounds (weighted in time) for higher order moments.

Theorem

Assume $a_{i,j} \leq C(i^\alpha j^\beta + i^\beta j^\alpha)$, with $0 \leq \alpha, \beta \leq 1$, and $B_i \geq C i^\gamma$. If

- $\gamma > \alpha + \beta$ and $\gamma > 1$,
- $\rho_1^{init} \in L^p(\Omega)$, for all $p < \infty$, and $\rho_2^{init} \in L^1(\Omega)$,
- $d_i > 0$, $d_i \underset{i\to\infty}{\longrightarrow} d_\infty > 0$,

then (under some technical assumptions), we have

$$\int_0^T t^{m-1} \int_\Omega \rho_{2+m(\gamma-1)} < \infty, \quad \forall\ m \in \mathbb{N}^*.$$

In particular, with $m = 1$ we have that the superlinear moment $\rho_{1+\gamma}$ lies in $L^1([0, T] \times \Omega)$, and therefore gelation cannot occur (i.e. the total mass is conserved).

Controlling the reaction terms

- Each c_i solves a heat equation

$$\partial_t c_i - d_i \Delta_x c_i = Q_i(c) + F_i(c), \quad \forall\, i \in \mathbb{N}^*,$$

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- However, as we saw on some examples, the reaction terms can be controlled by higher order moments.

Lemma

Assume $a_{i,j} \leq Cij$ and $B_i \leq Ci^{\delta}$. Then, for all $k \in \mathbb{N}$

$$\left\| i^k Q_i(c) \right\|_{W^{s,p}([0,T]\times\Omega)} \leq C_{s,k} \left\| \rho_{k+1} \right\|^2_{W^{s,2p}([0,T]\times\Omega)},$$

and

$$\left\| i^k F_i(c) \right\|_{W^{s,p}([0,T]\times\Omega)} \leq C_{s,k} \left\| \rho_{k+\delta} \right\|_{W^{s,p}([0,T]\times\Omega)}.$$

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- We can then use the regularizing properties of the heat equation to get $W^{1,p}$ estimates for $i^k c_i$ (uniform w.r.t. i, since the diffusion coefficients d_i are bounded away from 0).

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- This then implies $W^{1,p}$ estimates for the moments ρ_k, and we can bootstrap the argument to get higher Sobolev regularity.

Conclusions

- Under the assumption $d_i > 0$, $d_i \underset{i\to\infty}{\longrightarrow} d_\infty > 0$, duality lemmas can be used to obtain moments estimates for the coagulation-fragmentation equations with diffusion.
- We obtained new moments estimates in the sublinear coagulation case $a_{i,j} \leq C(i^\alpha j^\beta + i^\beta j^\alpha)$, $\alpha+\beta < 1$; as well as in the strong fragmentation case $B_i \geq Ci^\gamma$, $\gamma > \alpha + \beta$.
- These estimates imply mass conservation in the strong fragmentation case, as well as smoothness results.
- It would be interesting to extend these results to handle the case where $d_i \underset{i\to\infty}{\longrightarrow} 0$.
- The issue of mass conservation is still open for linear coagulation ($a_{i,j} = i + j$).

THANK YOU!